Quantum Algorithms for Scientific Computation

Lin Lin and Nathan Wiebe

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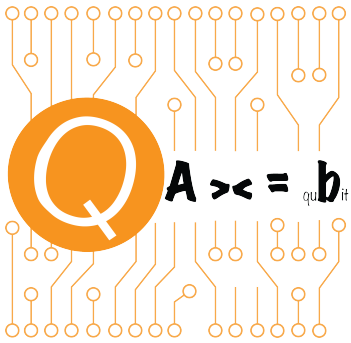


PRELIMINARY NOTES BEING CONTINUOUSLY UPDATED.

Contents

Part I

Background

Part I of this book sets the stage for our exploration of quantum algorithms for scientific computation by asking two questions: why should we expect quantum computers to offer a computational advantage, and what are the basic mathematical and physical principles that govern them?

Chapter 1 tackles the first question. We begin by tracing the conceptual origins of quantum computing and formalizes the notion of quantum speedup. We then introduce a quantum advantage hierarchy, which classifies applications based on the strength of evidence for quantum speedup.

Chapter 2 addresses the second question by providing a concise overview of elements of quantum computation. We introduce the postulates of quantum mechanics, the circuit model, and the density operator formalism. We also cover concepts such as the no-cloning theorem and the principles of deferred and implicit measurement. The chapter concludes by introducing the operator formalisms for spin, fermionic, and bosonic systems, which are essential for describing the physical problems encountered in scientific applications, and presents several example Hamiltonians that will serve as recurring illustrations throughout the book.

CHAPTER 1

Quantum advantage in scientific computation

In this chapter, we trace the conceptual origins of quantum computing and explain how the physical nature of information suggests that quantum mechanics may offer computational power beyond classical Turing machines. We then formalize the notion of quantum speedup. Any claim of quantum advantage requires accounting for all relevant computational costs, including data input and output. To structure this assessment, we introduce a quantum advantage hierarchy that categorizes problems based on the existing evidence for significant speedups. The chapter concludes with a brief discussion of quantum error correction, and why exponentially large state spaces do not force exponential error accumulation: in fault-tolerant computation, it suffices to implement each gate to an accuracy that scales inversely with the gate count.

1.1. Origin and justification for quantum computing

Our aim in this textbook is to provide a concrete understanding of not only how quantum algorithms work, but more importantly *why* they work and what impact scalable quantum computers are expected to yield in both the scientific and industrial worlds. Underlying this inquiry, however, is a deeper philosophical question about what it means to compute and why probing this question inevitably led to the idea of quantum computing.

Modern computer science traces its roots back to the early 20th century, with luminaries such as Alan Turing, John von Neumann, and Claude Shannon struggling to mathematically describe how information is stored and processed. Turing's great realization was that all such computers could be mathematically modeled by an abstract device called a "Turing Machine". The Turing machine was inspired strongly by the human "computers" (clerks) of the day: it possesses a tape for storing information and a read head that moves along the tape, updating the data on the tape in accordance with a stored program [Tur36].

John von Neumann is often credited with providing the first modern computer architecture that resembles modern computers, featuring dedicated memory, arithmetic and logic units, and input/output capabilities [VN93]. This architecture provided a far more realistic model of the postwar computers that were emerging, but conceptually these devices were no more powerful than the original Turing machine. Specifically, a machine is said to be "Turing Complete" if any function that a Turing machine can compute can be computed on the device. The von Neumann machine (given sufficient memory) can be shown to be Turing Complete, and in fact, a Turing machine can also simulate a machine implementing the von Neumann architecture. In this sense, the device is more than just Turing Complete: it is actually Turing Equivalent. Indeed, all known classical computational systems are Turing equivalent in this sense. This observation means that, effectively, every computational system in the universe could be understood as a Turing machine.

The formal study of algorithms revealed that not all tasks are fundamentally as easy for a Turing Machine. Some tasks, such as deciding whether a program halts, are strictly uncomputable [Tur36].

On the other hand, problems such as multiplying two n-bit numbers can be performed using a number of steps that scales polynomially in n. Still other problems, such as factoring an n-bit integer into a product of primes, can have their solution *verified* in polynomial time, but to date, no efficient algorithm has been found on a Turing machine that can *find* these factors in time that is polynomial in n (despite centuries of study). This suggested that a more fine-grained notion of computability needed to be considered than simply "computable" or "uncomputable". Instead, it was seen to be useful to categorize computational tasks that can be computed on a Turing Machine using a polynomial number of operations as "efficiently computable" and all others as inefficient.

This categorization led to a bold hypothesis, which we will later criticize, known as the **Extended Church-Turing Thesis**. This statement says that any reasonable model of computing can be simulated using a polynomial number of computational steps by a probabilistic Turing machine. The example of von Neumann's model of computing being simulatable in polynomial time by a Turing machine has indeed been reinforced by other models of computing based on physical phenomena, including billiard balls and the Game of Life. However, a challenge would emerge from an unlikely source: fundamental physics.

At the same time as computer science was being developed, a revolution was happening in physics. It had long been observed by physicists such as Planck and Einstein that classical physics could not be used to explain why heated objects (blackbodies) glowed red or how solar panels worked. Indeed, realistic models of these effects based on Newtonian principles failed to predict experimental observations. In the case of the stove elements, this failure was so radical that it predicted that infinite energy would be emitted by a stove burner (the "ultraviolet catastrophe"). A new type of model, formalized by von Neumann and others, was proposed to describe these systems that we now know as quantum mechanics (so named for its prediction that light should be emitted or absorbed in discrete quanta of energy). This language ultimately became the foundation of all fundamental physical law (gravitation being a notable exception).

Subsequent questions from Einstein, Podolsky, Rosen, and developments by Bell showed that quantum mechanics could not reasonably be described by classical local realism. Specifically, a phenomenon known as **entanglement**, which describes the correlations between measurement outcomes of coupled quantum systems, could not be described by classical mechanics without incorporating a non-local mechanism for updating measurement results. This work began to seriously question whether quantum systems could be plausibly described as mechanical systems. This, in turn, would much later be seen to question the Extended Church-Turing Thesis, as a Turing Machine is at its core a classical mechanical object that relies on local interactions.

A surprising feature of quantum mechanics is that its connection to computing seems to have taken several decades to be appreciated, despite us owing John von Neumann a great debt for formalizing both theories. With the benefit of hindsight, it is clear that with the appreciation of the fact that information is physical, quantum computing could have been developed as early as the 1940s.

The physical nature of information was elucidated most clearly by Shannon and Landauer. Shannon showed that the information content of a signal takes the same form as entropy, or disorder, in thermodynamics. Inspired by this connection, Shannon proposed that the two concepts were the same, establishing a link between his mathematical theory of information and thermal physics. Indeed, according to a widely circulated anecdote attributed to Shannon in an article by Tribus, von Neumann may have been agonizingly close to realizing the connection between physics and information processing [TM71]:

> *"What's in a name? In the case of Shannon's measure the naming was not accidental. In 1961 one of us (Tribus) asked Shannon what he had thought about when he had finally confirmed his famous measure. Shannon replied: 'My greatest concern was what to call it. I thought of calling it 'information', but the word was overly used, so I decided to call it 'uncertainty'. When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, 'You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name. In the second place, and more importantly, no one knows what entropy really is, so in a debate you will always have the advantage."*

Indeed, Shannon's work provided strong evidence that the two concepts are in fact the same and that thermodynamics had been telling us a secret lesson about information all along.

Landauer took this insight one step further by showing that thermodynamics places limitations on computers. Specifically, he showed that any computer that performs a calculation at finite temperature must pay an energy price for every bit of information erased to avoid violating the laws of thermodynamics [Lan61]. Similar work studying Maxwell's Demon, a hypothetical agent that can raise and lower a gate that allows fast gas molecules through while blocking slow molecules, revealed that if the thermodynamic cost of measuring and computing were ignored, the laws of thermodynamics could be violated by such an agent [Ben87]. These works showed a strong link between information and physics and laid the foundation for the link to quantum computing that would soon follow.

It took the insight that information is physical to begin to motivate incorporating the formalism of quantum mechanics into the language of computer science. Quantum computing was born of this synthesis and was articulated independently by Manin [Man80] and Feynman [Fey82]. The justification that they had was the fact that the description of the state space of even small quantum systems scales exponentially with the number of quantum bits. This means that a naïve simulation of the laws of quantum mechanics would require exponentially more time on a classical computer than the physical system itself requires to evolve. This work opened the possibility that a computer that exploited the full capabilities of quantum mechanics may be, for certain problems, exponentially more powerful than the Turing machine. This in turn caused the scientific community to begin to doubt that the Extended Church-Turing Thesis holds, and now the belief that any realistic model of computing is polynomially equivalent to a quantum computer has become widespread after the discovery of the fast factoring algorithm of Shor [Sho99], the quantum simulation algorithms of Lloyd and others [Llo96], as well as the quantum advantage proposals of Aaronson and Arkhipov [AA11].

At a high level though, quantum computing suggests something potentially even stronger. If the Extended Church-Turing Thesis is replaced by a quantum version, then all of nature could be described or simulated in polynomial time by a massive quantum computer. In this sense, the strong link between information and physics reaches a crescendo with quantum computing, which suggests that all of physical law could be thought of as an algorithm that is run on a quantum computer, and the set of tasks that a quantum computer cannot perform efficiently are precisely those that nature also cannot solve at scale. For this reason, the search for exponential algorithmic advantage plays a central role in quantum computing, not only because it provides us with new opportunities for our computers, but also because it reveals the limitations that physical systems impose on information processing, and in turn, the limitations that information processing places on physical systems. Indeed, the main purpose of this text is to shed light on the origin and utility of quantum speedups for scientific applications.

1.2. Quantum speedup

The primary aim of exploring quantum computation is to attain a **quantum speedup** or **quantum advantage**, thereby enhancing problem-solving capabilities in scientific computation. At first glance, it seems that n qubits can be used to represent a superposition over 2^n classical basis states, and significant quantum speedups should be expected everywhere. However, the situation is much more ambiguous: does the quantum algorithm require an exponential amount of classical information to be passed into the quantum computer? Does the quantum algorithm generate an exponential amount of information that needs to be extracted out of the quantum computer? If the size of the classical state space is 2^n, is it mandatory for the classical algorithm to go through all states in order to find an approximate solution to a desired precision? If the size of the classical state space is only n but the computational cost of an existing algorithm is 2^n, is it possible for a future classical algorithm to reduce this cost to poly(n)? Readers may be curious about how to evaluate and answer these questions before dedicating substantial time to learning quantum computation. Indeed, these discussions can occur at a relatively broad level, largely circumventing the need for intricate quantum jargon.

One way to formulate the quantum speedup (as a function of the system size n) is

$$\text{Quantum speedup} = \frac{\log(\min \text{Cost(classical)})}{\log \text{Cost(quantum)}}. \tag{1.1}$$

The presence of the logarithm can be intuitively understood as follows. For a task with a "system size" n, assume that the classical and quantum costs are (asymptotically) proportional to n^{α_c} and n^{α_q}, respectively. Then as $n \to \infty$, the quantum speedup defined according to Eq. (1.1) is α_c/α_q. For instance, a *quadratic* quantum speedup means $\alpha_c/\alpha_q = 2$, a *cubic* quantum speedup means $\alpha_c/\alpha_q = 3$, and so on. If $\alpha_c \to \infty$ as $n \to \infty$ but α_q remains bounded, the quantum speedup is *superpolynomial*. There is also a concept called "exponential quantum advantage" (EQA), which suggests that the classical cost increases at least exponentially in n but the quantum cost increases only polynomially.

Rigorous proof of EQA can be extraordinarily difficult for practical problems. For example, given two prime numbers p, q, the product $m = p \cdot q$ can be easily carried out on a classical computer. However, if we are only given the integer m, finding the prime factors p, q can be very challenging. This is called the prime factorization problem and has wide applications in cryptography. The difficulty of the prime factorization problem can be measured in terms of the number of bits in m. An integer m can always be expressed in binary format. For instance, $12 = 2^3 + 2^2$ can be represented as 1100 in binary format, where the number of bits n is 4. The most efficient classical algorithm, judged by asymptotic scaling in n, is the General Number Field Sieve method [Bri98]. The computational scaling is proportional to $\exp[cn^{\frac{1}{3}}(\log n)^{\frac{2}{3}}]$, which increases superpolynomially with n. Shor's celebrated algorithm [Sho94, Sho99] addresses the same problem on a quantum computer, with its cost being proportional to $n^2 \log n \log\log n$, i.e., only polynomial in n. On one hand, this provides a very clean (and so far the cleanest) quantum solution with a significant quantum speedup that is superpolynomial in n. On the other hand, even for this problem, the speedup is not yet exponential in the strict sense above. For practical purposes, we will be (more than) content with a superpolynomial quantum speedup.

In principle, the classical cost should be minimized with respect to *all* classical algorithms, including algorithms that exist today, and those that will ever be developed in the future. A useful lower bound of the cost of classical algorithms may be obtained for some simple problems. However, this undertaking is exceedingly challenging for the majority of scientific computing problems. For

instance, we do not know whether the problem of prime factorization can or cannot be performed in polynomial time. Therefore, for practical purposes, we will further be satisfied with an estimate of $\min \text{Cost}(\text{classical})$ by weighing both theoretical and empirical evidence, based on *existing* classical algorithms.

Although quantum mechanics is frequently described as a probabilistic theory, a key component is actually the quantum wavefunction (or quantum amplitude). This can be roughly equated to the square root of a probability density, along with phase information. This difference between probability density and quantum amplitude often forms the basis of the quadratic speedup, i.e., $\alpha_c/\alpha_q = 2$. The most prominent example of this is Grover's algorithm for unstructured search (see Chapter 11). Although a quadratic speedup is valuable, it is unlikely that this speedup alone will be the most groundbreaking application of early fault-tolerant quantum computers. Hence, we use the loose term *significant* quantum speedup to refer to speedups greater than quadratic (such as cubic or quartic), or better, to superpolynomial speedups.

The quantum cost can be roughly calculated as the total gate complexity multiplied by the number of repetitions due to the measurement process. It is also conceptually useful to divide it into the following three components:

(1) Input cost, or the cost for preparing the input quantum state. Without loss of generality, the quantum algorithm starts from a clean quantum state such as $|0^n\rangle$, and the input state to the quantum algorithm, denoted by $|\psi_I\rangle$, can be prepared using a unitary matrix U_I as $|\psi_I\rangle = U_I|0^n\rangle$. Then the input cost is the gate complexity for implementing U_I. Sometimes a quantum algorithm requires multiple accesses to the input oracle U_I in a coherent fashion. In this case, the input cost is given by the gate complexity for implementing U_I multiplied by the number of coherent initial state preparations.
(2) Output cost, or the cost of quantum measurement. Without loss of generality, after an appropriate basis change the measurement can be taken to be performed on one or multiple qubits in the computational basis at the end of an algorithm. Then the output cost is the number of repetitions M needed to run the quantum algorithm.
(3) Running cost, or the cost of coherently running the quantum algorithm once. This is given by the gate complexity for implementing the algorithm (excluding the cost for implementing U_I).

One reason for separating the total gate complexity into the input cost and the running cost is that it allows us to distinguish the case when the overall cost is dominated by preparing the input, rather than by coherently executing the rest of the algorithm. In many settings, the input information is classical, and the nature of its complexity can be very different from that in the quantum algorithm. There is also an important scenario in which the input state $|\psi_I\rangle$ is not generated by a known circuit U_I, but is produced by a quantum experiment. In this case, the relevant input cost is often the number of times the experiment must be repeated to prepare $|\psi_I\rangle$ (a sample complexity), rather than the gate complexity of a circuit. For instance, **quantum learning theory** studies how efficiently one can infer properties of an unknown quantum state from state preparations and measurements. Throughout this book, we focus on computational tasks in which quantum and classical algorithms have access to the same amount of classical input information and are required to output classical information, and we will not discuss quantum learning theory in detail (except basic concepts such as parameter estimation in Chapter 8).

Ultimately, all quantum algorithms must output information that can be processed through classical means via quantum measurements. If the quantum state itself is the end product, the procedure to recover the quantum state on a classical computer is called quantum state tomography.

The cost of the state tomography procedure usually grows exponentially relative to the size of the quantum system. Therefore, it is unlikely that significant quantum speedup can be achieved for problems involving a tomography procedure on a large number of qubits. Instead, we should focus on problems whose end result can be obtained by measuring a small number of observables related to the quantum state to a desired accuracy, for which the measurement overhead can sometimes be reduced substantially.

In summary, a quantum computer should not be viewed as an all-purpose computational device destined to replace classical computers. Rather, it should be seen as an accelerator, capable of providing significant speedups for specific computational tasks. As emphasized in [Aar14], one must "read the fine print" when evaluating claims of quantum advantage. Several criteria must be met: the problem under consideration should be computationally intensive on classical hardware; the task must be solvable efficiently on a quantum device; and the overhead associated with data input and output (i.e., loading and extracting data) should not dominate the overall cost. Furthermore, several proposed quantum speedups for linear algebra and machine learning on classical data rely on strong data-access assumptions, and in some cases comparable scaling can be achieved by quantum-inspired classical algorithms under similar assumptions. Meeting all of these conditions is far from trivial. It represents a significant theoretical, experimental, and algorithmic challenge for the entire scientific community.

1.3. Quantum advantage hierarchy

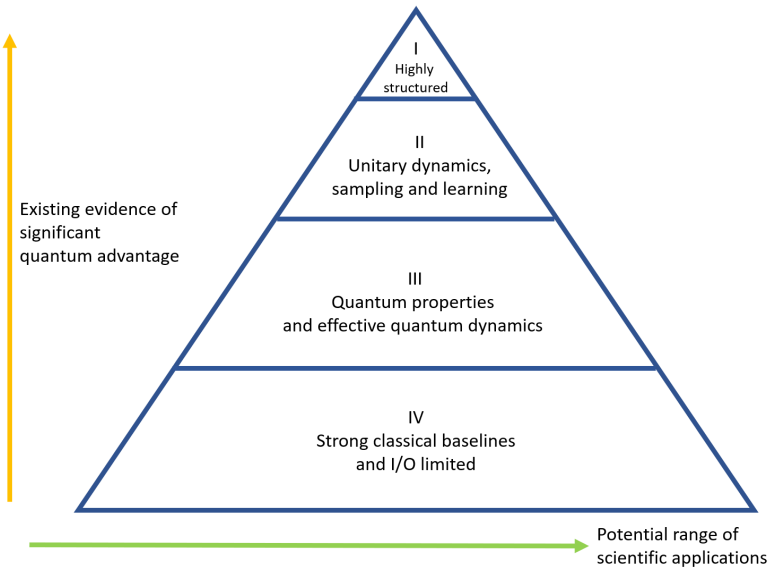


FIGURE 1.1. Quantum advantage hierarchy. The vertical level is determined by the most compelling application in each category, as demonstrated by the available evidence of quantum advantage.

Based on the aforementioned definition of quantum speedups, Fig. 1.1 organizes various quantum applications related to this book using a pyramid structure of 4 levels: Level I (Highly structured problems), Level II (Unitary dynamics, sampling, and learning problems), Level III (Quantum properties and effective dynamics problems), and Level IV (Strong classical baselines and I/O limited problems). Significant quantum speedups may exist across all levels. The vertical axis represents the *existing* amount of evidence supporting significant quantum speedups, while the horizontal axis represents the *potential* range of scientific applications. Besides gate complexity, for learning and sensing tasks the dominant cost can be the sample complexity (the number of experimental repetitions), which we treat as part of the running and output costs in this hierarchy. Now we give some examples at each level of the hierarchy, and the results are summarized in Table 1.1.

Level	Input Cost	Output Cost	Running Cost	Classical Cost	Examples
I Highly structured	✓	✓	✓	Provably expensive	Shor's algorithm for prime factorization and discrete logarithm, decoded quantum interferometry for structured optimization
II Unitary dynamics sampling and learning	✓	✓	✓	Empirically expensive	Hamiltonian simulation, random circuit sampling, learning with quantum memory
III Quantum properties and effective dynamics	?	?	✓	Empirically expensive	Ground state energy estimation, thermal state preparation, Green's function, open quantum system dynamics
IV Strong classical baselines and I/O limited	?	?	?	Efficient (except very large systems)	Classical partial differential equations, stochastic differential equations, unstructured optimization, classical machine learning

TABLE 1.1. Examples of problems in the quantum advantage hierarchy and existing amount of evidence justifying significant quantum speedups.

While prime factorization (and cryptography problems in general) are not typically classified as scientific computing problems, they occupy a unique position (Level I) at the peak of this hierarchy, and serves as a reference point for the ideal demonstration of quantum advantage in highly structured settings. These problems possess specific mathematical structures that allow quantum algorithms to bypass the exhaustive search often required by classical approaches. By describing the classical cost as "provably expensive," we mean that the problem is hard under reasonable complexity-theoretic conjectures or relative to the best-known classical algorithms. For example, Shor's algorithm exploits the periodicity of the modular exponentiation function, a property related

to the hidden subgroup problem. Another reason for placing Shor's algorithm at the top of the hierarchy is that these problems are "verifiable," meaning a candidate solution can be efficiently checked by classical means (e.g., by multiplying the returned factors). The recently developed decoded quantum interferometry (DQI) algorithm [JSW$^+$25] also solves highly structured optimization problems with superpolynomial speedups and has the potential to be classified in Level I. Unfortunately, such structures are rare in general scientific computing settings, as most problems in physics and engineering lack these clean, exploitable properties. To date, only a small number of applications have presented a comparable level of evidence supporting significant quantum speedups, and the list of credible candidates continues to evolve.

The most prominent example in Level II is the time evolution of a quantum state under a Hamiltonian, known as the Hamiltonian simulation problem. Many tasks in quantum physics and chemistry can be cast in this form. This category also includes sampling from unitary evolutions not explicitly defined by a Hamiltonian, such as random circuit sampling used in quantum supremacy experiments. For a physical Hamiltonian acting on n qubits, the description size is typically polynomial in n. We assume simple initial states, such as product states, which can be prepared with polynomial cost. The cost to simulate the dynamics for time t with precision ϵ then scales as $\mathrm{poly}(n, t, 1/\epsilon)$. Under these assumptions, no known classical algorithm is expected to reliably simulate generic many-body dynamics for long times. However, compared to Level I, the theoretical justification for speedup is often less rigorous, and verifying quantum advantage can be more difficult. For instance, verifying the output distribution of random circuit sampling typically demands exponential classical resources. Consequently, evidence for advantage relies heavily on the empirical hardness of classical simulation. Certain quantum learning tasks can demonstrate exponential advantage in sample complexity [HBC$^+$22]. These advantages primarily stem from the quantum nature of the input data and the availability of quantum memory [CCHL22]. This differs from the computational tasks addressed in this book, which focus on problems with classical inputs and outputs. Furthermore, the exponential advantage assumes that we have zero knowledge about the quantum system being learned, which is often not the case in physical applications.

Level III of the hierarchy includes a large class of problems in quantum physics, quantum chemistry, and materials science. By "quantum properties," we refer to static characteristics of the system, such as ground state energy, excited state energy, stationary states, and spectral properties. By "effective dynamics," we refer to processes that are not natively unitary, such as open system dynamics involving dissipation or imaginary time evolution used for cooling. Compared to Level II problems, the mapping from these non-unitary objects to the unitary logic of quantum hardware is indirect. This mapping often introduces overheads, such as the need for linear combinations of unitaries, post-selection, or many ancillary qubits. The amount of information that needs to be extracted from the quantum computer can be comparable to that in the quantum dynamics simulation and is at most polynomial in n. In the case of the ground-state energy estimation, the situation is even clearer since we only need to estimate a single number as the output. Compared to unitary dynamics, there exist a much larger number of powerful classical algorithms for these tasks. These are approximate methods and often cannot be used to converge to the true solution to arbitrary precision. However, for many practical problems, they have been shown to be sufficiently accurate. Input cost is also a major factor placing these problems at Level III. For example, ground state estimation often requires a good initial guess (an ansatz) to succeed; generating this ansatz can be computationally expensive or physically difficult, sometimes leading to QMA-hard bottlenecks. Finally, we may design quantum algorithms to solve problems that are entirely classical. For instance, we can consider quantum solvers for classical partial differential equations

(PDEs), stochastic differential equations, unstructured optimization problems, and sampling tasks. These cover a large variety of problems in scientific computing. However, many such classical problems fall into Level IV because they have strong classical baselines and/or are I/O limited. For example, many PDEs on a grid of size N can be solved classically in time polynomial in N (often approximately linear in N using fast algorithms). Even if a quantum algorithm offers a speedup in the processing stage, it faces the "I/O limit": merely loading an arbitrary input vector of size N into the quantum state takes time linear in N, which negates any potential exponential speedup. One exception arises when the classical data possesses significant structure that allows for efficient loading; a potential advantage in this regime was recently demonstrated for a quantum solver of a large number of classical oscillators [BBK+23]. Regarding unstructured search problems, while Grover's algorithm provides a quadratic speedup, this is often insufficient to overcome the significant constant-factor overheads of fault-tolerant quantum error correction compared to highly optimized classical heuristics. Thus, while the range of applications is vast, securing an end-to-end advantage is difficult. That being said, many cryptography problems can be formulated as classical optimization problems, and the next breakthrough in quantum algorithms *may* emerge from classical problems again.

The ongoing evaluation and pursuit of quantum advantage is a rapidly developing field. When discussing applications, we will only scratch the surface of the potential indications of quantum advantage by examining aspects such as quantum input cost, output cost, running cost, and the cost of classical algorithms, wherever possible. This approach is intended to encourage readers to seek out these elements in their own research. However, it is important to understand that the findings presented, while based on existing literature, are far from exhaustive or conclusive. The rapid pace of advancements means that future developments could significantly alter the current understanding and conclusions.

1.4. Quantum error correction and fault tolerant computation

All previous discussions assume that quantum operations can be perfectly performed. To this end, quantum error correction is necessary. The threshold theorem [ABO97] is a central result in the field of quantum error correction. The theorem essentially states that if the error rate of quantum operations (including gates and measurements) is below a certain threshold value (around 0.001, though the precise value depends on the detailed assumptions), then it is possible to perform quantum computation for an arbitrary length of time with arbitrarily high accuracy (see [NC00, Section 10.6]).

THEOREM 1.1 (Threshold theorem). *There exists an error threshold $p_t > 0$. If the physical error rate p per gate operation satisfies $p < p_t$, there exists a quantum error correction scheme such that the logical error rate q can be made as small as desired. In other words, $q = \mathcal{O}((p/p_t)^\ell)$ for any positive integer ℓ.*

We will not study the details of quantum error correction in this book. In classical computing, modern algorithm design generally does not take error correction into account. Similarly, in the long term, quantum error correction is expected to be largely a separate issue from the design of quantum algorithms. We always assume quantum error correction protocols have been implemented, physical noise has been eliminated, and the resulting quantum computer is **fault-tolerant**. For the purpose of this book, all errors come from either *approximation errors* at the mathematical level, or *Monte Carlo errors* in the readout process due to the probabilistic nature of the measurement process.

Quantum error correction is a dynamic and rapidly progressing field, and will significantly impact the development and potential of quantum algorithms, and the landscape of quantum computing. On a very coarse scale, we can categorize quantum algorithms based on the type of quantum computer architecture they are designed for.

(1) Noisy intermediate-scale quantum (NISQ) computers: These devices represent the current state of quantum computing technology. Characterized by a relatively small number (tens to a few hundreds) of physical qubits, these systems are prone to errors and lack full error correction capabilities. Quantum algorithms designed for NISQ devices, such as the Variational Quantum Eigensolver (VQE), need to be error resilient and must be capable of delivering meaningful results despite the presence of noise. Most of this book will not discuss NISQ algorithms.
(2) Fully fault-tolerant quantum computers: These are the ideal, long-term goal of quantum computing research. In these systems, quantum error correction protocols are fully implemented, allowing quantum algorithms to run for long durations without being overwhelmed by errors. This architecture will enable the execution of complex algorithms that require a large number of qubits and gate operations. Many of the algorithms discussed in this book are designed for this type of architecture. At the current stage, the goal of many fully fault-tolerant quantum algorithms is to minimize the total cost (in an *asymptotic* sense with respect to certain parameters, such as precision, system size etc.) for solving a given task.
(3) Early fault-tolerant quantum computers: This category represents a transitional phase between NISQ devices and fully fault-tolerant quantum computers. These systems would implement some form of quantum error correction, but they may have constraints such as a very limited number of logical ancilla qubits. This means that they can only run quantum algorithms within a certain complexity limit. Despite these constraints, early fault-tolerant quantum computers provide an opportunity to test and refine fault-tolerant designs and protocols, and to run quantum algorithms that are beyond the reach of NISQ devices but do not require the full capabilities of fault-tolerant quantum computers. Some of the algorithms in this book take such constraints into account and can be suitable on early fault-tolerant quantum computers.

1.5. Error accumulation mechanisms in classical and quantum computation

Quantum computation aims at processing objects whose natural dimension is exponential, such as vectors in $\mathbb{C}^{2^n}$ and matrices of size $2^n \times 2^n$. No computation can be carried out exactly, so will the error also accumulate exponentially with the system size? If that were the case, then quantum algorithms would become useless precisely in the regime where they are designed to operate. In this section we give a bird's-eye view of the relevant error accumulation mechanisms.

At first glance, deterministic numerical computation can look discouraging in this respect. Even a basic task such as forming an inner product involves many elementary operations, and Example 1.2 shows a worst-case bound for the accumulated rounding effects that is proportional to $N = 2^n$.

However, scientific computation has long dealt with exponentially large state spaces without requiring errors to grow linearly in the dimension. Randomized algorithms on n bits evolve a probability distribution on a space of size $N = 2^n$, yet the accuracy of the computation is governed by how many transition steps are composed, not by N itself: if each step is implemented to accuracy ϵ, then the overall error is at most $K\epsilon$, where K is the number of steps (see Proposition 3.30).

Quantum computation behaves in the same way at the level of circuit synthesis: a quantum algorithm is a product of elementary unitaries, and the accumulated implementation error is controlled by the number of gates. In particular, if the gate count is K and each gate can be implemented to precision ϵ/K, then the final error is $\mathcal{O}(\epsilon)$. In the fault-tolerant setting assumed above, achieving such per-gate accuracy is a realistic requirement, and the overhead of approximating elementary unitaries to a desired precision is discussed later (see Chapter 4). The distance notions used to make these comparisons precise are developed in Chapter 3, and the Monte Carlo errors arising at readout are discussed further in Chapter 8.

1.5.1. Deterministic classical computation. Modern scientific computation on classical computers is based on floating point arithmetic operations, which express a number in scientific notation. For instance, the number $-.271828 \times 10^5$ involves a sign $(-)$, fraction (271828), base (10), and exponent (5). In binary floating point, one stores a sign bit together with a fixed-length exponent and fraction. For instance, the IEEE single precision uses 1 bit for the sign, 8 bits for the exponent, and 23 bits for the fraction (32 bits long). The IEEE double precision uses 1 bit for the sign, 11 bits for the exponent, and 52 bits for the fraction (64 bits long). For instance, a double precision ranges from 2^{-1022} to 2^{1023}, or about 10^{-308} to 10^{308}. Numbers outside this range yield underflow or overflow error and need to be handled separately. This is much more efficient than the fixed point number representation (see Section 5.3), which would require more than 2046 bits (i.e., more than 2046 logical qubits for a single number) to cover the same range of numbers.

The basic assumption is that any real number a should be represented by $\mathrm{fl}(a)$ using a given number of bits. Similarly, any binary operation $a \odot b$ should be represented by $\mathrm{fl}(a \odot b)$, where $\odot$ is one of the four elementary binary operations $+, -, *, /$. The difference $a \odot b - \mathrm{fl}(a \odot b)$ is called the roundoff error. When the number is rounded correctly, i.e., $\mathrm{fl}(a \odot b)$ is a nearest floating point number to $a \odot b$, we have

$$\mathrm{fl}(a \odot b) = (a \odot b)(1 + \delta), \tag{1.2}$$

where $|\delta|$ is upper bounded by ϵ_{mach} (called the machine precision).

Example 1.2. Given $u, v \in \mathbb{R}^N$, consider the error accumulation of computing an inner product $\sum_{i=1}^N u_i v_i$. The error from each operation in the floating-point arithmetic needs to be counted separately. The floating-point representation of a product $u_i v_i$ is given by $u_i v_i(1 + \epsilon_i)$, where $|\epsilon_i| \leq \epsilon_{\mathrm{mach}}$, and ϵ_{mach} is the machine epsilon.

However, when summing these products, there is an additional error introduced at each addition step. Let us denote by δ'_j the relative rounding error incurred when adding the j-th term (so $|\delta'_j| \leq \epsilon_{\mathrm{mach}}$). Then the partial sums satisfy

$$\mathrm{fl}\big(s_{j-1} + u_j v_j(1 + \epsilon_j)\big) = \big(s_{j-1} + u_j v_j(1 + \epsilon_j)\big)(1 + \delta'_j), \tag{1.3}$$

where s_{j-1} denotes the computed partial sum from the previous step. After summing over all N terms, we may write

$$1 + \delta_i := (1 + \epsilon_i) \prod_{j=i+1}^{N} (1 + \delta'_j). \tag{1.4}$$

Therefore if overflow or underflow does not occur, then

$$\mathrm{fl}\left(\sum_{i=1}^N u_i v_i\right) = \sum_{i=1}^N u_i v_i(1 + \delta_i), \quad |\delta_i| \leq (1 + \epsilon_{\mathrm{mach}})^N - 1 \leq e^{N\epsilon_{\mathrm{mach}}} - 1. \tag{1.5}$$

◇

When $N\epsilon_{\text{mach}} < 1$, we have $|\delta_i| \leq 2N\epsilon_{\text{mach}}$. So the error grows linearly in N. This is due to the step of adding N numbers following a linear order. For computing the inner product, the error accumulation in the summation step can be significantly reduced using a technique called the pair summation (or cascade summation) to $\mathcal{O}((\log N)\epsilon_{\text{mach}})$. However, such a more accurate summation method is more difficult to implement in broader scenarios such as matrix-matrix multiplication. For most of the tasks, the poly(N) factor in the error accumulation is unavoidable. For instance, for solving a triangular linear system, the error accumulation is $\mathcal{O}(N\epsilon_{\text{mach}})$ [GVL13, Chapter 3.1]. For Gaussian elimination (or LU factorization), standard backward-error bounds involve the growth factor ρ and scale polynomially in N, typically of order $\mathcal{O}(N\rho\epsilon_{\text{mach}})$ [GVL13, Chapter 3.4].

That being said, not all deterministic computations involving vectors in $\mathbb{C}^N$ necessarily exhibit a poly(N) accumulation of numerical error. Error accumulation is governed not by the ambient dimension N itself, but by the number of elementary operations performed. For instance, tensor network methods provide settings in which certain computations on structured vectors in $\mathbb{C}^N$ can be carried out using only poly(n) operations, where $N = 2^n$. We will not discuss tensor network methods in this book, and classical probabilistic computation provides a more direct analogy to quantum computation for tackling high dimensional problems, as discussed next.

1.5.2. Probabilistic classical computation. A probabilistic computation on n bits evolves a probability distribution on a space of size $N = 2^n$, and hence it can be described by a vector in $\mathbb{R}^N$ acted on by stochastic matrices. The ambient dimension is exponential in n, but the computation is specified by a sequence of local update rules. As a result, neither the cost nor the accumulated implementation error needs to scale exponentially in N. This viewpoint also extends to the comparison between quantum and classical algorithms: a probability distribution can be viewed as a special quantum state, and a transition matrix can be associated with a special quantum channel (see Section 3.2).

If we can implement each transition matrix to precision ϵ, the global error of the overall transition matrix grows at most linearly with respect to the number of transition matrices and is at most $1, K\epsilon$ (see Proposition 3.30). Equivalently, if the gate complexity is K and we can implement each transition matrix to precision ϵ/K, then the final error is upper bounded by ϵ, independent of N. Compared to deterministic classical algorithms, randomized algorithms introduce another error mechanism: even when the transition rule is specified, one often estimates quantities of interest by sampling, and the output is therefore subject to Monte Carlo fluctuations. For example, estimating an expectation value by N_s independent samples typically incurs an error of order $\mathcal{O}(N_s^{-1/2})$, independent of the size of the underlying sample space. The statistical side of this issue is discussed further in Chapter 8.

1.5.3. Quantum computation. Quantum algorithms are designed to handle objects of size $N = 2^n$ without explicitly storing N numbers. As in probabilistic computation, error accumulation depends on how many steps are composed and on the metric used to compare channels (see Chapter 3), and they do not introduce an explicit dependence on N.

Every quantum circuit can be represented by a unitary U, decomposed into a series of simpler unitaries as $U = U_K \cdots U_1$. Each U_i can only be implemented approximately by some $\widetilde{U}_i$ to precision ϵ. The implementation cost of each simple unitary is independent of the Hilbert space dimension N (see Chapter 4). This implies that for any vector $|\psi\rangle$ of size N, the error between $U_i|\psi\rangle$ and $\widetilde{U}_i|\psi\rangle$ is less than ϵ with no explicit dependence on N.

If we can implement each local unitary to precision ϵ, the global error grows at most *linearly* with respect to the number of gates and is at most $K\epsilon$ (see Proposition 3.21). In other words, if the gate complexity is K and we can implement each gate to precision ϵ/K, then the final error is upper bounded by ϵ and is independent of N. The same statement holds for quantum channels (see Section 3.6).

CHAPTER 2

Elements of quantum computation

This chapter lays the groundwork for our journey into quantum algorithms for scientific computation. We will review the mathematical and physical principles that underpin quantum computing. While we assume a basic familiarity with quantum mechanics, our focus will be on establishing the specific concepts and notational conventions used throughout this book. This chapter is not intended as a comprehensive introduction to quantum computing, but rather as a targeted primer on the tools we will need to build and analyze sophisticated quantum algorithms. For a more comprehensive introduction to quantum computation, we refer the reader to standard textbooks such as [NC00, Wat18].

We start with the postulates of quantum mechanics, introducing the Dirac notation and the core principles governing quantum states and their evolution. We then move to the language of quantum circuits, which greatly simplifies the tensor manipulations inherent in multi-qubit systems. To handle scenarios involving noise and subsystems, we introduce the density operator formalism. We will also discuss the no-cloning theorem, which forbids the copying of arbitrary quantum states, and the principles of deferred and implicit measurement, which offer flexibility in circuit design. The latter part of the chapter introduces the representation of structured matrices, including sparse matrices and operators from fermionic and bosonic systems. We conclude with a selected list of Hamiltonians from physics, chemistry, and optimization that will serve as motivating examples in our exploration of quantum simulation and other applications.

2.1. Basic notation

The sets of real and complex numbers are denoted by $\mathbb{R}$ and $\mathbb{C}$, respectively. For a complex number $c \in \mathbb{C}$, the notation $\overline{c}$ or c^* denotes its complex conjugate.

A complex vector v of size N is an N-tuple of complex numbers, written as $v \in \mathbb{C}^N$, with its j-th component denoted by v_j. By default, we use 0-based indexing, that is, $j \in [N] := \{0, \ldots, N-1\}$. When 1-based indexing is used, we will explicitly write $j = 1, \ldots, N$.

The **vector 2-norm** of v is denoted by $\|v\| = \sqrt{\sum_{i\in[N]} |v_i|^2}$. Unless otherwise specified, a vector $v \in \mathbb{C}^N$ is considered unnormalized. A nonzero, normalized vector (viewed as a pure quantum state) is written as $|v\rangle = v/\|v\|$. To emphasize that a vector is unnormalized, we sometimes use the notation $|v\rangle$.

A matrix A of size $M \times N$ is denoted by $A \in \mathbb{C}^{M\times N}$, and its (i, j)-th entry is A_{ij} or a_{ij}. For $A \in \mathbb{C}^{M\times N}$, the complex conjugate of A, denoted by $\overline{A}$ or A^*, is obtained by replacing each entry of A with its complex conjugate. The inverse of A (if A is invertible) is denoted by A^{-1}. The transpose of A is denoted by $A^\top$. The Hermitian conjugate (or adjoint) of A, denoted by $A^\dagger$, is the complex conjugate of the transpose of A, which can be expressed as $A^\dagger = (A^\top)^*$. A matrix A is **Hermitian** if it is equal to its Hermitian conjugate, i.e., $A = A^\dagger$. A matrix A is **normal** if it commutes with its Hermitian conjugate, i.e., $AA^\dagger = A^\dagger A$. A matrix U is unitary if its Hermitian

conjugate is its inverse, i.e., $U^\dagger = U^{-1}$. The set of all $N \times N$ unitary matrices forms the unitary group, denoted by $\mathrm{U}(N)$. The set of all $N \times N$ unitary matrices with determinant 1 forms the special unitary group, denoted by $\mathrm{SU}(N)$.

If all eigenvalues of a Hermitian matrix $A \in \mathbb{C}^{N\times N}$ are nonnegative, A is called a **positive semidefinite** matrix, or **positive operator**, denoted by $A \succeq 0$. The notation $A \succeq B$ means $A - B \succeq 0$, and $A \preceq B$ means $B \succeq A$. Similarly, if all eigenvalues of A are positive, then A is called a **positive definite** matrix, denoted by $A \succ 0$. The notation $A \succ B$ means $A - B \succ 0$.

The **operator norm** (also called **induced vector 2-norm**)[1] of a matrix A is

$$\|A\| := \sup_{\|v\|=1} \|Av\| . \tag{2.1}$$

In quantum information theory, it is useful to consider the **Schatten p-norm** of A:

$$\|A\|_p := \left(\mathrm{Tr}(A^\dagger A)^{\frac{p}{2}}\right)^{\frac{1}{p}}, \quad p \geq 1. \tag{2.2}$$

The particularly useful one is the **Schatten 1-norm** (also called the **trace norm**)

$$\|A\|_1 := \mathrm{Tr}\sqrt{A^\dagger A}. \tag{2.3}$$

For instance, any quantum state (density operator) ρ is normalized with respect to the trace norm, i.e., $\|\rho\|_1 = 1$. Furthermore, the Schatten ∞-norm $\|A\|_\infty$ can be shown to coincide with the operator norm $\|A\|$. Many readers may not be familiar with the Schatten norms. We will discuss these norms in detail in Chapter 3.

We adopt the following **asymptotic notations**: Let $\mathbb{R}_+$ be the set of positive real numbers. Consider two functions $f : \mathbb{R} \to \mathbb{C}$ and $g : \mathbb{R} \to \mathbb{R}_+$. For any $a \in \mathbb{R} \cup \{\pm\infty\}$, if $\limsup_{x\to a} \frac{|f(x)|}{g(x)} < \infty$, then we write $f(x) = \mathcal{O}(g(x))$ as $x \to a$, or simply $f = \mathcal{O}(g)$[2] when $x \to a$ is clear from the context. We write $f = \Omega(g)$ if $g = \mathcal{O}(f)$; $f = \Theta(g)$ if $f = \mathcal{O}(g)$ and $g = \mathcal{O}(f)$. Note that $\mathcal{O}(g)$ can also be interpreted as a set, so it is also valid to write $f \in \mathcal{O}(g)$. Similarly we may write $f \in \Omega(g), f \in \Theta(g)$ etc.

The notation $\widetilde{\mathcal{O}}, \widetilde{\Omega}, \widetilde{\Theta}$ are used to suppress subdominant polylogarithmic factors. Specifically, $f = \widetilde{\mathcal{O}}(g)$ if $f = \mathcal{O}(g \,\mathrm{polylog}(g))$; $f = \widetilde{\Omega}(g)$ if $f = \Omega(g \,\mathrm{polylog}(g))$; $f = \widetilde{\Theta}(g)$ if $f = \Theta(g \,\mathrm{polylog}(g))$. Note that these tilde notations usually do not suppress dominant polylogarithmic factors. For instance, if $f = \mathcal{O}(\log g \log\log g)$, then we write $f = \widetilde{\mathcal{O}}(\log g)$ instead of $f = \widetilde{\mathcal{O}}(1)$. However, for simplicity of presentation, we may sometimes use the notation $\widetilde{\mathcal{O}}$ more casually to suppress dominant polylogarithmic factors. When we do so, we will make an explicit mention of this usage.

Throughout the book, the natural logarithm is denoted by ln, and is sometimes written as log without an explicit base when the context is clear. The logarithm to base 2 is denoted by $\log_2$. When N denotes the dimension of $\mathbb{C}^N$, and the notations N and n appear together, it is usually assumed that $N = 2^n$ for some positive integer n, referred to as the number of quantum bits (or **qubits**). Additional notations will be introduced in the book as needed.

---

[1] In matrix analysis, the operator norm is sometimes denoted by $\|A\|_2$ to indicate that this is the induced vector 2-norm. More generally, the induced vector p-norm is $\|A\|_p = \sup_{\|x\|_p=1} \|Ax\|_p$ where $\|x\|_p = \left(\sum_i |x_i|^p\right)^{1/p}$. For example, the induced vector 1-norm is $\|A\|_1 = \sup_{\|x\|_1=1} \|Ax\|_1 = \max_j \sum_i |a_{ij}|$. This book **does not** adopt such a notation.

[2] Sometimes $\mathcal{O}(g)$ is treated as a set of functions, and by this interpretation we can equivalently write $f \in \mathcal{O}(g)$.

2.2. Postulates of quantum mechanics

This section encapsulates some of the most important postulates of quantum mechanics. All postulates concern finite dimensional, closed quantum systems (i.e., systems isolated from environments). For more details, we refer readers to [NC00, Section 2.2].

2.2.1. State space postulate.

Definition 2.1 (Hilbert space)**.** *A (complex) Hilbert space denoted by $\mathcal{H}$ is a complex vector space equipped with an inner product $\langle\cdot|\cdot\rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ that satisfies the following properties for all $x, y, z \in \mathcal{H}$ and all $\alpha, \beta \in \mathbb{C}$:*

1. *(Conjugate Symmetry) $\langle x|y\rangle = \overline{\langle y|x\rangle}$.*
2. *(Linearity in the second argument) $\langle z|\alpha x + \beta y\rangle = \alpha\langle z|x\rangle + \beta\langle z|y\rangle$.*
3. *(Positive-definiteness) $\langle x|x\rangle \geq 0$ with equality if and only if $x = 0$.*

Furthermore, $\mathcal{H}$ is complete with respect to the norm induced by the inner product, where the norm of a vector $x \in \mathcal{H}$ is given by $\|x\| = \sqrt{\langle x|x\rangle}$.

The state space postulate assumes that the set of all quantum states of a quantum system, called the state space, is a Hilbert space. If the state space $\mathcal{H}$ is finite dimensional, it is isomorphic (i.e., there is a one-to-one mapping) to some $\mathbb{C}^N$, written as $\mathcal{H} \cong \mathbb{C}^N$. Throughout the book, unless otherwise specified, we only consider finite dimensional Hilbert spaces. A **state vector** (also called ket vector, wavefunction, or pure quantum state) $|\psi\rangle \in \mathcal{H}$ can be identified with a column vector in $\mathbb{C}^N$

$$\psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{N-1} \end{pmatrix}. \tag{2.4}$$

Let $\{e_i\}$ be the standard basis of $\mathbb{C}^N$. The i-th entry of ψ can be written as an inner product $\psi_i = \langle e_i|\psi\rangle$. We also use the Dirac notation, which uses $|\psi\rangle$ to denote a quantum state. We further postulate that two state vectors $|\psi\rangle$ and $c\,|\psi\rangle$ for some $0 \neq c \in \mathbb{C}$ always refer to the same physical state. Hence without loss of generality we always assume $|\psi\rangle$ is normalized to be a unit vector, i.e., $\langle\psi|\psi\rangle = 1$. Restricting to normalized state vectors, the complex number $c = e^{i\theta}$ for some $\theta \in [0, 2\pi)$ is called the global phase factor.

Throughout the book, unless otherwise specified, an unnormalized state vector is often denoted by ψ without the ket notation $|\cdot\rangle$, and $|\psi\rangle := \psi/\|\psi\|$ denotes the normalized counterpart.

The bra vector $\langle\psi|$ can be interpreted as a linear functional on $\mathcal{H}$, which maps any $|\varphi\rangle \in \mathcal{H}$ to a complex number $\langle\psi|\varphi\rangle$. When $\mathcal{H} = \mathbb{C}^N$, we have $\langle\psi|\varphi\rangle = \sum_{i\in[N]} \overline{\psi_i}\varphi_i$. It can be identified with a row vector, which is the Hermitian conjugate of the column vector ψ:

$$\psi^\dagger = \begin{pmatrix} \overline{\psi_0} & \overline{\psi_1} & \cdots & \overline{\psi_{N-1}} \end{pmatrix}. \tag{2.5}$$

The set of all bra vectors, or linear functionals on $\mathcal{H}$, is denoted by $\mathcal{H}^\star$[3].

Given a state space $\mathcal{H}$, let $L(\mathcal{H})$ denote the set of all linear operators on $\mathcal{H}$. When $\mathcal{H} = \mathbb{C}^N$, $L(\mathbb{C}^N)$ can be identified with the set of $N \times N$ matrices, denoted by $\mathbb{C}^{N\times N}$. The ketbra notation $|\psi\rangle\langle\varphi|$ is an element in $L(\mathcal{H})$, which maps any vector $|\xi\rangle \in \mathcal{H}$ to another state vector in $\mathcal{H}$ as

[3]The star $\star$ acting on a vector space does not mean the complex conjugation of $\mathcal{H}$. This notation is only used occasionally in the book. A Hilbert space satisfies $\mathcal{H} \cong \mathcal{H}^\star$ by the Riesz representation theorem.

$|\psi\rangle\langle\varphi|\xi\rangle$. The matrix representation of $|\psi\rangle\langle\varphi|$ is the product of the column vector ψ and the row vector $\varphi^\dagger$, i.e., $\psi\varphi^\dagger \in \mathbb{C}^{N\times N}$.

Example 2.2 (Single qubit system and Bloch sphere)**.** A (single) qubit corresponds to a state space $\mathbb{C}^2$. We also define

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}. \tag{2.6}$$

Since the state space of the spin-$\frac{1}{2}$ system is also isomorphic to $\mathbb{C}^2$, this is also called the single spin system, where $|0\rangle, |1\rangle$ are referred to as the spin-up and spin-down state, respectively. A general state vector in $\mathbb{C}^2$ takes the form

$$|\psi\rangle = a|0\rangle + b|1\rangle = \begin{pmatrix}a\\b\end{pmatrix}, \quad a, b \in \mathbb{C}, \tag{2.7}$$

and the normalization condition implies $|a|^2 + |b|^2 = 1$. So we may rewrite $|\psi\rangle$ as

$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right), \quad \theta, \varphi, \gamma \in \mathbb{R}. \tag{2.8}$$

If we ignore the irrelevant global phase $e^{i\gamma}$ (which also absorbs a minus sign in the coefficient of $|0\rangle$), then it holds

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle, \quad 0 \le \theta \le \pi, 0 \le \varphi < 2\pi. \tag{2.9}$$

So we may identify each single qubit quantum state with a unique point on the unit three-dimensional sphere (called the **Bloch sphere**) as

$$\mathbf{a} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^\top. \tag{2.10}$$

◇

2.2.2. Quantum operator postulate. The quantum operator postulate states that the evolution of a quantum state from $|\psi\rangle \to |\psi'\rangle \in \mathcal{H}$ is always achieved via a unitary operator U, i.e.,

$$|\psi'\rangle = U|\psi\rangle, \quad U^\dagger U = I. \tag{2.11}$$

Here $U^\dagger$ is the Hermitian conjugate of U, and I is the identity map that can be identified with a N-dimensional identity matrix. The set of all $N\times N$ unitary matrices is the unitary group, denoted by $\mathrm{U}(N)$. The set of all $N\times N$ unitary matrices with determinant 1 forms the special unitary group, denoted by $\mathrm{SU}(N)$.

This unitary evolution is derived from the system's **Hamiltonian** $H \in L(\mathcal{H})$, which is a Hermitian matrix that encapsulates the total energy of the system and thus governs its dynamics. For a time-independent Hamiltonian H, the state $|\psi(t)\rangle$ satisfies the Schrödinger equation

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle. \tag{2.12}$$

The corresponding time evolution operator is

$$U(t_2, t_1) = e^{-iH(t_2-t_1)}, \quad \forall t_2 \ge t_1. \tag{2.13}$$

In particular, $U(t_2, t_1) = U(t_2 - t_1, 0)$.

More generally, starting from an initial quantum state $|\psi(0)\rangle$, the quantum state can evolve in time, which gives a single parameter family of quantum states denoted by $\{|\psi(t)\rangle\}$. These quantum states are related to each other via a quantum evolution operator U:

$$|\psi(t_2)\rangle = U(t_2, t_1)\,|\psi(t_1)\rangle\,, \tag{2.14}$$

where $U(t_2, t_1)$ is unitary for any given t_1, t_2. Here $t_2 > t_1$ refers to quantum evolution forward in time, $t_2 < t_1$ refers to quantum evolution backward in time, and $U(t_1, t_1) = I$ for any t_1.

In quantum computation, a unitary matrix is often referred to as a **quantum gate**.

Example 2.3. For a single qubit, the **Pauli matrices** are

$$\sigma_x = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.15}$$

Together with the two-dimensional identity matrix, they form a basis of all linear operators on $\mathbb{C}^2$. ◇

Some other commonly used single qubit operators include, to name a few:

- **Hadamard gate**

$$\mathrm{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{2.16}$$

- **Phase gate**

$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \tag{2.17}$$

- T **gate**:

$$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} = \sqrt{S}. \tag{2.18}$$

When there are notational conflicts, we will use the roman font such as H, X for these single-qubit gates (for example, to distinguish the Hadamard gate H from a Hamiltonian H). An operator acting on an n-qubit quantum state space is called an n-qubit operator.

Example 2.4. For $P \in \{X, Y, Z\}$, the unitary evolution generated by the Hamiltonian $H = P$ is a rotation about the corresponding Bloch-sphere axis. Concretely,

$$\begin{aligned} R_x(2t) :=& e^{-itX} = \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix}, \\ R_y(2t) :=& e^{-itY} = \begin{pmatrix} \cos(t) & -\sin(t) \\ \sin(t) & \cos(t) \end{pmatrix}, \\ R_z(2t) :=& e^{-itZ} = \begin{pmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{pmatrix}. \end{aligned} \tag{2.19}$$

For instance, starting from an initial state $|\psi(0)\rangle = |0\rangle$, under $R_x(2t)$ at time $t = \pi/2$ the state evolves into $|\psi(\pi/2)\rangle = -i\,|1\rangle$, i.e., the $|1\rangle$ state up to a global phase. ◇

THEOREM 2.5 (Spectral theorem of normal matrices). *Given a matrix $A \in \mathbb{C}^{N\times N}$, the matrix A is normal (i.e., $A^\dagger A = AA^\dagger$), if and only if*

$$A = VDV^\dagger. \tag{2.20}$$

Here, $D \in \mathbb{C}^{N\times N}$ is a diagonal matrix containing the eigenvalues of A, and $V \in \mathrm{U}(N)$ is a unitary matrix whose columns are the eigenvectors of A.

A more general decomposition, which plays a key role throughout the book, is the **singular value decomposition** (SVD).

THEOREM 2.6 (Singular value decomposition). *Given any matrix $A \in \mathbb{C}^{M\times N}$, there exist unitary matrices $U \in \mathrm{U}(M)$ and $V \in \mathrm{U}(N)$, and a diagonal matrix $\Sigma \in \mathbb{C}^{M\times N}$ with non-negative real numbers on the diagonal, such that*

$$A = U\Sigma V^\dagger. \tag{2.21}$$

The diagonal entries of Σ are called the singular values of A, the columns of U are called the left singular vectors of A, and the columns of V are called the right singular vectors of A.

Operator exponentials, also called **matrix exponentials**, gives us a way to express gates as operator exponentials and because the algebra of exponentials makes this representation far easier to work with than explicitly writing the unitary in a matrix representation.

Definition 2.7 (Matrix function)**.** *For $A \in \mathbb{C}^{N\times N}$, and a complex valued function $f : \mathbb{C} \mapsto \mathbb{C}$, the matrix function $f(A)$ is defined as follows:*

1. *If f is an analytic function such that $f(x) = \sum_{j=0}^{\infty} a_j x^j$ then $f(A) := \sum_{j=0}^{\infty} a_j A^j$.*
2. *If f is a complex valued function and A is a normal matrix such that $A = VDV^\dagger$ where V is unitary and $D := \mathrm{diag}(\lambda_0, \ldots, \lambda_{N-1})$ where $f(\lambda_j) \in \mathbb{C}$. Then $f(A) := Vf(D)V^\dagger$ where $f(D) = \mathrm{diag}(f(\lambda_0), \ldots, f(\lambda_{N-1}))$.*

The definition of a matrix exponential can be seen as a direct consequence of either of the above definitions, and both definitions find extensive use in quantum computing. Specifically, using the former definition we have that for any matrix A

$$e^A := \sum_{j=0}^{\infty} \frac{A^j}{j!}. \tag{2.22}$$

Matrix function can also be defined for non-normal matrices using contour integrals (see [Hig08, Chapter 1]).

Lemma 2.8. *Let $A \in \mathbb{C}^{N\times N}$ and let $U \in \mathrm{U}(N)$ be a unitary matrix, then $Ue^AU^\dagger = e^{UAU^\dagger}$.*

The following result can be viewed as the simplest realization of the **Baker–Campbell–Hausdorff formula** (BCH).

Lemma 2.9. *For any $A, B \in \mathbb{C}^{N\times N}$, we have*

1. *if $[A, B] = 0$, then $e^A e^B = e^{A+B}$.*
2. *if $[A, [A, B]] = [B, [A, B]] = 0$, then $e^A e^B = e^{A+B+\frac{1}{2}[A,B]}$.*
3. *if $[A, B] \neq 0$, then $e^A e^B = e^{A+B+\frac{1}{2}[A,B]} + \mathcal{O}(\max(\|A\|, \|B\|)^3)$.*

In general, we can express any unitary operator as an exponential of a Hermitian operator. This result is a direct consequence of the definition of the operator exponential.

Lemma 2.10. *For any unitary matrix $U \in \mathrm{U}(N)$, there exists a Hermitian matrix $H \in \mathbb{C}^{N\times N}$ such that $U = e^{-iH}$.*

PROOF. A unitary matrix U is a normal matrix. According to Theorem 2.5, the unitary matrix U can be diagonalized as

$$U = VDV^\dagger, \tag{2.23}$$

where $V \in \mathbb{C}^{N\times N}$ is a unitary matrix and D is a diagonal matrix. The diagonal entries satisfy $|D_{ii}| = 1$. Without loss of generality we can write $D_{ii} = e^{-i\theta_i}$ where $\theta_i \in [0, 2\pi)$. Then define a diagonal matrix $\Theta_{ii} = \theta_i$, and $H = V\Theta V^\dagger$, we obtain $U = e^{-iH}$. Note that the matrix H is not unique since each θ_i can be chosen modulo 2π. □

In many scenarios such as the analysis of quantum simulation using Trotter-Suzuki formulas, we need to find Taylor series expansions of conjugated operators.

Lemma 2.11. *Let A, B be normal matrices in $\mathbb{C}^{N\times N}$ and let $t \in \mathbb{R}$. We then have that*

$$e^{At}Be^{-At} = B + \frac{[A,B]t}{1!} + \frac{[A,[A,B]]t^2}{2!} + \frac{[A,[A,[A,B]]]t^3}{3!} + \cdots \tag{2.24}$$

PROOF. We note that the above result is a power series in t, which must coincide with the Taylor series expansion of the function $f(t) = e^{At}Be^{-At}$ because the function is analytic. Thus the expression is true if the k-th derivative of $f(t)$ at $t = 0$ is given by the k-fold commutator. We prove by induction that

$$\partial_t^k(e^{At}Be^{-At}) = e^{At}[A,[A,[\cdots,[A,B]\cdots]]]e^{-At}, \tag{2.25}$$

where the commutator is applied k times. The base case $k = 0$ holds trivially. Assume the hypothesis holds for some $k \geq 0$. Then

$$\begin{aligned}\partial_t^{k+1}(e^{At}Be^{-At}) &= \partial_t\left(e^{At}[A,[A,[\cdots,[A,B]\cdots]]]e^{-At}\right)\\ &= e^{At}\left(A[A,[\cdots,[A,B]\cdots]] - [A,[\cdots,[A,B]\cdots]]A\right)e^{-At}\\ &= e^{At}[A,[A,[\cdots,[A,B]\cdots]]]e^{-At},\end{aligned} \tag{2.26}$$

where the final expression contains $k+1$ commutators. This confirms the inductive step. Evaluating at $t = 0$ yields the coefficients of the Taylor series, completing the proof. □

2.2.3. Quantum measurement postulate. In quantum mechanics, a **quantum observable** is always represented by a Hermitian matrix acting on the state space. The reason for using Hermitian matrices is that they have real eigenvalues, which correspond to the outcome of **quantum measurements**.

A quantum observable $O \in L(\mathcal{H})$ has the spectral decomposition

$$O = \sum_m \lambda_m P_m. \tag{2.27}$$

Here $\lambda_m \in \mathbb{R}$ are the eigenvalues of O, and $P_m \in L(\mathcal{H})$ is the projection operator onto the eigenspace associated with λ_m. The quantum measurement postulate states that when conducting a measurement on a quantum state $|\psi\rangle$ with respect to a quantum observable O, the eigenvalues λ_m represent all the possible results of the measurement. Furthermore, the probability of obtaining a particular outcome λ_m is

$$p_m = \langle\psi|P_m|\psi\rangle\,. \tag{2.28}$$

Following the measurement, the quantum state collapses to the corresponding eigenspace

$$|\psi\rangle \to \frac{P_m\,|\psi\rangle}{\sqrt{p_m}}. \tag{2.29}$$

The set of projection operators satisfies the resolution of identity:

$$\sum_m P_m = I. \tag{2.30}$$

This implies the normalization condition

$$\sum_m p_m = \sum_m \langle\psi|P_m|\psi\rangle = \langle\psi|\psi\rangle = 1, \quad \forall\, |\psi\rangle \in \mathcal{H}. \tag{2.31}$$

Together with $p_m \geq 0$, we find that $\{p_m\}$ is indeed a probability distribution.

The expectation value of the measurement outcome can be expressed as

$$\mathbb{E}_\psi(O) = \sum_m \lambda_m p_m = \sum_m \lambda_m \langle\psi|P_m|\psi\rangle = \left\langle \psi \middle| \left(\sum_m \lambda_m P_m\right) \middle| \psi \right\rangle = \langle\psi|O|\psi\rangle\,. \tag{2.32}$$

Example 2.12. Let $O = X$ be the Pauli X operator. From the spectral decomposition of X:

$$X\,|\pm\rangle = \lambda_\pm\,|\pm\rangle\,, \tag{2.33}$$

where $|\pm\rangle := \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$, $\quad \lambda_\pm = \pm 1$, we obtain the eigendecomposition

$$O = X = |+\rangle\langle+| - |-\rangle\langle-|\,. \tag{2.34}$$

Consider a quantum state $|\psi\rangle = |0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$, then

$$\langle\psi|P_+|\psi\rangle = \langle\psi|P_-|\psi\rangle = \frac{1}{2}. \tag{2.35}$$

Therefore the expectation value of the measurement is $\langle\psi|X|\psi\rangle = 0$. ◇

Exercise 2.1. Prove Eq. (2.34).

2.2.4. Tensor product postulate.

Definition 2.13 (Tensor product)**.** *The tensor product of two finite dimensional Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ is a complex vector space, denoted by $\mathcal{H}_1 \otimes \mathcal{H}_2$, spanned by vectors of the form $v \otimes w$ with $v \in \mathcal{H}_1$ and $w \in \mathcal{H}_2$. The bilinear map $\otimes : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathcal{H}_1 \otimes \mathcal{H}_2$ satisfies for all $v, v' \in \mathcal{H}_1$, $w, w' \in \mathcal{H}_2$, and scalars $\alpha, \beta \in \mathbb{C}$:*

1. *$(\alpha v + \beta v') \otimes w = \alpha(v \otimes w) + \beta(v' \otimes w)$ and $v \otimes (\alpha w + \beta w') = \alpha(v \otimes w) + \beta(v \otimes w')$.*
2. *$(\alpha v) \otimes w = \alpha(v \otimes w)$ and $v \otimes (\beta w) = \beta(v \otimes w)$.*

The tensor product is associative in the sense that the two vector spaces $(\mathcal{H}_1 \otimes \mathcal{H}_2) \otimes \mathcal{H}_3$ and $\mathcal{H}_1 \otimes (\mathcal{H}_2 \otimes \mathcal{H}_3)$ are isomorphic. Let $\mathcal{H}_1, \ldots, \mathcal{H}_k$ be finite-dimensional Hilbert spaces with inner products $\langle\cdot|\cdot\rangle_i$ for $i = 1, 2, \ldots, k$. The tensor product of these k spaces can be recursively defined as $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_k := \mathcal{H}_1 \otimes (\mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_k)$, which is spanned by all elements of the form $v_1 \otimes v_2 \otimes \cdots \otimes v_k$ called **product states**, where $v_i \in \mathcal{H}_i$ for $i = 1, 2, \ldots, k$. The inner product of two vectors $v = v_1 \otimes v_2 \otimes \cdots \otimes v_k$ and $w = w_1 \otimes w_2 \otimes \cdots \otimes w_k$ in the tensor product space $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_k$ is defined as

$$\langle v|w\rangle = \langle v_1|w_1\rangle_1 \cdot \langle v_2|w_2\rangle_2 \cdots \langle v_k|w_k\rangle_k.$$

This inner product is extended linearly to the entire tensor product space as

$$\left\langle \sum_i a_i v_i \middle| \sum_j b_j w_j \right\rangle = \sum_{i,j} \overline{a_i} b_j \langle v_i|w_j\rangle, \quad a_i, b_j \in \mathbb{C}.$$

The tensor product postulate states that the state space with k components $\mathcal{H}_1 \cong \mathbb{C}^{N_1}, \ldots, \mathcal{H}_k \cong \mathbb{C}^{N_k}$ is the tensor product of these spaces $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_k$. Let $\{|j_i\rangle\}_{j_i \in [N_i]}$ be the basis of $\mathbb{C}^{N_i}$, then a general state vector in $\mathcal{H}$ takes the form

$$|\psi\rangle = \sum_{j_1 \in [N_1], \ldots, j_k \in [N_k]} \psi_{j_1 \cdots j_k} |j_1\rangle \otimes \cdots \otimes |j_k\rangle . \tag{2.36}$$

Here $\psi_{j_1 \cdots j_k} \in \mathbb{C}$ is an entry of a k-way tensor. Given another state vector

$$|\varphi\rangle = \sum_{j_1 \in [N_1], \ldots, j_k \in [N_k]} \varphi_{j_1 \cdots j_k} |j_1\rangle \otimes \cdots \otimes |j_k\rangle , \tag{2.37}$$

the inner product takes the form

$$\langle \psi | \varphi \rangle = \sum_{j_1 \in [N_1], \ldots, j_k \in [N_k]} \overline{\psi_{j_1 \cdots j_k}} \varphi_{j_1 \cdots j_k} . \tag{2.38}$$

The state space of n-qubits is $\mathcal{H} = (\mathbb{C}^2)^{\otimes n} \cong \mathbb{C}^{2^n}$. We also use a shorthand notation: the tensor product $\otimes$ may be omitted when the context is clear.

$$|01\rangle \equiv |0, 1\rangle \equiv |0\rangle |1\rangle \equiv |0\rangle \otimes |1\rangle , \quad |0^{\otimes n}\rangle \equiv |0^n\rangle \equiv |0\rangle^{\otimes n} . \tag{2.39}$$

The tensor product operation provides us with a powerful way to describe two independent copies of different vector spaces as a single larger vector space. Further, the tensor product when viewed through this lens does not care about the nature of the form of the Hilbert spaces that are being combined. In fact a particularly important case that we need to consider is the tensor product between two operators.

Definition 2.14 (Tensor products of linear operators)**.** *Given two finite dimensional Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, the tensor product of $L(\mathcal{H}_1)$ and $L(\mathcal{H}_2)$, denoted by $L(\mathcal{H}_1) \otimes L(\mathcal{H}_2)$, is a complex vector space spanned by linear operators of the form $A \otimes B$ with $A \in L(\mathcal{H}_1)$ and $B \in L(\mathcal{H}_2)$. The bilinear map $\otimes : L(\mathcal{H}_1) \times L(\mathcal{H}_2) \to L(\mathcal{H}_1) \otimes L(\mathcal{H}_2)$ satisfies for all $A, B \in L(\mathcal{H}_1)$ and $C, D \in L(\mathcal{H}_2)$, $v \in \mathcal{H}_1$, $w \in \mathcal{H}_2$ and scalars $\alpha, \beta \in \mathbb{C}$:*

1. $(\alpha A + \beta B) \otimes C = \alpha A \otimes C + \beta B \otimes C$ *and* $A \otimes (\alpha C + \beta D) = \alpha A \otimes C + \beta A \otimes D$.
2. $(\alpha A) \otimes B = \alpha A \otimes B = A \otimes (\alpha B)$.

The space $L(\mathcal{H}_1) \otimes L(\mathcal{H}_2)$ is isomorphic to $L(\mathcal{H}_1 \otimes \mathcal{H}_2)$. The tensor product is also associative in the sense that $L(\mathcal{H}_1) \otimes (L(\mathcal{H}_2) \otimes L(\mathcal{H}_3))$ is isomorphic to $(L(\mathcal{H}_1) \otimes L(\mathcal{H}_2)) \otimes L(\mathcal{H}_3)$. A consequence of this definition is further that the application of multiple tensor products of linear operators on matching tensor products of vectors distributes across the tensor product via

$$(A_1 \otimes A_2 \otimes \cdots \otimes A_k)(v_1 \otimes v_2 \otimes \cdots \otimes v_k) = (A_1 v_1) \otimes (A_2 v_2) \otimes \cdots \otimes (A_k v_k). \tag{2.40}$$

Example 2.15 (Two qubit system)**.** The state space is $\mathcal{H} = (\mathbb{C}^2)^{\otimes 2} \cong \mathbb{C}^4$. The standard basis is (row-major order, i.e., last index is the fastest changing one)

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.41}$$

There are many important quantum operators on the two-qubit quantum system. One of them is the **CNOT gate**, with matrix representation

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{2.42}$$

In other words, when acting on the standard basis, we have

$$\text{CNOT} \begin{cases} |00\rangle & = |00\rangle \\ |01\rangle & = |01\rangle \\ |10\rangle & = |11\rangle \\ |11\rangle & = |10\rangle \end{cases}. \tag{2.43}$$

This can be compactly written as

$$\text{CNOT} \, |a\rangle \, |b\rangle = |a\rangle \, |a \oplus b\rangle \, . \tag{2.44}$$

Here $a \oplus b = (a + b) \mod 2$ is the "exclusive or" (XOR) operation. ◇

Definition 2.16 (Controlled unitaries)**.** *A controlled unitary operation is a quantum gate that applies a specified unitary operation U to a set of target qubits only when the control qubits are in a particular state, typically the $|1\rangle$ state for each control qubit. The single qubit controlled unitary operation can be represented as:*

$$CU = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U.$$

An n-qubit controlled unitary can be written as:

$$C^n U = (I - |1^n\rangle\langle 1^n|) \otimes I + |1^n\rangle\langle 1^n| \otimes U.$$

The CNOT gate is the same as CX. Controlled unitaries are ubiquitous in quantum algorithms. In particular, it enables conditional logic within quantum circuits.

Example 2.17 (Multi-qubit Pauli operators)**.** For a n-qubit quantum system, the Pauli operator acting on the i-th qubit is denoted by P_i ($P = X, Y, Z$), i.e.,

$$\begin{aligned} X_i &:= I^{\otimes(i-1)} \otimes X \otimes I^{\otimes(n-i)}, \\ Y_i &:= I^{\otimes(i-1)} \otimes Y \otimes I^{\otimes(n-i)}, \\ Z_i &:= I^{\otimes(i-1)} \otimes Z \otimes I^{\otimes(n-i)}. \end{aligned} \tag{2.45}$$

For example, in a 2-qubit system, following the row-major convention, the matrix representation of X_1, X_2 are

$$X_1 = X \otimes I = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad X_2 = I \otimes X = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{2.46}$$

◇

Definition 2.18 (Pauli group)**.** *The n-qubit Pauli group, denoted as $\mathcal{P}_n$, is a group that consists of all possible tensor products of n-qubit Pauli matrices along with multiplicative factors of ± 1 and $\pm i$. Each element of the n-qubit Pauli group can be represented as*

$$i^k(P_1 \otimes P_2 \otimes \cdots \otimes P_n),$$

where $k \in \{0, 1, 2, 3\}$, each P_i is one of the Pauli matrices X, Y, Z, or the identity matrix I, and $\otimes$ denotes the tensor product.

The n-qubit Pauli group contains 4^{n+1} elements due to the 4^n possible tensor products of Pauli matrices and identity matrices, each multiplied by one of the four possible phase factors $\pm 1, \pm i$. It plays a key role in quantum simulation and quantum error correction. Note that the product of any two elements is another element of the group (up to a phase factor), and every element is its own inverse (up to a phase factor).

Definition 2.19 (Clifford group)**.** *The n-qubit Clifford group, denoted as $\mathcal{C}_n$, is a group of unitary operators that normalizes the n-qubit Pauli group $\mathcal{P}_n$. This means that for every Clifford operator $C \in \mathcal{C}_n$ and every Pauli operator $P \in \mathcal{P}_n$, there exists a Pauli operator $P' \in \mathcal{P}_n$ such that*

$$CPC^\dagger = P'.$$

The Clifford group includes all elements of the Pauli group, the Hadamard gate H, the phase gate S, and the CNOT gate. It can be generated by $\{\mathrm{H}, S, \mathrm{CNOT}\}$.

Example 2.20. The single-qubit Pauli group $\mathcal{P}_1$ is defined as the group generated by the Pauli matrices X, Y, Z together with the phase factor i:

$$\mathcal{P}_1 = \{i^k P \mid k \in \{0, 1, 2, 3\}, P \in \{I, X, Y, Z\}\}.$$

We show that $\mathcal{P}_1$ can be generated by the set $\{\mathrm{H}, S\}$. First, we obtain the Pauli Z operator by squaring the phase gate:

$$S^2 = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = Z.$$

Next, we utilize the property that the Hadamard gate transforms Z into X under conjugation. Since H is Hermitian and unitary, we have:

$$X = \mathrm{H}\, Z\, \mathrm{H} = \mathrm{H}\, S^2\, \mathrm{H}\,.$$

The Pauli Y operator can be generated by conjugating X by S. We compute the conjugate transpose $S^\dagger = \mathrm{diag}(1, -i)$ and verify the relation:

$$\begin{aligned} SXS^\dagger &= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = Y. \end{aligned}$$

Since S is unitary and $S^4 = I$, we have $S^\dagger = S^{-1} = S^3$. Thus, $Y = SXS^3$.

Finally, since $XYZ = iI$, we conclude that $\{\mathrm{H}, S\}$ generates the entire Pauli group $\mathcal{P}_1$.

Since

$$T^2 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix} = S,$$

it immediately follows that $\{\mathrm{H}, T\}$ also generates $\mathcal{P}_1$. ◇

The Clifford group plays an important role in many areas. In quantum error correction, Clifford operations can transform certain errors into forms that are more easily correctable. This makes it desirable to choose Clifford gates to be part of a universal gate set (the most common one is Clifford + T). Additionally, the Gottesman–Knill theorem states that any quantum circuit using only Clifford gates on computational basis states and measurements in the computational basis can be efficiently simulated classically.

Example 2.21. We can concisely describe block matrices stored within a larger matrix. The matrix representation of $T \in L(\mathbb{C}^{NM} \otimes \mathbb{C}^{NM})$, when writing in the block form,

$$T = \begin{pmatrix} T_{0,0} & \cdots & T_{0,N-1} \\ \vdots & \ddots & \vdots \\ T_{N-1,0} & \cdots & T_{N-1,N-1} \end{pmatrix}, \quad T_{ij} \in \mathbb{C}^{M \times M}. \tag{2.47}$$

can be rewritten as

$$T = \sum_{i,j \in [N]} |e_i\rangle\langle e_j| \otimes T_{ij}. \tag{2.48}$$

◇

The notation for partial inner products and partial applications of operators is used throughout this book, particularly in the context of block-encoding.

Definition 2.22 (Partial inner product)**.** *Consider two finite dimensional Hilbert spaces $\mathcal{H}_A \cong \mathbb{C}^N$ with an orthonormal basis $\{|e_i\rangle\}_{i\in[N]}$, and $\mathcal{H}_B \cong \mathbb{C}^M$ with an orthonormal basis $\{|f_i\rangle\}_{i\in[M]}$. The partial inner product $\langle\cdot|\cdot\rangle$ is a map $\mathcal{H}_A \times (\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{H}_B$ defined as follows. For any $v \in \mathcal{H}_A$, $w \in \mathcal{H}_A \otimes \mathcal{H}_B$*

$$\langle v|w\rangle = \sum_{ij} \left(\langle v|e_i\rangle \langle e_i, f_j|w\rangle\right) |f_j\rangle \in \mathcal{H}_B. \tag{2.49}$$

With some abuse of notation, the partial inner product $\langle\cdot|\cdot\rangle$ also denotes a map: $(\mathcal{H}_A \otimes \mathcal{H}_B) \times \mathcal{H}_A \to \mathcal{H}_B^\star$ according to

$$\langle w|v\rangle = \sum_{ij} \left(\langle e_i|v\rangle \langle w|e_i, f_j\rangle\right) \langle f_j| \in \mathcal{H}_B^\star. \tag{2.50}$$

This definition of a partial inner product has been used in the literature in several works such as [LC17b]. A problem with the notation though is that it requires that the reader pay close attention to the dimensions of the objects in question in order to infer the dimension of the output with a partial inner product. This runs counter to the advantages of Dirac notation which can be confusing when used in the context of conventional Dirac notation where the inner product is always a scalar. While its brevity is an advantage, great care must be taken when using the above notation to avoid making mistakes about the shape of the output.

Example 2.23. Let $|v\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$ be a one-qubit state, $|w\rangle = |0\rangle \otimes (|00\rangle + |11\rangle) + |1\rangle \otimes (|01\rangle + |10\rangle)$ be a three-qubit state, then the partial inner product

$$\langle v|w\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) + \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \tag{2.51}$$

is a two-qubit state. ◇

Example 2.24. Let $w = \sum_{i\in[N]} |e_i\rangle \otimes |w_i\rangle$ be reshaped into a matrix

$$W = \begin{pmatrix} w_0 & \cdots & w_{N-1} \end{pmatrix} \in \mathbb{C}^{N\times M}. \tag{2.52}$$

Then the partial inner product $\langle e_i|w\rangle$ for $i \in [N]$ picks out the i-th column w_i. Similarly, the partial inner product $\langle w|e_i\rangle$ picks out the ith row of $W^\dagger$, which is $w_i^\dagger$. ⋄

The partial inner product between pure states provides a natural way to focus our attention on one of the subspaces involved. Sometimes however, we will wish to apply a transformation on the system in question. This generalizes the concept of the partial inner product, and will be vital in our later discussion on block-encoding in Chapter 9.

Definition 2.25 (Partial application of operators)**.** *Consider two finite dimensional Hilbert spaces $\mathcal{H}_A \cong \mathbb{C}^N$ with an orthonormal basis $\{|e_i\rangle\}_{i\in[N]}$, and $\mathcal{H}_B \cong \mathbb{C}^M$ with an orthonormal basis $\{|f_i\rangle\}_{i\in[M]}$. A partial application is a map $(\mathcal{H}_A^\star \otimes L(\mathcal{H}_B)) \times (\mathcal{H}_A \otimes \mathcal{H}_B) \to \mathcal{H}_B$ so that for $|v\rangle \in \mathcal{H}_A$, $C \in L(\mathcal{H}_B)$, $|u\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$,*

$$(\langle v| \otimes C)\,|u\rangle = \sum_{jk} \left(\langle v|e_j\rangle \langle e_j, f_k|u\rangle\right)(C\,|f_k\rangle) \in \mathcal{H}_B. \tag{2.53}$$

Similarly we define

$$\langle u|\,(|v\rangle \otimes C) = \sum_{jk} \left(\langle e_j|v\rangle \langle u|e_j, f_k\rangle\right)(\langle f_k|\,C) \in \mathcal{H}_B^\star. \tag{2.54}$$

Example 2.26. The partial inner product can also be viewed as a partial application of the identity gate, i.e., for $|v\rangle \in \mathcal{H}_A$, $I \in L(\mathcal{H}_B)$, $|u\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$

$$\langle v|u\rangle = (\langle v| \otimes I)\,|u\rangle\,, \quad \langle u|v\rangle = \langle u|\,(|v\rangle \otimes I). \tag{2.55}$$

For $T = \sum_{jk} |e_j\rangle\langle e_k| \otimes T_{jk}$, the quantity $(\langle e_i| \otimes I)T$ can be represented as a rectangular matrix that consists of the i-th block row of T:

$$\begin{aligned}(\langle e_i| \otimes I)T &= (\langle e_i| \otimes I) \sum_{jk} |e_j\rangle\langle e_k| \otimes T_{jk} \\ &= \sum_k \langle e_k| \otimes T_{ik} \equiv \begin{pmatrix} T_{i,0} & \cdots & T_{i,N-1} \end{pmatrix},\end{aligned} \tag{2.56}$$

Similarly, $T(|e_j\rangle \otimes I)$ picks out the j-th block column of the matrix T.

$$\begin{aligned}T(|e_j\rangle \otimes I) &= \sum_{ik} \delta_{jk}\,|e_i\rangle \otimes T_{ik} \\ &= \sum_i |e_i\rangle \otimes T_{ij} \equiv \begin{pmatrix} T_{0,j} \\ \vdots \\ T_{N-1,j} \end{pmatrix},\end{aligned} \tag{2.57}$$

and $(\langle e_i| \otimes I)T(|e_j\rangle \otimes I)$ returns the (i,j)-th block T_{ij} as can be seen via

$$(\langle e_i| \otimes I)T(|e_j\rangle \otimes I) = (\langle e_i| \otimes I) \sum_k |e_k\rangle \otimes T_{kj} = T_{ij}. \tag{2.58}$$

With some abuse of notation, we may omit the $\otimes I$ notation, so $(\langle e_i| \otimes I)T(|e_j\rangle \otimes I)$ may be written simply as $\langle e_i|\,T\,|e_j\rangle$. ⋄

2.3. Density operator

So far all quantum states encountered have been described by a single state vector $|\psi\rangle$. How to describe a classical mixture of state vectors, such as the state after a measurement process? How can the state of a subsystem within a larger quantum system be defined? The answer to these questions requires the formulation of the density operator (also called density matrix).

Definition 2.27 (Density operator)**.** *A linear operator $\rho \in L(\mathbb{C}^N)$ is called a density operator, if $\rho \succeq 0$, and $\operatorname{Tr}\rho = 1$. The set of all density operators is denoted by $\mathcal{D}(\mathbb{C}^N)$.*

The density operator corresponding to a state vector $|\psi\rangle$ is a rank-1 matrix

$$\rho = |\psi\rangle\langle\psi|. \tag{2.59}$$

Recall that quantum mechanics postulates that $|\psi\rangle$ and $|\psi'\rangle = e^{i\theta}|\psi\rangle$ represent the same physical state. This statement is more natural from the perspective of the density operator, since

$$\rho' = |\psi'\rangle\langle\psi'| = e^{i\theta}|\psi\rangle\, e^{-i\theta}\langle\psi| = \rho. \tag{2.60}$$

In physics, such an irrelevant phase factor is referred to as a gauge degree of freedom. The density operator ρ encapsulates the same physical information as is present in $|\psi\rangle$, but with the added benefit of being invariant to the gauge choice.

With some abuse of terminology, throughout this book, both the density operator ρ and the state vector $|\psi\rangle$ are called quantum states. A rank-1 density operator is called a **pure state**.

Exercise 2.2. Prove that all eigenvalues of a density operator ρ belong to $[0, 1]$. Furthermore, $\rho^2 \preceq \rho$, and the equality holds if and only if ρ is a pure state.

If ρ is not a pure state, then it is called a **mixed state**. We can diagonalize the density matrix as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| =: \sum_i p_i \rho_i, \tag{2.61}$$

where all state vectors $|\psi_i\rangle$ are orthogonal to each other, and each ρ_i is a pure state. On the other hand, if we have the ability to prepare each pure state ρ_i, then to create the mixed state ρ, all we need to do is prepare a state ρ_i randomly, with the probability of preparing each state given by p_i. In essence, a mixed state can be seen as a **classical ensemble** of pure quantum states. In particular, an n-qubit state $\rho = \frac{I}{2^n}$ is called the **maximally mixed state**.

Let $\{\rho_j\}$ be a set of density operators. With any discrete probability distribution $\{p_j\}$, define $\rho' = \sum_j p_j \rho_j$. Then $\rho' \succeq 0$ and $\operatorname{Tr}[\rho'] = \sum_j p_j \operatorname{Tr}[\rho_j] = \sum_j p_j = 1$. Therefore ρ' is a density operator. In other words, a classical ensemble of (pure or mixed) density operators is also a density operator.

Example 2.28 (Expectation value of a quantum observable)**.** Let us consider the expectation value of an observable O with respect to a mixed state ρ. Since the expectation value with respect to a pure state is

$$\langle O\rangle_{\rho_i} = \langle\psi_i|O|\psi_i\rangle = \operatorname{Tr}[O\rho_i], \tag{2.62}$$

if we obtain the expectation value for a mixed state that obtains a pure state ρ_i with probability p_i, the expectation value is concisely written as

$$\langle O\rangle_{\rho} = \sum_i p_i \operatorname{Tr}[O\rho_i] = \operatorname{Tr}[O\rho]. \tag{2.63}$$

◇

The measurement process can be described without referring to a quantum observable. A quantum measurement can be described by a set of measurement operators $\{M_m\}$, where m labels the different possible outcomes of the measurement. The operators M_m act on the state space $\mathcal{H}$ of the system and satisfy the completeness relation: $\sum_m M_m^\dagger M_m = I$. After a measurement described by M_m is made on a quantum system in a state ρ, the probability of getting result m is given by

$$p_m = \mathrm{Tr}[M_m \rho M_m^\dagger]. \tag{2.64}$$

If outcome m occurs, then the state of the quantum system collapses to a new state

$$\rho'_m = \frac{M_m \rho M_m^\dagger}{\mathrm{Tr}[M_m \rho M_m^\dagger]}. \tag{2.65}$$

The density operator of the resulting ensemble is

$$\rho' = \sum_m p_m \rho'_m = \sum_m M_m \rho M_m^\dagger. \tag{2.66}$$

If each M_m is a projection operator denoted by P_m, then $\{P_m\}$ is called a **projective measurement**. When a quantum observable is measured, the action that is performed on the quantum system is a projective measurement. That is, the state of the system is projected onto an eigenstate of the observable, corresponding to the obtained result of the measurement.

Example 2.29 (Projective measurement)**.** Let the initial state $\rho = |\psi\rangle\langle\psi|$ be a pure state subject to a projective measurement $\{P_m\}_m$. After measurement, the system collapses into a state $|\psi_m\rangle = P_m|\psi\rangle / \sqrt{p_m}$ with probability $p_m = \langle\psi|P_m|\psi\rangle$. If we attempt to represent it by a pure state, one natural choice seems to be $|\psi'\rangle = \sum_m \sqrt{p_m}|\psi_m\rangle$. However, using the normalization condition of the projective measurement in Eq. (2.30)

$$\sum_m \sqrt{p_m}|\psi_m\rangle = \sum_m \sqrt{p_m} P_m|\psi\rangle / \sqrt{p_m} = \sum_m P_m|\psi\rangle = |\psi\rangle. \tag{2.67}$$

In other words, state before and after the measurement is exactly the same! This clearly does not make sense.

Instead, the resulting state should be be represented by a mixed state

$$\rho' = \sum_m p_m |\psi_m\rangle\langle\psi_m| = \sum_m P_m|\psi\rangle\langle\psi| P_m = \sum_m P_m \rho P_m. \tag{2.68}$$

◇

The partial trace is an operation on a joint quantum state (often representing a composite system), which effectively "traces out" one or more subsystems to leave a reduced density operator for the remaining subsystem(s). The operation is widely used in quantum mechanics, especially in the study of open quantum systems, quantum information, and quantum computation.

Definition 2.30 (Partial trace)**.** *Consider two finite dimensional Hilbert spaces $\mathcal{H}_A \cong \mathbb{C}^N$ with an orthonormal basis $\{|e_i\rangle\}_{i\in[N]}$, and $\mathcal{H}_B \cong \mathbb{C}^M$, and $T \in L(\mathcal{H}_A \otimes \mathcal{H}_B)$. The partial trace over $\mathcal{H}_A$, denoted by $\mathrm{Tr}_A(T)$ is an element in $L(\mathcal{H}_B)$ defined as:*

$$\mathrm{Tr}_A(T) = \sum_{i\in[N]} (\langle e_i| \otimes I) T (|e_i\rangle \otimes I). \tag{2.69}$$

The partial trace $\mathrm{Tr}_B(T)$ is defined similarly.

Example 2.31. The matrix representation of $T \in L(\mathbb{C}^N \otimes \mathbb{C}^M)$ takes the form of a block matrix

$$T = \begin{pmatrix} T_{0,0} & \cdots & T_{0,N-1} \\ \vdots & \ddots & \vdots \\ T_{N-1,0} & \cdots & T_{N-1,N-1} \end{pmatrix}, \quad T_{ij} \in \mathbb{C}^{M\times M}. \tag{2.70}$$

Then

$$\mathrm{Tr}_A(T) = \sum_{i\in[N]} T_{ii} \tag{2.71}$$

is the sum of all diagonal blocks. ◇

Given a density operator $\rho \in \mathcal{D}(\mathcal{H}_A \otimes \mathcal{H}_B)$, the partial trace

$$\rho_A = \mathrm{Tr}_B[\rho] \in \mathcal{D}(\mathcal{H}_A), \quad \rho_B = \mathrm{Tr}_A[\rho] \in \mathcal{D}(\mathcal{H}_B) \tag{2.72}$$

are called **reduced density operators**. In particular, if $\rho = \rho_1 \otimes \rho_2$, then

$$\mathrm{Tr}_B[\rho] = \rho_1, \quad \mathrm{Tr}_A[\rho] = \rho_2. \tag{2.73}$$

Note that even if ρ is a pure state, in general, the reduced density operators ρ_A, ρ_B are mixed states.

If a quantum observable is defined only on the subsystem A, i.e., $O = O_A \otimes I_B$ and $O_A = \sum_m \lambda_m P_m$, then when measuring a quantum state ρ with respect to O, the probability of obtaining λ_m, and the expectation value only depend on the reduced density matrix ρ_A:

$$p_m = \mathrm{Tr}[(P_m \otimes I)\rho] = \mathrm{Tr}[P_m \,\mathrm{Tr}_B[\rho]] = \mathrm{Tr}[P_m \rho_A], \quad \mathbb{E}_\rho[O] = \mathrm{Tr}[(O_A \otimes I)\rho] = \mathrm{Tr}[O_A \rho_A]. \tag{2.74}$$

Exercise 2.3. The **Bell state** (also called the EPR pair) is defined to be

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{2.75}$$

Use the partial trace over the second qubit to prove that the Bell state cannot be written as any product state $|a\rangle \otimes |b\rangle$.

Example 2.32 (Purification of mixed state)**.** Any mixed state can always be dilated to a pure state using ancilla qubits. In particular, any n-qubit mixed state ρ can be expressed as $\sum_j p_j |\lambda_j\rangle\langle\lambda_j|$ where $|\lambda_j\rangle$ are the eigenvectors of ρ, and p_j is the corresponding eigenvalue. Given this we can construct a $2n$-qubit pure state

$$|\rho\rangle := \sum_j \sqrt{p_j}\, |\lambda_j\rangle_A \, |\lambda_j\rangle_B \,. \tag{2.76}$$

Then $\mathrm{Tr}_B(|\rho\rangle\langle\rho|) = \rho$. ◇

A more general concept than projective measurement is called **generalized measurement**, also called positive operator-valued measure (POVM).

Definition 2.33. *A **positive operator-valued measure** (POVM) is a set of positive semidefinite operators $\{E_m\}$ that sum to the identity:*

$$\sum_m E_m = I, \quad E_m \succeq 0. \tag{2.77}$$

If a quantum system is in state ρ, the probability of obtaining outcome m is given by

$$p_m = \mathrm{Tr}[E_m \rho]. \tag{2.78}$$

Unlike projective measurements, the elements E_m of a POVM are not necessarily orthogonal, nor are they required to be projection operators (i.e., E_m^2 need not equal E_m). However, POVMs provide the most general description of quantum measurements. On the other hand, the Naimark's dilation theorem (see e.g. [Wat18, Chapter 2.3]) tells us that any generalized measurement can be implemented by coupling the system of interest to an ancilla system and performing a standard projective measurement on the composite system.

THEOREM 2.34 (Naimark's dilation theorem). *Every POVM can be realized as a projective measurement on a larger Hilbert space. Specifically, given a POVM $\{E_m\}$ on $\mathcal{H}_A$, there exists an auxiliary Hilbert space $\mathcal{H}_B$, a pure state $|0\rangle_B \in \mathcal{H}_B$, and a projective measurement $\{P_m\}$ on $\mathcal{H}_A \otimes \mathcal{H}_B$ such that for any state ρ on $\mathcal{H}_A$:*

$$\mathrm{Tr}[E_m \rho] = \mathrm{Tr}[P_m(\rho \otimes |0\rangle\langle 0|_B)]. \tag{2.79}$$

PROOF. Since each E_m is positive semidefinite, we can define $M_m = \sqrt{E_m}$ such that $M_m^\dagger M_m = E_m$. Let $\mathcal{H}_B$ be a Hilbert space with an orthonormal basis $\{|m\rangle\}$ corresponding to the indices of the POVM elements. We define a linear operator $V : \mathcal{H}_A \to \mathcal{H}_A \otimes \mathcal{H}_B$ by its action on an arbitrary state $|\psi\rangle \in \mathcal{H}_A$:

$$V|\psi\rangle = \sum_m M_m |\psi\rangle \otimes |m\rangle_B . \tag{2.80}$$

This operator is an isometry because

$$\langle V\psi|V\psi\rangle = \sum_{m,n} \langle\psi| M_m^\dagger M_n |\psi\rangle \langle m|n\rangle = \sum_m \langle\psi| M_m^\dagger M_m |\psi\rangle = \langle\psi| \left(\sum_m E_m\right) |\psi\rangle = \langle\psi|\psi\rangle . \tag{2.81}$$

We can extend this isometry to a unitary operator U acting on $\mathcal{H}_A \otimes \mathcal{H}_B$ such that $U(|\psi\rangle \otimes |0\rangle_B) = V|\psi\rangle$. Now, define the projective measurement on the composite system by the projectors $\Pi_m = I_A \otimes |m\rangle\langle m|_B$. Let $P_m = U^\dagger \Pi_m U$. Since U is unitary and $\{\Pi_m\}$ are orthogonal projectors summing to identity, $\{P_m\}$ is a valid projective measurement. Finally, we verify the probability condition:

$$\begin{aligned} \mathrm{Tr}[P_m(\rho \otimes |0\rangle\langle 0|_B)] &= \mathrm{Tr}[U^\dagger \Pi_m U(\rho \otimes |0\rangle\langle 0|_B)] \\ &= \mathrm{Tr}[\Pi_m U(\rho \otimes |0\rangle\langle 0|_B)U^\dagger] \\ &= \mathrm{Tr}[(I_A \otimes |m\rangle\langle m|_B) V \rho V^\dagger]. \end{aligned} \tag{2.82}$$

Using the definition of V, we have $V\rho V^\dagger = \sum_{k,l} M_k \rho M_l^\dagger \otimes |k\rangle\langle l|_B$. Substituting this back,

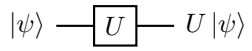
$$\begin{aligned} \mathrm{Tr}[P_m(\rho \otimes |0\rangle\langle 0|_B)] &= \mathrm{Tr}\left[(I_A \otimes |m\rangle\langle m|_B) \sum_{k,l} M_k \rho M_l^\dagger \otimes |k\rangle\langle l|_B\right] \\ &= \mathrm{Tr}[M_m \rho M_m^\dagger] = \mathrm{Tr}[M_m^\dagger M_m \rho] = \mathrm{Tr}[E_m \rho]. \end{aligned} \tag{2.83}$$

□

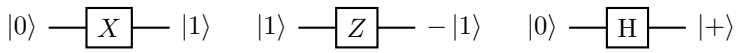
2.4. Quantum circuit

Nearly all quantum algorithms operate on multi-qubit quantum systems. When quantum operators operate on two or more qubits, writing down quantum states in terms of its components as in Eq. (2.36) quickly becomes cumbersome. The language of **quantum circuit** offers a graphical and compact manner for writing down the procedure of applying a sequence of quantum operators to a quantum state. For more details see [NC00, Section 4.2, 4.3].

In the quantum circuit language, time flows from the left to right, i.e., the input quantum state appears on the left, and the quantum operator appears on the right, and each "wire" represents a qubit i.e.,



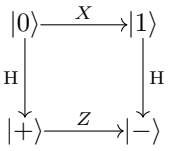
Here are a few examples:



which is a graphical way of writing

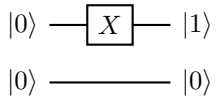
$$X|0\rangle = |1\rangle\,, \quad Z|1\rangle = -|1\rangle\,, \quad \mathrm{H}|0\rangle = |+\rangle\,. \tag{2.84}$$

The relation between these states can be expressed in terms of the following diagram



(2.85)

Also verify that

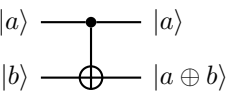


which is a graphical way of writing

$$(X \otimes I)|00\rangle = |10\rangle\,. \tag{2.86}$$

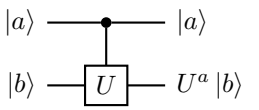
Note that the input state can be general, and in particular does not need to be a product state. For example, if the input is a Bell state (2.75), we just apply the quantum operator to $|00\rangle$ and $|11\rangle$, respectively and multiply the results by $1/\sqrt{2}$ and add together. To distinguish with other symbols, these single qubit gates may be either written as X, Y, Z, H or (using the roman font) $\mathrm{X}, \mathrm{Y}, \mathrm{Z}, \mathrm{H}$.

The quantum circuit for the CNOT gate is

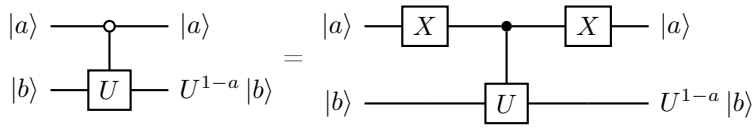


Here the "dot" means that the quantum gate connected to the dot only becomes active if the state of the qubit 0 (called the control qubit) is $a = 1$. This justifies the name of the CNOT gate (controlled NOT).

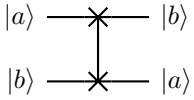
Similarly,



is the controlled U gate for some unitary U. Here $U^a = I$ if $a = 0$. The CNOT gate can be obtained by setting $U = X$. Sometimes we want to control a unitary only if the control qubit is zero rather than 1. In this case, we represent the control using a hollow circle as shown below.

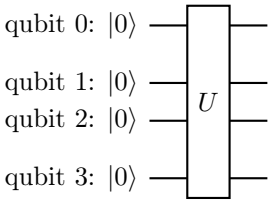


Another commonly used two-qubit gate is the **SWAP gate**, which swaps the state in the 0-th and the 1-st qubits.



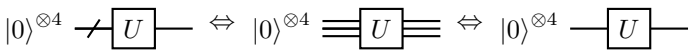
Exercise 2.4. Write down the matrix representation of the SWAP gate.

Quantum operators applied to multiple qubits can be written in a similar manner:

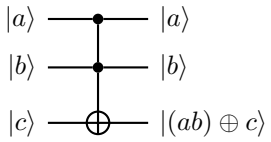


For a multi-qubit quantum circuit, unless stated otherwise, the first qubit will be referred to as the qubit 0, and the second qubit as the qubit 1, etc.

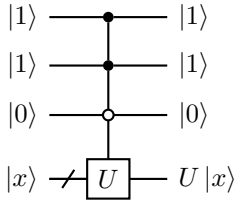
When the context is clear, we may also use a more compact notation for the multi-qubit quantum operators:



One useful multiple qubit gate is the **Toffoli gate** (or controlled-controlled-NOT, CCNOT gate).



We may also want to apply a n-qubit unitary U only when certain conditions are met

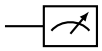


where the empty circle means that the gate being controlled only becomes active when the value of the control qubit is 0. This can be used to write down the quantum "if" statements, i.e., when the qubits $0, 1$ are at the $|1\rangle$ state and the qubit 2 is at the $|0\rangle$ state, then apply U to $|x\rangle$.

A set of qubits is often called a **quantum register** (or register for short). For example, in the picture above, the main quantum state of interest (an n qubit quantum state $|x\rangle$) is called the system register. The first 3 qubits can be called the control register. When multiple registers are present, we can distinguish them by writing $|x\rangle_A |y\rangle_B$, so that we can refer to the quantum state associated with the qubits in registers A and B, respectively.

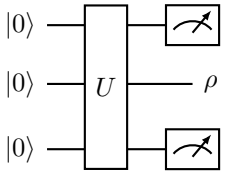
In quantum computation, a classical bit-string is denoted as $x \in \{0,1\}^n$, and the corresponding $|x\rangle$ is called a **classical state**. The set of all classical states form the **computational basis** of an n-qubit system. It is worth noting that $\{|x\rangle \langle x| \, | x \in \{0,1\}^n\}$ forms a set of projective measurement operators, which can be identified with the simultaneous measurement with respect to Pauli-Z operators $Z_1, \ldots, Z_n$. Consequently, when a measurement is performed with respect to the Pauli-Z operator, it is called a measurement in the computational basis.

The circuit symbol for the quantum measurement with respect to a single Pauli-Z is



Example 2.35 (Measure Pauli-Z operators)**.** For a quantum state $|\psi\rangle$, the measurement of a multi-qubit Pauli-Z operator of the form $(Z_1)^{a_1} \cdots (Z_n)^{a_n}$, where $a_1, \ldots, a_n \in \{0,1\}$ can be directly implemented at the circuit level. For example, for a 3-qubit system, the following circuit

(2.87)



measures the outcome of Z_1 and Z_3, yielding 4 possible outcomes $\{00, 01, 10, 11\}$ with respective probabilities $\{p(00), p(01), p(10), p(11)\}$. Now consider an observable $O = Z_1 Z_3$ whose eigenvalues are 1 and -1. The probability of obtaining each eigenvalue is

$$p(O = 1) = p(00) + p(11), \quad p(O = -1) = p(01) + p(10). \tag{2.88}$$

◇

Example 2.36 (**Hadamard test circuit**)**.** The Hadamard test is a useful tool for computing the expectation value of an unitary operator with respect to a state, i.e., $\langle\psi|U|\psi\rangle$. It can be used to solve the phase estimation problem. The Hadamard test uses two circuits to estimate the real and imaginary part of the expectation value separately.

The (real) Hadamard test is the quantum circuit in Fig. 2.1 for estimating $\mathrm{Re}\,\langle\psi|U|\psi\rangle$.

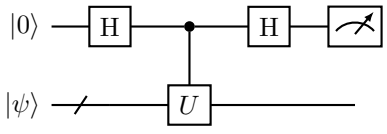


FIGURE 2.1. Hadamard test for $\mathrm{Re}\,\langle\psi|U|\psi\rangle$.

To verify this, we find that the circuit transforms $|0\rangle|\psi\rangle$ as

$$\begin{aligned}|0\rangle|\psi\rangle &\xrightarrow{\mathrm{H}\otimes I} \frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)|\psi\rangle \\ &\xrightarrow{c\text{-}U} \frac{1}{\sqrt{2}}(|0\rangle|\psi\rangle+|1\rangle U|\psi\rangle) \\ &\xrightarrow{\mathrm{H}\otimes I} \frac{1}{2}|0\rangle(|\psi\rangle+U|\psi\rangle)+\frac{1}{2}|1\rangle(|\psi\rangle-U|\psi\rangle).\end{aligned}$$

The probability of measuring the qubit 0 to be in state $|0\rangle$ is

$$p(0)=\frac{1}{2}(1+\operatorname{Re}\langle\psi|U|\psi\rangle). \tag{2.89}$$

This is well defined since $-1\le \operatorname{Re}\langle\psi|U|\psi\rangle\le 1$.

To obtain the imaginary part, we can use the circuit in Fig. 2.2 called the (imaginary) Hadamard test, where

$$S=\begin{pmatrix}1&0\\0&i\end{pmatrix} \tag{2.90}$$

is called the phase gate.

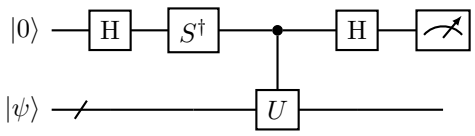


FIGURE 2.2. Hadamard test for $\operatorname{Im}\langle\psi|U|\psi\rangle$.

Similar calculation shows the circuit transforms $|0\rangle|\psi\rangle$ to the state

$$\frac{1}{2}|0\rangle(|\psi\rangle-iU|\psi\rangle)+\frac{1}{2}|1\rangle(|\psi\rangle+iU|\psi\rangle). \tag{2.91}$$

Therefore the probability of measuring the qubit 0 to be in state $|0\rangle$ is

$$p(0)=\frac{1}{2}(1+\operatorname{Im}\langle\psi|U|\psi\rangle). \tag{2.92}$$

Combining the results from the two circuits, we obtain the estimate to $\langle\psi|U|\psi\rangle$.

◇

Example 2.37 (Overlap estimate using the SWAP test)**.** A special case of the Hadamard test is called the **SWAP test**, which can be used to estimate the overlap of two quantum states $|\langle\varphi|\psi\rangle|$. The quantum circuit for the swap test is

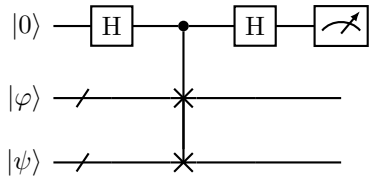


FIGURE 2.3. Circuit for the SWAP test.

Note that this is exactly the Hadamard test with U being the swap gate. Direct calculation shows that the probability of measuring the first qubit and obtaining outcome 0 is

$$p(0) = \frac{1}{2}(1 + \mathrm{Re}\,\langle\varphi, \psi|\psi, \varphi\rangle) = \frac{1}{2}(1 + |\langle\varphi|\psi\rangle|^2). \tag{2.93}$$

◇

2.5. Copy operation and no-cloning theorem

Most computer programs on classical computers have an assignment of the form $y = x$, or $y = \mathrm{copy}(x)$, which stores the value in the variable x in a new location in memory as a variable y. In scientific computation, this is the foundation of iterative methods, which solve a problem by making progress gradually. For example, classical iterative algorithms for solving linear systems require storing intermediate variables. It is therefore striking that such a basic step is explicitly ruled out by quantum mechanics.

The **no-cloning theorem** is an early result in quantum computation: it forbids a universal quantum copy operation (see also [NC00, Section 12.1]).

THEOREM 2.38 (No cloning). *Given a fixed state $|s\rangle$ (e.g. $|s\rangle = |0^n\rangle$), there is no unitary operator U that acts as a copy operation, in the sense that for every state $|x\rangle$,*

$$U|x\rangle \otimes |s\rangle = |x\rangle \otimes |x\rangle\,. \tag{2.94}$$

PROOF. Assume such a U exists. Take two states $|x_1\rangle, |x_2\rangle$ such that $0 < |\langle x_1|x_2\rangle| < 1$. Then

$$U\big(|x_1\rangle \otimes |s\rangle\big) = |x_1\rangle \otimes |x_1\rangle\,, \quad U\big(|x_2\rangle \otimes |s\rangle\big) = |x_2\rangle \otimes |x_2\rangle\,. \tag{2.95}$$

Taking the inner product of the two equations and using unitarity,

$$\langle x_1|x_2\rangle = \langle x_1, s|x_2, s\rangle = \langle x_1, s|U^\dagger U|x_2, s\rangle = \langle x_1, x_1|x_2, x_2\rangle = \langle x_1|x_2\rangle^2\,. \tag{2.96}$$

Hence $\langle x_1|x_2\rangle \in \{0, 1\}$, contradicting $0 < |\langle x_1|x_2\rangle| < 1$. □

There are two important special cases in which copying is possible without contradicting Theorem 2.38. The first is that $|x\rangle$ is not arbitrary: it is a specific state for which we know a preparation procedure, i.e., $|x\rangle = U_x|s\rangle$ for a known unitary U_x and some fixed state $|s\rangle$. Then we can prepare a second copy of $|x\rangle$ via

$$(I \otimes U_x)|x\rangle \otimes |s\rangle = |x\rangle \otimes |x\rangle\,. \tag{2.97}$$

The second is copying classical information in the computational basis, using the CNOT gate. i.e.,

$$\mathrm{CNOT}\,|x, 0\rangle = |x, x\rangle\,, \quad x \in \{0, 1\}. \tag{2.98}$$

The same principle applies to copying classical information from multiple qubits. Fig. 2.4 gives an example of copying the classical information stored in 3 bits.

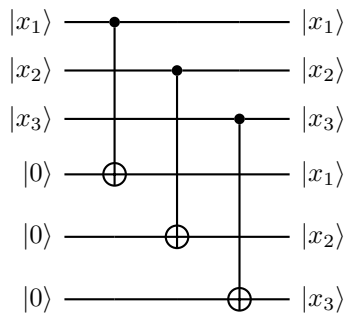


FIGURE 2.4. Copying classical information using multi-qubit CNOT gates.

In general, multi-qubit CNOT operations can be used to perform classical copying in the computational basis. Note that in the circuit model, this can be implemented with a depth-1 circuit, since these CNOT gates act on disjoint sets of qubits.

The copying of classical information is compatible with Theorem 2.38 in the following sense. The proof of Theorem 2.38 uses two non-orthogonal states $|x_1\rangle, |x_2\rangle$ to obtain a contradiction. However, all states in the computational basis are orthogonal to each other. Therefore, there exist unitaries that copy a specified orthonormal set of states, but a universal quantum copy operation is impossible.

Example 2.39. Let us verify that the CNOT gate does not violate the no-cloning theorem, i.e., it cannot be used to copy a general superposition $|x\rangle = a|0\rangle + b|1\rangle$. Direct calculation shows

$$\text{CNOT}\,|x\rangle \otimes |0\rangle = a|00\rangle + b|11\rangle \neq |x\rangle \otimes |x\rangle \tag{2.99}$$

unless $ab = 0$. In particular, if $|x\rangle = |+\rangle$, then CNOT creates a Bell state. ◇

Similar to the quantum no-cloning theorem, there does not exist a unitary U that performs a "deleting" operation which resets an unknown state $|x\rangle$ to $|0^n\rangle$:

$$U|0^n\rangle \otimes |x\rangle = |0^n\rangle \otimes |0^n\rangle \tag{2.100}$$

for all $|x\rangle$. Indeed, if $|x_1\rangle, |x_2\rangle$ are orthogonal, then unitarity implies

$$0 = \langle 0^n, x_1|0^n, x_2\rangle = \langle 0^n, x_1|U^\dagger U|0^n, x_2\rangle = \langle 0^n, 0^n|0^n, 0^n\rangle = 1, \tag{2.101}$$

a contradiction.

A more general version of the no-deleting theorem is as follows: given two copies of an arbitrary quantum state, it is impossible to delete one of the copies. Specifically, there is no unitary U performing the following operation using fixed known states $|s\rangle, |s'\rangle$,

$$U|x\rangle|x\rangle|s\rangle = |x\rangle|0^n\rangle|s'\rangle \tag{2.102}$$

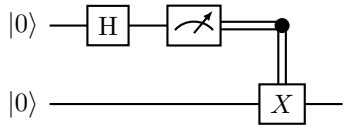
for an arbitrary unknown state $|x\rangle$.

Exercise 2.5. Prove the version of the no-deleting theorem in Eq. (2.102).

2.6. Deferred and implicit measurements

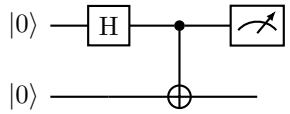
There are two important principles related to quantum measurements: the principle of deferred measurement, and the principle of implicit measurement. At first glance, both principles may seem counterintuitive.

Example 2.40 (Deferring quantum measurements)**.** Consider the circuit



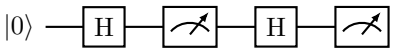
Here the double line denotes a classical control operation. The outcome is that qubit 0 has probability 1/2 of outputting 0, and qubit 1 is in the state $|0\rangle$. Qubit 0 also has probability 1/2 of outputting 1, and qubit 1 is in the state $|1\rangle$.

However, we may replace the classical control operation after the measurement by a quantum controlled X (i.e. CNOT), and measure qubit 0 afterwards:

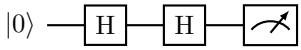


It can be verified that the result is the same. In this sense, CNOT copies the measurement outcome of qubit 0 to qubit 1 in the computational basis. ◇

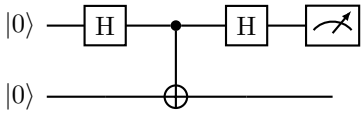
Example 2.41 (Deferring measurement requires extra qubits)**.** The procedure of deferring quantum measurements using CNOTs is general, and important. Consider the following circuit:



The probability of obtaining 0 or 1 is 1/2. However, if we simply "defer" the measurement to the end by removing the intermediate measurement, we obtain

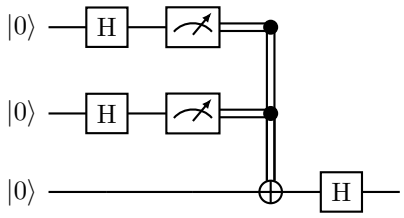


The result of the measurement is deterministically 0! The correct way of deferring the intermediate quantum measurement is to introduce another qubit



Measuring the qubit 0, we obtain 0 or 1 w.p. 1/2, respectively. Hence when deferring quantum measurements, it is necessary to store the intermediate information in extra (ancilla) qubits, even if such information is not used afterwards. ◇

Exercise 2.6. Consider a quantum circuit with three qubits, initially all in state $|0\rangle$. The circuit is as follows:

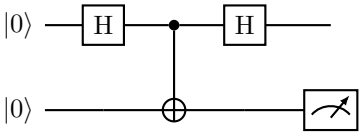


Design a quantum circuit that defers the measurements of the first two qubits to the end, using two additional ancilla qubits to store the intermediate measurement information. After the deferred measurements, describe the final states of all qubits. Ensure the overall effect on the ancilla qubits is the same as if the measurements were performed immediately.

The **principle of deferred measurement** states that in a quantum circuit, measurement operations can be postponed from an intermediate stage to the end of the circuit. This remains true even when a measurement at an intermediate step determines the conditional control of subsequent gates: such classical controls can be replaced by quantum controls. One use of this principle is to simplify quantum circuits and their analysis, by expressing the computation as a unitary circuit (possibly using ancilla qubits) followed by measurements at the end.

The **principle of implicit measurements** states that, for predicting the statistics of the qubits that are measured at the end of a circuit, it is irrelevant whether other qubits are explicitly measured at the end or simply left unmeasured.

Example 2.42. Consider the circuit:



Before the measurement, the final state is $\frac{1}{2}(|00\rangle + |01\rangle) + \frac{1}{2}(|10\rangle - |11\rangle)$. So measuring qubit 1 yields 0 and 1 with equal probability.

If we measure qubit 0 first, verify that qubit 1 will be in the mixed state

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|, \tag{2.103}$$

so if we measure qubit 1 afterwards, we again obtain 0 and 1 with equal probability. ◇

Why does the principle of implicit measurement hold? Assume the quantum system consists of two subsystems A and B. Recall from Eq. (2.74) that a measurement on subsystem A only depends on the reduced density matrix ρ_A. Thus it suffices to show that ρ_A does not depend on whether B is measured. Let $\{P_i\}$ be the projectors onto the computational basis of B, and let the joint state be ρ. If we measure subsystem B and discard the outcome, the joint state becomes

$$\rho' = \sum_i (I \otimes P_i)\rho(I \otimes P_i). \tag{2.104}$$

Then

$$\rho'_A = \mathrm{Tr}_B[\rho'] = \sum_i \mathrm{Tr}_B[(I \otimes P_i)\rho(I \otimes P_i)] = \sum_i \mathrm{Tr}_B[\rho(I \otimes P_i)] = \mathrm{Tr}_B\left[\rho\big(I \otimes \sum_i P_i\big)\right] = \mathrm{Tr}_B[\rho] = \rho_A. \tag{2.105}$$

Therefore, if the qubits in A are to be measured at the end of the circuit, the measurement statistics do not depend on whether the qubits in B are measured or not.

2.7. Sparse matrix, Majorana, fermionic, and bosonic operators

Sparse matrices are among the most important examples of very large matrices that can be efficiently encoded on quantum computers. They are also closely related to many physical Hamiltonians in practical applications.

Definition 2.43 (s-sparse matrix)**.** *A matrix $A \in \mathbb{C}^{M\times N}$ is called s-sparse if each row and column of the matrix contains at most s non-zero entries.*

Example 2.44. A diagonal matrix is 1-sparse. Any diagonal matrix $A \in \mathbb{C}^{2^n\times 2^n}$ can be written as a linear combination of Pauli Z-operators

$$A = \sum_{i_1,\ldots,i_n\in\{0,1\}} J_{i_1,\ldots,i_n}\sigma_{i_1,1}\cdots\sigma_{i_n,n}, \tag{2.106}$$

where $\sigma_{s,k}$ is equal to Z_k if $s = 1$ and I if $s = 0$. Any permutation matrix Π is 1-sparse. A row and column permutation of a 1-sparse matrix is 1-sparse. Any 1-sparse matrix A can be written as ΠD or $D\Pi'$, where D is a diagonal matrix and Π, Π' are permutation matrices. A tridiagonal matrix is 3-sparse. The following matrix

$$A = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \\ \vdots & & & \vdots \\ 1 & 0 & \cdots & 0 \end{pmatrix} = \left(\sum_{i=1}^{N} e_i\right) e_1^\top \in \mathbb{R}^{N\times N} \tag{2.107}$$

has only one nonzero entry per row, but it is **not** 1-sparse since the first column has N nonzero entries. ◇

Definition 2.45. *The maximal absolute value of the entries of $A \in \mathbb{C}^{M\times N}$, also called the **max norm**, is defined as:*

$$\|A\|_{\max} := \max_{i,j} |A_{ij}| . \tag{2.108}$$

Lemma 2.46. *Let $A \in \mathbb{C}^{N\times N}$ be s-sparse. Then*

$$\|A\| \le s \|A\|_{\max} . \tag{2.109}$$

Proof. For any row i of A, the set of nonzero column indices is denoted by $\mathcal{C}_i$. By Cauchy-Schwarz,

$$|(Ax)_i|^2 = \left|\sum_{j\in\mathcal{C}_i} A_{ij}x_j\right|^2 \le \sum_{j\in\mathcal{C}_i} |A_{ij}|^2 \sum_{j\in\mathcal{C}_i} |x_j|^2 \le s \|A\|_{\max}^2 \sum_{j\in\mathcal{C}_i} |x_j|^2 . \tag{2.110}$$

Then

$$\|Ax\|^2 \le s \|A\|_{\max}^2 \sum_i \sum_{j\in\mathcal{C}_i} |x_j|^2 . \tag{2.111}$$

The condition that A is s-sparse implies that for each j, there are at most s indices i such that $A_{ij} \neq 0$, i.e., j belongs to at most s sets among $\{\mathcal{C}_i\}_i$. Therefore each j can appear at most s times in the double sum. This means

$$\|Ax\|^2 \leq s^2 \|A\|_{\max}^2 \sum_j |x_j|^2 = s^2 \|A\|_{\max}^2 \|x\|^2 . \tag{2.112}$$

Taking the supremum over $x \neq 0$ yields $\|A\| \leq s \|A\|_{\max}$. □

The equality in Lemma 2.46 can be reached by considering a matrix B whose upper left $s \times s$ block is $\|A\|_{\max} ee^\top$, where e is an all 1 vector of length s. Direct computation shows that $\|B\| = s \|A\|_{\max}$.

A useful lemma is that the product of any 1-sparse matrices is 1-sparse.

Lemma 2.47. *Let A and B be $N \times N$ 1-sparse matrices. Then $C = AB$ is also 1-sparse.*

Proof. Since A, B are 1-sparse, there exists permutation matrices Π, Π' and diagonal matrices D, D' so that $A = \Pi D, B = D'\Pi'$. Therefore

$$C = \Pi(DD')\Pi' \tag{2.113}$$

is a permutation of a diagonal matrix, and is therefore 1-sparse. □

Example 2.48. All Pauli gates in $\mathcal{P}_n$ are 1-sparse. This can be proved by induction. First, all Pauli matrices I, X, Y, Z are 1-sparse matrices. Assume all Pauli gates in $\mathcal{P}_{n-1}$ are 1-sparse, then an element in $\mathcal{P}_n$ can always be constructed (up to a reordering of qubits) as

$$P \otimes P_1, \quad P \in \mathcal{P}_{n-1}, P_1 \in \mathcal{P}_1. \tag{2.114}$$

This replaces a nonzero entry in P by a 2×2 matrix that is 1-sparse, so the overall matrix is still 1-sparse. ◇

Example 2.49 (Majorana operator)**.** For a fermionic system defined on n modes, the state space $\mathcal{F} = \otimes_{i=1}^n \mathbb{C}^2 \cong \mathbb{C}^{2^n}$ is called the Fock space. The Majorana fermion operators (or Majorana operators for short) denoted by $\{\gamma_i\}_{i=1}^{2n}$, are Hermitian operators in $L(\mathbb{C}^{2^n})$ satisfying the anticommutation relations:

$$\{\gamma_i, \gamma_j\} := \gamma_i\gamma_j + \gamma_j\gamma_i = 2\delta_{ij}, \quad i, j = 1, \ldots, 2n. \tag{2.115}$$

The canonical realization of Majorana operators is through Pauli operators. When $n = 1$, we simply have

$$\gamma_1 = X, \quad \gamma_2 = Y. \tag{2.116}$$

For the n mode system, the Majorana operators can be defined using the **Jordan–Wigner transformation**,

$$\gamma_{2j-1} = \left(\prod_{k=1}^{j-1} Z_k\right) X_j, \quad \gamma_{2j} = \left(\prod_{k=1}^{j-1} Z_k\right) Y_j, \quad j = 1, \ldots, n. \tag{2.117}$$

So Majorana operators are also 1-sparse matrices. Furthermore, any product of Majorana operators $\gamma_{i_1} \cdots \gamma_{i_k}$, $i_1, \cdots, i_k \in \{1, \ldots, 2n\}$ is 1-sparse. ◇

Example 2.50 (Fermionic operator)**.** For a fermionic system defined on n modes with the Fock space $\mathcal{F} = \otimes_{i=1}^{n} \mathbb{C}^2 \cong \mathbb{C}^{2^n}$, the fermionic creation and annihilation operators, denoted by $a_i^\dagger$ and a_i respectively, are operators in $L(\mathbb{C}^{2^n})$ that satisfy the **canonical anticommutation relations** (CAR):

$$\{a_i, a_j^\dagger\} := a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij},\ \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0, \quad i, j = 1, \ldots, n. \tag{2.118}$$

The creation operator $a_i^\dagger$ adds a fermion to the mode i, while the annihilation operator a_i removes a fermion from the mode i.

For a single mode system,

$$a = X^+ = \frac{1}{2}(X + iY) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad a^\dagger = X^- = \frac{1}{2}(X - iY) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{2.119}$$

In this convention $a^\dagger |0\rangle = |1\rangle, a^\dagger |1\rangle = 0$, $a |1\rangle = |0\rangle, a |0\rangle = 0$. Here $|s\rangle$ denotes the state with s fermions ($s = 0, 1$). The number operator $\hat{n} = a^\dagger a = \frac{1}{2}(1 - Z)$ satisfies $\hat{n} |s\rangle = s |s\rangle$.

For an n-mode system, the fermionic operators are related to the Majorana operators according to the relation:

$$a_i = \frac{1}{2}(\gamma_{2i-1} + i\gamma_{2i}), \quad a_i^\dagger = \frac{1}{2}(\gamma_{2i-1} - i\gamma_{2i}), \quad i = 1, \ldots, n, \tag{2.120}$$

where γ_{2i-1} and γ_{2i} are the Majorana operators associated with the i-th fermionic mode. Therefore any operator defined using a linear combination of fermionic creation and annihilation operators can be expressed as a linear combination of Majorana operators, and vice versa.

From the Jordan–Wigner transformation,

$$a_j = \left(\prod_{k=1}^{j-1} Z_k\right) X_j^+, \quad a_j^\dagger = \left(\prod_{k=1}^{j-1} Z_k\right) X_j^-, \tag{2.121}$$

with

$$X_j^+ = \frac{1}{2}(X_j + iY_j), \quad X_j^- = \frac{1}{2}(X_j - iY_j). \tag{2.122}$$

Since $X^\pm$ are 1-sparse matrices, $a_j^\dagger, a_j, a_j^\dagger a_j, a_j a_j^\dagger$ are also 1-sparse. Furthermore, any product of fermionic operators $a_{i_1}^\dagger \cdots a_{i_k}^\dagger a_{j_1} \cdots a_{j_l}$ is 1-sparse. ◇

Example 2.51 (Bosonic operator)**.** For an n-mode bosonic systems, the bosonic creation and annihilation operators, denoted by $b_i^\dagger$ and b_i respectively, are operators that satisfy the **canonical commutation relations** (CCR):

$$[b_i, b_j^\dagger] := b_i b_j^\dagger - b_j^\dagger b_i = \delta_{ij}, \quad [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0, \quad i, j = 1, \ldots, n. \tag{2.123}$$

The creation operator $b_i^\dagger$ adds a boson to the mode i, while the annihilation operator b_i removes a boson from the mode i.

When $n = 1$, these operators satisfy

$$b |0\rangle = 0, \quad b |s\rangle = \sqrt{s} |s - 1\rangle, s = 1, 2, \ldots, \tag{2.124}$$

and

$$b^\dagger |s\rangle = \sqrt{s + 1} |s + 1\rangle, s = 0, 1, 2, \ldots. \tag{2.125}$$

Here $|s\rangle$ denotes a state with s bosons. We also have

$$b^\dagger b |s\rangle = s |s\rangle. \tag{2.126}$$

In the matrix form, we can write

$$b = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad b^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{2.127}$$

These operators are infinite dimensional operators, i.e., operators defined in an infinite dimensional space. They are also 1-sparse. Furthermore, $\|b\|, \left\|b^\dagger\right\| = \infty$, so unlike any finite dimensional matrices, these operators are unbounded. The physical reason is that a single bosonic mode can accommodate an infinite number of bosons, and the energy of a system with an infinite number of bosons in a single mode is infinity.

Due to the commutation relation, multi-mode bosonic operators can be defined using tensor products:

$$b_i = I^{\otimes(i-1)} \otimes b \otimes I^{\otimes(n-i)}, \quad b_i^\dagger = I^{\otimes(i-1)} \otimes b^\dagger \otimes I^{\otimes(n-i)}, \quad i = 1, \ldots, n, \tag{2.128}$$

where the identity operator $I |s\rangle = |s\rangle$ also acts on an infinite dimensional space.

The precise characterization of the Hilbert space for unbounded operators is beyond the scope of this book. However, if we truncate the state space of each bosonic mode to a finite dimensional space with d levels, i.e., $\mathbb{C}^d$, the state space of a bosonic system defined on n modes with d levels per mode is $\mathcal{F} = \otimes_{i=1}^n \mathbb{C}^d \cong \mathbb{C}^{d^n}$ and is finite dimensional.

In a single-mode truncated bosonic system, $b, b^\dagger$ are finite dimensional matrices:

$$b = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & \sqrt{2} & 0 & \cdots & 0 \\ 0 & 0 & 0 & \sqrt{3} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \sqrt{d-1} \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad b^\dagger = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ \sqrt{1} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \sqrt{2} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \sqrt{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \sqrt{d-1} & 0 \end{pmatrix}. \tag{2.129}$$

These are 1-sparse matrices of size $d \times d$. Then the multi-mode operators defined in Eq. (2.128) are 1-sparse matrices. Using Lemma 2.47, the product of any multi-mode bosonic operators $b_{i_1}^\dagger \cdots b_{i_k}^\dagger b_{j_1} \cdots b_{j_l}$, where $b, b^\dagger$ are truncated bosonic creation and annihilation operators defined in Eq. (2.129) are 1-sparse matrices. ◇

Exercise 2.7. Prove that the truncated bosonic creation and annihilation operators defined in Eq. (2.129) satisfy the modified commutation relation

$$[b, b^\dagger] = 1 - \frac{d}{(d-1)!} \left(b^\dagger\right)^{d-1} (b)^{d-1}. \tag{2.130}$$

2.8. Selected examples of Hamiltonians in physics, chemistry, and optimization

With the introduction of spin, Majorana, fermionic, and bosonic operators, we can provide several examples of Hamiltonians encountered in applications. Although we will not use all of these examples to illustrate the performance of quantum algorithms, the algorithms in this book can be applied to any of them.

2.8.1. Condensed matter physics.

Example 2.52 (Transverse field Ising model)**.** The Hamiltonian for the one dimensional transverse field Ising model (TFIM) with nearest neighbor interaction of length n is

$$H = -\sum_{i=1}^{n-1} Z_i Z_{i+1} - g\sum_{i=1}^{n} X_i, \tag{2.131}$$

where g is the coupling constant. ◇

Example 2.53 (1D Heisenberg model)**.** The Hamiltonian for the 1D Heisenberg model with nearest neighbor interaction is given by

$$H = -J\sum_{i=1}^{n-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{2.132}$$

where J is the interaction strength and $\mathbf{S}_i$ represents the spin operator at site i, defined as

$$\mathbf{S}_i = \frac{1}{2}\begin{pmatrix} X_i \\ Y_i \\ Z_i \end{pmatrix}. \tag{2.133}$$

We can decompose this Hamiltonian into three terms, each associated with the x, y, and z components of the spins:

$$H_x = -\frac{J}{4}\sum_{i=1}^{n-1} X_i X_{i+1}, \quad H_y = -\frac{J}{4}\sum_{i=1}^{n-1} Y_i Y_{i+1}, \quad H_z = -\frac{J}{4}\sum_{i=1}^{n-1} Z_i Z_{i+1}. \tag{2.134}$$

When $J > 0$ the problem is called ferromagnetic, and when $J < 0$ it is called anti-ferromagnetic. ◇

Example 2.54 (2D Heisenberg model)**.** The Hamiltonian for the 2D Heisenberg model on a square lattice is given by:

$$H = -J\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}(\mathbf{S}_{i,j} \cdot \mathbf{S}_{i+1,j} + \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1}) \tag{2.135}$$

We decompose this Hamiltonian into three terms associated with the x, y, and z components of the spins:

$$\begin{aligned} H_x &= -\frac{J}{4}\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}(X_{i,j}X_{i+1,j} + X_{i,j}X_{i,j+1}), \\ H_y &= -\frac{J}{4}\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}(Y_{i,j}Y_{i+1,j} + Y_{i,j}Y_{i,j+1}), \\ H_z &= -\frac{J}{4}\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}(Z_{i,j}Z_{i+1,j} + Z_{i,j}Z_{i,j+1}). \end{aligned} \tag{2.136}$$

◇

Example 2.55 (k-Local Hamiltonian)**.** A k-local Hamiltonian is a quantum Hamiltonian where each term acts nontrivially on at most k qubits. One convenient way to write such a Hamiltonian on n qubits is as a linear combination of Pauli strings of weight at most k. For example, one may write

$$H = \sum_{S\subseteq[n],\,|S|\leq k} \sum_{\alpha\in\{0,1,2,3\}^S} J_{S,\alpha} \prod_{i\in S} \sigma_{\alpha(i),i}, \tag{2.137}$$

where $\sigma_{0,i} = I$, $\sigma_{1,i} = X_i$, $\sigma_{2,i} = Y_i$, and $\sigma_{3,i} = Z_i$.

For example, consider a 2-local Hamiltonian for an n-qubit system:

$$H = \sum_{i<j} J_{ij}\sigma_i\sigma_j, \tag{2.138}$$

where σ_i, σ_j are Pauli operators acting on qubits i and j, respectively. Transverse Ising models and Heisenberg models are 2-local Hamiltonians. ◇

Example 2.56 (Quadratic fermionic Hamiltonians)**.** Consider the following n-mode fermionic Hamiltonian

$$H = \sum_{k=1}^{n} \lambda_k c_k^\dagger c_k = \sum_{k=1}^{n} \frac{\lambda_k}{2}(1 - Z_k), \tag{2.139}$$

where $c_k^\dagger$ and c_k are new fermionic creation and annihilation operators, and λ_k are real eigenvalues representing the energy levels of the system. The Hamiltonian H is a linear combination of Pauli Z operators and is thus a diagonal matrix.

Now, consider a general quadratic fermionic Hamiltonian of the form:

$$H = \sum_{i,j=1}^{n} A_{ij} a_i^\dagger a_j, \tag{2.140}$$

where A is a Hermitian matrix. Since A is Hermitian, we can diagonalize it using a unitary transformation U such that:

$$U^\dagger A U = \Lambda, \tag{2.141}$$

where Λ is a diagonal matrix containing the eigenvalues λ_k. Then define

$$c_k = \sum_{i=1}^{n} (U^\dagger)_{ki} a_i, \quad c_k^\dagger = \sum_{i=1}^{n} a_i^\dagger U_{ik}, \quad k = 1, \ldots, n. \tag{2.142}$$

Direct calculation shows that the new set of creation and annihilation operators $\{c_k^\dagger, c_k\}$ satisfy the canonical anticommutation relation. Substituting these transformations into the Hamiltonian,

$$H = \sum_{i,j,k} U_{ik}\lambda_k (U^\dagger)_{kj} a_i^\dagger a_j = \sum_{k=1}^{n} \lambda_k c_k^\dagger c_k, \tag{2.143}$$

we have transformed H into a diagonal Hamiltonian. ◇

Example 2.57 (1D spinless Hubbard model)**.** The Hamiltonian for the 1D spinless Hubbard model with nearest-neighbor interaction is given by:

$$H = -t \sum_{i=1}^{n-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) + U \sum_{i=1}^{n-1} n_i n_{i+1}, \tag{2.144}$$

where t is the hopping parameter, representing the kinetic energy term, and U is the nearest-neighbor interaction strength. The operators $a_i^\dagger$ and a_i are the fermionic creation and annihilation operators at site i, respectively, and $n_i = a_i^\dagger a_i$ is the number operator at site i. When $U = 0$, the Hamiltonian is a quadratic in the fermionic operators and can be turned into a diagonalized form. When $U \neq 0$, the Hamiltonian is no longer quadratic and cannot be turned into a diagonalized Hamiltonian using the same strategy. ◇

Example 2.58 (Uniform electron gas in a plane wave basis)**.** In a plane wave basis, the Hamiltonian for a box of uniform electron gas can be expressed in second quantization as follows:

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} V(\mathbf{q}) c_{\mathbf{k}_1+\mathbf{q}}^\dagger c_{\mathbf{k}_2-\mathbf{q}}^\dagger c_{\mathbf{k}_2} c_{\mathbf{k}_1}, \tag{2.145}$$

where $c_{\mathbf{k}}^\dagger$ and $c_{\mathbf{k}}$ are fermionic creation and annihilation operators for an electron with wave vector $\mathbf{k} \in \mathbb{R}^3$, $\epsilon_{\mathbf{k}} = |\mathbf{k}|^2/2$ is the kinetic energy. The interaction potential $V(\mathbf{q}) = 4\pi/\mathbf{q}^2$ in a plane wave basis is the Fourier transform of the Coulomb potential. ◇

Example 2.59 (Harmonic oscillator)**.** The Hamiltonian for a quantum harmonic oscillator in the first quantization (i.e., real space representation) is given by

$$H = \frac{p^2 + x^2}{2}, \tag{2.146}$$

where $p = -i\partial_x$ is the momentum operator and x is the position operator. Define

$$b = \frac{1}{\sqrt{2}}(x + ip), \quad b^\dagger = \frac{1}{\sqrt{2}}(x - ip), \tag{2.147}$$

then $b, b^\dagger$ satisfy the canonical commutation relation $[b, b^\dagger] = 1$. Furthermore, the Hamiltonian takes the form

$$H = b^\dagger b + \frac{1}{2}. \tag{2.148}$$

If we truncate the bosonic mode to include d levels, the state space is $\mathcal{F} = \mathbb{C}^d$, and H is a diagonal matrix of size $d \times d$. ◇

2.8.2. Quantum chemistry.

Example 2.60 (Quantum chemistry in first quantization)**.** In first quantization, the Hamiltonian for a many-electron system is given in terms of the coordinates and momenta of the electrons. The non-relativistic electronic Hamiltonian for a molecule in atomic units can be expressed as:

$$H = -\sum_{i=1}^{N} \frac{\nabla_i^2}{2} - \sum_{i=1}^{N} \sum_{A=1}^{M} \frac{Z_A}{|\mathbf{r}_i - \mathbf{R}_A|} + \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{A<B} \frac{Z_A Z_B}{|\mathbf{R}_A - \mathbf{R}_B|}, \tag{2.149}$$

where N is the number of electrons, M is the number of nuclei, $\mathbf{r}_i$ and $\mathbf{R}_A$ are the positions of the i-th electron and the A-th nucleus, respectively, Z_A is the atomic number of the A-th nucleus. This is an unbounded operator. ◇

Example 2.61 (Quantum chemistry in second quantization)**.** In quantum chemistry, the electronic structure of molecules can be described using the formalism of second quantization with n molecular orbitals. The state space $\mathcal{F} = \otimes_{i=1}^n \mathbb{C}^2$ is finite dimensional. The use of second quantization allows

for a compact and efficient representation of the Hamiltonian and facilitates the expression of the Hamiltonian on quantum computers via the Jordan–Wigner transformation. The Hamiltonian of a many-electron system in second quantization is given by

$$H = \sum_{p,q=1}^{n} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s=1}^{n} V_{pqrs} a_p^\dagger a_q^\dagger a_r a_s, \tag{2.150}$$

where $a_p^\dagger$ and a_q are fermionic creation and annihilation operators, respectively. The creation operator $a_p^\dagger$ adds an electron to the molecular orbital p, and the annihilation operator a_q removes an electron from the molecular orbital q. For simplicity we only consider the spatial part of the orbital and omit the spin part. The indices p, q, r, and s label the molecular orbitals, h_{pq} are the one-electron integrals, and V_{pqrs} are the two-electron integrals.

The one-electron integrals h_{pq} are given by

$$h_{pq} = \int \psi_p^*(\mathbf{r}) \left(-\frac{\nabla^2}{2} + V_{\text{ext}}(\mathbf{r}) \right) \psi_q(\mathbf{r})\, d\mathbf{r}, \tag{2.151}$$

where $\psi_p(\mathbf{r})$ is the spatial part of the molecular orbital and $V_{\text{ext}}(\mathbf{r}) = -\sum_{A=1}^{M} \frac{Z_A}{|\mathbf{r}-\mathbf{R}_A|}$ is the external potential due to the nuclei. The two-electron integrals V_{pqrs} are given by

$$V_{pqrs} = \int \int \psi_p^*(\mathbf{r}_1) \psi_q^*(\mathbf{r}_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_r(\mathbf{r}_2) \psi_s(\mathbf{r}_1)\, d\mathbf{r}_1 d\mathbf{r}_2. \tag{2.152}$$

The nuclei-nuclei interaction is a constant and is dropped for simplicity. ◇

Example 2.62 (PPP Model)**.** The Pariser-Parr-Pople (PPP) model is used in quantum chemistry to describe the π-electron systems in conjugated organic molecules. The Hamiltonian for the PPP model can be written as

$$H = \sum_{p,q=1}^{n} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q=1}^{n} V_{pq} n_p n_q, \tag{2.153}$$

where h_{pq} are hopping integral elements, V_{pq} are Coulomb interaction elements, $a_p^\dagger$ and a_p are the fermionic creation and annihilation operators at site p, and $n_p = a_p^\dagger a_p$ is the number operator. The Hubbard model is a special case of the PPP model with short ranged hopping and Coulomb interaction elements. Compared to the full chemistry Hamiltonian in second quantization, the two-body interaction coefficients V_{pq} have only $\mathcal{O}(n^2)$ entries but can still represent long range interactions. ◇

2.8.3. Quantum field theory.

Example 2.63 (Schwinger Model in 1D)**.** The Schwinger model describes quantum electrodynamics in $1+1$ dimensions. The state space for the Schwinger model is the tensor product of two spaces: a tensor product of $n+1$ fermionic spaces and a product of n gauge field spaces. The total Fock space is given by

$$\mathcal{F} = \left(\bigotimes_{i=1}^{n+1} \mathbb{C}^2 \right) \otimes \left(\bigotimes_{j=1}^{n} \mathbb{C}^d \right), \tag{2.154}$$

where $d = 2L+1$ is the number of levels the gauge field can take. There are two operators that we need to define that act on the gauge field space. The first is E_j^2, which is a diagonal operator that

counts the energy stored in the gauge field with index $j \in \{1, \ldots, n\}$. The second is U_j, which adds one to the value stored in the gauge field register and is analogous to a bosonic creation operator. The action of these operators is given formally below:

$$E_j^2 = \sum_{\varepsilon=-L}^{L} \varepsilon^2 \left|\varepsilon\right\rangle_j \left\langle\varepsilon\right|_j, \quad U_j = \sum_{\varepsilon=-L}^{L} \left|\varepsilon+1\right\rangle_j \left\langle\varepsilon\right|_j, \quad U_j^\dagger = \sum_{\varepsilon=-L}^{L} \left|\varepsilon-1\right\rangle_j \left\langle\varepsilon\right|_j. \tag{2.155}$$

Here we assume for U_j and its adjoint that the gauge field satisfies periodic boundary conditions at the cutoff located at $\varepsilon = \pm L$.

The Hamiltonian for the Schwinger model is given by:

$$H = \sum_{j=1}^{n} E_j^2 \otimes I_2^{\otimes(n+1)} + \nu \sum_{j=1}^{n} \left[U_j \otimes a_j^\dagger a_{j+1} - U_j^\dagger \otimes a_j a_{j+1}^\dagger\right] + \mu \sum_{j=1}^{n} (-1)^j I_d^{\otimes n} \otimes a_j^\dagger a_j, \tag{2.156}$$

where a_i and $a_i^\dagger$ are the fermionic annihilation and creation operators at site i, and I_m denotes the identity operator of dimension m. The parameters μ, ν are related to parameters such as the lattice spacing. ◇

Example 2.64 (Quadratic Majorana operators)**.** From the Jordan–Wigner transformation in Eq. (2.117), and use the fact that $XY = iZ$, we find that

$$H = -i \sum_{k=1}^{n} \lambda_k \gamma_{2k-1} \gamma_{2k} = \sum_{k=1}^{n} \lambda_k Z_k, \quad \lambda_k \in \mathbb{R} \tag{2.157}$$

is a diagonal Hamiltonian.

Consider a quadratic Hamiltonian of the form:

$$H = -i \sum_{1 \le p < q \le 2n} A_{pq} \zeta_p \zeta_q = -\frac{i}{2} \sum_{p,q=1}^{2n} A_{pq} \zeta_p \zeta_q, \tag{2.158}$$

where A is a real antisymmetric matrix, and $\{\zeta_p\}_{p=1}^{2n}$ is a set of Majorana operators. There exists an orthogonal matrix O such that:

$$O^\top A O = \bigoplus_{k=1}^{n} \begin{pmatrix} 0 & \lambda_k \\ -\lambda_k & 0 \end{pmatrix} =: \Lambda \tag{2.159}$$

where λ_k are the singular values of A. Now define a set of transformed Majorana operators

$$\gamma_j = \sum_p \zeta_p O_{pj} = \sum_p (O^\top)_{jp} \zeta_p, \quad j = 1, \ldots, 2n, \tag{2.160}$$

then we still have

$$\{\gamma_j, \gamma_{j'}\} = 2\delta_{j,j'}. \tag{2.161}$$

The transformed Hamiltonian takes a diagonal form

$$H = -\frac{i}{2} \sum_{1 \le j, j' \le 2n} \gamma_j (\Lambda)_{jj'} \gamma_{j'} = -i \sum_{k=1}^{n} \lambda_k \gamma_{2k-1} \gamma_{2k}. \tag{2.162}$$

The quadratic fermionic Hamiltonian in Example 2.56 is a special case of this example. ◇

Example 2.65 (SYK Model)**.** The Sachdev-Ye-Kitaev (SYK) model is a quantum mechanical model of n Majorana fermions with random all-to-all interactions. The Hamiltonian for the SYK model is given by

$$H = \sum_{1 \le i < j < k < l \le 2n} J_{ijkl} \gamma_i \gamma_j \gamma_k \gamma_l, \tag{2.163}$$

where γ_i are the Majorana fermion operators, and J_{ijkl} are random coupling constants, typically drawn from a Gaussian distribution. The SYK model is of particular interest due to its connections to quantum chaos, holography, and black hole physics. ◇

2.8.4. Optimization.

Example 2.66 (k-SAT problem)**.** Classical optimization problems, such as the k-SAT problem, can be represented using a Hamiltonian. The k-SAT problem is a type of Boolean satisfiability problem where each clause contains exactly k literals. The goal is to find an assignment to the Boolean variables that satisfies all the clauses. The most famous examples are 2-SAT (classically easy), and 3-SAT (NP-complete).

Consider a k-SAT problem with n Boolean variables $x_1, x_2, \ldots, x_n$ and m clauses $C_1, C_2, \ldots, C_m$. Each clause C_i is a disjunction of exactly k literals.

We can construct a Hamiltonian H such that its ground state corresponds to the solution of the k-SAT problem. The Hamiltonian for the k-SAT problem can be written as:

$$H = \sum_{i=1}^{m} H_{C_i}, \tag{2.164}$$

where H_{C_i} is the Hamiltonian for the i-th clause. Each clause Hamiltonian H_{C_i} is designed to be zero if the clause is satisfied and positive otherwise. For clauses involving single literals, such as $C_k = (x_p)$ or $C_l = (\bar{x}_q)$, the Hamiltonians H_{C_k} and H_{C_l} are:

$$H_{C_k} = \frac{1}{2}\left(1 + Z_p\right), \quad H_{C_l} = \frac{1}{2}\left(1 - Z_q\right). \tag{2.165}$$

For a clause $C_i = (x_p \vee \bar{x}_q)$, the corresponding Hamiltonian H_{C_i} can be written using the product

$$H_{C_i} = \frac{1}{4}\left(1 + Z_p\right)\left(1 - Z_q\right). \tag{2.166}$$

For a general clause $C_i = (l_1 \vee l_2 \vee \cdots \vee l_k)$, where l_j represents either x_{p_j} or $\bar{x}_{p_j}$, the corresponding Hamiltonian H_{C_i} can be written using the Pauli-Z operator Z:

$$H_{C_i} = \prod_{j=1}^{k} \frac{1 + z_j Z_{p_j}}{2}, \tag{2.167}$$

where $z_j = +1$ if $l_j = x_{p_j}$ and $z_j = -1$ if $l_j = \bar{x}_{p_j}$. The Hamiltonian H is diagonal and positive semidefinite. If the smallest eigenvalue (called the ground state energy) of H is 0, then the associated eigenvector (called the ground state, which may not be unique) corresponds to the Boolean variable assignment that satisfies all the clauses of the k-SAT problem. ◇

Example 2.67 (MAX-CUT problem)**.** The MAX-CUT problem is a well-known combinatorial optimization problem. Given a graph $G = (V, E)$ with a set of vertices V and a set of edges E, the

goal is to partition the vertices into two subsets such that the number of edges between the subsets is maximized. Assume the graph has n vertices, and the Hamiltonian for the MAX-CUT problem can be written as:

$$H = -\sum_{(i,j)\in E} \frac{1}{2}\left(1 - Z_i Z_j\right). \tag{2.168}$$

Each term $-\frac{1}{2}(1 - Z_i Z_j)$ equals -1 if vertices i and j are in different subsets and 0 if they are in the same subset. Therefore, minimizing H is equivalent to maximizing the number of edges that are cut by the partition. ◇

Part II

Foundation

CHAPTER 3

Probability, quantum channel, and distances

We begin by reviewing basic concepts in classical probability theory, which provides intuition for how errors propagate in randomized processes. We then introduce quantum channels as the general framework for quantum dynamics. Unlike ideal quantum circuits which are unitary, real-world quantum processes often involve noise and decoherence. Quantum channels allow us to model these effects, as well as measurements and interactions with the environment. We explain the requirements (specifically, the concept of complete positivity) for a map to be a valid quantum channel and describe standard representations such as the Kraus and Stinespring forms.

With this framework in place, we introduce distance measures for quantum states. For pure states, we use norms that account for the global phase. For mixed states, we introduce the trace distance and fidelity. These two measures are complementary: trace distance relates to the distinguishability of states via measurement, while fidelity captures their overlap and behaves well under quantum operations.

Finally, we discuss how to compare quantum channels. This requires norms that are stable even when the channels act on part of an entangled system. This leads us to the diamond norm, which is the standard metric for quantifying the error of quantum operations.

3.1. Basic notions in probability theory

Probability theory is a subject that carries nearly as many profound surprises as quantum theory itself. In this section, we introduce some basic concepts in probability theory, focusing on finite-dimensional spaces. In quantum computing, the probability distributions associated with an n-qubit system reside in 2^n-dimensional spaces.

Definition 3.1. *Let Σ be a finite set called a state space, or sample space, where each element of Σ is called an event. A **probability distribution** is a function $\mathbb{P} : \Sigma \to [0, 1]$, which can be represented as a vector in a Euclidean space, and satisfies $\sum_{s\in\Sigma} \mathbb{P}(s) = 1$.*

Let Σ_A and Σ_B be sample spaces and let $\mathbb{P}_A$ and $\mathbb{P}_B$ be probability distributions on the two sample spaces. These distributions are said to be independent if the joint distribution, $\mathbb{P}_{AB}$ on the set $\Sigma_A \times \Sigma_B$ obeys $\mathbb{P}_{AB} = \mathbb{P}_A \otimes \mathbb{P}_B$. The expectation value (or average value) of a function mapping $f : \Sigma \mapsto \mathbb{C}$ is defined to be $\mathbb{E}(f) := \sum_{s\in\Sigma} f(s)\mathbb{P}(s) = \langle f, \mathbb{P}\rangle$.

Example 3.2. As an example, let us consider rolling a four-sided die. Here the random variable is the outcome of the experiment; the sample space is $\{1, 2, 3, 4\}$ and the probability distribution (for a fair die) is $1/4$ for each of these outcomes. The random variable, x, in this case corresponds to the result of the die.

In the event that we wanted to find the probability that the sample is a prime number, we could redefine the sample space and the underlying distribution but it is easier to use the indicator-function property of the distribution to see that

$$\mathbb{P}(x \in \{2,3\}) = \mathbb{E}(\mathbf{1}_{\{2,3\}}) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}. \tag{3.1}$$

In general, this approach is often the easiest way to compute a probability because it constructs an indicator function which projects onto the fraction of the sample space that we want to measure. Note this is also true in quantum theory wherein the probability of measuring a mixed state, ρ, to be a pure state $|\psi\rangle$ is

$$\mathbb{P}(|\psi\rangle) = \mathrm{Tr}(|\psi\rangle\langle\psi|\rho) = \langle\psi|\,\rho\,|\psi\rangle\,. \tag{3.2}$$

Here the projector $|\psi\rangle\langle\psi|$ plays the same role as the indicator function used above, and further illustrates the close ties between probability theory and quantum theory. ⋄

Similar to the amplitude of the wave function in quantum theory, there is not a single unifying interpretation of probability. For this reason we recommend that the reader be well versed in both interpretations as each can convey useful intuitions.

The following bound, known as the union bound, is very useful for estimating probabilities of events. We provide it as well as its proof as an elementary example of probability theory.

THEOREM 3.3 (Union Bound). *Let Σ be a sample space and let $A, B \subseteq \Sigma$ and let $\mathbb{P}$ be a probability distribution on Σ. We then have*

$$\mathbb{P}(A \cup B) = \mathbb{E}(\mathbf{1}_A + \mathbf{1}_B - \mathbf{1}_A\mathbf{1}_B) \leq \mathbb{P}(A) + \mathbb{P}(B). \tag{3.3}$$

PROOF. Intuitively, by looking at a Venn diagram for events A and B it is clear that the region $A \cup B$ contains region A and region B but also may include region $A \cap B$. Thus the upper bound given above overcounts the probability in the intersection and therefore it is an upper bound. Formally, we use linearity of expectation:

$$\mathbb{E}(\mathbf{1}_A + \mathbf{1}_B - \mathbf{1}_A\mathbf{1}_B) = \mathbb{E}(\mathbf{1}_A) + \mathbb{E}(\mathbf{1}_B) - \mathbb{E}(\mathbf{1}_A\mathbf{1}_B). \tag{3.4}$$

Next, $\mathbb{E}(\mathbf{1}_A\mathbf{1}_B) = \sum_{s\in\Sigma} \mathbb{P}(s)(\mathbf{1}_A(s)\mathbf{1}_B(s)) \geq 0$, and $\mathbb{E}(\mathbf{1}_A) = \mathbb{P}(A)$, $\mathbb{E}(\mathbf{1}_B) = \mathbb{P}(B)$. Combining these gives the claim. □

Example 3.4 (Failure Propagation Bound)**.** Consider the following problem: you have a quantum algorithm that succeeds with probability $1 - \delta$ and fails with probability δ. Suppose we run the algorithm independently N times; determine a value of δ that guarantees the probability of at least one failure is at most $1/3$. This problem appears ubiquitously in quantum computing in problems such as phase estimation or quantum error correction where the probability of failure needs to be considered and extra computational resources are needed to suppress them.

The N events each have a probability of δ assigned to them and so we expect that the total probability of at least one error happening will be from the union bound $N\delta$. We can validate this inductively. For the base case we see trivially that the claim holds for $N = 1$. For the induction step, let us assume that the probability of at least one error occuring in the first $N-1$ steps is at most $(N-1)\delta$. From the union bound the probability of failing in the next sample is δ and thus the total failure probability is at most $(N-1)\delta + \delta = N\delta$. Thus if we want to see a failure probability of $1/3$ it suffices to take

$$\delta \leq \frac{1}{3N}. \tag{3.5}$$

This example shows that worst case scenario that the failure probability for our algorithm grows linearly. This actually might seem strange to the reader since the error probability compounds exponentially in practice; however, linear growth of error is actually in this context worse than exponential because for large enough N the union bound will be greater than 1 whereas the exponential upper bound is always less than 1. In this context, surprisingly, linear growth is worse than exponential but nonetheless the simplicity and generality of union bounds often provide good enough bounds that are easy to manipulate. ◇

The natural operations on probability distributions are stochastic transformations, which can be represented as transition matrices. We define these transformations below.

Definition 3.5. *Let Σ be a sample space of size N and let $p \in \mathbb{R}^N$ be the column vector representation of a probability distribution. A valid transformation on the state space of the register X to itself has a matrix representation $P : \mathbb{R}^N \to \mathbb{R}^N$, which maps p to Pp. The matrix P is called a* ***transition matrix*** *and satisfies*

(1) $P_{ij} \geq 0, \quad \forall i, j \in [N]$,
(2) $\sum_{i \in [N]} P_{ij} = 1, \quad \forall j \in [N]$.

Remark 3.6. In classical probability theory, the probability distribution is often written as a row vector. Then the transition matrix is applied from the right as pP, and the transition matrix needs to be **right stochastic** or **row stochastic**, i.e., $\sum_{j \in [N]} P_{ij} = 1$ for all $i \in [N]$. Given a probability distribution $p \in \mathbb{R}^N$, a natural quantum state encoding the distribution p (also called a coherent version of p) is

$$|\sqrt{p}\rangle = \sum_i \sqrt{p_i}\, |i\rangle \,. \tag{3.6}$$

This is a normalized state. It is thus more natural to view p as a column vector so that the usual rule of applying an operator to a state vector applies. A matrix satisfying the properties in Definition 3.5 is also called **left stochastic** or **column stochastic**. Any j-th column of P, denoted by $P_{:,j}$, is a probability distribution. If P is both left and right stochastic, then it is called a **doubly stochastic** matrix. ◇

Example 3.7. Let us consider how we would represent an AND gate in this language. The AND gate has the property that for any $x, y \in \{0, 1\}$, $\mathrm{AND}(x, y) = xy$. This operation is an example of an irreversible operation, meaning that it cannot be inverted from the outputs to find the inputs. In this case the natural vector space for probability distributions for two bits can be represented as a probability vector in $\mathbb{R}^2 \otimes \mathbb{R}^2$. As we are using square matrices to represent these transformations we will take $\mathrm{AND}(e_x \otimes e_y) = e_0 \otimes e_{xy}$ for computational basis vectors e_0, e_1 and $x, y \in \{0, 1\}$. Specifically then we have that the gate can be represented as a stochastic matrix P_{AND}

$$P_{\mathrm{AND}} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.7}$$

We see that the matrix representation is stochastic, but not doubly stochastic.

If we consider taking two distributions for our bits $p_x = [a, 1-a]^\top$ and $p_y = [b, 1-b]^\top$ for $a, b \in [0, 1]$ then we can see that the distribution that we get from applying the AND operation to

the distribution on the bits is

$$P_{\mathrm{AND}}(p_x \otimes p_y) = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} ab \\ a(1-b) \\ b(1-a) \\ (1-a)(1-b) \end{pmatrix} = \begin{bmatrix} (a+b)-ab \\ 1-(a+b)+ab \\ 0 \\ 0 \end{bmatrix}. \tag{3.8}$$

This output distribution makes intuitive sense. The AND output is 1 only if both inputs are 1, which occurs with probability $(1-a)(1-b)$, corresponding to the second entry above. Equivalently, the probability that the AND output is 0 is the probability that at least one input is 0, namely $a+b-ab$, corresponding to the first entry. ◇

3.2. Quantum channels

The concept of a quantum channel generalizes both the unitary evolution of isolated quantum systems, as governed by the Schrödinger equation, and the stochastic evolution of classical probability distributions. It provides a unified framework for describing the most general physically permissible evolution of quantum states, encompassing coherent dynamics (e.g., unitary transformations) and incoherent processes such as measurement, decoherence, and interactions with an environment.

We begin by defining the mathematical objects under consideration. A **superoperator** is a linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$. We denote the action of $\mathcal{Q}$ on an operator $A \in L(\mathbb{C}^N)$ by $\mathcal{Q}[A]$ or $\mathcal{Q}(A)$.

Given two superoperators $\mathcal{Q}_1 : L(\mathbb{C}^{N_1}) \to L(\mathbb{C}^{M_1})$ and $\mathcal{Q}_2 : L(\mathbb{C}^{N_2}) \to L(\mathbb{C}^{M_2})$, their **tensor product** $\mathcal{Q}_1 \otimes \mathcal{Q}_2$ is the unique linear map $L(\mathbb{C}^{N_1} \otimes \mathbb{C}^{N_2}) \to L(\mathbb{C}^{M_1} \otimes \mathbb{C}^{M_2})$ satisfying

$$(\mathcal{Q}_1 \otimes \mathcal{Q}_2)[A_1 \otimes A_2] = \mathcal{Q}_1[A_1] \otimes \mathcal{Q}_2[A_2] \tag{3.9}$$

for all $A_1 \in L(\mathbb{C}^{N_1})$ and $A_2 \in L(\mathbb{C}^{N_2})$. This definition extends to all operators by linearity.

Just as a unitary transformation maps a state vector to another state vector while preserving its norm, a **quantum channel** is a superoperator intended to map a density operator to another density operator. A fundamental example is the **identity channel** $\mathcal{I} : L(\mathbb{C}^N) \to L(\mathbb{C}^N)$, defined by $\mathcal{I}[A] = A$ for any $A \in L(\mathbb{C}^N)$.

Example 3.8. The action of the tensor product of superoperators is particularly important when analyzing local operations on composite systems. Let $\mathcal{I}_K : L(\mathbb{C}^K) \to L(\mathbb{C}^K)$ be the identity map and $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ be a linear map. Consider an operator $A \in L(\mathbb{C}^K \otimes \mathbb{C}^N)$. We can represent A in block form with respect to an orthonormal basis $\{|i\rangle\}$ of $\mathbb{C}^K$:

$$A = \sum_{i,j \in [K]} |i\rangle\langle j| \otimes A_{ij}, \quad A_{ij} \in L(\mathbb{C}^N). \tag{3.10}$$

The action of $\mathcal{I}_K \otimes \mathcal{Q}$ is given by applying $\mathcal{Q}$ to each block:

$$(\mathcal{I}_K \otimes \mathcal{Q})[A] = \sum_{i,j \in [K]} |i\rangle\langle j| \otimes \mathcal{Q}[A_{ij}]. \tag{3.11}$$

For instance, if $K = 2$, the matrix representation is

$$(\mathcal{I}_2 \otimes \mathcal{Q}) \left[\begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} \right] = \begin{pmatrix} \mathcal{Q}[A_{00}] & \mathcal{Q}[A_{01}] \\ \mathcal{Q}[A_{10}] & \mathcal{Q}[A_{11}] \end{pmatrix} \in L(\mathbb{C}^2 \otimes \mathbb{C}^M). \tag{3.12}$$

◇

To ensure that a superoperator maps density operators (which are positive semidefinite and have unit trace) to density operators, it must satisfy certain constraints.

Definition 3.9. *A linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ is called:* ***positive*** *if $\mathcal{Q}[A]$ is positive semidefinite for every positive semidefinite $A \in L(\mathbb{C}^N)$. $\mathcal{Q}$ is called* ***trace preserving*** *(TP) if $\mathrm{Tr}(\mathcal{Q}[A]) = \mathrm{Tr}(A)$ for every $A \in L(\mathbb{C}^N)$.*

While it might seem sufficient to define a quantum channel simply as a positive, trace-preserving map, the structure of quantum mechanics demands a stronger condition. Quantum systems often exist as subsystems of larger, composite systems. If $\mathcal{Q}$ describes the evolution of a system S, and S is potentially entangled with an ancillary system A, the evolution of the joint system is described by $\mathcal{I}_A \otimes \mathcal{Q}$. For this joint evolution to be physically valid, $\mathcal{I}_A \otimes \mathcal{Q}$ must also map density operators to density operators, meaning it must be a positive map, regardless of the dimension of the ancilla A. This requirement leads to the concept of complete positivity.

Definition 3.10. *A linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ is* ***completely positive*** *(CP) if for all integers $K \geq 1$, the map $\mathcal{I}_K \otimes \mathcal{Q} : L(\mathbb{C}^K \otimes \mathbb{C}^N) \to L(\mathbb{C}^K \otimes \mathbb{C}^M)$ is positive.*

It is worth noting that the ordering of the tensor product in the definition is immaterial. One could equivalently require that $\mathcal{Q} \otimes \mathcal{I}_K$ be positive for all K. Physically, this reflects the fact that the labeling of the ancillary system is arbitrary. Mathematically, the maps $\mathcal{I} \otimes \mathcal{Q}$ and $\mathcal{Q} \otimes \mathcal{I}$ are related via the SWAP operator (the isomorphism that exchanges the tensor factors). Specifically, they are unitarily equivalent:

$$\mathcal{Q} \otimes \mathcal{I} = \mathcal{U}_{\mathrm{SWAP}} \circ (\mathcal{I} \otimes \mathcal{Q}) \circ \mathcal{U}_{\mathrm{SWAP}}^{-1}, \tag{3.13}$$

where the superoperator $\mathcal{U}_{\mathrm{SWAP}}$ acts as $\mathcal{U}_{\mathrm{SWAP}}[X] = \mathrm{SWAP} \cdot X \cdot \mathrm{SWAP}^\dagger$. Since $X \succeq 0$ if and only if $UXU^\dagger \succeq 0$ for any unitary U, it follows that $\mathcal{I} \otimes \mathcal{Q}$ is positive if and only if $\mathcal{Q} \otimes \mathcal{I}$ is positive.

While positivity ensures that the channel acts correctly on the system itself, complete positivity is strictly stronger, ensuring correct action even when the system is entangled with an ancilla.

Example 3.11 (Positive map that is not completely positive)**.** Consider the transpose map $\mathcal{T} : L(\mathbb{C}^2) \to L(\mathbb{C}^2)$, defined by $\mathcal{T}[A] = A^\top$ with respect to the computational basis. If A is positive, its eigenvalues are non-negative. Since A and $A^\top$ share the same spectrum, $A^\top$ is also positive. Thus, $\mathcal{T}$ is a positive map.

However, $\mathcal{T}$ is not completely positive. To illustrate this, consider a two-qubit system in the maximally entangled Bell state $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. The corresponding density operator is:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|). \tag{3.14}$$

We apply the map $\mathcal{I} \otimes \mathcal{T}$ (the partial transpose with respect to the second subsystem) to this state:

$$(\mathcal{I} \otimes \mathcal{T})[\rho] = \frac{1}{2}(|00\rangle\langle 00| + |01\rangle\langle 10| + |10\rangle\langle 01| + |11\rangle\langle 11|). \tag{3.15}$$

In the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, the matrix representation is

$$\frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.16}$$

This matrix has eigenvalues $\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\}$. Since one eigenvalue is negative, the resulting operator is not positive. Thus, $\mathcal{T}$ is not completely positive. ◇

We now arrive at the formal definition of a quantum channel.

Definition 3.12 (Quantum channel, or CPTP map)**.** *A **quantum channel** $\mathcal{Q}$ is a linear map $L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ that is completely positive (CP) and trace preserving (TP).*

If $\mathcal{Q}$ is a quantum channel, it maps any density operator $\rho \in \mathcal{D}(\mathbb{C}^N)$ to a density operator $\mathcal{Q}[\rho] \in \mathcal{D}(\mathbb{C}^M)$. The complete positivity condition ensures that if $\mathcal{Q}$ acts locally on a subsystem of a larger entangled state $\widetilde{\rho} \in \mathcal{D}(\mathbb{C}^K \otimes \mathbb{C}^N)$, the resulting state $(\mathcal{I}_K \otimes \mathcal{Q})[\widetilde{\rho}]$ remains a valid density operator in $\mathcal{D}(\mathbb{C}^K \otimes \mathbb{C}^M)$. This property is fundamental to the consistency of quantum mechanics.

Example 3.13. A fundamental class of quantum channels is the **unitary channel**. This requires the input and output dimensions to be equal, $N = M$. Given a unitary matrix $U \in \mathrm{U}(N)$, the corresponding channel $\mathcal{U} : L(\mathbb{C}^N) \to L(\mathbb{C}^N)$ acts by conjugation:

$$\mathcal{U}[\rho] = U\rho U^\dagger. \tag{3.17}$$

This map is trace-preserving, as $\mathrm{Tr}[U\rho U^\dagger] = \mathrm{Tr}[\rho U^\dagger U] = \mathrm{Tr}[\rho]$. It is also completely positive, as we will see shortly. The identity channel $\mathcal{I}$ is a unitary channel with $U = I$. ◇

A powerful way to characterize and construct quantum channels is through the Kraus representation.

Proposition 3.14. *Let $\{K_j\}_{j\in[R]}$ be a set of matrices in $\mathbb{C}^{M\times N}$ satisfying the completeness relation*

$$\sum_{j\in[R]} K_j^\dagger K_j = I_N. \tag{3.18}$$

Then the linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ defined by

$$\mathcal{Q}[\rho] = \sum_{j\in[R]} K_j \rho K_j^\dagger \tag{3.19}$$

is a quantum channel (CPTP).

Proof. We first verify complete positivity. Let L be an arbitrary integer and consider any positive operator $X \in L(\mathbb{C}^L \otimes \mathbb{C}^N)$. The action of the extended map is

$$(\mathcal{I}_L \otimes \mathcal{Q})[X] = \sum_{j\in[R]} (I_L \otimes K_j) X (I_L \otimes K_j)^\dagger. \tag{3.20}$$

For any operator A, if X is positive, then $AXA^\dagger$ is also positive. Thus, each term in the summation is a positive operator. Since the sum of positive operators is positive, $\mathcal{I}_L \otimes \mathcal{Q}$ is a positive map for all L. Thus, $\mathcal{Q}$ is completely positive.

Next, we verify the trace-preserving property. For any $\rho \in L(\mathbb{C}^N)$, using the linearity and the cyclic property of the trace, we have

$$\mathrm{Tr}[\mathcal{Q}[\rho]] = \sum_{j\in[R]} \mathrm{Tr}[K_j \rho K_j^\dagger] = \mathrm{Tr}\left[\rho \left(\sum_{j\in[R]} K_j^\dagger K_j\right)\right]. \tag{3.21}$$

Substituting the completeness relation $\sum_{j\in[R]} K_j^\dagger K_j = I_N$, we obtain $\mathrm{Tr}[\rho I_N] = \mathrm{Tr}[\rho]$. Therefore, $\mathcal{Q}$ is trace-preserving. □

The representation in Eq. (3.19) is called the **Kraus form** or the **operator sum representation** of the channel. The operators $\{K_j\}$ are known as Kraus operators. For example, the unitary channel in Example 3.13 is in Kraus form with a single Kraus operator $K_0 = U$.

We can now explore the connection between classical stochastic evolution and quantum channels. This correspondence highlights that quantum mechanics is a generalization of classical probability theory.

For any probability distribution $p \in \mathbb{R}^N$, we can embed it into a quantum state

$$\rho = \sum_{i\in[N]} p_i |i\rangle\langle i|. \tag{3.22}$$

This diagonal density matrix is called a **classical state** or **probabilistic state**.

Given a (column) stochastic matrix $P \in \mathbb{R}^{M\times N}$ (i.e., $P_{ij} \geq 0$ and $\sum_{i\in[M]} P_{ij} = 1$ for all $j \in [N]$), which defines a classical Markov process mapping distribution p to $p' = Pp$, we can construct a corresponding **classical channel** $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ defined by

$$\mathcal{Q}[\rho] = \sum_{i\in[M],j\in[N]} P_{ij} |i\rangle\langle j|\rho|j\rangle\langle i|. \tag{3.23}$$

If ρ is a classical state, $\mathcal{Q}[\rho]$ is also a classical state corresponding to the evolved probability distribution p'.

Exercise 3.1. Prove that the classical channel $\mathcal{Q}$ defined in Eq. (3.23) is indeed a quantum channel (CPTP).

The fact that classical channels are a subset of quantum channels suggests that any advantage offered by quantum computation must stem from the utilization of the off-diagonal entries of the density matrix (coherence) and the structure of non-classical channels.

We now present several examples of important quantum channels, typically modeling different types of noise processes in qubits ($N = M = 2$).

Example 3.15 (Bit flip and phase flip channels)**.** The bit flip channel $\mathcal{Q}_{\text{bf}}$ describes a process where the qubit state is flipped (i.e., X gate applied) with probability $1-p$, and remains unchanged with probability p:

$$\mathcal{Q}_{\text{bf}}[\rho] = p\rho + (1-p)X\rho X, \quad 0 \leq p \leq 1. \tag{3.24}$$

This is in Kraus form with $K_0 = \sqrt{p}I$ and $K_1 = \sqrt{1-p}X$.

Similarly, the phase flip channel $\mathcal{Q}_{\text{pf}}$ flips the relative phase (i.e., Z gate applied) with probability $1-p$:

$$\mathcal{Q}_{\text{pf}}[\rho] = p\rho + (1-p)Z\rho Z, \quad 0 \leq p \leq 1. \tag{3.25}$$

This channel is also known as the **dephasing channel**, as it suppresses coherences while leaving populations unchanged. ◇

Example 3.16 (Depolarizing channel)**.** The depolarizing channel $\mathcal{Q}_{\text{dp}} : L(\mathbb{C}^N) \to L(\mathbb{C}^N)$ models a process where the state remains intact with probability p, and is replaced by the maximally mixed state I/N with probability $1-p$:

$$\mathcal{Q}_{\text{dp}}[\rho] = p\rho + \frac{1-p}{N} I, \quad 0 \leq p \leq 1. \tag{3.26}$$

◇

Example 3.17 (Amplitude damping channel)**.** The amplitude damping channel $\mathcal{Q}_{\text{ad}} : L(\mathbb{C}^2) \to L(\mathbb{C}^2)$ models energy dissipation, such as spontaneous emission, where an excited state $|1\rangle$ decays to the ground state $|0\rangle$ with probability γ. It is described by the Kraus operators

$$K_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-\gamma} \end{pmatrix}, \quad K_1 = \begin{pmatrix} 0 & \sqrt{\gamma} \\ 0 & 0 \end{pmatrix}, \quad 0 \leq \gamma \leq 1. \tag{3.27}$$

◇

Perhaps surprisingly, the converse of Proposition 3.14 is also true: every quantum channel can be written in the Kraus form. This fundamental result demonstrates that the abstract definition of a CPTP map is equivalent to the constructive definition provided by the operator sum representation.

THEOREM 3.18 (Choi–Kraus Representation). *A linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ is a quantum channel if and only if there exists a set of matrices $\{K_j\}_{j\in[R]}$ in $\mathbb{C}^{M\times N}$, with $R \leq NM$, satisfying the completeness relation $\sum_{j\in[R]} K_j^\dagger K_j = I_N$, such that $\mathcal{Q}$ takes the form*

$$\mathcal{Q}(\rho) = \sum_{j\in[R]} K_j \rho K_j^\dagger. \tag{3.28}$$

PROOF. The "if" part is established by Proposition 3.14. We now prove the "only if" part using a technique known as the **Choi-Jamiołkowski isomorphism**.

Let $\mathcal{Q}$ be a quantum channel. Define an unnormalized maximally entangled vector on $\mathbb{C}^N \otimes \mathbb{C}^N$:

$$|\gamma\rangle\!\rangle = \sum_{i\in[N]} |i\rangle \otimes |i\rangle\,. \tag{3.29}$$

Let $\mathcal{I}_N$ denote the identity map on the first N-dimensional register (the ancilla). By the complete positivity of $\mathcal{Q}$, the map $\mathcal{I}_N \otimes \mathcal{Q}$ is positive. Therefore, the **Choi matrix** defined as

$$\sigma = (\mathcal{I}_N \otimes \mathcal{Q})[|\gamma\rangle\!\rangle\langle\!\langle\gamma|] \in L(\mathbb{C}^N \otimes \mathbb{C}^M) \tag{3.30}$$

is a positive operator.

The Choi matrix completely characterizes the channel $\mathcal{Q}$. To see this, we use a key property of the maximally entangled vector. Let $|\psi\rangle = \sum_i \psi_i |i\rangle \in \mathbb{C}^N$ be a normalized state, so $\sum_i |\psi_i|^2 = 1$. Let $|\widetilde{\psi}\rangle = \sum_i \overline{\psi_i} |i\rangle$ be its element-wise conjugate in the computational basis; this vector is also normalized. We can verify the identity:

$$(\langle\widetilde{\psi}| \otimes I_N)|\gamma\rangle\!\rangle = \sum_{i,j} \psi_j (\langle j|i\rangle \otimes |i\rangle) = \sum_i \psi_i |i\rangle = |\psi\rangle\,. \tag{3.31}$$

We can recover the action of the channel on $|\psi\rangle\langle\psi|$ by taking the partial inner product of σ with $|\widetilde{\psi}\rangle$ on the first register. By the definition of the tensor product map and the identity above, we have:

$$\begin{aligned} (\langle\widetilde{\psi}| \otimes I_M)\sigma(|\widetilde{\psi}\rangle \otimes I_M) &= (\langle\widetilde{\psi}| \otimes I_M)(\mathcal{I}_N \otimes \mathcal{Q})[|\gamma\rangle\!\rangle\langle\!\langle\gamma|](|\widetilde{\psi}\rangle \otimes I_M) \\ &= \mathcal{Q}\left[(\langle\widetilde{\psi}| \otimes I_N)|\gamma\rangle\!\rangle\langle\!\langle\gamma|(|\widetilde{\psi}\rangle \otimes I_N)\right] \\ &= \mathcal{Q}(|\psi\rangle\langle\psi|). \end{aligned} \tag{3.32}$$

Since σ is positive, we can perform its eigendecomposition. Let $R = \operatorname{rank}(\sigma) \leq NM$. We write

$$\sigma = \sum_{j\in[R]} |s_j\rangle\!\rangle\langle\!\langle s_j|, \tag{3.33}$$

where $|s_j\rangle\!\rangle \in \mathbb{C}^N \otimes \mathbb{C}^M$ are, in general, unnormalized vectors obtained by scaling normalized eigenvectors by the square roots of the corresponding eigenvalues.

For each $j \in [R]$, we define a linear operator $K_j : \mathbb{C}^N \to \mathbb{C}^M$ via the relation (sometimes called vectorization or flattening):

$$K_j |\psi\rangle := (\langle\widetilde{\psi}| \otimes I_M)|s_j\rangle\!\rangle . \tag{3.34}$$

Substituting the decomposition of σ back into the recovery formula:

$$\begin{aligned} \mathcal{Q}(|\psi\rangle\langle\psi|) &= (\langle\widetilde{\psi}| \otimes I_M) \left(\sum_{j\in[R]} |s_j\rangle\!\rangle\langle\!\langle s_j| \right) (|\widetilde{\psi}\rangle \otimes I_M) \\ &= \sum_{j\in[R]} \left[(\langle\widetilde{\psi}| \otimes I_M)|s_j\rangle\!\rangle \right] \left[\langle\!\langle s_j|(|\widetilde{\psi}\rangle \otimes I_M) \right] \\ &= \sum_{j\in[R]} (K_j |\psi\rangle)(K_j |\psi\rangle)^\dagger = \sum_{j\in[R]} K_j |\psi\rangle\langle\psi| K_j^\dagger. \end{aligned} \tag{3.35}$$

Since this holds for arbitrary $|\psi\rangle$, by linearity it holds for all operators $\rho \in L(\mathbb{C}^N)$.

Finally, we must verify the completeness relation. The trace-preserving property $\mathrm{Tr}[\mathcal{Q}(\rho)] = \mathrm{Tr}[\rho]$ implies

$$\mathrm{Tr}\left[\sum_{j\in[R]} K_j \rho K_j^\dagger \right] = \mathrm{Tr}\left[\left(\sum_{j\in[R]} K_j^\dagger K_j \right) \rho \right] = \mathrm{Tr}[I_N \rho]. \tag{3.36}$$

Since this equality holds for all ρ, we must have $\sum_{j\in[R]} K_j^\dagger K_j = I_N$. □

The definition of complete positivity in Definition 3.10 requires verifying positivity for all dimensions K, which is operationally cumbersome. However, the proof of the Choi–Kraus theorem reveals that a much simpler criterion suffices. Let $\mathcal{I}_N$ denote the identity channel on $L(\mathbb{C}^N)$. If we assume only that the map $\mathcal{I}_N \otimes \mathcal{Q}$ is positive, then the Choi matrix σ (defined in the proof of Theorem 3.18) must be positive, as it is the image of the positive operator $|\gamma\rangle\!\rangle\langle\!\langle\gamma|$ under this map. As shown in the proof, the positivity of σ guarantees the existence of a Kraus representation for $\mathcal{Q}$. Finally, by Proposition 3.14, any map with a Kraus representation is completely positive (i.e., $\mathcal{I}_K \otimes \mathcal{Q}$ is positive for all K). This establishes the equivalence between the original definition and a condition involving only an ancilla of the input dimension:

Proposition 3.19 (Choi's Theorem)**.** *A linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ is completely positive if and only if its Choi matrix σ is positive semidefinite. Equivalently, $\mathcal{Q}$ is CP if and only if the map $\mathcal{I}_N \otimes \mathcal{Q}$ is positive.*

The Kraus representation provides deep insight into the structure of quantum channels. Another fundamental structural result is the Stinespring dilation theorem, which connects general quantum channels (which may involve decoherence or dissipation) to coherent evolution on a larger Hilbert space.

THEOREM 3.20 (Stinespring dilation). *Given any quantum channel $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$, there exists an ancilla system A of dimension $R \leq NM$, and an isometry $V : \mathbb{C}^N \to \mathbb{C}^M \otimes \mathbb{C}^R$ (i.e., $V^\dagger V = I_N$) such that*

$$\mathcal{Q}(\rho) = \mathrm{Tr}_A \left[V \rho V^\dagger \right]. \tag{3.37}$$

Furthermore, this isometry can always be realized by a unitary evolution U on a sufficiently large joint system initialized with the ancilla in a fixed state $|0\rangle$:

$$\mathcal{Q}(\rho) = \mathrm{Tr}_A \left[U(\rho \otimes |0\rangle\langle 0|)U^\dagger \right]. \tag{3.38}$$

Proof. By the Choi–Kraus theorem (Theorem 3.18), $\mathcal{Q}$ has a Kraus representation $\mathcal{Q}(\rho) = \sum_{j\in[R]} K_j \rho K_j^\dagger$, where $R \le NM$.

We construct the isometry $V : \mathbb{C}^N \to \mathbb{C}^M \otimes \mathbb{C}^R$. Let $\{|j\rangle\}$ be an orthonormal basis for the ancilla space $\mathbb{C}^R$. Define V by

$$V|\psi\rangle = \sum_{j\in[R]} (K_j|\psi\rangle) \otimes |j\rangle. \tag{3.39}$$

We verify that V is an isometry. For any $|\psi\rangle \in \mathbb{C}^N$:

$$\begin{aligned} \langle\psi|V^\dagger V|\psi\rangle &= \|V|\psi\rangle\|^2 = \sum_{j\in[R]} \|K_j|\psi\rangle\|^2 \\ &= \sum_{j\in[R]} \langle\psi|K_j^\dagger K_j|\psi\rangle = \langle\psi| \left(\sum_j K_j^\dagger K_j \right) |\psi\rangle. \end{aligned} \tag{3.40}$$

By the completeness relation, this equals $\langle\psi|\psi\rangle$. Thus $V^\dagger V = I_N$.

Now we verify the representation in Eq. (3.37). We compute $V\rho V^\dagger$. It is helpful to view V formally as $V = \sum_j K_j \otimes |j\rangle$. Then

$$V\rho V^\dagger = \left(\sum_i K_i \otimes |i\rangle \right) \rho \left(\sum_j K_j^\dagger \otimes \langle j| \right) = \sum_{i,j} (K_i \rho K_j^\dagger) \otimes |i\rangle\langle j|. \tag{3.41}$$

Tracing over the ancilla (the second register) yields

$$\mathrm{Tr}_A[V\rho V^\dagger] = \sum_{i,j} (K_i \rho K_j^\dagger) \,\mathrm{Tr}[|i\rangle\langle j|] = \sum_j K_j \rho K_j^\dagger = \mathcal{Q}(\rho). \tag{3.42}$$

To realize this via a unitary evolution, we define U such that its action on the subspace corresponding to the initial state $\rho \otimes |0\rangle\langle 0|$ matches the isometry V. Let the joint space be large enough (e.g., dimension $D = \max(N, M)R$). We define U such that

$$U(|\psi\rangle \otimes |0\rangle) = V|\psi\rangle, \quad \forall |\psi\rangle \in \mathbb{C}^N. \tag{3.43}$$

(We might need to embed $\mathbb{C}^N$ and $\mathbb{C}^M \otimes \mathbb{C}^R$ into the larger space $\mathbb{C}^D$). Since V is an isometry, this definition is norm-preserving. We can always extend this definition to a full unitary U on the joint space.

Finally, we verify the representation in Eq. (3.38). Let $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ be the spectral decomposition.

$$\begin{aligned} U(\rho \otimes |0\rangle\langle 0|)U^\dagger &= \sum_k p_k U(|\psi_k\rangle \otimes |0\rangle)(\langle\psi_k| \otimes \langle 0|)U^\dagger \\ &= \sum_k p_k (V|\psi_k\rangle)(V|\psi_k\rangle)^\dagger = V\rho V^\dagger. \end{aligned} \tag{3.44}$$

Therefore, $\mathcal{Q}(\rho) = \mathrm{Tr}_A[V\rho V^\dagger] = \mathrm{Tr}_A \left[U(\rho \otimes |0\rangle\langle 0|)U^\dagger \right]$. □

Theorem 3.20 states that any quantum channel, no matter how noisy or irreversible it appears, can always be modeled as a unitary interaction between the system and an environment (ancilla), followed by discarding the environment. This provides a powerful conceptual tool, showing that all quantum evolution is fundamentally unitary if we consider a large enough closed system.

3.3. Distance between state vectors and unitaries

A **distance** (also called a **metric**) on a set X is a function $d : X \times X \to \mathbb{R}$ that assigns a real number $d(x, y)$ to each pair of points $x, y \in X$. This function satisfies the following properties for all $x, y, z \in X$:

(1) (Non-negativity) $d(x, y) \geq 0$.
(2) (Identity of indiscernibles) $d(x, y) = 0$ if and only if $x = y$.
(3) (Symmetry) $d(x, y) = d(y, x)$.
(4) (Triangle inequality) $d(x, y) \leq d(x, z) + d(z, y)$.

For example, the vector 2-norm defines a metric on $\mathbb{C}^N : (x, y) \to \|x - y\|$, and the operator norm defines a metric on $\mathrm{U}(N)$: $(U, V) \to \|U - V\|$.

The difference for the product of K unitaries can be bounded using a simple technique sometimes referred to as a "hybrid argument". This technique is used to bound the distance between two states by considering a sequence of "hybrid" unitaries, each of which differs from the next in the sequence by a small amount.

Proposition 3.21 (Linear error growth for products of unitaries)**.** *Given unitaries* $U_1, \widetilde{U}_1, \ldots, U_K, \widetilde{U}_K \in \mathrm{U}(N)$ *satisfying*

$$\left\|U_i - \widetilde{U}_i\right\| \leq \epsilon, \quad \forall i = 1, \ldots, K, \tag{3.45}$$

we have

$$\left\|U_K \cdots U_1 - \widetilde{U}_K \cdots \widetilde{U}_1\right\| \leq K\epsilon. \tag{3.46}$$

Proof. Use a telescoping series

$$\begin{aligned} & U_K \cdots U_1 - \widetilde{U}_K \cdots \widetilde{U}_1 \\ =& (U_K \cdots U_2 U_1 - U_K \cdots U_2 \widetilde{U}_1) + (U_K \cdots U_3 U_2 \widetilde{U}_1 - U_K \cdots U_3 \widetilde{U}_2 \widetilde{U}_1) + \cdots \\ & + (U_K U_{K-1} \cdots \widetilde{U}_1 - \widetilde{U}_K \widetilde{U}_{K-1} \cdots \widetilde{U}_1) \\ =& U_K \cdots U_2 (U_1 - \widetilde{U}_1) + U_K \cdots U_3 (U_2 - \widetilde{U}_2) \widetilde{U}_1 + \cdots + (U_K - \widetilde{U}_K) \widetilde{U}_{K-1} \cdots \widetilde{U}_1. \end{aligned} \tag{3.47}$$

Since all $U_i, \widetilde{U}_i$ are unitary matrices, we readily have

$$\left\|U_K \cdots U_1 - \widetilde{U}_K \cdots \widetilde{U}_1\right\| \leq \sum_{i=1}^{K} \left\|U_i - \widetilde{U}_i\right\| \leq K\epsilon. \tag{3.48}$$

□

It is worth mentioning that the **Duhamel principle** (also called the variation of constants) can be viewed as a continuous-time analogue of the linear error growth property in discrete-time settings.

Proposition 3.22 (Duhamel's principle for Hamiltonian simulation)**.** *Let $H \in \mathbb{C}^{N\times N}$ be a Hermitian matrix and let $B(t) \in \mathbb{C}^{N\times N}$ be an arbitrary time-dependent matrix. Suppose $U(t), \widetilde{U}(t) \in \mathbb{C}^{N\times N}$ form the solutions to the following initial value problems:*

$$i\partial_t U(t) = HU(t), \quad i\partial_t \widetilde{U}(t) = H\widetilde{U}(t) + B(t), \quad \text{with } U(0) = \widetilde{U}(0) = I. \tag{3.49}$$

Then, the solution $\widetilde{U}(t)$ satisfies the integral equation

$$\widetilde{U}(t) = U(t) - i\int_0^t U(t-s)B(s)\,\mathrm{d}s. \tag{3.50}$$

Furthermore, the difference between the propagators is bounded by

$$\left\|\widetilde{U}(t) - U(t)\right\| \le \int_0^t \|B(s)\|\,\mathrm{d}s. \tag{3.51}$$

Proof. We verify Eq. (3.50) by direct differentiation. Let $V(t)$ denote the right-hand side of Eq. (3.50). At $t = 0$, the integral vanishes, so $V(0) = U(0) = I$, which satisfies the initial condition.

Next, we differentiate $V(t)$ with respect to time. Using $\partial_t U(t) = -iHU(t)$ and Leibniz's integral rule, we obtain:

$$\begin{aligned}
\partial_t V(t) &= \partial_t U(t) - i\left(U(0)B(t) + \int_0^t \left[\partial_t U(t-s)\right] B(s)\,\mathrm{d}s\right) \\
&= -iHU(t) - iB(t) - i\int_0^t \left[-iHU(t-s)\right] B(s)\,\mathrm{d}s \\
&= -iH\left(U(t) - i\int_0^t U(t-s)B(s)\,\mathrm{d}s\right) - iB(t) \\
&= -iHV(t) - iB(t).
\end{aligned} \tag{3.52}$$

Multiplying by i, we obtain $i\partial_t V(t) = HV(t) + B(t)$. Thus, $V(t)$ satisfies the defining differential equation for $\widetilde{U}(t)$.

Taking the norm of the integral term yields

$$\left\|\widetilde{U}(t) - U(t)\right\| = \left\|-i\int_0^t U(t-s)B(s)\,\mathrm{d}s\right\| \le \int_0^t \|U(t-s)\|\,\|B(s)\|\,\mathrm{d}s = \int_0^t \|B(s)\|\,\mathrm{d}s, \tag{3.53}$$

which completes the proof. □

An important application of Proposition 3.22 arises when the inhomogeneity takes the form $B(t) = E(t)\widetilde{U}(t)$, where $E(t)$ represents an error term or perturbation. In this case, Eq. (3.50) becomes

$$\widetilde{U}(t) = U(t) - i\int_0^t U(t-s)E(s)\widetilde{U}(s)\,\mathrm{d}s. \tag{3.54}$$

If the perturbed dynamics remains unitary (for example, if $\widetilde{U}$ solves $i\partial_t\widetilde{U}(t) = (H + E(t))\widetilde{U}(t)$ with $E(t)$ Hermitian), then $\left\|\widetilde{U}(s)\right\| = 1$ and the error bound simplifies to

$$\left\|\widetilde{U}(t) - U(t)\right\| \le \int_0^t \left\|E(s)\widetilde{U}(s)\right\|\,\mathrm{d}s \le \int_0^t \|E(s)\|\,\mathrm{d}s. \tag{3.55}$$

This is a continuous-time analogue of Proposition 3.21.

For most of this book, the vector 2-norm and the operator norm distances are both convenient and sufficient. However, they are only applicable to pure states. For measuring the distance between mixed states, new tools will be needed. Even for pure states, unitaries may differ by a phase which should be inconsequential for measuring physical observables. These require the introduction of new metrics.

Two state vectors $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^N$ are physically indistinguishable if they only differ by a global phase. Similarly, two unitary matrices $U, V \in \mathrm{U}(N)$ induce the same evolution on density operators if they only differ by a global phase. Consider the matrices

$$I_+ := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad I_- := \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.56}$$

We have in this case that $\|I_+ - I_-\| = 2$. However, for an arbitrary density matrix ρ, the induced evolution of the density operator under these two operators is

$$\|I_+ \rho I_+ - I_- \rho I_-\| = \left\|\rho - (-1)^2 \rho\right\| = 0. \tag{3.57}$$

This motivates the definition of the global phase invariant distance for vectors and unitary matrices. The subscript p in D_p stands for phase.

Definition 3.23. *Let $|\psi\rangle, |\varphi\rangle \in \mathbb{C}^N$ be two state vectors, their **global phase invariant distance** is*

$$D_p(|\psi\rangle, |\varphi\rangle) := \min_{\phi \in \mathbb{R}} \left\| |\psi\rangle - e^{i\phi} |\varphi\rangle \right\|. \tag{3.58}$$

Definition 3.24. *For two unitaries $U, V \in \mathrm{U}(N)$, their global phase invariant distance is*

$$D_p(U, V) = \min_{\phi \in \mathbb{R}} \left\| U - e^{i\phi} V \right\|. \tag{3.59}$$

An **equivalence relation** on a set X is a binary relation $\sim$ that satisfies the following three properties for all $a, b, c \in X$:

(1) (Reflexivity) $a \sim a$.
(2) (Symmetry) If $a \sim b$, then $b \sim a$.
(3) (Transitivity) If $a \sim b$ and $b \sim c$, then $a \sim c$.

A relation that satisfies these properties is called an equivalence relation, and it partitions the set X into disjoint equivalence classes.

Definition 3.25. *Let X be a set and $\sim$ be an equivalence relation on X. The quotient space (or quotient set) $X/\sim$ is defined as the set of equivalence classes of X under the relation $\sim$. An equivalence class $[x]$ of an element $x \in X$ is the set of all elements in X that are equivalent to x, i.e.,*

$$[x] = \{y \in X \mid y \sim x\}. \tag{3.60}$$

The quotient space $X/\sim$ is the set of all such equivalence classes:

$$X/\sim = \{[x] \mid x \in X\}. \tag{3.61}$$

Example 3.26. Define an equivalence relation on $\mathbb{C}^N$:

$$x \sim y \iff x = \lambda y \text{ for some } \lambda \in \mathbb{C} \setminus \{0\}, \quad x, y \in \mathbb{C}^N \setminus \{0\}. \tag{3.62}$$

Then $\mathrm{P}\mathbb{C}^N := \mathbb{C}^N \setminus \{0\}/\sim$ is called the **complex projective space**, which is isomorphic to the set of all nonzero physical states. The **real dimension** of a manifold M is the number of real coordinates needed to locally describe the manifold. For example, the real dimension of $\mathbb{C}^N$ is $2N$, and the real dimension of $\mathrm{P}\mathbb{C}^N$ is $2N-2$.

We may identify each single qubit quantum state with a unique point on the Bloch sphere as

$$\mathbf{a} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)^\top, \quad \theta, \varphi \in \mathbb{R}. \tag{3.63}$$

This agrees with the previous statement that the real dimension of $\mathrm{P}\mathbb{C}^2$ is 2. ◇

Exercise 3.2. Prove that the global phase invariant distance is a distance on the complex projective space $\mathrm{P}\mathbb{C}^N$.

Example 3.27. Define an equivalence relation on $\mathrm{U}(N)$:

$$U \sim V \iff U = e^{i\theta}V \text{ for some } \theta \in \mathbb{R}, \quad U, V \in \mathrm{U}(N). \tag{3.64}$$

Then $\mathrm{PU}(N) := \mathrm{U}(N)/\sim$ is called the **projective unitary group**. The real dimension of $\mathrm{U}(N)$ is N^2, and the real dimension of $\mathrm{PU}(N)$ is N^2-1.

Recall that the special unitary group $\mathrm{SU}(N)$ consists of all unitary matrices with determinant 1. So the real dimension of $\mathrm{SU}(N)$ is N^2-1. However, the equivalence relation on $\mathrm{SU}(N)$ is

$$U \sim V \iff U = e^{i2\pi k/N}V \text{ for some } k \in [N], \quad U, V \in \mathrm{SU}(N). \tag{3.65}$$

So each equivalence class only consists of N discrete elements and does not reduce the dimension. Therefore the real dimension of the projective special unitary group denoted by $\mathrm{PSU}(N)$ is still N^2-1. ◇

Exercise 3.3. Prove that the global phase invariant distance is a distance on the projective unitary group $\mathrm{PU}(N)$.

Exercise 3.4. Given unitaries $U_1, \widetilde{U}_1, \ldots, U_K, \widetilde{U}_K \in \mathrm{U}(N)$ satisfying

$$D_p(U_i, \widetilde{U}_i) \le \epsilon, \quad \forall i = 1, \ldots, K, \tag{3.66}$$

prove that

$$D_p(U_K \cdots U_1, \widetilde{U}_K \cdots \widetilde{U}_1) \le K\epsilon. \tag{3.67}$$

Let $|\varphi\rangle = e^{i\alpha}\cos\theta\,|\psi\rangle + \sin\theta\,|\perp\rangle$, where $\langle\psi|\perp\rangle = 0$ and $0 \le \theta \le \pi/2$. Then $\cos\theta = |\langle\varphi|\psi\rangle|$ is the overlap between the two vectors. We can perform a unitary operation that rotates $e^{i\alpha}|\psi\rangle$ to $|0\rangle$ and $|\perp\rangle$ to $|1\rangle$. Direct calculation shows

$$D_p(|\psi\rangle, |\varphi\rangle) = \min_{\phi\in\mathbb{R}} \big\| |0\rangle - e^{i\phi}(e^{i\alpha}\cos\theta\,|0\rangle + \sin\theta\,|1\rangle)\big\| = \sqrt{2(1-\cos\theta)} = \sqrt{2(1-|\langle\varphi|\psi\rangle|)}. \tag{3.68}$$

Therefore the global phase invariant distance between two vectors can be directly computed from the overlap.

Exercise 3.5. For $U, V \in \mathrm{U}(N)$, prove that

$$D_p(U, V) = 2\min_{\phi}\max_{j}\left|\sin\frac{\lambda_j - \phi}{2}\right|, \tag{3.69}$$

where $\{e^{i\lambda_j}\}$ are eigenvalues of $V^\dagger U$.

Exercise 3.6. For $U, V \in \mathrm{U}(N)$, another distance that is invariant to the global phase is

$$D_{p,F}(U,V) = \frac{1}{\sqrt{2N}} \min_{\phi} \left\| U - e^{i\phi} V \right\|_F . \tag{3.70}$$

Prove that

$$D_{p,F}(U,V) = \sqrt{1 - \frac{|\mathrm{Tr}[U^\dagger V|}{N}}. \tag{3.71}$$

3.4. Distance between classical states and classical channels

In this section, we provide a connection between concepts in classical probabilistic computation and density operators and quantum channels in quantum computation. For two probability distributions $p, q \in \mathbb{R}^N$, the **total variation distance** is

$$D(p,q) := \frac{1}{2} \sum_{i \in [N]} |p_i - q_i| . \tag{3.72}$$

The name total variation distance comes from that it measures the largest difference between p and q for some subset (also called event) S. The total variation distance is the default metric we will use between probability distributions and will be denoted by D without subscripts.

Proposition 3.28. *For any two classical probability distributions $p, q \in \mathbb{R}^N$,*

$$D(p,q) = \max_S (p(S) - q(S)) := \max_S \left(\sum_{i \in S} p_i - \sum_{i \in S} q_i \right), \tag{3.73}$$

where the maximization is over all subsets S.

Proof. For any subset S, let $\overline{S}$ be its complement. Then

$$0 = \sum_i p_i - \sum_i q_i = \sum_{i \in S} (p_i - q_i) + \sum_{i \in \overline{S}} (p_i - q_i). \tag{3.74}$$

Hence

$$\sum_{i \in S} p_i - \sum_{i \in S} q_i = \frac{1}{2} \left(\sum_{i \in S} (p_i - q_i) - \sum_{i \in \overline{S}} (p_i - q_i) \right) \leq D(p,q). \tag{3.75}$$

Now let $S = \{i | p_i \geq q_i\}$. Then

$$\frac{1}{2} \left(\sum_{i \in S} (p_i - q_i) - \sum_{i \in \overline{S}} (p_i - q_i) \right) = \frac{1}{2} \sum_i |p_i - q_i| = D(p,q), \tag{3.76}$$

and the equality is achieved. □

We now prove that the application of a transition matrix does not increase the total variation distance.

Proposition 3.29. *Given a transition matrix $P \in \mathbb{R}^{N \times N}$, and any two classical probability distributions $p, q \in \mathbb{R}^N$,*

$$D(Pp, Pq) \leq D(p,q). \tag{3.77}$$

If the equality holds for any $p, q \in \mathbb{R}^N$, then P is a permutation matrix.

PROOF. Use the left stochasticity of the transition matrix, we have

$$D(Pp, Pq) = \frac{1}{2}\sum_i \left|\sum_j P_{ij}(p_j - q_j)\right| \leq \frac{1}{2}\sum_i \sum_j P_{ij}\,|p_j - q_j| = \frac{1}{2}\sum_j |p_j - q_j| = D(p, q). \tag{3.78}$$

If the equality holds for any $p, q \in \mathbb{R}^N$, we prove that each row of P has only one nonzero entry. If this is not the case, assume that there exists a row index i and two distinct column indices $j_1 \neq j_2$ such that $P_{ij_1} > 0$ and $P_{ij_2} > 0$. Choose $p = e_{j_1}$ and $q = e_{j_2}$. Then for this row i,

$$\left|\sum_j P_{ij}(p_j - q_j)\right| = |P_{i,j_1} - P_{i,j_2}| < P_{i,j_1} + P_{i,j_2} = \sum_j P_{ij}\,|p_j - q_j|\,, \tag{3.79}$$

which contradicts equality in the triangle inequality step above. Hence each row has exactly one nonzero entry. By left stochasticity, each column must also have exactly one nonzero entry, which must equal 1. This proves that P is a permutation matrix. □

The **induced total variation distance** between two transition matrices $P, Q \in \mathbb{R}^{N\times N}$ is defined as

$$D(P, Q) = \max_{j\in[N]} D(P_{:,j}, Q_{:,j}). \tag{3.80}$$

Exercise 3.7. Prove that $D(\cdot,\cdot)$ is a distance on the set of $N \times N$ transition matrices.

Finally, we prove that the difference for the composition of K classical channels grows linearly.

Proposition 3.30 (Linear error growth for product of transition matrices)**.** *Given the transition matrices $P_1, \widetilde{P}_1, \ldots, P_K, \widetilde{P}_K \in \mathbb{R}^{N\times N}$, the induced total variation distance satisfies*

$$D(P_K \cdots P_1, \widetilde{P}_K \cdots \widetilde{P}_1) \leq \sum_{i=1}^{K} D(P_i, \widetilde{P}_i). \tag{3.81}$$

PROOF. Using the telescope series Proposition 3.21, it is sufficient to consider the case for $K = 2$. Then

$$\begin{aligned}
D(P_2P_1, \widetilde{P}_2\widetilde{P}_1) \leq& D(P_2P_1, P_2\widetilde{P}_1) + D(P_2\widetilde{P}_1, \widetilde{P}_2\widetilde{P}_1)\\
=& \max_{j\in[N]} D((P_2P_1)_{:,j}, (P_2\widetilde{P}_1)_{:,j}) + \max_{j\in[N]} D((P_2\widetilde{P}_1)_{:,j}, (\widetilde{P}_2\widetilde{P}_1)_{:,j})\\
\leq& \max_{j\in[N]} D((P_1)_{:,j}, (\widetilde{P}_1)_{:,j}) + \max_{j\in[N]} \left(\max_{l\in[N]} D((P_2)_{:,l}, (\widetilde{P}_2)_{:,l})\right) \sum_k (\widetilde{P}_1)_{kj}\\
\leq& \max_{j\in[N]} D((P_1)_{:,j}, (\widetilde{P}_1)_{:,j}) + \max_{l\in[N]} D((P_2)_{:,l}, (\widetilde{P}_2)_{:,l})\\
=& D(P_1, \widetilde{P}_1) + D(P_2, \widetilde{P}_2).
\end{aligned} \tag{3.82}$$

Here we have used Proposition 3.29 and the left stochasticity of $\widetilde{P}_1$. □

3.5. Distance between quantum states

Quantifying the similarity or difference between quantum states is fundamental to quantum information theory. It allows us to analyze the performance of quantum algorithms, assess the errors in quantum communication protocols, and understand the distinguishability of quantum states through measurements. In this section, we introduce the two most widely used measures: the trace distance and the fidelity. These generalize the corresponding concepts for classical probability distributions, such as the total variation distance discussed in Section 3.4. For a comprehensive treatment, we refer readers to [NC00, Chapter 9] and [Wat18, Chapter 3].

3.5.1. Schatten norms and the trace norm. To define distances between density operators, which are matrices, we first need appropriate matrix norms. The Schatten norms provide a family of norms generalizing the ℓ^p norms for vectors to the space of operators.

Let $A \in \mathbb{C}^{M\times N}$. The singular values of A, denoted $\sigma_i(A)$, are the square roots of the non-negative eigenvalues of $A^\dagger A$. The matrix norm!Schatten p-norm of A for $p \geq 1$ is defined as the ℓ^p norm of its singular values:

$$\|A\|_p := \left(\sum_i \sigma_i(A)^p\right)^{\frac{1}{p}}. \tag{3.83}$$

This can also be expressed using the trace function. Let $|A| := \sqrt{A^\dagger A}$ denote the positive semidefinite square root of $A^\dagger A$. Then

$$\|A\|_p = \left(\mathrm{Tr}[|A|^p]\right)^{\frac{1}{p}}. \tag{3.84}$$

The following choices of p are particularly important:

- The Schatten 1-norm, also known as the trace norm, is the sum of the singular values:

$$\|A\|_1 = \mathrm{Tr}[|A|] = \sum_i \sigma_i(A). \tag{3.85}$$

  If A is positive semidefinite, $|A| = A$, so $\|A\|_1 = \mathrm{Tr}[A]$.
- The Schatten 2-norm (also called the Hilbert-Schmidt norm or Frobenius norm) is the Euclidean norm of the singular values:

$$\|A\|_2 = \sqrt{\mathrm{Tr}[A^\dagger A]} = \left(\sum_i \sigma_i(A)^2\right)^{\frac{1}{2}}. \tag{3.86}$$

- The Schatten ∞-norm is the maximum singular value:

$$\|A\|_\infty = \lim_{p\to\infty} \|A\|_p = \max_i \sigma_i(A). \tag{3.87}$$

  This is identical to the standard operator norm (the induced $\ell^2 \to \ell^2$ norm), often denoted $\|A\|$ (equivalently $\|A\|_\infty$).

A basic but useful property relates the trace of a matrix to its trace norm.

Proposition 3.31. *For any square matrix $A \in L(\mathbb{C}^N)$,*

$$|\mathrm{Tr}[A]| \leq \|A\|_1. \tag{3.88}$$

PROOF. Consider the singular value decomposition $A = U\Sigma V^\dagger$, where U, V are unitary and $\Sigma = \mathrm{diag}(\sigma_i)$ contains the singular values. Using the cyclic property of the trace:

$$\mathrm{Tr}[A] = \mathrm{Tr}[U\Sigma V^\dagger] = \mathrm{Tr}[\Sigma V^\dagger U]. \tag{3.89}$$

Let $W = V^\dagger U$. Since W is unitary, its entries satisfy $|W_{ii}| \leq 1$ for all i. Therefore, by the triangle inequality,

$$|\mathrm{Tr}[A]| = \left|\sum_i \sigma_i W_{ii}\right| \leq \sum_i \sigma_i |W_{ii}| \leq \sum_i \sigma_i = \|A\|_1 . \tag{3.90}$$

□

The Schatten norms share many properties with the ℓ^p norms for vectors, including the triangle inequality and Hölder's inequality. We state these fundamental results without proof, referring the reader to texts on matrix analysis such as [Bha97].

Proposition 3.32 (Properties of Schatten p-norms)**.** *Let A, B be operators.*

1. *(Triangle inequality) For $1 \leq p \leq \infty$, $\|A + B\|_p \leq \|A\|_p + \|B\|_p$.*
2. *(Hölder's inequality, [Bha97, Corollary IV.2.6]) For $1 \leq p, q \leq \infty$ satisfying $\frac{1}{p} + \frac{1}{q} = 1$, if the product AB is defined, then $\|AB\|_1 \leq \|A\|_p \|B\|_q$.*

We are primarily interested in the trace norm ($p = 1$) and the operator norm ($p = \infty$). An important specialization of Hölder's inequality is the case $p = \infty, q = 1$:

$$\|AB\|_1 \leq \|A\|_\infty \|B\|_1 . \tag{3.91}$$

This inequality is frequently used to bound the trace norm of a product. Another useful variation involves the trace of a product, which can be viewed as a generalization of the Cauchy-Schwarz inequality. We provide a self-contained proof of this specific case.

Lemma 3.33 (Hölder's inequality for trace)**.** *For any operators $A, B \in L(\mathbb{C}^N)$, the following inequality holds:*

$$\left|\mathrm{Tr}(A^\dagger B)\right| \leq \|A\|_\infty \|B\|_1 . \tag{3.92}$$

PROOF. Let $B = U\Sigma V^\dagger$ be the SVD of B, with singular values s_i. By definition, $\|B\|_1 = \sum_i s_i$. Using the cyclic property of the trace:

$$\mathrm{Tr}(A^\dagger B) = \mathrm{Tr}(A^\dagger U\Sigma V^\dagger) = \mathrm{Tr}(V^\dagger A^\dagger U\Sigma). \tag{3.93}$$

Let $W = V^\dagger A^\dagger U$. Since U and V are unitary, the operator norm is invariant under unitary multiplication: $\|W\|_\infty = \left\|A^\dagger\right\|_\infty$. Furthermore, $\left\|A^\dagger\right\|_\infty = \|A\|_\infty$ as they share the same singular values. The trace is the sum of the diagonal elements of W weighted by the singular values:

$$\mathrm{Tr}(W\Sigma) = \sum_i W_{ii} s_i. \tag{3.94}$$

We can now bound the magnitude of the trace using the triangle inequality:

$$\begin{aligned} \left|\mathrm{Tr}(A^\dagger B)\right| &= \left|\sum_i W_{ii} s_i\right| \leq \sum_i |W_{ii}| s_i \\ &\leq \sum_i \|W\|_\infty s_i = \|A\|_\infty \sum_i s_i = \|A\|_\infty \|B\|_1 . \end{aligned} \tag{3.95}$$

□

We now consider how the trace norm behaves under the partial trace operation, which often arises when dealing with composite systems.

Exercise 3.8. Let $|u\rangle, |v\rangle$ be normalized state vectors in $\mathcal{H}_A \otimes \mathcal{H}_B$. Show that

$$\|\mathrm{Tr}_B |u\rangle\langle v|\|_1 \leq 1. \tag{3.96}$$

(Hint: use Hölder's inequality for the Schatten 2-norm.)

More generally, the partial trace is a contraction with respect to the trace norm.

Proposition 3.34 (Partial trace does not increase the trace norm)**.** *For any operator $O \in L(\mathcal{H}_A \otimes \mathcal{H}_B)$,*

$$\|\mathrm{Tr}_B O\|_1 \leq \|O\|_1 . \tag{3.97}$$

Proof. Consider the singular value decomposition of the operator O:

$$O = \sum_k \sigma_k |u_k\rangle\langle v_k|, \tag{3.98}$$

where $\sigma_k > 0$ are the singular values, and $\{|u_k\rangle\}, \{|v_k\rangle\}$ are sets of orthonormal vectors in $\mathcal{H}_A \otimes \mathcal{H}_B$. The trace norm is $\|O\|_1 = \sum_k \sigma_k$.

Applying the partial trace and using the triangle inequality (Proposition 3.32):

$$\|\mathrm{Tr}_B O\|_1 = \left\| \sum_k \sigma_k \,\mathrm{Tr}_B |u_k\rangle\langle v_k| \right\|_1 \leq \sum_k \sigma_k \|\mathrm{Tr}_B |u_k\rangle\langle v_k|\|_1 . \tag{3.99}$$

By Exercise 3.8, $\|\mathrm{Tr}_B |u_k\rangle\langle v_k|\|_1 \leq 1$. Therefore,

$$\|\mathrm{Tr}_B O\|_1 \leq \sum_k \sigma_k = \|O\|_1 . \tag{3.100}$$

□

The trace norm and the operator norm are dual to each other with respect to the trace inner product, a property that is frequently exploited in optimization problems and for deriving operational interpretations of these norms.

Lemma 3.35 (Duality of Trace and Operator Norms)**.** *For any operator $Y \in L(\mathbb{C}^N)$, the following identities hold:*

$$\|Y\|_1 = \sup_{\|Z\|_\infty \leq 1} |\mathrm{Tr}(Z^\dagger Y)|, \tag{3.101}$$

and

$$\|Y\|_\infty = \sup_{\|X\|_1 \leq 1} |\mathrm{Tr}(Y^\dagger X)|. \tag{3.102}$$

Proof. We first prove Eq. (3.101). Let S_1 denote the right-hand side. Applying Hölder's inequality (Lemma 3.33), we have $|\mathrm{Tr}(Z^\dagger Y)| \leq \|Z\|_\infty \|Y\|_1$. If we restrict the optimization to $\|Z\|_\infty \leq 1$, then $|\mathrm{Tr}(Z^\dagger Y)| \leq \|Y\|_1$. Taking the supremum yields $S_1 \leq \|Y\|_1$.

To show $S_1 \geq \|Y\|_1$, we construct an operator Z that achieves the bound. Let $Y = U\Sigma V^\dagger$ be the SVD of Y. Define $Z = UV^\dagger$. Since Z is unitary, $\|Z\|_\infty = 1$. We compute the trace:

$$\begin{aligned} \mathrm{Tr}(Z^\dagger Y) &= \mathrm{Tr}((UV^\dagger)^\dagger (U\Sigma V^\dagger)) = \mathrm{Tr}(VU^\dagger U\Sigma V^\dagger) \\ &= \mathrm{Tr}(V\Sigma V^\dagger) = \mathrm{Tr}(\Sigma) = \|Y\|_1 . \end{aligned} \tag{3.103}$$

Thus, $S_1 \geq \|Y\|_1$.

Next, we prove Eq. (3.102). Let S_∞ denote the right-hand side. Applying Lemma 3.33, we have $|\operatorname{Tr}(Y^\dagger X)| \leq \|Y\|_\infty \|X\|_1$. Restricting to $\|X\|_1 \leq 1$ and taking the supremum yields $S_\infty \leq \|Y\|_\infty$.

To show $S_\infty \geq \|Y\|_\infty$, we construct an optimal X. Let $Y = \sum_i s_i |u_i\rangle\langle v_i|$ be the SVD of Y, ordered such that $s_1 = \|Y\|_\infty$. Define the rank-1 operator $X = |u_1\rangle\langle v_1|$. Since $|u_1\rangle, |v_1\rangle$ are normalized, $\|X\|_1 = 1$. We compute the trace:

$$\begin{aligned} \operatorname{Tr}(Y^\dagger X) &= \operatorname{Tr}\left(\left(\sum_i s_i |v_i\rangle\langle u_i|\right)|u_1\rangle\langle v_1|\right) \\ &= \operatorname{Tr}\left(\sum_i s_i |v_i\rangle\langle v_1| \langle u_i|u_1\rangle\right). \end{aligned} \tag{3.104}$$

Due to the orthonormality of $\{|u_i\rangle\}$, only the $i = 1$ term survives:

$$\operatorname{Tr}(Y^\dagger X) = \operatorname{Tr}(s_1 |v_1\rangle\langle v_1|) = s_1 = \|Y\|_\infty . \tag{3.105}$$

Thus, $S_\infty \geq \|Y\|_\infty$. □

When the operator Y is Hermitian, the optimization domains in these duality relations can also be restricted to Hermitian operators.

Lemma 3.36 (Duality for Hermitian Operators)**.** *Let $H \in L(\mathbb{C}^N)$ be a Hermitian operator.*

(1) *The trace norm is achieved by maximizing over Hermitian operators in the unit operator-norm ball (i.e., $-I \preceq Z \preceq I$):*

$$\|H\|_1 = \sup\{|\operatorname{Tr}(ZH)| : Z = Z^\dagger, \|Z\|_\infty \leq 1\}. \tag{3.106}$$

(2) *The operator norm is achieved by maximizing over density operators:*

$$\|H\|_\infty = \sup\{|\operatorname{Tr}(H\rho)| : \rho \in \mathcal{D}(\mathbb{C}^N)\}. \tag{3.107}$$

Proof. In both cases, the inequality $\leq$ (for the left-hand side) follows immediately from Lemma 3.35, as the restricted optimization domains are subsets of the original domains. We only need to show that the bounds can be achieved within these restricted domains.

1. Proof of Eq. (3.106). Let $H = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ be the spectral decomposition, where $\lambda_i \in \mathbb{R}$. The trace norm is $\|H\|_1 = \sum_i |\lambda_i|$. Define the sign operator $Z = \sum_i \operatorname{sgn}(\lambda_i)|\psi_i\rangle\langle\psi_i|$. Z is Hermitian, and its eigenvalues are in $\{-1, 0, 1\}$, so $\|Z\|_\infty \leq 1$.

$$\operatorname{Tr}(ZH) = \sum_i \operatorname{sgn}(\lambda_i)\lambda_i = \sum_i |\lambda_i| = \|H\|_1 . \tag{3.108}$$

2. Proof of Eq. (3.107). The operator norm is $\|H\|_\infty = \max_i |\lambda_i|$. Let k be an index achieving the maximum. Define the pure state $\rho = |\psi_k\rangle\langle\psi_k|$, which is a density operator.

$$|\operatorname{Tr}(H\rho)| = |\langle\psi_k|H|\psi_k\rangle| = |\lambda_k| = \|H\|_\infty . \tag{3.109}$$

□

3.5.2. Trace distance. The trace norm provides a natural way to define a distance metric on the space of quantum states, generalizing the classical total variation distance.

Definition 3.37 (Trace distance)**.** *The **trace distance** between two quantum states $\rho, \sigma \in \mathcal{D}(\mathbb{C}^N)$ is defined as*

$$D(\rho, \sigma) := \frac{1}{2} \|\rho - \sigma\|_1 . \tag{3.110}$$

The factor of $1/2$ ensures that the distance lies in the range $[0, 1]$. Since $\|\rho\|_1 = 1$ and $\|\sigma\|_1 = 1$, the triangle inequality (Proposition 3.32) gives $\|\rho - \sigma\|_1 \leq \|\rho\|_1 + \|\sigma\|_1 = 2$.

Example 3.38 (Trace distance for classical states)**.** Consider classical probability distributions $p, s \in \mathbb{R}^N$ embedded as classical states:

$$\rho = \sum_{i \in [N]} p_i |i\rangle\langle i|, \quad \sigma = \sum_{i \in [N]} s_i |i\rangle\langle i|. \tag{3.111}$$

The difference $\rho - \sigma$ is a diagonal matrix with entries $p_i - s_i$. The trace norm is the sum of the absolute values of the eigenvalues:

$$D(\rho, \sigma) = \frac{1}{2} \|\rho - \sigma\|_1 = \frac{1}{2} \sum_i |p_i - s_i| . \tag{3.112}$$

This is exactly the total variation distance $D(p, s)$ between the probability distributions p and s. $\diamond$

The trace distance has an operational interpretation related to the distinguishability of quantum states through measurement. This is the quantum generalization of Proposition 3.28.

Proposition 3.39 (Operational interpretation of trace distance)**.** *For any quantum states $\rho, \sigma \in \mathcal{D}(\mathbb{C}^N)$, the trace distance satisfies*

$$D(\rho, \sigma) = \max_{0 \preceq M \preceq I} \operatorname{Tr}[M(\rho - \sigma)]. \tag{3.113}$$

The maximum is achieved when M is the projector onto the subspace where $\rho - \sigma$ is positive.

Proof. Let $\Delta = \rho - \sigma$. Δ is Hermitian and $\operatorname{Tr}[\Delta] = 0$. We want to maximize $\operatorname{Tr}[M\Delta]$ over $0 \preceq M \preceq I$.

We utilize the duality results established earlier. Consider an operator M such that $0 \preceq M \preceq I$. Define $Z = 2M - I$. Then Z is Hermitian, and $-I \preceq Z \preceq I$, which means $\|Z\|_\infty \leq 1$. We have

$$\operatorname{Tr}[Z\Delta] = \operatorname{Tr}[(2M - I)\Delta] = 2 \operatorname{Tr}[M\Delta]. \tag{3.114}$$

By the Hermitian duality relation (Lemma 3.36, Eq. (3.106)), $\|\Delta\|_1 = \sup\{|\operatorname{Tr}(Z'\Delta)| : Z' = Z'^\dagger, \|Z'\|_\infty \leq 1\}$. Since Z is admissible for this optimization, we have

$$2 \operatorname{Tr}[M\Delta] = \operatorname{Tr}[Z\Delta] \leq \|\Delta\|_1 . \tag{3.115}$$

Thus, $\operatorname{Tr}[M\Delta] \leq \frac{1}{2} \|\Delta\|_1 = D(\rho, \sigma)$.

To show equality, we construct an optimal M. Let $\Delta = \Delta_+ - \Delta_-$, where Δ_+, Δ_- are positive semidefinite operators with orthogonal support. Since $\operatorname{Tr}[\Delta] = 0$, we have $\operatorname{Tr}[\Delta_+] = \operatorname{Tr}[\Delta_-]$. The trace norm is

$$\|\Delta\|_1 = \operatorname{Tr}[\Delta_+] + \operatorname{Tr}[\Delta_-] = 2 \operatorname{Tr}[\Delta_+]. \tag{3.116}$$

So $D(\rho, \sigma) = \operatorname{Tr}[\Delta_+]$.

Let P be the projector onto the support of Δ_+ with $P\Delta_+ = \Delta_+$. We evaluate the trace:

$$\mathrm{Tr}[P\Delta] = \mathrm{Tr}[P(\Delta_+ - \Delta_-)] = \mathrm{Tr}[\Delta_+] = D(\rho, \sigma). \tag{3.117}$$

Therefore, the maximum is achieved. □

Proposition 3.39 implies that $D(\rho, \sigma)$ is the maximum difference in the probability of obtaining a specific measurement outcome when measuring ρ versus σ.

A fundamental property of the trace distance is that it cannot increase under the action of a quantum channel. This reflects the physical intuition that noise or information loss (modeled by the channel) makes states harder to distinguish. This result parallels Proposition 3.29 for classical channels.

THEOREM 3.40 (Quantum channels are contractive). *Let $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ be a quantum channel. For any $\rho, \sigma \in \mathcal{D}(\mathbb{C}^N)$,*

$$D(\mathcal{Q}[\rho], \mathcal{Q}[\sigma]) \leq D(\rho, \sigma). \tag{3.118}$$

PROOF. Let $\rho' = \mathcal{Q}[\rho]$ and $\sigma' = \mathcal{Q}[\sigma]$. By Proposition 3.39, there exists a projector P (specifically, onto the positive subspace of $\rho' - \sigma'$) such that

$$D(\rho', \sigma') = \mathrm{Tr}[P(\rho' - \sigma')] = \mathrm{Tr}[P\mathcal{Q}[\rho - \sigma]]. \tag{3.119}$$

Consider the decomposition $\rho - \sigma = \Delta_+ - \Delta_-$, where $\Delta_+, \Delta_- \succeq 0$ are the positive and negative parts, respectively. As shown in the proof of Proposition 3.39, $D(\rho, \sigma) = \mathrm{Tr}[\Delta_+] = \mathrm{Tr}[\Delta_-]$.

Substituting the decomposition and using linearity:

$$D(\rho', \sigma') = \mathrm{Tr}[P\mathcal{Q}[\Delta_+ - \Delta_-]] = \mathrm{Tr}[P\mathcal{Q}[\Delta_+]] - \mathrm{Tr}[P\mathcal{Q}[\Delta_-]]. \tag{3.120}$$

We analyze the two terms. Since $\mathcal{Q}$ is a positive map, and $\Delta_- \succeq 0$, the output $\mathcal{Q}[\Delta_-]$ is positive semidefinite. Since $P \succeq 0$, the trace of the product of two positive operators is non-negative: $\mathrm{Tr}[P\mathcal{Q}[\Delta_-]] \geq 0$. Therefore,

$$D(\rho', \sigma') \leq \mathrm{Tr}[P\mathcal{Q}[\Delta_+]]. \tag{3.121}$$

Next, since $\mathcal{Q}[\Delta_+] \succeq 0$ and $P \preceq I$, we have $I - P \succeq 0$. Thus $\mathrm{Tr}[(I - P)\mathcal{Q}[\Delta_+]] \geq 0$, which implies $\mathrm{Tr}[P\mathcal{Q}[\Delta_+]] \leq \mathrm{Tr}[\mathcal{Q}[\Delta_+]]$. Therefore,

$$D(\rho', \sigma') \leq \mathrm{Tr}[\mathcal{Q}[\Delta_+]]. \tag{3.122}$$

Finally, since $\mathcal{Q}$ is trace-preserving, $\mathrm{Tr}[\mathcal{Q}[\Delta_+]] = \mathrm{Tr}[\Delta_+]$. Combining the inequalities, we obtain

$$D(\mathcal{Q}[\rho], \mathcal{Q}[\sigma]) \leq \mathrm{Tr}[\Delta_+] = D(\rho, \sigma). \tag{3.123}$$

□

3.5.3. Fidelity. While the trace distance is an operationally useful metric for the distance between quantum states, another widely used measure is the fidelity. Fidelity quantifies the "overlap" between two quantum states, and generalizes the inner product between pure state vectors.

Definition 3.41 (Fidelity)**.** *The **fidelity** between two quantum states $\rho, \sigma \in \mathcal{D}(\mathbb{C}^N)$ is defined as*

$$F(\rho, \sigma) := \mathrm{Tr}\left[\sqrt{\rho^{\frac{1}{2}}\sigma\rho^{\frac{1}{2}}}\right]. \tag{3.124}$$

This definition can be rewritten using the trace norm. A more symmetric expression involves the operator $A = \rho^{1/2}\sigma^{1/2}$. Recall that the trace norm of A is $\|A\|_1 = \mathrm{Tr}[|A|] = \mathrm{Tr}[\sqrt{A^\dagger A}]$. Here $A^\dagger A = \sigma^{1/2}\rho\sigma^{1/2}$. The singular values of A are the square roots of the eigenvalues of $A^\dagger A$ (and also $AA^\dagger = \rho^{1/2}\sigma\rho^{1/2}$). Thus,

$$F(\rho,\sigma) = \left\|\rho^{1/2}\sigma^{1/2}\right\|_1. \tag{3.125}$$

This immediately establishes that fidelity is symmetric: $F(\rho,\sigma) = F(\sigma,\rho)$, since $\|A\|_1 = \left\|A^\dagger\right\|_1$.

Remark 3.42. Nomenclature can be confusing. Sometimes the quantity defined above is called the square root fidelity, and $F(\rho,\sigma)^2$ is called the fidelity. The **infidelity** is then defined as $1-F(\rho,\sigma)^2$. We will adhere to Definition 3.41. ◇

Fidelity satisfies $0 \le F(\rho,\sigma) \le 1$. The upper bound follows from Hölder's inequality (Proposition 3.32, $p = q = 2$):

$$F(\rho,\sigma) = \left\|\rho^{1/2}\sigma^{1/2}\right\|_1 \le \left\|\rho^{1/2}\right\|_2 \left\|\sigma^{1/2}\right\|_2. \tag{3.126}$$

Since $\left\|\rho^{1/2}\right\|_2^2 = \mathrm{Tr}[\rho^{1/2}\rho^{1/2}] = \mathrm{Tr}[\rho] = 1$, we have $F(\rho,\sigma) \le 1$. Furthermore, $F(\rho,\sigma) = 1$ if and only if $\rho = \sigma$.

Fidelity itself is not a distance metric (it does not satisfy the triangle inequality). However, it can be converted into a metric known as the angle or Bures angle.

Definition 3.43 (Angle between quantum states)**.** *The **angle** between two quantum states $\rho,\sigma \in \mathcal{D}(\mathbb{C}^N)$ is*

$$\theta(\rho,\sigma) := \arccos(F(\rho,\sigma)) \in [0,\pi/2]. \tag{3.127}$$

Example 3.44 (Pure states)**.** If $\rho = |\psi\rangle\langle\psi|$ and $\sigma = |\varphi\rangle\langle\varphi|$ are two pure states.

$$\rho^{1/2}\sigma\rho^{1/2} = |\psi\rangle\langle\psi||\varphi\rangle\langle\varphi||\psi\rangle\langle\psi| = |\langle\psi|\varphi\rangle|^2|\psi\rangle\langle\psi|. \tag{3.128}$$

This is a rank-1 operator. Its only non-zero eigenvalue is $|\langle\psi|\varphi\rangle|^2$. The square root of this eigenvalue is $|\langle\psi|\varphi\rangle|$. Thus,

$$F(\rho,\sigma) = |\langle\psi|\varphi\rangle|. \tag{3.129}$$

The fidelity is the absolute value of the overlap between the state vectors.

More generally, if only one state is pure, say $\rho = |\psi\rangle\langle\psi|$, then

$$F(\rho,\sigma) = \sqrt{\langle\psi|\sigma|\psi\rangle}. \tag{3.130}$$

It is the square root of the overlap between the pure state $|\psi\rangle$ and the mixed state σ.

Let us relate the trace distance and fidelity for pure states ρ,σ. Let the angle be $\theta = \theta(\rho,\sigma)$, so $F(\rho,\sigma) = \cos\theta$. We can choose a basis such that $|\psi\rangle = |0\rangle$ and $|\varphi\rangle = \cos\theta\,|0\rangle + \sin\theta\,|1\rangle$ (by adjusting global phase). In this 2D subspace, the difference $\rho - \sigma$ is represented by the matrix:

$$\Delta = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} \cos^2\theta & \cos\theta\sin\theta \\ \cos\theta\sin\theta & \sin^2\theta \end{pmatrix} = \begin{pmatrix} \sin^2\theta & -\cos\theta\sin\theta \\ -\cos\theta\sin\theta & -\sin^2\theta \end{pmatrix}. \tag{3.131}$$

The eigenvalues of Δ are $\pm\sin\theta$. The trace norm is $\|\Delta\|_1 = |\sin\theta| + |-\sin\theta| = 2\sin\theta$ (since $0 \le \theta \le \pi/2$).

$$D(\rho,\sigma) = \frac{1}{2}\|\rho-\sigma\|_1 = \sin\theta. \tag{3.132}$$

We can express this in terms of fidelity $F = \cos\theta$:

$$D(\rho, \sigma) = \sqrt{1 - F(\rho, \sigma)^2}. \tag{3.133}$$

◇

Example 3.45 (Classical states)**.** Let ρ, σ be classical states corresponding to probability distributions p, q (see Example 3.38). Since the operators are diagonal, the definition simplifies:

$$F(\rho, \sigma) = \sum_j \sqrt{p_j q_j}. \tag{3.134}$$

This is the classical Bhattacharyya coefficient. The relationship between trace distance and fidelity for classical states is characterized by the inequality:

$$\begin{aligned} D(\rho, \sigma) &= \frac{1}{2} \sum_j |p_j - q_j| \geq \frac{1}{2} \sum_j (\sqrt{p_j} - \sqrt{q_j})^2 \\ &= \frac{1}{2} \sum_j (p_j + q_j - 2\sqrt{p_j q_j}) = 1 - \sum_j \sqrt{p_j q_j} = 1 - F(\rho, \sigma). \end{aligned} \tag{3.135}$$

The inequality step uses $|a^2 - b^2| \geq (a - b)^2$ for $a, b \geq 0$. ◇

We have seen two extremes: for pure states $D = \sqrt{1 - F^2}$, while for classical states $D \geq 1 - F$. These relationships are generalized by the Fuchs–van de Graaf inequalities (see [NC00, Section 9.2]), which provide tight bounds relating the two measures for arbitrary quantum states.

THEOREM 3.46 (Fuchs–van de Graaf inequalities). *For any $\rho, \sigma \in \mathcal{D}(\mathbb{C}^N)$,*

$$1 - F(\rho, \sigma) \leq D(\rho, \sigma) \leq \sqrt{1 - F(\rho, \sigma)^2}. \tag{3.136}$$

We state a few important properties of fidelity without proof. Their proofs typically rely on a powerful result known as Uhlmann's theorem, which relates the fidelity between two mixed states to the maximum overlap between their purifications (see [NC00, Chapter 9], [Wat18, Chapter 3]).

Proposition 3.47 (Properties of Fidelity and Angle)**.** *Let $\rho, \sigma \in \mathcal{D}(\mathbb{C}^N)$.*

1. *(Metric property) The angle $\theta(\rho, \sigma)$ is a distance metric on $\mathcal{D}(\mathbb{C}^N)$.*
2. *(Contractivity) For any quantum channel $\mathcal{Q}$, the angle is contractive:*

$$\theta(\mathcal{Q}[\rho], \mathcal{Q}[\sigma]) \leq \theta(\rho, \sigma). \tag{3.137}$$

Equivalently, fidelity increases (or stays the same) under quantum channels:

$$F(\mathcal{Q}[\rho], \mathcal{Q}[\sigma]) \geq F(\rho, \sigma). \tag{3.138}$$

The Fuchs–van de Graaf inequalities (Theorem 3.46) can be rewritten in terms of the angle $\theta = \theta(\rho, \sigma)$:

$$2\sin^2\frac{\theta}{2} \leq D(\rho, \sigma) \leq \sin\theta. \tag{3.139}$$

When the states are close ($\theta 1$), we can use the approximations $\sin\theta \approx \theta$ and $2\sin^2(\theta/2) \approx \theta^2/2$. This gives

$$\frac{1}{2}\theta^2 \lesssim D(\rho, \sigma) \lesssim \theta. \tag{3.140}$$

This quadratic difference in scaling suggests that while the different distance metrics are related, they can behave very differently.

Example 3.48. Consider a target state $\rho = |0\rangle\langle 0|$. Let $\theta \in [0, \pi/2]$ and define two pure states:

$$|\theta_+\rangle = \cos\theta\,|0\rangle + \sin\theta\,|1\rangle\,, \quad |\theta_-\rangle = \cos\theta\,|0\rangle - \sin\theta\,|1\rangle\,. \tag{3.141}$$

Let σ_+ and σ_- be the corresponding density operators. We also consider the mixed state $\sigma_M = \frac{1}{2}(\sigma_+ + \sigma_-)$.

$$\sigma_M = \cos^2\theta|0\rangle\langle 0| + \sin^2\theta|1\rangle\langle 1|. \tag{3.142}$$

We compare the fidelities and trace distances to the target state ρ. The fidelities are identical:

$$F(\rho, \sigma_+) = F(\rho, \sigma_-) = F(\rho, \sigma_M) = \cos\theta. \tag{3.143}$$

However, the trace distances differ significantly. For the pure states (using Example 3.44):

$$D(\rho, \sigma_\pm) = \sin\theta. \tag{3.144}$$

For the mixed state σ_M (using Example 3.38):

$$D(\rho, \sigma_M) = \sin^2\theta. \tag{3.145}$$

If θ is small, $D(\rho, \sigma_\pm) \approx \theta$ while $D(\rho, \sigma_M) \approx \theta^2$. The mixed state is quadratically closer to the target state in trace distance than its pure components, even though they all share the same fidelity. The coherent superpositions in σ_+ and σ_- (the off-diagonal terms) cancel out in the incoherent mixture σ_M, leading to a state that is statistically closer to ρ. ◇

Which measure, fidelity or trace distance, is more physically relevant? The answer depends on the context. Fidelity can often be estimated experimentally (e.g., via the SWAP test), while estimating the trace distance generally requires full quantum state tomography.

On the other hand, the trace distance directly bounds the difference in measurement statistics. According to Proposition 3.39, the maximum difference in the probability of any measurement outcome M is bounded by the trace distance:

$$|\mathrm{Tr}[M\rho] - \mathrm{Tr}[M\sigma]| \leq D(\rho, \sigma). \tag{3.146}$$

If the trace distance is small, the states are statistically indistinguishable by any measurement.

3.6. Distance between quantum channels

Quantifying the distance between quantum channels is important for analyzing the precision of quantum gates, the robustness of quantum algorithms, and the distinguishability of physical processes. This section introduces the primary tools used for this purpose: the induced trace norm and the diamond norm.

3.6.1. Induced trace norm. We begin by considering norms induced on the space of linear maps (superoperators) by the Schatten norms on the input and output spaces.

Definition 3.49. *For a linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$, the **induced trace norm** (or the induced $1 \to 1$ norm) is defined as*

$$\|\mathcal{Q}\|_{1\to 1} := \sup_{X \in L(\mathbb{C}^N), \|X\|_1 \leq 1} \|\mathcal{Q}[X]\|_1\,. \tag{3.147}$$

This norm quantifies the maximum amplification of the trace norm under the action of $\mathcal{Q}$.

*Analogously, the **induced operator norm** (or the induced $\infty \to \infty$ norm) is defined using the operator norm $\|\cdot\|_\infty$:*

$$\|\mathcal{Q}\|_{\infty\to\infty} := \sup_{X \in L(\mathbb{C}^N), \|X\|_\infty \leq 1} \|\mathcal{Q}[X]\|_\infty\,. \tag{3.148}$$

Induced norms are inherently submultiplicative, a property useful when analyzing compositions of maps.

Proposition 3.50 (Submultiplicativity)**.** *Let $\mathcal{R} : L(\mathbb{C}^N) \to L(\mathbb{C}^{N'})$ and $\mathcal{Q} : L(\mathbb{C}^{N'}) \to L(\mathbb{C}^M)$ be linear maps. Then*

$$\|\mathcal{Q} \circ \mathcal{R}\|_{1\to 1} \leq \|\mathcal{Q}\|_{1\to 1} \|\mathcal{R}\|_{1\to 1} . \tag{3.149}$$

Proof. For any $X \in L(\mathbb{C}^N)$, by the definition of the induced norm:

$$\|(\mathcal{Q} \circ \mathcal{R})(X)\|_1 = \|\mathcal{Q}[\mathcal{R}[X]]\|_1 \leq \|\mathcal{Q}\|_{1\to 1} \|\mathcal{R}[X]\|_1 \leq \|\mathcal{Q}\|_{1\to 1} \|\mathcal{R}\|_{1\to 1} \|X\|_1 . \tag{3.150}$$

Taking the supremum over X with $\|X\|_1 \leq 1$ yields the result. □

To analyze these norms, we introduce the concept of the adjoint map. The space of linear operators $L(\mathbb{C}^N)$ forms a Hilbert space under the Hilbert-Schmidt inner product $\langle A, B\rangle = \mathrm{Tr}(A^\dagger B)$. The **adjoint map** $\mathcal{Q}^\dagger : L(\mathbb{C}^M) \to L(\mathbb{C}^N)$ is uniquely defined by the relation

$$\langle Y, \mathcal{Q}(X)\rangle = \langle \mathcal{Q}^\dagger(Y), X\rangle, \tag{3.151}$$

for all $X \in L(\mathbb{C}^N)$ and $Y \in L(\mathbb{C}^M)$.

The induced trace norm and the induced operator norm exhibit a duality relationship analogous to the duality between the trace norm and operator norm for matrices (Lemma 3.35).

Proposition 3.51 (Duality of Induced Norms)**.** *For any linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$, the following duality relation holds:*

$$\|\mathcal{Q}\|_{1\to 1} = \left\|\mathcal{Q}^\dagger\right\|_{\infty\to\infty} . \tag{3.152}$$

Proof. We begin with the definition of the induced trace norm and apply the variational characterization of the trace norm (Lemma 3.35, Eq. (3.101)):

$$\begin{aligned} \|\mathcal{Q}\|_{1\to 1} &= \sup_{\|X\|_1 \leq 1} \|\mathcal{Q}(X)\|_1 \\ &= \sup_{\|X\|_1 \leq 1} \left(\sup_{\|Y\|_\infty \leq 1} |\,\mathrm{Tr}(Y^\dagger \mathcal{Q}[X])| \right). \end{aligned} \tag{3.153}$$

We exchange the order of the suprema and employ the definition of the adjoint map (Eq. (3.151)):

$$\|\mathcal{Q}\|_{1\to 1} = \sup_{\|Y\|_\infty \leq 1} \left(\sup_{\|X\|_1 \leq 1} |\,\mathrm{Tr}((\mathcal{Q}^\dagger(Y))^\dagger X)| \right). \tag{3.154}$$

The inner supremum is the characterization of the operator norm via duality (Lemma 3.35, Eq. (3.102)), applied to the operator $W = \mathcal{Q}^\dagger(Y)$. That is, $\sup_{\|X\|_1 \leq 1} |\,\mathrm{Tr}(W^\dagger X)| = \|W\|_\infty$.

$$\|\mathcal{Q}\|_{1\to 1} = \sup_{\|Y\|_\infty \leq 1} \left\|\mathcal{Q}^\dagger(Y)\right\|_\infty = \left\|\mathcal{Q}^\dagger\right\|_{\infty\to\infty} . \tag{3.155}$$

□

To compute the induced trace norm, it is helpful to characterize the inputs that achieve the maximum. We first establish that for general linear maps, the maximum is attained on rank-1 operators.

Lemma 3.52. *For any linear map $\mathcal{Q}$, the induced $1 \to 1$ norm is achieved by a rank-1 operator:*

$$\|\mathcal{Q}\|_{1\to 1} = \sup\{\|\mathcal{Q}(|u\rangle\langle v|)\|_1 : \|u\|_2 = 1, \|v\|_2 = 1\}. \tag{3.156}$$

PROOF. Let $C_1 = \{X : \|X\|_1 \leq 1\}$ be the unit ball in the trace norm. The function $f(X) = \|\mathcal{Q}(X)\|_1$ is convex. Since C_1 is a compact, convex set, the maximum of $f(X)$ over C_1 must be achieved at an extreme point of C_1. The extreme points of C_1 are precisely the rank-1 operators of the form $|u\rangle\langle v|$ with normalized vectors $|u\rangle, |v\rangle$.

Explicitly, let X maximize the norm, with $\|X\|_1 = 1$. Its SVD $X = \sum_i s_i |u_i\rangle\langle v_i|$ is a convex combination (since $\sum s_i = 1, s_i > 0$) of the rank-1 operators $X_i = |u_i\rangle\langle v_i|$. By the triangle inequality:

$$\|\mathcal{Q}(X)\|_1 = \left\| \sum_i s_i \mathcal{Q}(X_i) \right\|_1 \leq \sum_i s_i \|\mathcal{Q}(X_i)\|_1 \leq \max_i \|\mathcal{Q}(X_i)\|_1 . \tag{3.157}$$

Thus, the maximum is achieved by one of the rank-1 operators X_i. □

We now investigate how these norms behave for positive maps. We first state the following result for positive maps without proof [Wat18, Eq. (3.329)].

Lemma 3.53. *Let $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ be a positive linear map. Then*

$$\|\mathcal{Q}\|_{1\to 1} = \left\|\mathcal{Q}^\dagger(I_M)\right\|_\infty . \tag{3.158}$$

A celebrated result known as the Russo–Dye theorem [Wat18, Theorem 3.39] simplifies the calculation of the induced norm for such maps.

THEOREM 3.54 (Russo–Dye). *Let $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ be a positive linear map. Then*

$$\|\mathcal{Q}\|_{1\to 1} = \max_{\|u\|_2 = 1} \mathrm{Tr}\left(\mathcal{Q}\left(|u\rangle\langle u|\right)\right). \tag{3.159}$$

PROOF. Since $\mathcal{Q}^\dagger(I_M)$ is Hermitian (in fact positive semidefinite), its operator norm is the largest eigenvalue:

$$\left\|\mathcal{Q}^\dagger(I_M)\right\|_\infty = \sup_{\|u\|_2 = 1} \langle u| \mathcal{Q}^\dagger(I_M) |u\rangle = \sup_{\|u\|_2 = 1} \mathrm{Tr}(\mathcal{Q}(|u\rangle\langle u|)). \tag{3.160}$$

The result follows from Lemma 3.53. □

As an immediate consequence, if $\mathcal{Q}$ is a quantum channel, it is positive and trace-preserving. Thus,

$$\|\mathcal{Q}\|_{1\to 1} = \max_u \mathrm{Tr}\left(\mathcal{Q}\left(|u\rangle\langle u|\right)\right) = \max_u \mathrm{Tr}\left(|u\rangle\langle u|\right) = 1. \tag{3.161}$$

The fact that quantum channels have an induced trace norm of 1 leads to an important stability property for compositions of channels.

Proposition 3.55. *Let $\mathcal{Q}_1, \ldots, \mathcal{Q}_K$ and $\widetilde{\mathcal{Q}}_1, \ldots, \widetilde{\mathcal{Q}}_K$ be sequences of quantum channels. Then*

$$\left\| \mathcal{Q}_K \circ \cdots \circ \mathcal{Q}_1 - \widetilde{\mathcal{Q}}_K \circ \cdots \circ \widetilde{\mathcal{Q}}_1 \right\|_{1\to 1} \leq \sum_{i=1}^K \left\| \mathcal{Q}_i - \widetilde{\mathcal{Q}}_i \right\|_{1\to 1} . \tag{3.162}$$

PROOF. We use a telescoping sum argument. For $K = 2$:

$$\mathcal{Q}_2 \circ \mathcal{Q}_1 - \widetilde{\mathcal{Q}}_2 \circ \widetilde{\mathcal{Q}}_1 = (\mathcal{Q}_2 - \widetilde{\mathcal{Q}}_2) \circ \mathcal{Q}_1 + \widetilde{\mathcal{Q}}_2 \circ (\mathcal{Q}_1 - \widetilde{\mathcal{Q}}_1). \tag{3.163}$$

By the triangle inequality and submultiplicativity (Proposition 3.50):

$$\begin{aligned} \left\| \mathcal{Q}_2 \circ \mathcal{Q}_1 - \widetilde{\mathcal{Q}}_2 \circ \widetilde{\mathcal{Q}}_1 \right\|_{1\to 1} \leq & \left\| \mathcal{Q}_2 - \widetilde{\mathcal{Q}}_2 \right\|_{1\to 1} \|\mathcal{Q}_1\|_{1\to 1} \\ & + \left\| \widetilde{\mathcal{Q}}_2 \right\|_{1\to 1} \left\| \mathcal{Q}_1 - \widetilde{\mathcal{Q}}_1 \right\|_{1\to 1} . \end{aligned} \tag{3.164}$$

Since $\mathcal{Q}_1$ and $\widetilde{\mathcal{Q}}_2$ are quantum channels, their induced trace norms are 1.

$$\left\|\mathcal{Q}_2 \circ \mathcal{Q}_1 - \widetilde{\mathcal{Q}}_2 \circ \widetilde{\mathcal{Q}}_1\right\|_{1\to 1} \leq \left\|\mathcal{Q}_2 - \widetilde{\mathcal{Q}}_2\right\|_{1\to 1} + \left\|\mathcal{Q}_1 - \widetilde{\mathcal{Q}}_1\right\|_{1\to 1}. \tag{3.165}$$

The general case follows by induction. □

3.6.2. The diamond norm. The induced trace norm quantifies how much a map $\mathcal{Q}$ acting on a system S changes the state of S. However, this is insufficient in quantum mechanics due to entanglement. If S is entangled with an auxiliary system A, the action of $\mathcal{Q}$ on S (described by $\mathcal{Q} \otimes \mathcal{I}_A$) might alter the joint state of SA significantly more than predicted by $\|\mathcal{Q}\|_{1\to 1}$. To capture the true behavior of the map in the presence of arbitrary entanglement, we must consider its stabilized action. This leads to the **diamond norm**, also known as the **completely bounded trace norm**.

Definition 3.56 (Diamond Norm)**.** *Let $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$ be a linear map. The diamond norm of $\mathcal{Q}$ is defined as*

$$\|\mathcal{Q}\|_\diamond := \sup_{k\geq 1} \|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1} = \sup_{k\geq 1} \|\mathcal{I}_k \otimes \mathcal{Q}\|_{1\to 1}, \tag{3.166}$$

where $\mathcal{I}_k$ denotes the identity map on $L(\mathbb{C}^k)$.

If $\mathcal{Q}$ is a quantum channel, then for every k the map $\mathcal{Q} \otimes \mathcal{I}_k$ is also a quantum channel, and hence has induced trace norm 1. Therefore,

$$\|\mathcal{Q}\|_\diamond = \sup_{k\geq 1} \|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1} = 1. \tag{3.167}$$

While the definition involves a supremum over all dimensions k, a remarkable result shows that the supremum is achieved when the auxiliary dimension matches the input dimension of the map.

Proposition 3.57 (Stabilization of the Diamond Norm)**.** *For any linear map $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^M)$, the supremum in Eq.* (3.166) *is achieved for $k = N$. That is,*

$$\|\mathcal{Q}\|_\diamond = \|\mathcal{Q} \otimes \mathcal{I}_N\|_{1\to 1}. \tag{3.168}$$

Proof. We aim to show that for any $k \geq 1$, $\|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1} \leq \|\mathcal{Q} \otimes \mathcal{I}_N\|_{1\to 1}$.

Let $k \geq 1$. By Lemma 3.52, the induced norm is achieved by a rank-1 input. There exist normalized vectors $|\alpha\rangle, |\beta\rangle \in \mathbb{C}^N \otimes \mathbb{C}^k$ such that

$$\|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1} = \|(\mathcal{Q} \otimes \mathcal{I}_k)(|\alpha\rangle\langle\beta|)\|_1. \tag{3.169}$$

Consider the Schmidt decompositions of $|\alpha\rangle$ and $|\beta\rangle$. The Schmidt ranks r, s are at most N.

$$|\alpha\rangle = \sum_{i=1}^{r} \sqrt{p_i}\,|a_i\rangle \otimes |x_i\rangle, \quad |\beta\rangle = \sum_{j=1}^{s} \sqrt{q_j}\,|b_j\rangle \otimes |y_j\rangle. \tag{3.170}$$

Here, $\{|a_i\rangle\}, \{|b_j\rangle\} \subset \mathbb{C}^N$ and $\{|x_i\rangle\}, \{|y_j\rangle\} \subset \mathbb{C}^k$ are orthonormal sets. Let $Y = (\mathcal{Q} \otimes \mathcal{I}_k)(|\alpha\rangle\langle\beta|)$.

$$Y = \sum_{i,j} \sqrt{p_i q_j}\,\mathcal{Q}(|a_i\rangle\langle b_j|) \otimes |x_i\rangle\langle y_j|. \tag{3.171}$$

We construct corresponding vectors in $\mathbb{C}^N \otimes \mathbb{C}^N$. Let $\{|e_i\rangle\}_{i=1}^N$ be a basis for $\mathbb{C}^N$. Define normalized vectors $|\alpha'\rangle, |\beta'\rangle \in \mathbb{C}^N \otimes \mathbb{C}^N$ by replacing $|x_i\rangle$ with $|e_i\rangle$ and $|y_j\rangle$ with $|e_j\rangle$. Let $Y' = (\mathcal{Q} \otimes \mathcal{I}_N)(|\alpha'\rangle\langle\beta'|)$.

$$Y' = \sum_{i,j} \sqrt{p_i q_j}\,\mathcal{Q}(|a_i\rangle\langle b_j|) \otimes |e_i\rangle\langle e_j|. \tag{3.172}$$

We show that $\|Y\|_1 = \|Y'\|_1$. Define partial isometries $V, W : \mathbb{C}^N \to \mathbb{C}^k$. Let V map $\text{span}\{|e_i\rangle\}_{i=1}^r$ isometrically onto $\text{span}\{|x_i\rangle\}_{i=1}^r$, and similarly for W and $\{|y_j\rangle\}$. We can relate Y and Y':

$$Y = (I_M \otimes V)Y'(I_M \otimes W^\dagger). \tag{3.173}$$

Extend V and W to unitaries $\widetilde{V}, \widetilde{W}$ on $\mathbb{C}^k$ (by choosing orthonormal complements). Since Y' only has support on the subspaces where V and W act isometrically, we have

$$Y = (I_M \otimes \widetilde{V})Y'(I_M \otimes \widetilde{W}^\dagger). \tag{3.174}$$

By unitary invariance of the trace norm, $\|Y\|_1 = \|Y'\|_1$.

We have established $\|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1} = \|Y'\|_1$. Since $\||\alpha'\rangle\langle\beta'|\|_1 = 1$, we have $\|Y'\|_1 \leq \|\mathcal{Q} \otimes \mathcal{I}_N\|_{1\to 1}$. This completes the proof. □

The diamond norm inherits the submultiplicativity property from the induced trace norm.

Proposition 3.58 (Submultiplicativity of the Diamond Norm)**.** *Let $\mathcal{R} : L(\mathbb{C}^N) \to L(\mathbb{C}^{N'})$ and $\mathcal{Q} : L(\mathbb{C}^{N'}) \to L(\mathbb{C}^M)$ be linear maps. Then*

$$\|\mathcal{Q} \circ \mathcal{R}\|_\diamond \leq \|\mathcal{Q}\|_\diamond \|\mathcal{R}\|_\diamond . \tag{3.175}$$

Proof. We use the definition of the diamond norm and the property that $(\mathcal{Q} \circ \mathcal{R}) \otimes \mathcal{I}_k = (\mathcal{Q} \otimes \mathcal{I}_k) \circ (\mathcal{R} \otimes \mathcal{I}_k)$.

$$\|\mathcal{Q} \circ \mathcal{R}\|_\diamond = \sup_k \|(\mathcal{Q} \otimes \mathcal{I}_k) \circ (\mathcal{R} \otimes \mathcal{I}_k)\|_{1\to 1} . \tag{3.176}$$

By the submultiplicativity of the induced trace norm (Proposition 3.50):

$$\begin{aligned} \|\mathcal{Q} \circ \mathcal{R}\|_\diamond &\leq \sup_k \left(\|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1} \|\mathcal{R} \otimes \mathcal{I}_k\|_{1\to 1}\right) \\ &\leq \left(\sup_k \|\mathcal{Q} \otimes \mathcal{I}_k\|_{1\to 1}\right)\left(\sup_k \|\mathcal{R} \otimes \mathcal{I}_k\|_{1\to 1}\right) \\ &= \|\mathcal{Q}\|_\diamond \|\mathcal{R}\|_\diamond . \end{aligned} \tag{3.177}$$

□

We can derive useful bounds on the diamond norm for specific types of maps. We start with maps defined by a single Kraus operator.

Lemma 3.59. *Let $\mathcal{Q}_A(X) = AXA^\dagger$ and $\mathcal{Q}_B(X) = BXB^\dagger$. Then the diamond norm of their difference is bounded by*

$$\|\mathcal{Q}_A - \mathcal{Q}_B\|_\diamond \leq (\|A\|_\infty + \|B\|_\infty) \|A - B\|_\infty . \tag{3.178}$$

Proof. Let $\Phi = \mathcal{Q}_A - \mathcal{Q}_B$. By stabilization (Proposition 3.57), we evaluate $\|\Phi \otimes \mathcal{I}_N\|_{1\to 1}$. Let X_{SR} be an input operator with $\|X_{SR}\|_1 = 1$.

$$(\Phi \otimes \mathcal{I}_N)(X_{SR}) = (A \otimes I)X_{SR}(A^\dagger \otimes I) - (B \otimes I)X_{SR}(B^\dagger \otimes I). \tag{3.179}$$

We use the identity $AA^\dagger - BB^\dagger = A(A^\dagger - B^\dagger) + (A - B)B^\dagger$.

$$\begin{aligned} (\Phi \otimes \mathcal{I}_N)(X_{SR}) = &(A \otimes I)X_{SR}((A^\dagger - B^\dagger) \otimes I) \\ &+ ((A - B) \otimes I)X_{SR}(B^\dagger \otimes I). \end{aligned} \tag{3.180}$$

We bound the trace norm using the triangle inequality and Hölder's inequality ($\|Y_1 X Y_2\|_1 \leq \|Y_1\|_\infty \|X\|_1 \|Y_2\|_\infty$). Since $\|X_{SR}\|_1 = 1$ and $\|Y \otimes I\|_\infty = \|Y\|_\infty$:

$$\|(\Phi \otimes \mathcal{I}_N)(X_{SR})\|_1 \leq \|A\|_\infty \left\|A^\dagger - B^\dagger\right\|_\infty + \|A - B\|_\infty \left\|B^\dagger\right\|_\infty . \tag{3.181}$$

Using $\left\|A^\dagger - B^\dagger\right\|_\infty = \|A - B\|_\infty$ and $\left\|B^\dagger\right\|_\infty = \|B\|_\infty$, we obtain the bound. □

Example 3.60 (Distance between unitary channels)**.** Consider unitary channels $\mathcal{U}(X) = UXU^\dagger$ and $\mathcal{V}(X) = VXV^\dagger$. Since $\|U\|_\infty = \|V\|_\infty = 1$, Lemma 3.59 yields the bound:

$$\|\mathcal{U} - \mathcal{V}\|_\diamond \leq 2 \|U - V\|_\infty . \tag{3.182}$$

◇

While the bound in Eq. (3.182) is widely used, it is not always tight. Furthermore, one might expect that stabilization is necessary for unitary channels. However, the difference between unitary channels exhibits a special structure that renders stabilization unnecessary.

Proposition 3.61. *Let $\mathcal{U}, \mathcal{V}$ be two unitary channels defined by unitaries U and V. Then the diamond norm of their difference is equal to the induced trace norm:*

$$\|\mathcal{U} - \mathcal{V}\|_\diamond = \|\mathcal{U} - \mathcal{V}\|_{1\to 1} . \tag{3.183}$$

This norm can be computed explicitly using the numerical range of $W = U^\dagger V$:

$$\|\mathcal{U} - \mathcal{V}\|_\diamond = 2\sqrt{1 - d_{\min}^2}, \tag{3.184}$$

where $d_{\min} = \inf\{|z| : z \in \mathcal{W}(W)\}$ is the minimum distance from the origin to the numerical range $\mathcal{W}(W) = \{\langle x| W |x\rangle : \|x\|_2 = 1\}$.

Proof. Let $\Phi = \mathcal{U} - \mathcal{V}$. We first establish a lower bound for the induced trace norm $\|\Phi\|_{1\to 1}$. According to Lemma 3.52, the induced trace norm is defined by the supremum over rank-1 inputs. Restricting the optimization to pure states $\rho = |x\rangle\langle x|$ yields a lower bound:

$$\|\Phi\|_{1\to 1} \geq \sup_{|x\rangle} \|\Phi(|x\rangle\langle x|)\|_1 . \tag{3.185}$$

The output is

$$\Phi(|x\rangle\langle x|) = U|x\rangle\langle x|U^\dagger - V|x\rangle\langle x|V^\dagger = |\psi_U\rangle\langle\psi_U| - |\psi_V\rangle\langle\psi_V|, \tag{3.186}$$

where $|\psi_U\rangle = U|x\rangle$ and $|\psi_V\rangle = V|x\rangle$. The trace norm of the difference between two pure states is determined by their overlap (see Example 3.44):

$$\||\psi_U\rangle\langle\psi_U| - |\psi_V\rangle\langle\psi_V|\|_1 = 2\sqrt{1 - |\langle\psi_U|\psi_V\rangle|^2}. \tag{3.187}$$

The overlap is $\langle\psi_U|\psi_V\rangle = \langle x| U^\dagger V |x\rangle = \langle x| W |x\rangle$. To maximize the norm, we must minimize the magnitude of the overlap. The set of values $\{\langle x| W |x\rangle : \|x\|_2 = 1\}$ is the numerical range $\mathcal{W}(W)$. Thus, the supremum over pure states is

$$2\sqrt{1 - \inf_{z\in\mathcal{W}(W)} |z|^2} = 2\sqrt{1 - d_{\min}^2}. \tag{3.188}$$

Next, we consider the diamond norm $\|\Phi\|_\diamond$. By the stabilization property (Proposition 3.57), $\|\Phi\|_\diamond = \|\Phi \otimes \mathcal{I}_N\|_{1\to 1}$. Unlike the induced trace norm, the diamond norm is achieved on pure states (see [Wat18, Theorem 3.51]). Let $|\Psi\rangle \in \mathbb{C}^N \otimes \mathbb{C}^N$ be a normalized pure state. The action of the map

on $\rho = |\Psi\rangle\langle\Psi|$ yields the difference of two pure states $|\Psi_U\rangle = (U \otimes I)|\Psi\rangle$ and $|\Psi_V\rangle = (V \otimes I)|\Psi\rangle$. The norm is again given by $2\sqrt{1 - |\langle\Psi_U|\Psi_V\rangle|^2}$. The overlap is

$$\langle\Psi_U|\Psi_V\rangle = \langle\Psi|(U^\dagger \otimes I)(V \otimes I)|\Psi\rangle = \langle\Psi|(W \otimes I)|\Psi\rangle. \tag{3.189}$$

We express this overlap in terms of the reduced density operator $\rho_A = \mathrm{Tr}_B[|\Psi\rangle\langle\Psi|]$:

$$\langle\Psi|(W \otimes I)|\Psi\rangle = \mathrm{Tr}[(W \otimes I)|\Psi\rangle\langle\Psi|] = \mathrm{Tr}[W\rho_A]. \tag{3.190}$$

As $|\Psi\rangle$ varies over all pure states in the joint space, ρ_A varies over all density operators in $\mathcal{D}(\mathbb{C}^N)$. The set of achievable overlaps is therefore the set of expectation values $\{\mathrm{Tr}[W\rho] : \rho \in \mathcal{D}(\mathbb{C}^N)\}$. This set is the convex hull of the numerical range $\mathcal{W}(W)$. By the Toeplitz–Hausdorff theorem (see [Bha97, Chapter 1]), the numerical range $\mathcal{W}(W)$ is a convex set. Therefore, the convex hull of $\mathcal{W}(W)$ is $\mathcal{W}(W)$ itself. This implies that allowing entanglement does not extend the range of possible overlaps:

$$\inf_{\||\Psi\rangle\|_2=1} |\langle\Psi|(W \otimes I)|\Psi\rangle| = \inf_{z \in \mathcal{W}(W)} |z| = d_{\min}. \tag{3.191}$$

Consequently,

$$\|\Phi\|_\diamond = 2\sqrt{1 - d_{\min}^2}. \tag{3.192}$$

Combining this with Eq. (3.188) and the inequality $\|\Phi\|_{1\to1} \le \|\Phi\|_\diamond$, we conclude $\|\Phi\|_\diamond = \|\Phi\|_{1\to1}$. □

Example 3.62. Consider the 2×2 unitaries $U = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and $V = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. We calculate the operator norm of their difference:

$$U - V = \begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}. \tag{3.193}$$

The singular values are the square roots of the eigenvalues of $(U-V)^\dagger(U-V) = \mathrm{diag}(2,2)$. Thus, $\|U - V\|_\infty = \sqrt{2}$. The general bound in Eq. (3.182) gives $\|\mathcal{U} - \mathcal{V}\|_\diamond \le 2\sqrt{2} \approx 2.828$.

However, as $W = U^\dagger = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, the eigenvalues of W are i and $-i$. Since W is normal, $\mathcal{W}(W)$ is the convex hull of the eigenvalues, i.e., the segment $[-i, i]$ on the imaginary axis. The minimum distance to the origin is $d_{\min} = 0$. Thus, the exact diamond norm is $2\sqrt{1 - 0^2} = 2$. ⋄

Example 3.63 (Qubit Phase Shift Channel)**.** We illustrate the computation using a single-qubit example. Consider the identity channel $\mathcal{I}$ ($U = I$) and the phase shift channel $\mathcal{P}_\theta$, defined by the unitary $V = P_\theta = \mathrm{diag}(1, e^{i\theta})$. We wish to compute $\|\mathcal{I} - \mathcal{P}_\theta\|_\diamond$.

We apply Proposition 3.61. We compute $W = U^\dagger V = P_\theta$. We need to determine the numerical range $\mathcal{W}(P_\theta)$. Since P_θ is a normal operator, its numerical range is the convex hull of its eigenvalues, $\{1, e^{i\theta}\}$. This is the line segment (chord) connecting 1 and $e^{i\theta}$ in the complex plane.

We seek the minimum distance $d_{\min}$ from the origin to this segment. Geometrically, this distance is the altitude of the isosceles triangle formed by the origin and the two eigenvalues.

The length of the base of the triangle (the chord) is $|1 - e^{i\theta}| = \sqrt{(1-\cos\theta)^2 + \sin^2\theta} = \sqrt{2 - 2\cos\theta} = 2|\sin(\theta/2)|$. The area of the triangle is $\frac{1}{2}|\sin\theta|$. Let h be the altitude, which corresponds to $d_{\min}$. The area is also $\frac{1}{2} \cdot \text{base} \cdot h$.

$$d_{\min} = h = \frac{|\sin\theta|}{2|\sin(\theta/2)|} = \frac{2|\sin(\theta/2)\cos(\theta/2)|}{2|\sin(\theta/2)|} = |\cos(\theta/2)|. \tag{3.194}$$

Substituting this minimum value into Eq. (3.184):

$$\|\mathcal{I} - \mathcal{P}_\theta\|_\diamond = 2\sqrt{1-\cos^2(\theta/2)} = 2\sqrt{\sin^2(\theta/2)} = 2|\sin(\theta/2)|. \tag{3.195}$$

By Proposition 3.61, the induced trace norm is identical: $\|\mathcal{I} - \mathcal{P}_\theta\|_{1\to 1} = 2|\sin(\theta/2)|$.

For instance, if $\theta = \pi$, the channel is the Pauli-Z channel $\mathcal{Z}$. The diamond norm is $2|\sin(\pi/2)| = 2$. The minimum overlap is $d_{\min} = 0$. This is achieved by the input state $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, since $\langle +| Z |+\rangle = 0$. ⋄

The following example illustrates that the standard induced trace norm can drastically underestimate the "size" of a map that is not completely positive.

Example 3.64 (Transpose Map)**.** Let $\mathcal{T} : \mathbb{C}^{N\times N} \to \mathbb{C}^{N\times N}$ be the transpose map, $\mathcal{T}(X) = X^\top$, defined in a fixed basis. Since the transpose preserves the eigenvalues of Hermitian matrices and maps density matrices to density matrices, it preserves the 1-norm for positive inputs. It can be shown that $\|\mathcal{T}\|_{1\to 1} = 1$.

However, consider the action of $\mathcal{T} \otimes \mathcal{I}_N$ on the unnormalized maximally entangled state $|\Omega\rangle = \sum_{i=1}^N |i\rangle \otimes |i\rangle$. The corresponding density matrix is $\omega = \sum_{i,j} |i\rangle\langle j| \otimes |i\rangle\langle j|$. Applying the partial transpose yields

$$(\mathcal{T} \otimes \mathcal{I}_N)(\omega) = \sum_{i,j} |j\rangle\langle i| \otimes |i\rangle\langle j|, \tag{3.196}$$

which is the SWAP operator. The eigenvalues of the SWAP operator on $\mathbb{C}^N \otimes \mathbb{C}^N$ are $+1$ (on the symmetric subspace of dimension $N(N+1)/2$) and -1 (on the antisymmetric subspace of dimension $N(N-1)/2$). The trace norm is the sum of singular values (absolute values of eigenvalues):

$$\|(\mathcal{T} \otimes \mathcal{I}_N)(\omega)\|_1 = \frac{N(N+1)}{2} + \frac{N(N-1)}{2} = N^2. \tag{3.197}$$

Since $\|\omega\|_1 = \||\Omega\rangle\|^2 = N$, we find that for this specific state, the ratio of output norm to input norm is N. Thus $\|\mathcal{T}\|_\diamond \geq N$. ⋄

3.6.3. Induced trace distance and diamond distance. The **induced trace distance** between two linear maps $\mathcal{Q}, \mathcal{R}$ is

$$D(\mathcal{Q}, \mathcal{R}) := \frac{1}{2}\|\mathcal{Q} - \mathcal{R}\|_{1\to 1}. \tag{3.198}$$

Example 3.65 (Trace distance for classical channel)**.** Given two transition matrices $Q, R \in \mathbb{R}^{N\times N}$, the corresponding classical channels are

$$\mathcal{Q}[\rho] = \sum_{i,j\in[N]} Q_{ij}|i\rangle\langle j|\rho|j\rangle\langle i|, \quad \mathcal{R}[\rho] = \sum_{i,j\in[N]} R_{ij}|i\rangle\langle j|\rho|j\rangle\langle i|. \tag{3.199}$$

Then

$$\begin{aligned} D(\mathcal{Q},\mathcal{R}) =& \frac{1}{2}\sup_{\|\rho\|_1=1}\|\mathcal{Q}[\rho]-\mathcal{R}[\rho]\|_1 \\ =& \frac{1}{2}\sup_{\|\rho\|_1=1}\sum_i\left|\sum_j(Q_{ij}-R_{ij})\rho_{jj}\right| \\ \leq& \frac{1}{2}\sup_{\|\rho\|_1=1}\left(\max_j\sum_i|Q_{ij}-R_{ij}|\right)\operatorname{Tr}|\rho| \\ \leq& \frac{1}{2}\sup_{\|\rho\|_1=1}\left(\max_j\sum_i|Q_{ij}-R_{ij}|\right)\|\rho\|_1 \\ =& D(Q,R), \end{aligned} \tag{3.200}$$

which is the induced total variation distance between the transition matrices Q, R. Here we have used Proposition 3.31 in the last inequality. On the other hand, choosing $\rho = |j'\rangle\langle j'|$ with $j' = \arg\max_j \sum_i |Q_{ij} - R_{ij}|$, we have $D(\mathcal{Q},\mathcal{R}) \geq D(Q,R)$. This proves that the induced trace distance is consistent with the induced total variation distance on classical channels:

$$D(\mathcal{Q},\mathcal{R}) = D(Q,R). \tag{3.201}$$

◇

The metric induced by the diamond norm is known as the diamond distance. The factor of $1/2$ normalizes the metric such that perfectly distinguishable channels have a distance of 1, analogous to the trace distance for quantum states.

Definition 3.66 (Diamond Distance)**.** *Let $\mathcal{Q},\mathcal{R} : \mathbb{C}^{N\times N} \to \mathbb{C}^{M\times M}$ be two linear maps. The **diamond distance** between them is defined as*

$$D_\diamond(\mathcal{Q},\mathcal{R}) := \frac{1}{2}\|\mathcal{Q}-\mathcal{R}\|_\diamond. \tag{3.202}$$

Quantum channels satisfy the linear error growth property with respect to the diamond distance. The proof is also very similar to Proposition 3.55.

Proposition 3.67. *Let $\{\mathcal{U}_i\}_{i=1}^K$ and $\{\widetilde{\mathcal{U}}_i\}_{i=1}^K$ be sequences of unitary channels generated by the unitary operators $\{U_i\}_{i=1}^K$ and $\{\widetilde{U}_i\}_{i=1}^K$, respectively. The diamond distance between the composite channels is bounded by*

$$D_\diamond(\mathcal{U}_K\cdots\mathcal{U}_1, \widetilde{\mathcal{U}}_K\cdots\widetilde{\mathcal{U}}_1) \leq \sum_{i=1}^K \left\|U_i-\widetilde{U}_i\right\|_\infty. \tag{3.203}$$

Proof. First, we observe that quantum channels satisfy a linear error growth property with respect to the diamond distance. The proof of this property relies on a telescoping sum argument, which is strictly analogous to the proof of Proposition 3.55 and is therefore omitted. This yields the bound

$$D_\diamond(\mathcal{U}_K\cdots\mathcal{U}_1, \widetilde{\mathcal{U}}_K\cdots\widetilde{\mathcal{U}}_1) \leq \frac{1}{2}\sum_{i=1}^K \left\|\widetilde{\mathcal{U}}_i-\mathcal{U}_i\right\|_\diamond. \tag{3.204}$$

It suffices to bound the diamond norm difference for a single step. Recalling Eq. (3.182), we have the general bound $\left\|\widetilde{\mathcal{U}}_i - \mathcal{U}_i\right\|_\diamond \leq 2\left\|U_i - \widetilde{U}_i\right\|$. Substituting this estimate into the linear error growth inequality completes the proof. □

Notes and further reading

The formalism of quantum channels rests on foundational results in operator theory. The operator-sum representation (Theorem 3.18) is due to Kraus [KBDW83], while the dilation theorem (Theorem 3.20) was established by Stinespring [Sti55]. The isomorphism characterizing completely positive maps via their action on entangled states is attributed to Choi [Cho75] and Jamiołkowski [Jam72].

The induced trace distance provides a useful way to compare two channels via their action on input states. It is worth noting that the contractivity properties of the trace distance used in this context rely on positivity and trace preservation, and do not require complete positivity. By contrast, complete positivity is required to ensure that a channel remains positive when extended by an identity map on an arbitrary ancillary register. This distinction becomes operationally visible in the channel discrimination task: for some pairs of channels, optimal discrimination is only possible when the input is entangled with an ancillary register. This motivates the use of stabilized distances such as the diamond norm (the completely bounded trace norm), which explicitly accounts for ancillary extensions. For distance measures, Helstrom [Hel69] provided the operational interpretation of the trace distance in terms of state discrimination. Fidelity was studied by Uhlmann [Uhl76] as transition probability. The tight relationship between these two measures (Theorem 3.46) was established by Fuchs and van de Graaf [FVDG02]. The diamond norm was introduced to quantum computing by Kitaev [Kit97] to quantify the accuracy of quantum gates in a manner robust to entanglement, and is closely related to the completely bounded norm in operator algebra. We refer readers to [Wat18, Chapter 3.3] for further discussion.

Most of the discussions in this book will be restricted to unitary channels, and these unitary channels are often applied to pure states. Nevertheless, the concept of a quantum channel is helpful for understanding the probabilistic nature of quantum algorithms. For a systematic treatment of density operators and quantum channels, we refer readers to [Wat18, Chapter 2] and [NC00, Section 2.4, 8.2]. We refer readers to [Wat18, Chapter 3] for properties of the norms and distances introduced here, and their applications in discrimination-type problems. For matrix analysis tools, such as Schatten norms, we refer to [Bha97].

CHAPTER 4

Universality of quantum circuits

CHAPTER 5

Quantum processing of classical information

Quantum algorithms often require classical data to be loaded, processed, and manipulated within a quantum circuit. This chapter explores how classical information can be encoded and operated on in a quantum computing framework. We begin with the reversible simulation of classical logic gates, a prerequisite for embedding classical computation into quantum circuits. We then discuss uncomputation, which is very useful for cleaning up intermediate states without disturbing the computation's outcome. The chapter proceeds to cover fixed-point number representation and quantum random access memory (QRAM). Finally, we present methods for implementing certain classical arithmetic operations within quantum circuits.

5.1. Reversible simulation of classical gates

How can we compare the computational power of quantum computers to that of classical computers? While it remains extremely difficult to prove that quantum computers are fundamentally more powerful than classical ones, it is well established that quantum computers are at least as powerful. More precisely, any classical circuit can be simulated asymptotically efficiently by a quantum circuit.

The key idea is that all classical gates can be simulated in a reversible way. Some classical logic gates, such as the NOT gate, are already reversible and can be directly implemented by the Pauli X gate. However, many commonly used gates, including AND, OR, and NAND, are not reversible and cannot be directly translated into unitary transformations.

Reversible computation, which predates quantum computing, was originally studied in the context of thermodynamics and the fundamental limits of energy dissipation [Lan61]. In this model of computation, each operation can be reversed, and information is preserved throughout the process. To simulate arbitrary classical circuits in a reversible form, it is sufficient to construct reversible versions of universal gates such as the NAND gate. Once a reversible version of a universal gate is available, the entire classical computation can be lifted into a reversible framework, which can then be embedded into a quantum circuit using unitary operations.

Example 5.1 (Toffoli is universal for classical computation)**.** All boolean logic can be implemented using only NAND gates. NAND and FANOUT (i.e., making a copy of a classical bit x) are together universal for classical computation. The Toffoli gate is a controlled-controlled-NOT gate, and with an ancilla initialized to $|0\rangle$ it computes x AND y into the target register. We can use the Toffoli gate to simulate NAND and FANOUT. Therefore the Toffoli gate is universal for classical computation.

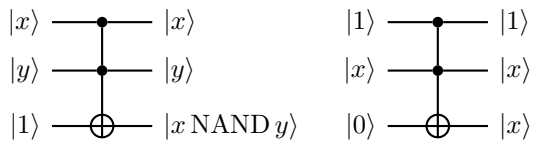


FIGURE 5.1. Using the Toffoli gate to implement NAND and FANOUT

◇

Exercise 5.1. Give explicit expressions for using Toffoli gates to implement AND, NOT, XOR, and OR.

A classical computation procedure can be expressed as the evaluation of a boolean map $f : \{0,1\}^n \to \{0,1\}^m$, which may be irreversible. However, it can be made into a reversible classical gate

$$(z, x) \mapsto (z \oplus f(x), x). \tag{5.1}$$

In particular, $(0^m, x) \mapsto (f(x), x)$ is a reversible map that can then be implemented using unitary operations. Efficient implementation of $x \mapsto f(x)$ on a classical computer means that the number of elementary classical gates (e.g., AND, NOT, NAND gates) is at most $\mathrm{poly}(n)$, and the classical implementation of the map uses at most $\mathrm{poly}(n)$ additional bits for storage. By converting each of the elementary classical gate into a reversible gate, we can implement

$$U_f : |0\rangle^{\otimes w} |0\rangle^{\otimes m} |x\rangle \mapsto |g(x)\rangle |f(x)\rangle |x\rangle . \tag{5.2}$$

Using $w = \mathrm{poly}(n)$ ancilla qubits, the depth of the quantum circuit is $\mathrm{poly}(n)$.

THEOREM 5.2. *Any irreversible classical computation using* $\mathrm{poly}(n)$ *classical gates can be simulated on a quantum computer using* $\mathrm{poly}(n)$ *simple quantum gates and* $\mathrm{poly}(n)$ *qubits.*

Up to a polynomial slowdown, a quantum computer is at least as powerful as classical computers. It should be noted that such a procedure is likely to be extremely inefficient. Thus the construction used in Theorem 5.2 is not expected to be practically useful beyond the simplest scenario.

5.2. Uncomputation

Unlike classical bits, qubits can exist in superpositions of computational basis states, which enables interference effects in computation. However, qubits are also prone to interference and can easily lose their coherence, causing computational errors. When a quantum computer performs a computation, it can create a large number of ancilla qubits (also called working qubits, or garbage register) that are entangled with the qubits carrying the actual result of the computation. If these ancilla qubits are not properly reset back to their initial state (usually $|0\rangle^{\otimes a}$), they can interfere with subsequent computations and cause errors. This resetting process is called **uncomputation**. Other than avoiding interference, uncomputation is also important for the purpose of resource management. Quantum systems available today have a limited number of qubits. By uncomputing, we can reuse qubits more efficiently.

Uncomputation needs to be done in a very specific way to maintain the integrity of the quantum computation. Simply resetting qubits (for example, by measuring the ancilla qubits and resetting them to $|0\rangle$) is not sufficient, as it can destroy the superposition and entanglement of the other

qubits in the system. Furthermore, due to the no-deleting theorem, there is no generic unitary operator that can set a black-box state to $|0\rangle^{\otimes w}$.

Let us now consider how to perform uncomputation when implementing a classical mapping. In quantum computing, an **oracle** means a black box operation that for a given input provides an output, usually the result of evaluating a function on that input. With the help of a working register, we assume that the oracle implementing Eq. (5.2) is available.

In order to set the working register back to $|0\rangle^{\otimes w}$ while keeping the input and output state, we must use the information stored in U_f explicitly. We introduce yet another m-qubit ancilla register initialized at $|0\rangle^{\otimes m}$. Then we can use an m-qubit CNOT controlled on the output register and obtain

$$|0\rangle^{\otimes m}|g(x)\rangle|f(x)\rangle|x\rangle \mapsto \underbrace{|f(x)\rangle}_{\text{ancilla}}\underbrace{|g(x)\rangle}_{\text{working}}\underbrace{|f(x)\rangle}_{\text{output}}\underbrace{|x\rangle}_{\text{input}}. \tag{5.3}$$

It is important to remember that in the operation above, the multi-qubit CNOT gate only performs the classical copying operation in the computational basis, and does not violate the no-cloning theorem.

Recall that $U_f^{-1} = U_f^\dagger$, so

$$(I^{\otimes m} \otimes U_f^\dagger)|f(x)\rangle|g(x)\rangle|f(x)\rangle|x\rangle = |f(x)\rangle|0\rangle^{\otimes w}|0\rangle^{\otimes m}|x\rangle. \tag{5.4}$$

Finally we apply an m-qubit SWAP operator on the ancilla and output registers to obtain

$$|f(x)\rangle|0\rangle^{\otimes w}|0\rangle^{\otimes m}|x\rangle \mapsto |0\rangle^{\otimes m}|0\rangle^{\otimes w}|f(x)\rangle|x\rangle. \tag{5.5}$$

After this procedure, both the ancilla and the working register are set to the initial state. They are no longer entangled to the input or output register, and can be reused for other purposes. The circuit for this uncomputation step is shown in Fig. 5.2.

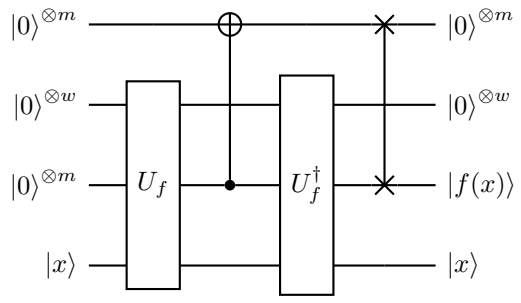


FIGURE 5.2. Circuit for uncomputation. The CNOT and SWAP operators indicate the multi-qubit copy and swap operations, respectively.

Remark 5.3 (Discarding working registers)**.** After the uncomputation as shown in Fig. 5.2, the first two registers are unchanged before and after the application of the circuit (though they are changed during the intermediate steps). Therefore Fig. 5.2 effectively implements a unitary

$$(I^{\otimes(m+w)} \otimes V_f)|0\rangle^{\otimes m}|0\rangle^{\otimes w}|0\rangle^{\otimes m}|x\rangle = |0\rangle^{\otimes m}|0\rangle^{\otimes w}|f(x)\rangle|x\rangle, \tag{5.6}$$

or equivalently

$$V_f \left|0\right\rangle^{\otimes m} \left|x\right\rangle = \left|f(x)\right\rangle \left|x\right\rangle . \tag{5.7}$$

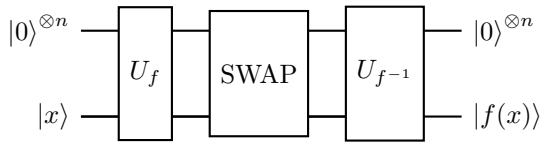
In the definition of V_f, all working registers have been discarded. This allows us to simplify the notation and focus on the essence of the quantum algorithms under study. Using the technique of uncomputation, if the map $x \mapsto f(x)$ can be efficiently implemented on a classical computer, then we can implement this map efficiently on a quantum computer as well with a controllable amount of quantum resources. ◇

Example 5.4. Given $f : \{0,1\}^n \to \{0,1\}^n$, in general, the transformation $\left|x\right\rangle \mapsto \left|f(x)\right\rangle$ is not unitary. However, when f is a bijection, and we have access to both f, f^{-1} as follows:

$$U_f : \left|z\right\rangle \left|x\right\rangle \mapsto \left|z \oplus f(x)\right\rangle \left|x\right\rangle , \quad U_{f^{-1}} : \left|z\right\rangle \left|x\right\rangle \mapsto \left|z \oplus f^{-1}(x)\right\rangle \left|x\right\rangle , \tag{5.8}$$

we can use them to construct the unitary transformation $U'_f : \left|x\right\rangle \mapsto \left|f(x)\right\rangle$.

To implement U'_f, we will use an ancilla register initialized in the $\left|0\right\rangle^{\otimes n}$ state to hold the result of applying f or f^{-1}. Apply U_f to the state $\left|0\right\rangle^{\otimes n} \left|x\right\rangle$ to get $\left|f(x)\right\rangle \left|x\right\rangle$. This setup now contains the desired mapping in the first register, but it is entangled with the input in the second register. Next apply SWAP to the two registers and the state becomes $\left|x\right\rangle \left|f(x)\right\rangle$. Apply $U_{f^{-1}}$ to the state $\left|x\right\rangle \left|f(x)\right\rangle$ to get $\left|x \oplus f^{-1}(f(x))\right\rangle \left|f(x)\right\rangle = \left|x \oplus x\right\rangle \left|f(x)\right\rangle = \left|0\right\rangle^{\otimes n} \left|f(x)\right\rangle$. The ancilla register is restored to $\left|0\right\rangle^{\otimes n}$ and can be discarded. This gives our desired U'_f. The circuit is as follows.



◇

Example 5.5. Another common usage of the uncomputation is to disentangle two registers. Consider the following sequence of operations

$$\begin{aligned} \sum_j c_j \left|v_j\right\rangle \left|0\right\rangle^{\otimes a} \left|0\right\rangle^{\otimes b} &\xrightarrow{U_a} \sum_j c_j \left|v_j\right\rangle \left|u_j\right\rangle \left|0\right\rangle^{\otimes b} \\ &\xrightarrow{U_b} \sum_j c_j \left|v_j\right\rangle \left|u_j\right\rangle (\beta_j \left|0\right\rangle^{\otimes b} + \sqrt{1 - \left|\beta_j\right|^2} \left|\perp_j\right\rangle). \end{aligned} \tag{5.9}$$

Here U_a only acts on the first and second register, U_b only acts on the second and third register, and $\left|\perp_j\right\rangle$ is a state that is orthogonal to $\left|0\right\rangle^{\otimes b}$. Our goal is to obtain a state proportional to

$$\sum_j c_j \beta_j \left|v_j\right\rangle \left|0\right\rangle^{\otimes a} \left|0\right\rangle^{\otimes b} . \tag{5.10}$$

This cannot be done by measuring the third register and check whether the outcome is 0^b, since it will lead to $\sum_j c_j \beta_j \left|v_j\right\rangle \left|u_j\right\rangle \left|0\right\rangle^{\otimes b}$, which entangles the first two registers. The correct procedure is to perform uncomputation by applying $U_a^\dagger$ to the first two registers, which gives a state

$$\sum_j c_j \left|v_j\right\rangle \left|0\right\rangle^{\otimes a} (\beta_j \left|0\right\rangle^{\otimes b} + \sqrt{1 - \left|\beta_j\right|^2} \left|\perp_j\right\rangle). \tag{5.11}$$

Then measuring the third register produces the desired state. ◇

5.3. Fixed point number representation and quantum random access memory

When we want to perform arithmetic operations on a quantum computer, such as addition, multiplication, or more complex functions, we need to encode the numbers we are working with into qubit states. On classical computers, floating point number representations are an efficient way to represent numbers with a wide numerical range. However, on quantum computers, it is often convenient to encode numbers into amplitudes or phases (e.g., via phase kickback). Therefore it is difficult in general to handle numbers that are too large or too small (e.g., $3.14 \times 10^{\pm 12}$). The standard practice is to use a binary fixed point representation of real numbers.

Any integer $k \in [N]$ where $N = 2^n$ can be expressed as an n-bit string as $k = (k_{n-1} \cdots k_0)$ with $k_i \in \{0, 1\}$. This is called the binary representation of the integer k. It should be interpreted as

$$k = \sum_{i=0}^{n-1} k_i 2^i. \tag{5.12}$$

The number k divided by 2^m $(0 \le m \le n)$ can be written as (note that the binary point is shifted to be after k_m):

$$a = \frac{k}{2^m} = \sum_{i=0}^{n-1} k_i 2^{i-m} =: (k_{n-1} \cdots k_m . k_{m-1} \cdots k_0). \tag{5.13}$$

The most common case is $m = n$, where

$$a = \frac{k}{2^n} = \sum_{i=0}^{n-1} k_i 2^{i-n} =: (0.k_{n-1} \cdots k_0) \equiv (.k_{n-1} \cdots k_0). \tag{5.14}$$

Sometimes we may also write $a = 0.k_1 \cdots k_n$, which is simply a relabeling of the digits. For a given real number $0 \le a < 1$ written as

$$a = (0.k_1 \cdots k_n k_{n+1} \cdots), \tag{5.15}$$

the number $(0.k_1 \cdots k_n)$ is called the n-bit **fixed point representation** (or n-bit binary representation) of a. Therefore to represent a to additive precision ϵ, we will need $n = \lceil \log_2(1/\epsilon) \rceil$ bits of precision. If the sign of a is also important, we may reserve one extra bit $s \in \{0, 1\}$ to indicate its sign and interpret $(s.k_1 \cdots k_n)$ as $(-1)^s (0.k_1 \cdots k_n)$. A complex number z can be represented using two real numbers as $z = a + ib$, where $a, b \in \mathbb{R}$ are given in the fixed point number representation.

Definition 5.6. *For a length $N = 2^n$ classical data vector x, assume that each component x_i has a d-bit representation. Then the **quantum random access memory** (QRAM) is a unitary U_{QRAM} acting on $n + d$ qubits:*

$$U_{\mathrm{QRAM}} |i\rangle |y\rangle = |i\rangle |y \oplus x_i\rangle . \tag{5.16}$$

The implementation of U_{QRAM} often uses working registers, and such a dependence is hidden in Eq. (5.16) after the uncomputation step. Sometimes QRAM is called the quantum random access classical memory (QRACM). Ideally, the cost for implementing QRAM is poly(n), but this may not be possible if x represents an unstructured classical data set, and the cost for implementing QRAM may be as high as poly(N).

5.4. Classical arithmetic operations

Using the fixed point number representation and reversible computation, we can approximately implement classical arithmetic operations on quantum computers. The map $x \mapsto f(x)$ can be implemented as $U_f |\widetilde{x}\rangle |y\rangle = |\widetilde{x}\rangle |y \oplus \widetilde{f}(x)\rangle$ using e.g., a QRAM. Here $\widetilde{x}$ and $\widetilde{f}(x)$ are n-bit fixed point representation of $x, f(x)$ in the computational basis of the quantum register, respectively. However, it may be much more efficient to implement certain classical arithmetic operations on-the-fly on quantum computers without referring to a QRAM. For instance, $x \mapsto 2x$ can be implemented as a shift operation in the binary format that can be implemented via a sequence of SWAP gates. Other arithmetic mappings, such as $x \mapsto x^2$, as well as binary operations $(x, y) \mapsto x + y$, $(x, y) \mapsto xy$ are harder to implement. Furthermore, these operations can be implemented on quantum computers without going through the process of the reversible implementation of elementary classical gates. Some other classical functions, such as $x \mapsto \arccos(x)$ can be even more difficult to implement. In general, implementation of classical arithmetic operations on quantum computers will incur a significant overhead, both in terms of the number of ancilla qubits and the circuit depth.

Many arithmetic operations involve a procedure called the controlled rotation, which transforms the information stored in a register from a fixed point representation to the amplitude of the wavefunction.

Proposition 5.7 (Controlled rotation given rotation angles)**.** *Let $0 \leq \theta < 1$ have exact d-bit fixed point representation $\theta = (.\theta_{d-1} \cdots \theta_0)$. Then there is a $(d+1)$-qubit unitary U_θ such that*

$$U_\theta : |0\rangle|\theta\rangle \mapsto (\cos(\pi\theta)|0\rangle + \sin(\pi\theta)|1\rangle)|\theta\rangle. \tag{5.17}$$

Proof. First (by e.g. Taylor expansion)

$$\exp(-i\tau\sigma_y) = \begin{pmatrix} \cos(\tau) & -\sin(\tau) \\ \sin(\tau) & \cos(\tau) \end{pmatrix} =: R_y(2\tau). \tag{5.18}$$

Here $R_y(\cdot)$ performs a single-qubit rotation around the y-axis. For any $j \in [2^d]$ with its binary representation $j = j_{d-1} \cdots j_0$, we have

$$j/2^d = (.j_{d-1} \cdots j_0). \tag{5.19}$$

So choose $\tau = \pi(.j_{d-1} \cdots j_0)$, and define

$$U_\theta = \sum_{j \in [2^d]} \exp(-i\pi(.j_{d-1} \cdots j_0)\sigma_y) \otimes |j\rangle\langle j|. \tag{5.20}$$

Applying U_θ to $|0\rangle|\theta\rangle$ gives the desired results. This is a sequence of single-qubit rotations on the signal qubit, each controlled by a single qubit. □

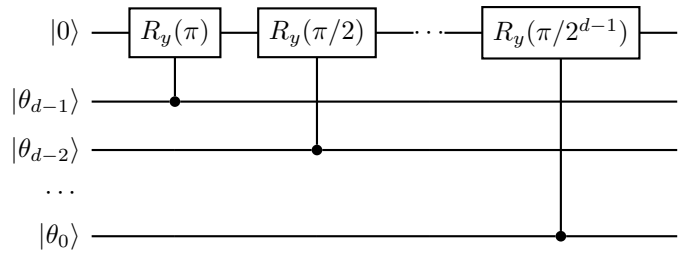


FIGURE 5.3. Quantum circuit for the controlled rotation operation U_θ.

Example 5.8 (Diagonal matrix multiplication using controlled rotation)**.** Let $0 \le a < 1$ be given by an d-bit fixed point representation using an d-qubit register, $f : \mathbb{R} \to \mathbb{R}$ be a function satisfying $|f(a)| \le 1$ for all $0 \le a < 1$. For simplicity assume $f(a) \ge 0$; the case of signed $f(a)$ can be handled by additionally computing the sign of $f(a)$ and applying a controlled phase flip on the $|1\rangle$ branch. We would like to construct a circuit that approximately implements

$$|a\rangle \to f(a)\,|a\rangle\,. \tag{5.21}$$

More generally, the state $|\psi\rangle = \sum_a \psi_a\,|a\rangle$ is mapped to $\sum_a \psi_a f(a)\,|a\rangle$. This can be viewed as multiplying a diagonal matrix $D = \mathrm{diag}\{f(a)\}$ to $|\psi\rangle$.

To implement such a mapping, we first define

$$\theta(a) = \frac{1}{\pi}\arccos f(a). \tag{5.22}$$

Note that even though a is exactly given by d-bits, $\theta(a)$ may not be. So we assume that it can be *rounded* to an d'-bit number $\widetilde{\theta}(a)$. For simplicity we assume d' is large enough so that the error of the fixed point representation is negligible in this step. To implement the mapping $a \mapsto \widetilde{\theta}(a)$, we can construct a classical arithmetics circuit

$$U_{\mathrm{angle}}\,|0^{d'}\rangle\,|a\rangle = |\widetilde{\theta}(a)\rangle\,|a\rangle\,, \tag{5.23}$$

whose construction may require $\mathrm{poly}(\max\{d, d'\})$ gates and an additional working register of $\mathrm{poly}(\max\{d, d'\})$ qubits, which are not displayed here. Therefore, the entire controlled rotation operation needed is given by the circuit in Fig. 5.4.

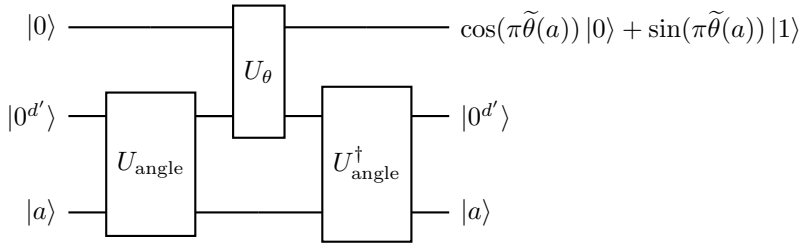


FIGURE 5.4. Circuit for using controlled rotation to implement the multiplication of a diagonal matrix (not including additional working register for classical arithmetic operations).

Note that through the uncomputation $U_{\text{angle}}^\dagger$, the d' ancilla qubits also become a working register. After uncomputation, the ancillas are returned to $|0^{d'}\rangle$ (together with any additional workspace used in U_{angle}), so they may be reused. We obtain a unitary U_{CR} satisfying

$$U_{\text{CR}}\,|0\rangle\,|a\rangle = \Big(\cos(\pi\widetilde{\theta}(a))\,|0\rangle + \sin(\pi\widetilde{\theta}(a))\,|1\rangle\Big)\,|a\rangle \approx \Big(f(a)\,|0\rangle + \sqrt{1-f(a)^2}\,|1\rangle\Big)\,|a\rangle\,. \tag{5.24}$$

Measure the single ancilla qubit. If the result is 0, the data register is projected onto a state proportional to $\sum_a \psi_a f(a)\,|a\rangle$, i.e., the mapping in Eq. (5.21) up to renormalization. If the input state is $|\psi\rangle = \sum_a \psi_a\,|a\rangle$, the probability of obtaining 0 after measuring the ancilla qubit is

$$\mathbb{P}(0) \approx \sum_a |\psi_a|^2\,|f(a)|^2\,. \tag{5.25}$$

◇

Example 5.9 (Use of arithmetic operations in the HHL algorithm)**.** The last step of the Harrow–Hassidim–Lloyd (HHL) algorithm for solving a linear system of equations $Ax = b$ with a Hermitian matrix A involves the following arithmetic operations. For simplicity assume λ_j (eigenvalues of A) are given exactly in a d-bit fixed point number representation, and $\lambda_j \in [\delta, 1]$ for some $\delta > 0$. Start from a linear combination of states $|\psi\rangle = \sum_j \beta_j\,|0\rangle\,|\lambda_j\rangle\,|v_j\rangle$, we would like to construct a state

$$|\psi'\rangle = \sum_j \frac{C\beta_j}{\lambda_j}\,|1\rangle\,|\lambda_j\rangle\,|v_j\rangle + |0\rangle\,|\perp\rangle\,. \tag{5.26}$$

Here C is a normalization constant chosen so that $|C/\lambda_j| < 1$ for all $\lambda_j \in [\delta, 1]$, and $|\perp\rangle$ is an irrelevant unnormalized state. Viewing this as a diagonal matrix multiplication problem, the function of interest is

$$f(a) = \frac{C}{a}, \quad a \in [\delta, 1]. \tag{5.27}$$

The implementation involves the classical arithmetic circuit for computing

$$\theta(a) = \frac{1}{\pi}\arcsin f(a) = \frac{1}{\pi}\arcsin(C/a) \tag{5.28}$$

using d' bits ($d' > d$).

Once $|\psi'\rangle$ is prepared, we can uncompute $|\lambda_j\rangle$ to obtain a state

$$\sum_j \frac{C\beta_j}{\lambda_j} |1\rangle |0^d\rangle |v_j\rangle + |0\rangle |\perp'\rangle \tag{5.29}$$

to disentangle the λ_j register from the v_j register. If we measure the first ancilla register and obtain 1, we obtain the desired form of the solution in the HHL algorithm. ◇

Notes and further reading

Reversible computation predates quantum computing and has both physical and algorithmic motivations. For background on reversible embeddings of classical circuits into unitary dynamics, see [NC00, Section 3.2.5]. For fixed-point encodings and reversible arithmetic (addition, multiplication, and function evaluation), a detailed treatment is given in [RP11, Chapter 6]. For standard universal classical gate constructions and decompositions into elementary quantum gates, see [BBC$^+$95]. There is also opportunity to optimize the cost of the uncomputation stage. An example is Gidney's construction [Gid18] of the quantum adder circuit. The QRAM model [GLM08] should be interpreted as an assumption about data access rather than an automatic feature of a fault-tolerant architecture.

CHAPTER 6

Query complexity and quantum complexity theory

CHAPTER 7

Perturbation theory

Numerical computation is inexact: errors in the input data, discretization error, and roundoff errors can all affect the final output. Analogous error sources in quantum algorithms include finite-precision state preparation, approximate arithmetic, and imperfect implementations of primitives such as block encodings or Hamiltonian simulation. This chapter provides tools that allow us to isolate the part of the error that is intrinsic to the mathematical task itself, by asking how much the output can change under small perturbations of the input.

Perturbation theory provides a streamlined way to separate the error from data from the error from algorithms. Once the sensitivity of the underlying problem is quantified, one can treat the available input as exact and focus on how a chosen algorithm propagates or amplifies perturbations. This viewpoint is closely aligned with backward error analysis in classical computation.

We first introduce basic concepts such as forward error, backward error and condition number, and then apply the perturbation analysis to two prototypical problems: linear systems of equations, and eigenvalue problems. Some perturbation tools will also be used later in quantum phase estimation, Hamiltonian simulation, quantum singular value transformation, and related primitives.

7.1. Forward and backward error

For simplicity, consider a smooth function $f : \mathbb{R}^d \to \mathbb{R}$. Let $a \in \mathbb{R}^d$ be the input, let $f(a)$ denote the exact value, and let $\mathrm{alg}(f)(a)$ denote the output produced by an algorithm intended to approximate $f(a)$. The quantity $|\mathrm{alg}(f)(a) - f(a)|$ is called the **forward error**. It is the end-to-end discrepancy between the quantity we want and the quantity we actually compute, so it is the most direct measure of accuracy. However, forward error alone does not identify the source of the discrepancy. When it is large, it may be unclear whether the problem itself is highly sensitive to perturbations of the input or whether the algorithm has introduced substantial additional error.

This ambiguity is the reason to consider backward error. If there exists a perturbation δa such that $\mathrm{alg}(f)(a) = f(a+\delta a)$, then δa is called a **backward perturbation**. When such a representation exists, one defines the **backward error** as the (typically minimal) size $\|\delta a\|$. Backward error asks whether the computed output is the exact answer to a nearby problem. If $\|\delta a\|$ is small, then the algorithm has changed the data only slightly, and a large forward error should be attributed primarily to the sensitivity of f. If every such perturbation must be large, then the algorithm itself is significantly distorting the problem, and the loss of accuracy should be blamed on the algorithm.

Thus forward error typically mixes two effects: sensitivity of the problem and error introduced by the algorithm, whereas backward error helps separate them. The following examples illustrate this distinction. Suppose $d = 1$ and the goal is to compute $f(a) = e^a$ at $a = 100$ to some absolute precision. Then an input perturbation δa produces $|f(a + \delta a) - f(a)| \approx e^{100}\,|\delta a|$ for small δa, regardless of the algorithm. A more complex example is the prediction of trajectories in chaotic dynamics, where a tiny perturbation of the initial state a can lead to a macroscopically different

trajectory $f(a)$. In such cases, a large forward error may be unavoidable because it reflects the sensitivity of the problem itself rather than a defect of the algorithm.

Conversely, even for a well-posed problem, a poor algorithmic choice can produce a large forward error. Consider approximating $f(a) = g'(x)|_{x=a}$ for a smooth function g via a forward difference quotient:

$$\mathrm{alg}(f)(a) = \frac{(g(a+h)+u_1)-(g(a)+u_2)}{h} = g'(a) + \frac{1}{2}g''(a)h + \frac{u_1-u_2}{h} + \mathcal{O}(h^2). \tag{7.1}$$

Here h is the step size, and u_1, u_2 model the (absolute) evaluation errors in finite precision. The truncation term $\frac{1}{2}g''(a)h+\mathcal{O}(h^2)$ decreases with h, whereas the roundoff term $(u_1-u_2)/h$ is amplified when h is small. If h is chosen too small relative to the evaluation errors, then the roundoff term dominates and the forward error can become $\mathcal{O}(1)$ even when g is smooth. Since h is an algorithmic parameter, this is an algorithm-induced loss of accuracy.

When $g''(a) \neq 0$, this instability can also be expressed in terms of a backward perturbation by solving for δa such that

$$g'(a+\delta a) = g'(a) + \frac{1}{2}g''(a)h + \frac{u_1-u_2}{h}, \tag{7.2}$$

which yields to leading order:

$$\delta a \approx \frac{h}{2} + \frac{u_1-u_2}{g''(a)h}. \tag{7.3}$$

This makes explicit that taking h too small can force $\|\delta a\|$ to be large, so in this case the failure is attributable to the algorithm rather than to unusual sensitivity of the underlying problem.

More generally, suppose the input data itself is inexact. Let $\widetilde{a}$ denote the available input with $\|\widetilde{a}-a\| \leq \epsilon'$. Then the total error admits the decomposition

$$|\mathrm{alg}(f)(\widetilde{a}) - f(a)| \leq |\mathrm{alg}(f)(\widetilde{a}) - f(\widetilde{a})| + |f(\widetilde{a}) - f(a)|\,. \tag{7.4}$$

The first term is the algorithmic error for the (putative) exact input $\widetilde{a}$, while the second term is the error induced by data uncertainty. By the mean value theorem,

$$|f(\widetilde{a}) - f(a)| \leq \sup_{0\leq\theta\leq 1} \left\|\nabla f\big(a+\theta(\widetilde{a}-a)\big)\right\| \, \|\widetilde{a}-a\|\,. \tag{7.5}$$

For small ϵ', this is often approximated by $\|\nabla f(a)\|\,\epsilon'$. In this scalar-output setting, $\|\nabla f(a)\|$ is a natural local **condition number**: it measures the sensitivity of $f(a)$ to perturbations of the input.

This decomposition provides several insights. First, when $\|\nabla f(a)\|$ is large, even a small input uncertainty can produce a large forward error, indicating that the problem is locally ill-conditioned. Second, when the input data has inherent uncertainty, there is limited benefit in refining the algorithm beyond the scale of that uncertainty: if $|\mathrm{alg}(f)(\widetilde{a}) - f(\widetilde{a})|\,|f(\widetilde{a}) - f(a)|$, then further reductions in algorithmic error yield diminishing returns in the total error. This perspective is especially relevant in quantum algorithms, where the input (for example, a matrix provided via block encoding or a Hamiltonian given through a simulation procedure) is itself constructed approximately.

To relate this to backward error analysis, suppose that for a given input a one can write

$$\mathrm{alg}(f)(a) = f(a+\delta a), \tag{7.6}$$

for some backward perturbation δa. Then

$$|\mathrm{alg}(f)(a) - f(a)| = |f(a+\delta a) - f(a)| \approx \|\nabla f(a)\|\,\|\delta a\|\,. \tag{7.7}$$

Combining this with Eq. (7.4), we see that there is typically no practical benefit in guaranteeing a backward error $\|\delta a\|$ that is far smaller than the uncertainty already present in the input data. An algorithm is called **backward stable** if it admits backward perturbations that remain small for all admissible inputs.

Throughout this book, we will not generally prove backward stability explicitly. Instead, once perturbation theory confirms that the problem is not inherently ill-conditioned, we will focus on proving that the forward error of the quantum algorithm is small.

Example 7.1 (s-sparse matrices)**.** In matrix computations, let A denote the exact input matrix and $\widetilde{A} = A + E$ its numerical approximation. The perturbation E may arise from various sources, such as roundoff errors introduced during the loading of matrix entries into QRAM. If A is unstructured, the resulting norm $\|E\|$ may scale with the dimension of A, and thus become prohibitively large for high-dimensional systems.

Now consider the case where A is an s-sparse matrix, and assume that the perturbation E is also s-sparse with entrywise bound $\|E\|_{\max} \leq \epsilon$. Then, as shown in Lemma 2.46, the operator norm of the perturbation satisfies $\|E\| \leq s\epsilon$, which is independent of the overall dimension of A.

Perturbation results in matrix analysis often take the form of a condition number multiplied by $\|E\|$. This simple estimate demonstrates that such results remain meaningful in the quantum setting, even for matrices of exponentially large size 2^n, provided the matrix is sparse. ◇

Example 7.2. Let A, B be $N \times N$ matrices, and assume A, B commute with their commutator, i.e., $[A, [A, B]] = [B, [A, B]] = 0$. We would like to evaluate the matrix exponential $f(A, B) = e^{(A+B)t}$ for some small t. The algorithm we are using is

$$\mathrm{alg}(f)(A, B) = e^{At} e^{Bt}, \tag{7.8}$$

which introduces an error. The Baker–Campbell–Hausdorff formula (BCH) states that

$$\mathrm{alg}(f)(A, B) = e^{At} e^{Bt} = e^{(A+B)t + \frac{t^2}{2}[A,B]} = f\left(A + \frac{t}{2}[A, B], B\right). \tag{7.9}$$

Thus the algorithmic output coincides exactly with the true value of f evaluated on a perturbed input $(A + \delta A, B + \delta B)$, for instance with $\delta A = \frac{t}{2}[A, B]$ and $\delta B = 0$. In this sense the backward perturbation has size $\mathcal{O}(t)$ (more precisely, $\|\delta A\| = \frac{t}{2}\|[A, B]\|$ in operator norm). The backward perturbation is not unique: one may equally write $\mathrm{alg}(f)(A, B) = f(A, B + \frac{t}{2}[A, B])$, and thereby attribute the perturbation to B instead. ◇

Remark 7.3. Backward error analysis might not always be applicable. For instance, in computing the outer product $M = aa^\top$, the exact output has rank 1, whereas an algorithm may produce an approximation $\widetilde{M} = \mathrm{alg}(M)$ of rank larger than 1. In this case there need not exist any δa such that $\widetilde{M} = (a + \delta a)(a + \delta a)^\top$. ◇

7.2. Perturbation theory for linear systems of equations

Consider the linear systems $Ax = b$ and $(A + \delta A)\widetilde{x} = b + \delta b$. We would like to bound the solution error $\delta x := \widetilde{x} - x$ in terms of the perturbations δA and δb. Subtracting the two equations gives

$$A\delta x = -(\delta A)\widetilde{x} + \delta b. \tag{7.10}$$

Assume that A is invertible and that $\|\delta A\|$ and $\|\delta b\|$ are small. In this linear regime, we discard all second-order terms in δA and δb and obtain

$$\delta x = -A^{-1}(\delta A)x + A^{-1}\delta b. \tag{7.11}$$

Therefore,

$$\|\delta x\| \leq \left\|A^{-1}\right\| \left(\|\delta A\| \, \|x\| + \|\delta b\|\right), \tag{7.12}$$

and hence

$$\frac{\|\delta x\|}{\|x\|} \leq \left\|A^{-1}\right\| \|A\| \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|A\| \, \|x\|}\right) \leq \left\|A^{-1}\right\| \|A\| \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|}\right). \tag{7.13}$$

Here we used $\|A\| \, \|x\| \geq \|Ax\| = \|b\|$. The quantity $\kappa(A) := \left\|A^{-1}\right\| \|A\|$ is called the condition number of A. It controls the amplification of **relative error** in the solution by relative error in the input data.

The analysis above omits second-order contributions in δA and δb. For larger perturbations, a similar argument can be made rigorous, but it requires controlling these higher-order terms. First, we rewrite Eq. (7.10) as

$$(A + \delta A)\delta x = -(\delta A)x + \delta b. \tag{7.14}$$

This gives

$$\frac{\|\delta x\|}{\|x\|} \leq \left\|(A + \delta A)^{-1}\right\| \|A\| \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|}\right). \tag{7.15}$$

Exercise 7.1. For any square matrix A satisfying $\|A\| < 1$, prove that the matrix $I - A$ is invertible, and

$$\left\|(I - A)^{-1}\right\| \leq (1 - \|A\|)^{-1}. \tag{7.16}$$

Now apply Eq. (7.16). Assume $\left\|A^{-1}\right\| \|\delta A\| < 1$. Then

$$\left\|(A + \delta A)^{-1}\right\| \leq \left\|(I + A^{-1}\delta A)^{-1}\right\| \left\|A^{-1}\right\| \leq \frac{1}{1 - \|A^{-1}\delta A\|} \left\|A^{-1}\right\| \leq \frac{1}{1 - \|A^{-1}\| \, \|A\| \, \frac{\|\delta A\|}{\|A\|}} \left\|A^{-1}\right\|. \tag{7.17}$$

Therefore

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\kappa(A)}{1 - \kappa(A)\frac{\|\delta A\|}{\|A\|}} \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|}\right). \tag{7.18}$$

There is an interesting generalization of the perturbation analysis above to the quantum setting. When solving linear systems on a quantum computer, because a quantum state has to be normalized, we cannot directly obtain an approximation to the solution vector x. Instead we can only aim at preparing the normalized state $|x\rangle := x/\|x\|$, and likewise $|\widetilde{x}\rangle := \widetilde{x}/\|\widetilde{x}\|$. According to the relation

??, the trace distance is upper bounded by the error of the normalized solution:

$$\begin{aligned} D(|x\rangle\langle x|, |\widetilde{x}\rangle\langle\widetilde{x}|) =& \sin\theta(|x\rangle\langle x|, |\widetilde{x}\rangle\langle\widetilde{x}|) \\ \leq& D_p(|x\rangle, |\widetilde{x}\rangle) \leq \||x\rangle - |\widetilde{x}\rangle\| \\ =& \left\| \frac{x}{\|x\|} - \frac{\widetilde{x}}{\|\widetilde{x}\|} \right\| \\ \leq& \left\| \frac{x}{\|x\|} - \frac{\widetilde{x}}{\|x\|} \right\| + \left\| \frac{\widetilde{x}}{\|x\|} - \frac{\widetilde{x}}{\|\widetilde{x}\|} \right\| \\ =& \frac{\|\delta x\|}{\|x\|} + \left| \frac{\|\widetilde{x}\|}{\|x\|} - 1 \right| \\ \leq& 2\frac{\|\delta x\|}{\|x\|} \\ \leq& \frac{2\kappa(A)}{1 - \kappa(A)\frac{\|\delta A\|}{\|A\|}} \left(\frac{\|\delta A\|}{\|A\|} + \frac{\|\delta b\|}{\|b\|} \right). \end{aligned} \tag{7.19}$$

In the last inequality we used Eq. (7.18). So compared to the standard problem of solving $Ax = b$, the relative error for computing the normalized solution is amplified by at most a factor of 2.

7.3. Perturbation theory for Hermitian eigenvalue problems

Consider the eigenvalue problem $A|x\rangle = \lambda|x\rangle$ for a Hermitian matrix A. Then the eigenvalue λ is real. We would like to estimate the perturbations of the eigenvalue and eigenvector in the perturbed problem $(A + \delta A)|\widetilde{x}\rangle = \widetilde{\lambda}|\widetilde{x}\rangle$. For simplicity, assume that λ and $\widetilde{\lambda}$ are simple eigenvalues of A and $A + \delta A$, respectively. Let $\widetilde{\lambda} = \lambda + \delta\lambda$ and $|\widetilde{x}\rangle = |x\rangle + \delta x$. The use of the ket notation implies that $|x\rangle$ and $|\widetilde{x}\rangle$ are normalized, but δx need not be. In the linear regime, assume that $\|\delta A\|$ is small and drop second and higher order terms. Then

$$A\delta x + \delta A|x\rangle = \lambda\delta x + \delta\lambda|x\rangle. \tag{7.20}$$

Applying $\langle x|$ to both sides of the equation, we have

$$\langle x|A\delta x + \langle x|\delta A|x\rangle = \lambda\langle x|\delta x + \delta\lambda\langle x|x\rangle. \tag{7.21}$$

Since $\langle x|A = \lambda\langle x|$, we obtain the perturbation of the eigenvalue

$$\delta\lambda = \langle x|\delta A|x\rangle = \mathrm{Tr}[\delta A|x\rangle\langle x|]. \tag{7.22}$$

In particular,

$$|\delta\lambda| \leq \|\delta A\|. \tag{7.23}$$

For example, if $A(\alpha)$ depends smoothly on a parameter α, then

$$\frac{\mathrm{d}\lambda}{\mathrm{d}\alpha} = \langle x|A'(\alpha)|x\rangle. \tag{7.24}$$

This is an example of the Hellmann–Feynman theorem.

The perturbation of the eigenvector satisfies the equation

$$(\lambda I - A)\delta x = (\delta A - \delta\lambda)|x\rangle. \tag{7.25}$$

Since $\lambda I - A$ is not invertible, the solution to this linear system of equations is not unique. The unique solution can be obtained by minimizing the global-phase-invariant distance between $|x\rangle$ and $|\widetilde{x}\rangle$, which fixes the phase and leads to the constraint $\langle x|\,\delta x = 0$. We obtain

$$\delta x = Q(\lambda I - A)^{-1} Q(\delta A - \delta\lambda)\,|x\rangle = Q(\lambda I - A)^{-1} Q\delta A\,|x\rangle\,. \tag{7.26}$$

where $Q = I - |x\rangle\langle x|$ is a projection operator. Therefore in the linear regime,

$$D(|x\rangle\langle x|, |\widetilde{x}\rangle\langle\widetilde{x}|) = \sin\theta(|x\rangle\langle x|, |\widetilde{x}\rangle\langle\widetilde{x}|) \le \||x\rangle - |\widetilde{x}\rangle\| = \|\delta x\| \le \left\|Q(\lambda I - A)^{-1}Q\right\| \|\delta A\| \le \frac{\|\delta A\|}{\Delta} = \frac{\|A\|}{\Delta}\cdot\frac{\|\delta A\|}{\|A\|}. \tag{7.27}$$

Here Δ is the minimal distance between λ and the rest of the eigenvalues of A, and is often called the (absolute) spectral gap. The ratio $\Delta/\|A\|$ is called the relative spectral gap, which describes the spectral gap when A is normalized. Here the inverse of the relative gap, i.e., $\|A\|/\Delta$, plays the role of the condition number for the eigenvector x.

Exercise 7.2. Let $A\,|x_k\rangle = \lambda_k\,|x_k\rangle$ and $\lambda = \lambda_l$ be a simple eigenvalue of A. Show that Eq. (7.26) can be as

$$\delta x = \sum_{k\neq l} |x_k\rangle\,\frac{1}{\lambda_l - \lambda_k}\,\langle x_k|\delta A|x_l\rangle\,. \tag{7.28}$$

So far we have assumed that λ is a simple eigenvalue and the perturbation δA is infinitesimally small. The rigorous version of the bound for eigenvalues is given by **Weyl's inequality**, which holds for any A and δA. The following statement is a simplified version of Weyl's inequality [HJ91, Theorem 4.3.1].

THEOREM 7.4 (Weyl). *Let A and E be $n\times n$ Hermitian matrices. Denote the ordered eigenvalues of $A, A+E$ by $\lambda_i(A), \lambda_i(A+E)$ respectively, where $i = 1, 2, \ldots, n$, and the eigenvalues are arranged in non-increasing order. Then*

$$|\lambda_i(A+E) - \lambda_i(A)| \le \|E\|\,, \quad i = 1, \ldots, n. \tag{7.29}$$

PROOF. Given A and E are $n \times n$ Hermitian matrices, and $\lambda_i(A)$ and $\lambda_i(A+E)$ are their ordered eigenvalues. By the **Courant-Fischer min-max principle** [Bha97, Theorem 3.1.2] the i-th eigenvalue of a Hermitian matrix M can be characterized as follows:

$$\lambda_i(M) = \max_{\substack{S\subseteq\mathbb{C}^n \\ \dim(S)=i}} \min_{\substack{x\in S \\ \|x\|=1}} x^\dagger M x = \min_{\substack{S\subseteq\mathbb{C}^n \\ \dim(S)=n-i+1}} \max_{\substack{x\in S \\ \|x\|=1}} x^\dagger M x. \tag{7.30}$$

Let $S \subseteq \mathbb{C}^n$ be the subspace with $\dim(S) = n - i + 1$ corresponding to $\lambda_i(A)$. Then

$$\lambda_i(A+E) \le \max_{\substack{x\in S \\ \|x\|=1}} x^\dagger(A+E)x \le \max_{\substack{x\in S \\ \|x\|=1}} x^\dagger A x + \|E\| = \lambda_i(A) + \|E\|\,. \tag{7.31}$$

Similarly, let $S \subseteq \mathbb{C}^n$ be the subspace with $\dim(S) = n - i + 1$ corresponding to $\lambda_i(A+E)$. Then the same argument shows

$$\lambda_i(A) \le \lambda_i(A+E) + \|E\|\,. \tag{7.32}$$

This completes the proof. □

What about the perturbation of eigenvectors? A rigorous version of Eq. (7.27) is called the **Davis-Kahan** $\sin\theta$ **theorem**. We state a version without proof, which is a direct consequence of a more general result in [Bha97, Theorem VII.3.1].

THEOREM 7.5 (Davis-Kahan $\sin\theta$ theorem). *Let A and $A+\delta A$ be $N\times N$ Hermitian matrices. Let P be a spectral projector of A associated with eigenvalues in an interval $[a,b]$, and $\widetilde{P}$ be a spectral projector of $A+\delta A$ associated with eigenvalues in an interval $[a-\Delta, b+\Delta]$, respectively. Then*

$$\left\|P(I-\widetilde{P})\right\| \leq \frac{\|\delta A\|}{\Delta}. \tag{7.33}$$

To see how $\sin\theta$ appears, let us revisit the case of a single isolated eigenvalue, where $P = |x\rangle\langle x|, \widetilde{P} = |\widetilde{x}\rangle\langle\widetilde{x}|$ are spectral projectors associated with the eigenvalue $\lambda, \widetilde{\lambda}$ of $A, A+\delta A$, respectively. Choose the phase factor so that $\langle x|\widetilde{x}\rangle = \cos\theta > 0$. Then $P\widetilde{P} = |x\rangle\langle x|\widetilde{x}\rangle\langle\widetilde{x}| = |x\rangle\cos(\theta)\langle\widetilde{x}|$, and

$$\left\|P(I-\widetilde{P})\right\| = \||x\rangle - \cos\theta\,|\widetilde{x}\rangle\| = \sqrt{1-\cos^2\theta} = \sin\theta = D(P,\widetilde{P}), \tag{7.34}$$

which is the trace distance between the pure states $P, \widetilde{P}$. We refer to [Bha97, Chapter VII.1] for a more general connection between $P(I-\widetilde{P})$ and the principal angle of the two associated subspaces.

Example 7.6. An interesting connection between the linear system solver and a Hermitian eigenvalue problem in the quantum setting is as follows. For simplicity, let A be Hermitian positive definite with $A \succeq \Delta I$ for some $\Delta > 0$, and assume $\|b\| = 1$. Write $|b\rangle := b$. Then an alternative formulation of finding $|x\rangle = x/\|x\|$ such that $Ax = b$ can be stated as an eigenvalue problem:

$$\mathcal{A}\begin{pmatrix}|x\rangle\\0\end{pmatrix} = 0, \quad \mathcal{A} = \begin{pmatrix}0 & AQ_b\\ Q_bA & 0\end{pmatrix}, \quad Q_b = I - |b\rangle\langle b|. \tag{7.35}$$

Now consider a perturbed problem

$$\widetilde{\mathcal{A}} := \begin{pmatrix}0 & (A+\delta A)Q_b\\ Q_b(A+\delta A) & 0\end{pmatrix} \tag{7.36}$$

and suppose that

$$\widetilde{\mathcal{A}}\begin{pmatrix}|\widetilde{x}\rangle\\0\end{pmatrix} = 0. \tag{7.37}$$

Let $\langle x|\widetilde{x}\rangle = \cos\theta > 0$. All nonzero eigenvalues of $\mathcal{A}$ have magnitude at least Δ. Apply Theorem 7.5 and we find

$$D(|x\rangle\langle x|, |\widetilde{x}\rangle\langle\widetilde{x}|) = \sin\theta \leq \frac{\|\delta A\|}{\Delta} = \frac{\|A\|}{\Delta}\frac{\|\delta A\|}{\|A\|}. \tag{7.38}$$

Note that $\|A\|/\Delta = \|A\|\left\|A^{-1}\right\| = \kappa(A)$ is precisely the condition number of A. ◇

7.4. Additional perturbation theorems

Definition 7.7 (Optimal matching distance)**.** *The **optimal matching distance** between $x, y \in \mathbb{C}^N$ is*

$$D_m(x,y) = \min_{\sigma\in S_N}\max_i \left|x_i - y_{\sigma(i)}\right|, \tag{7.39}$$

where S_N denotes the symmetric group on N elements.

Exercise 7.3. If $x, y \in \mathbb{R}^N$, and $x_1 \leq x_2 \leq \cdots \leq x_N$, $y_1 \leq y_2 \leq \cdots \leq y_N$, prove that the optimal matching distance is equal to $\max_i |x_i - y_i|$.

Using Exercise 7.3, Weyl's inequality can also be stated as

$$D_m(\lambda(A), \lambda(A+E)) \leq \|E\|, \tag{7.40}$$

where $\lambda(A)$ denotes the set of eigenvalues of A.

There is a nontrivial generalization of Weyl's inequality to unitary matrices. The following theorem is a restatement of [Bha97, Theorem VI.3.11].

THEOREM 7.8 (Perturbation of eigenvalues for unitary matrices). *For any two unitary matrices $U, V \in \mathbb{C}^{N\times N}$,*

$$D_m(\lambda(U), \lambda(V)) \leq \|U - V\|, \tag{7.41}$$

where $\lambda(A)$ denotes the set of eigenvalues of A.

This is useful, for example, in the context of phase estimation (see Chapter 16), to bound the phase errors in terms of the error in the input unitary. To control perturbations of eigenvectors, we will use the following Davis–Kahan type bound, restated from [Bha97, Theorem VII.3.3] for unitary matrices.

THEOREM 7.9. *Let $U, V \in \mathrm{U}(N)$. Let P be a spectral projector of U associated with eigenvalues in a subset $S \subset \mathbb{C}$, and let $\widetilde{Q}$ be a spectral projector of V associated with eigenvalues in a subset $\widetilde{S} \subset \mathbb{C}$. Assume that* $\operatorname{dist}(S, \widetilde{S}) = \Delta > 0$. *Then there exists a universal constant $C < 2.91$ such that*

$$\left\| P\widetilde{Q} \right\| \leq \frac{C\,\|U - V\|}{\Delta}. \tag{7.42}$$

If U has a simple eigenvalue $e^{i\lambda}$ with a spectral projector P, and V has a simple eigenvalue in the disk $B(e^{i\lambda}, \Delta)$ in the complex plane with a spectral projector $\widetilde{P}$, then

$$D(P, \widetilde{P}) = \left\| P(I - \widetilde{P}) \right\| \leq \frac{C\,\|U - V\|}{\Delta}. \tag{7.43}$$

There is a counterpart of Weyl's theorem for singular values. The following result, restated from [Bha97, Problem III.6.13], will be useful when we analyze singular value transformations in Chapter 12.

THEOREM 7.10 (Perturbation of singular values). *For any two matrices $A, B \in \mathbb{C}^{N\times N}$,*

$$D_m(\Sigma(A), \Sigma(B)) \leq \|A - B\|, \tag{7.44}$$

where $\Sigma(A)$ denotes the set of singular values of A.

For general matrices, the **Gershgorin circle theorem** provides a simple and efficient way to estimate the range in which all eigenvalues must lie.

THEOREM 7.11 (Gershgorin circle theorem, see e.g. [GVL13, Theorem 7.2.1]). *Let $A \in \mathbb{C}^{N\times N}$ with entries a_{ij}. For each $i = 1, \ldots, N$, define*

$$R_i = \sum_{j \neq i} |a_{ij}|. \tag{7.45}$$

Let

$$D_i = \{z \in \mathbb{C} : |z - a_{ii}| \leq R_i\}, \tag{7.46}$$

be a closed disc centered at a_{ii} with radius R_i, called a Gershgorin disc. Then every eigenvalue of A lies within at least one of the Gershgorin discs D_i.

Notes and further reading

Many of the perturbation bounds used in quantum algorithm design are inherited directly from classical numerical linear algebra and matrix analysis. General discussions of forward and backward error, condition numbers, and stability can be found in standard texts on numerical computation and linear algebra; see, for instance, [HJ91, TB97, Dem97, Hig02, GVL13]. For a systematic treatment of matrix inequalities and perturbation theorems for eigenvalues, singular values, spectral subspaces, and matrix functions, see Bhatia [Bha97]; for a focused account of eigenvalue and singular value sensitivity, see Stewart and Sun [SS90]. For a more general operator-theoretic perspective, including unbounded and infinite-dimensional settings, see Kato [Kat76].

CHAPTER 8

Statistical estimates

Quantum algorithms return classical information only through measurement, and in many cases the object of interest is not a single outcome but a parameter of the induced distribution. Consequently, the cost of a quantum algorithm is often controlled not only by state preparation and unitary evolution, but also by the number of samples needed to extract means, probabilities, phases, or other derived quantities to a prescribed accuracy. This chapter develops the statistical tools needed to quantify that sampling cost and to identify the limits that any estimation procedure must obey.

We begin with concentration inequalities because they give finite-sample control of fluctuations and therefore translate directly into confidence bounds and repetition counts. This leads naturally to statistical amplification and to basic estimation tasks arising from single-qubit measurements and Hadamard-test circuits, where one sees how the dependence on precision, variance, and failure probability enters concretely. We then turn to parameter estimation and the Cramér-Rao bound, which characterize the best variance achievable by unbiased estimators for a fixed statistical model. The chapter closes by lifting this viewpoint to quantum measurements themselves, as shown in the quantum Cramér-Rao bound, where the optimization is no longer only over estimators but also over the measurement strategy.

8.1. Elementary concentration inequalities

We first state a few **concentration inequalities**, which provide an upper bound for the probability that a random variable differs from its expected value by more than a certain value. This allows us to derive, for instance, confidence intervals.

THEOREM 8.1 (**Markov's inequality**). *Let X be a non-negative random variable and $t > 0$. Then the probability that X is at least t is*

$$\mathbb{P}(X \geq t) \leq \frac{\mathbb{E}[X]}{t}. \tag{8.1}$$

PROOF. Since $X \geq 0$, we have

$$X \geq t \cdot \mathbf{1}_{X \geq t}, \tag{8.2}$$

where $\mathbf{1}_{X \geq t}$ is the indicator function of the event $X \geq t$. Taking expectations on both sides, we get

$$\mathbb{E}[X] \geq t \cdot \mathbb{E}\left[\mathbf{1}_{X \geq t}\right] = t \cdot \mathbb{P}(X \geq t). \tag{8.3}$$

Therefore,

$$\mathbb{P}(X \geq t) \leq \frac{\mathbb{E}[X]}{t}. \tag{8.4}$$

□

THEOREM 8.2 (**Chebyshev's inequality**). *Let X be a random variable with finite expected value $\mathbb{E}X$ and finite non-zero variance $\mathbb{V}X$. Then for any real number $t > 0$,*

$$\mathbb{P}(|X - \mathbb{E}X| \geq t) \leq \frac{\mathbb{V}X}{t^2}. \tag{8.5}$$

PROOF. For any $t > 0$, we have

$$\mathbb{P}(|X - \mathbb{E}X| \geq t) = \mathbb{P}\left((X - \mathbb{E}X)^2 \geq t^2\right). \tag{8.6}$$

Since $(X - \mathbb{E}X)^2$ is a non-negative random variable, by Markov's inequality,

$$\mathbb{P}\left((X - \mathbb{E}X)^2 \geq t^2\right) \leq \frac{\mathbb{E}\left[(X - \mathbb{E}X)^2\right]}{t^2}. \tag{8.7}$$

Recognizing that $\mathbb{E}\left[(X - \mathbb{E}X)^2\right] = \mathbb{V}X$, we obtain

$$\mathbb{P}(|X - \mathbb{E}X| \geq t) \leq \frac{\mathbb{V}X}{t^2}. \tag{8.8}$$

□

THEOREM 8.3 (**Hoeffding's inequality**). *Let $X_1, X_2, ..., X_n$ be independent random variables, where each X_i is bounded such that $a_i \leq X_i \leq b_i$. Let $\bar{X} = \frac{1}{n}\sum_{i=1}^n X_i$ be the sample mean of these variables. Then for any $t > 0$, the following inequalities hold:*

$$\mathbb{P}(\bar{X} - \mathbb{E}[\bar{X}] \geq t) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right), \tag{8.9}$$

and

$$\mathbb{P}(\bar{X} - \mathbb{E}[\bar{X}] \leq -t) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^n (b_i - a_i)^2}\right). \tag{8.10}$$

PROOF. Let $Y_i = X_i - \mathbb{E}[X_i]$. Then each Y_i is a centered random variable bounded as $a_i - \mathbb{E}[X_i] \leq Y_i \leq b_i - \mathbb{E}[X_i]$.

Consider the sum $S = \sum_{i=1}^n Y_i$. Then $\bar{X} - \mathbb{E}[\bar{X}] = \frac{S}{n}$.

For any $\lambda > 0$, by the exponential version of the Markov inequality,

$$\mathbb{P}(S \geq nt) = \mathbb{P}\left(e^{\lambda S} \geq e^{\lambda nt}\right) \leq \frac{\mathbb{E}[e^{\lambda S}]}{e^{\lambda nt}}. \tag{8.11}$$

Since the Y_i are independent,

$$\mathbb{E}[e^{\lambda S}] = \prod_{i=1}^n \mathbb{E}[e^{\lambda Y_i}]. \tag{8.12}$$

The following inequality, also due to Hoeffding, states that for any zero-mean random variable Y such that $Y \in [a, b]$,

$$\mathbb{E}[e^{\lambda Y}] \leq \exp\left(\frac{\lambda^2(b-a)^2}{8}\right), \tag{8.13}$$

we apply it to each Y_i:

$$\mathbb{E}[e^{\lambda Y_i}] \leq \exp\left(\frac{\lambda^2(b_i - a_i)^2}{8}\right). \tag{8.14}$$

This gives

$$\mathbb{E}[e^{\lambda S}] \leq \exp\left(\frac{\lambda^2}{8}\sum_{i=1}^{n}(b_i - a_i)^2\right). \tag{8.15}$$

Substituting back,

$$\mathbb{P}(S \geq nt) \leq \exp\left(-\lambda nt + \frac{\lambda^2}{8}\sum_{i=1}^{n}(b_i - a_i)^2\right). \tag{8.16}$$

To minimize the bound, choose $\lambda = \frac{4nt}{\sum_{i=1}^{n}(b_i-a_i)^2}$. Plugging this optimal λ back in,

$$\mathbb{P}(S \geq nt) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right). \tag{8.17}$$

Thus,

$$\mathbb{P}\left(\bar{X} - \mathbb{E}[\bar{X}] \geq t\right) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right). \tag{8.18}$$

Similarly, we can show that

$$\mathbb{P}\left(\bar{X} - \mathbb{E}[\bar{X}] \leq -t\right) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^{n}(b_i - a_i)^2}\right). \tag{8.19}$$

□

A Bernoulli random variable is a random variable which takes the value 1 with probability p and the value 0 with probability $1-p$. An application of Hoeffding's inequality gives the Hoeffding bound (also referred to as the Chernoff bound) for Bernoulli random variables.

Example 8.4 (Hoeffding bound for Bernoulli random variables)**.** Let $X_1, X_2, \ldots, X_n$ be independent Bernoulli random variables, each with expectation p. Let $S = \sum_{i=1}^{n} X_i$. Then for any $t > 0$, using Hoeffding's inequality,

$$\mathbb{P}(S - pn \geq tn) = \mathbb{P}(\bar{X} - \mathbb{E}[\bar{X}] \geq t) \leq \exp\left(-\frac{2n^2t^2}{\sum_{i=1}^{n} 1}\right) = \exp\left(-2t^2n\right). \tag{8.20}$$

Similarly

$$\mathbb{P}(S - pn \leq -tn) = \mathbb{P}(\bar{X} - \mathbb{E}[\bar{X}] \leq -t) \leq \exp\left(-2t^2n\right). \tag{8.21}$$

The two equations together give

$$\mathbb{P}(|S - pn| \geq tn) \leq 2\exp\left(-2t^2n\right). \tag{8.22}$$

We will refer to this as the Hoeffding bound for Bernoulli variables. ◇

A sharper estimate that incorporates the variance is given by Bernstein's inequality specialized to Bernoulli random variables.

THEOREM 8.5 (Bernstein bound for Bernoulli random variables). *Let $X_1, X_2, \ldots, X_n$ be independent Bernoulli random variables, each with expectation p. Let $S = \sum_{i=1}^{n} X_i$. Then for any $t > 0$,*

$$\mathbb{P}(|S - pn| \geq tn) \leq 2\exp\left(-\frac{nt^2}{2p(1-p) + 2t/3}\right). \tag{8.23}$$

PROOF. Let $X_1, X_2, \ldots, X_n$ be independent Bernoulli random variables with $\mathbb{E}[X_i] = p$. Define $S = \sum_{i=1}^n X_i$.

Let $Y_i = X_i - p$, so that $\mathbb{E}[Y_i] = 0$ and $Y_i \in [-p, 1-p]$. In particular, $|Y_i| \leq 1$, and the variance of each Y_i is $\mathbb{V}[Y_i] = p(1-p)$.

Bernstein's inequality for independent centered random variables bounded in absolute value by 1 states that for any $u > 0$,

$$\mathbb{P}\left(\sum_{i=1}^n Y_i \geq u\right) \leq \exp\left(-\frac{u^2}{2\sum_{i=1}^n \mathbb{V}[Y_i] + 2u/3}\right). \tag{8.24}$$

Since $\sum_{i=1}^n \mathbb{V}[Y_i] = np(1-p)$, choosing $u = tn$ yields

$$\mathbb{P}\left(S - pn \geq tn\right) = \mathbb{P}\left(\sum_{i=1}^n Y_i \geq tn\right) \leq \exp\left(-\frac{nt^2}{2p(1-p) + 2t/3}\right). \tag{8.25}$$

The desired result can be obtained by combining this with the same inequality applied to $-Y_i$. □

8.2. Statistical amplification

Consider a quantum algorithm with a success probability $p > \frac{1}{2}$ per execution to produce the correct answer (represented by 1, but we do not know whether the correct answer is 0 or 1 in advance). This implies a failure probability $1 - p$ for each run, where an incorrect outcome (represented by 0) might be produced. To reduce this failure rate, we can apply concentration inequalities to obtain a technique known as **statistical amplification**.

Let X_i denote the outcome of the i-th independent execution of the algorithm, with $X_i = 1$ indicating a successful run with probability p. By conducting n independent executions, we aggregate the results into a sum $S = \sum_{i=1}^n X_i$ and decide by majority vote. For simplicity, assume that n is even and that ties are counted as failures, so the algorithm succeeds when $S > \frac{n}{2}$. The expected value of S, denoted by $\mathbb{E}[S]$, equals np. Our objective is therefore to assess the likelihood that $S \leq \frac{n}{2}$.

The first way to bound the failure probability uses the Hoeffding bound for Bernoulli variables:

$$\mathbb{P}(S \leq n/2) = \mathbb{P}(S - pn \leq -(p - \tfrac{1}{2})n) \leq \exp\left(-2(p - \tfrac{1}{2})^2 n\right), \tag{8.26}$$

For $p > \frac{1}{2}$, this bound shows that the probability of the majority of the runs being unsuccessful decreases exponentially with the number of runs n. Thus, by increasing n, we can make this probability arbitrarily small, effectively amplifying the probability of success of the quantum algorithm. However, as $p \to 1$, the Hoeffding bound states

$$\mathbb{P}(S \leq n/2) \leq \exp\left(-\frac{n}{2}\right). \tag{8.27}$$

This is not sharp since the failure probability should approach 0 as $p \to 1$.

The second way uses the Bernstein bound. Applying the one-sided Bernstein inequality to $-Y_i$ with $t = p - \frac{1}{2}$ gives

$$\mathbb{P}(S \leq n/2) = \mathbb{P}(S - pn \leq -(p - \tfrac{1}{2})n) \leq \exp\left(-\frac{n(p - \frac{1}{2})^2}{2p(1-p) + 2(p - \frac{1}{2})/3}\right). \tag{8.28}$$

This is sharper than the Hoeffding bound for moderate values of p, but it is still not sharp as $p \to 1$ because the term $2(p - \frac{1}{2})/3$ in the denominator remains bounded away from 0.

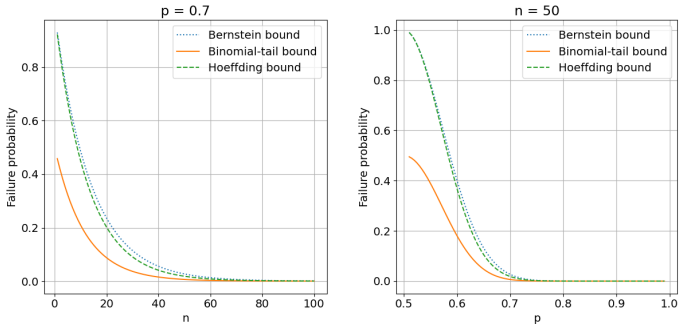


FIGURE 8.1. Comparison of the Bernstein, binomial-tail, and Hoeffding bounds for statistical amplification.

This problem can be solved using the following binomial-tail bound for majority vote. Note that $p > \frac{1}{2}$ implies $(1-p)/p < 1$ and $2\sqrt{p(1-p)} < 1$. Then the failure probability is upper bounded by

$$\begin{aligned} \mathbb{P}(S \leq n/2) &= \sum_{k=\frac{n}{2}}^{n} (1-p)^k p^{n-k} \binom{n}{k} = p^n \sum_{k=\frac{n}{2}}^{n} \left(\frac{1-p}{p}\right)^k \binom{n}{k} \\ &\leq p^n \left(\frac{1-p}{p}\right)^{\frac{n}{2}} \sum_{k=\frac{n}{2}}^{n} \binom{n}{k} = p^n \left(\frac{1-p}{p}\right)^{\frac{n}{2}} 2^{n-1} = \frac{1}{2}(2\sqrt{p(1-p)})^n. \end{aligned} \tag{8.29}$$

Fig. 8.1 compares the performance of three bounds in different settings. Even though all bounds decrease exponentially in n, both the Hoeffding bound and the Bernstein bound are loose for a fixed $p = 0.7$. The binomial-tail bound also captures the limit $p \to 1$ much more accurately.

Example 8.6 (Median concentration)**.** Given a sequence of i.i.d. real numbers $\{x_k\}_{k=1}^n$, let M_n be the median of $\{x_k\}$. For any interval $I \subseteq \mathbb{R}$, assume

$$\mathbb{P}(x_k \notin I) = \epsilon < \frac{1}{2}. \tag{8.30}$$

Then statistical amplification (using the binomial-tail bound for majority vote) states

$$\mathbb{P}(M_n \notin I) \leq \frac{1}{2}\left(2\sqrt{\epsilon(1-\epsilon)}\right)^n. \tag{8.31}$$

As a result, when using a quantum algorithm to solve a decision problem of whether x_k belongs to I, we only need to make sure the algorithm succeeds with probability at least e.g., $2/3$, and taking the median of x_k allows us to exponentially suppress the failure probability. ◇

8.3. Example: Single qubit measurement and Hadamard test circuit

Consider a single qubit state $|\psi\rangle$ measured with respect to the computational basis, and we are interested in estimating the success probability of obtaining 1 denoted by p. Consider the random variable X that takes the value 1 when the outcome of the measurement is $|1\rangle$, and the value 0 when the outcome of the measurement is $|0\rangle$. The expectation value is therefore $\mathbb{E}X = p$. Let us compare the performance of the concentration inequalities for this problem.

To estimate the success probability p within a certain precision ϵ, we could use the Hoeffding bound for Bernoulli variables, which states that for any $\epsilon > 0$,

$$\mathbb{P}(|\bar{X}_n - p| \geq \epsilon) \leq 2\exp(-2n\epsilon^2), \tag{8.32}$$

where $\bar{X}_n$ is the empirical mean of n independent samples from the distribution of X. If we want the difference between the true success probability p and our estimate to be less than ϵ with probability at least $1-\delta$, we can set the right-hand side to δ, and solve for n. This gives:

$$2\exp(-2n\epsilon^2) \leq \delta. \tag{8.33}$$

Taking the logarithm of both sides and solving for n gives the minimum number of samples we need to ensure our estimate of p is within ϵ of the true value with probability at least $1-\delta$:

$$n \geq \frac{\log(2/\delta)}{2\epsilon^2}. \tag{8.34}$$

This $n = \Omega(\epsilon^{-2})$ scaling is very common in quantum computing, and is called the **standard quantum limit** (sometimes called the **shot-noise- limited scaling**).

The number of samples from the Hoeffding bound is independent of p. This is counter-intuitive, since if $p = 0$ or $p = 1$, we know the outcome with near certainty and intuitively it should be easy to estimate p. Chebyshev's inequality improves the result along this aspect.

The variance of this Bernoulli-distributed random variable X is given by $\mathbb{V}[X] = p - p^2 = p(1-p)$. The variance of $\bar{X}_n$ is $\mathbb{V}[\bar{X}_n] = \frac{1}{n^2}\sum_{i=1}^{n}\mathbb{V}[X_i] = \frac{p(1-p)}{n}$, since the X_i are independent. We can use Chebyshev's inequality to obtain an upper bound of the failure probability $\frac{p(1-p)}{n\epsilon^2}$. So to succeed with probability at least $1-\delta$, we need

$$n \geq \frac{p(1-p)}{\epsilon^2\delta}. \tag{8.35}$$

Indeed, the required number of samples vanishes as p approaches 0 or 1.

The above example shows that the number of repetitions always scales as $\mathcal{O}(1/\epsilon^2)$ with respect to the precision ϵ. However, this Hoeffding bound is not sharp when p is close to 0 or 1, and the Chebyshev bound is not sharp with respect to the failure probability δ.

On the other hand, Bernstein's inequality for Bernoulli variables states that in order to estimate p to precision ϵ with probability at least $1-\delta$, it is sufficient to choose

$$n \geq \frac{(2p(1-p) + 2\epsilon/3)\log(2/\delta)}{\epsilon^2}. \tag{8.36}$$

Fig. 8.2 compares the performance of the Bernstein, Hoeffding, and Chebyshev bounds for the failure probability to estimate p to precision ϵ. Bernstein improves on the Hoeffding estimate by incorporating the variance, while in the pre-asymptotic regime the failure probability from the Chebyshev bound can be slightly smaller.

Example 8.7 (Multiplicative error)**.** The discussion so far estimates p to **additive** error ϵ. If we are interested in estimating p to **multiplicative** accuracy ϵ, Chebyshev's inequality gives

$$\mathbb{P}(|\bar{X}_n - p| \geq \epsilon p) \leq \frac{p(1-p)/n}{\epsilon^2 p^2} \leq \delta. \tag{8.37}$$

Then the number of samples satisfies

$$n \geq \frac{(1-p)}{\epsilon^2 p\delta}. \tag{8.38}$$

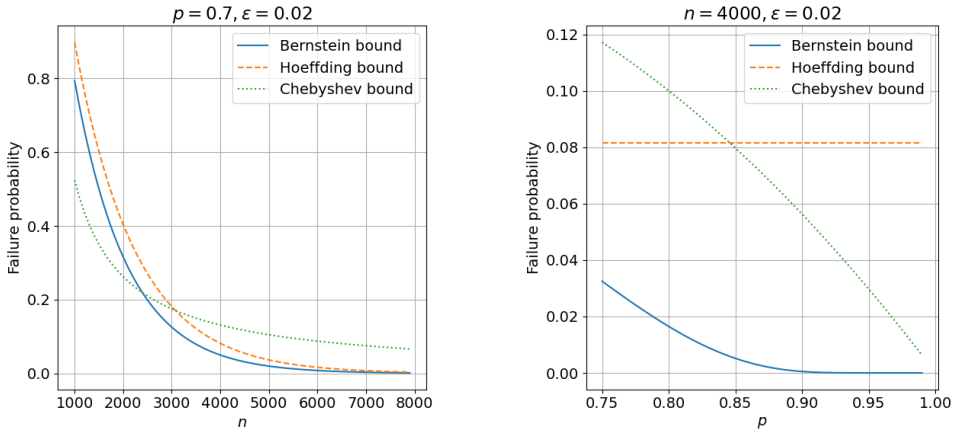


FIGURE 8.2. Comparison of the Bernstein, Hoeffding, and Chebyshev bounds for the failure probability to estimate p to precision $\epsilon = 0.02$.

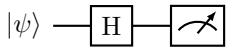
Therefore the task becomes increasingly more difficult when p approaches 0. ◇

Since most quantum computers implement measurement in the computational basis, measuring other observables requires expressing the observable in the computational basis as well. The general principle is that if an observable $O = U^\dagger O_Z U$, where O_Z is a multi-qubit Pauli-Z operator, then we can first apply the circuit U and measure in the computational basis.

Example 8.8. If we want to estimate the expectation value of the Pauli-X operator on a state $|\psi\rangle$, which is given by $\langle\psi|X|\psi\rangle$, and we only have the ability to measure in the computational basis, we can use the relation

$$\mathrm{H}\, Z\, \mathrm{H} = X. \tag{8.39}$$

This equality signifies that measuring X is equivalent to first applying a Hadamard gate and then measuring in the computational basis. The circuit is as follows



Similar to before, we can define a random variable Ξ to represent the transformed measurement outcome that takes the value $+1$ with probability p and -1 with probability $1 - p$. The analysis is the same. ◇

Example 8.9. If the goal is to compute the expectation value of a quantum observable M_A acting on a subsystem A, then its variance is

$$\mathbb{V}_\rho[M_A] = \mathrm{Tr}[M_A^2 \rho_A] - (\mathrm{Tr}[M_A \rho_A])^2. \tag{8.40}$$

By Chebyshev's inequality, the number of samples n needed to estimate $\mathrm{Tr}[M_A\rho_A]$ to additive precision ϵ with probability at least $1 - \delta$ satisfies

$$n \geq \frac{\mathbb{V}_\rho[M_A]}{\epsilon^2 \delta}, \tag{8.41}$$

which only depends on ρ_A. ◇

Example 8.10 (Shot-Noise Limited Phase estimation using one ancilla qubit)**.** Apply the Hadamard test in Fig. 2.1 to $U = e^{i2\pi H}$ with $U|\psi\rangle = e^{i2\pi\varphi}|\psi\rangle$. Then the probability of measuring the qubit 0 to be in state $|1\rangle$ is

$$p(1) = \frac{1}{2}(1 - \mathrm{Re}\,\langle\psi|U|\psi\rangle) = \frac{1}{2}(1 - \cos(2\pi\varphi)). \tag{8.42}$$

For simplicity, assume $0 < \varphi < \frac{1}{2}$ and the mapping between φ and $p(1)$ is a one to one. Therefore

$$\varphi = \frac{\arccos(1 - 2p(1))}{2\pi}. \tag{8.43}$$

In order to quantify the efficiency of the procedure, we first use the procedure described in **??** to estimate $p(1)$ to precision ϵ'. Using the Hoeffding bound for Bernoulli variables, the number of repetitions satisfies $n \geq \log(2/\delta)/(2\epsilon'^2)$, where δ is the failure probability. Choosing $\epsilon' = \pi\,|\sin(2\pi\varphi)|\,\epsilon$ allows us to estimate φ to additive precision ϵ.

Using this estimate, the cost becomes very large if φ is close to 0 or $\frac{1}{2}$. We can improve the Hoeffding estimate by using the Bernstein bound for Bernoulli variables. Let us consider the case when φ is close to 0. Then $p(1) \approx (\pi\varphi)^2$, $1 - p(1) \approx 1$, and the first-order estimate gives $\epsilon' \approx 2\pi^2\varphi\epsilon$. Applying Eq. (8.36), the number of repetitions satisfies

$$n \geq \frac{(2p(1-p) + 2\epsilon'/3)\log(2/\delta)}{\epsilon'^2} \approx \left(\frac{1}{2\pi^2\epsilon^2} + \frac{1}{3\pi^2\varphi\epsilon}\right)\log(2/\delta), \tag{8.44}$$

This shows that Bernstein improves the Hoeffding estimate. However, the term proportional to $1/(\varphi\epsilon)$ comes from the first-order relation $\epsilon' \approx 2\pi^2\varphi\epsilon$, which is not uniform as $\varphi \to 0$. A simple way to recover the correct endpoint behavior is to use the exact increment

$$\frac{1}{2}(1 - \cos(2\pi(\varphi + \epsilon))) - \frac{1}{2}(1 - \cos(2\pi\varphi)) = \sin(\pi\epsilon)\sin(2\pi\varphi + \pi\epsilon). \tag{8.45}$$

If $0 < \epsilon \leq \frac{1}{4}$ and $0 < \varphi \leq \epsilon$, then the right-hand side is at least $\sin^2(\pi\epsilon) \geq 4\epsilon^2$, and also $p(1) = \mathcal{O}(\epsilon^2)$. Therefore it suffices to estimate $p(1)$ to precision $\epsilon' = 2\epsilon^2$, and applying Eq. (8.36) gives $n = \mathcal{O}(\epsilon^{-2}\log(2/\delta))$, which recovers the optimal scaling as $\varphi \to 0$. When $\varphi \gg \epsilon$, the first-order estimate above is the relevant one. The case when φ is close to $1/2$ is similar. ⋄

Other than phase estimation, the Hadamard test has a few other useful applications such as estimating the overlap of two quantum states.

Example 8.11 (Overlap estimate with relative phase information)**.** In the swap test (see Example 2.37), the quantum states $|\varphi\rangle, |\psi\rangle$ can be black-box states, and in such a scenario obtaining an estimate to $|\langle\varphi|\psi\rangle|$ is the best one can do. In order to retrieve the relative phase information and to obtain $\langle\varphi|\psi\rangle$, we need to have access to the unitary circuit preparing $|\varphi\rangle, |\psi\rangle$, i.e.,

$$U_\varphi|0^n\rangle = |\varphi\rangle, \quad U_\psi|0^n\rangle = |\psi\rangle. \tag{8.46}$$

Then we have $\langle\varphi|\psi\rangle = \langle 0^n|U_\varphi^\dagger U_\psi|0^n\rangle$.

The SWAP test also is interesting from a statistical perspective as it provides an example of a one-sided test where if the SWAP test returns 0 then we cannot determine whether or not $|\psi\rangle = |\varphi\rangle$. This is because if the two states are the same then the probability of measuring 0 is 1, but even if $\langle\psi|\varphi\rangle = 0$ then $\mathbb{P}(0) = 1/2$. Conversely, if we measure 1 then we know with certainty that $|\psi\rangle \neq |\varphi\rangle$. Thus the SWAP test can be used to decide whether $|\psi\rangle = |\varphi\rangle$ or whether $|\langle\psi|\varphi\rangle|^2 \leq 1 - \Delta$ for some $\Delta > 0$. Such a separation is needed in order to make such a decision problem tractable. ⋄

8.4. Parameter estimation and Cramér-Rao bound

Parameter estimation is a fundamental task in statistical inference. It involves using observed data, generated according to a parameterized family of probability distributions, to determine the best estimate of the underlying parameters of the system that produced the data. This task is even more important in quantum computing than in classical computing. The output of a quantum algorithm is typically encoded in the parameters of a quantum state; accessing this information requires a measurement, resulting in a probability distribution dependent on these parameters. Consequently, extracting the result of a quantum computation often takes the form of a parameter estimation problem, underlying algorithms such as phase estimation, amplitude estimation, and tasks such as Hamiltonian learning.

Consider for concreteness a finite sample space Σ (the set of possible outcomes) and a scalar parameter space $\Theta \subset \mathbb{R}$. We assume a statistical model defined by a family of probability distributions $\{\mathbb{P}(\nu|\theta) : \nu \in \Sigma, \theta \in \Theta\}$, which is continuously differentiable in θ and satisfies $\mathbb{P}(\nu|\theta) > 0$ for all $\nu \in \Sigma$ and $\theta \in \Theta$. An event $\nu \in \Sigma$ is assumed to be generated according to $\mathbb{P}(\nu|\theta)$, governed by an unknown parameter $\theta \in \Theta$. In practice, we often draw N independent samples $\nu_1, \ldots, \nu_N$ from the same sample space Σ. In this case, the joint outcome is $D = (\nu_1, \ldots, \nu_N) \in \Sigma^N$, and the corresponding sample space is the **product space** Σ^N. The joint probability of the data under parameter θ is $\mathbb{P}(D|\theta) = \prod_{i=1}^N \mathbb{P}(\nu_i|\theta)$. The goal of parameter estimation is to infer the true parameter θ. An **estimator** $\hat{\theta}$ is a function that maps the observed data D to a point estimate in the parameter space.

Given data D, the function $\mathcal{L}(\theta|D) = \mathbb{P}(D|\theta) = \prod_{i=1}^N \mathbb{P}(\nu_i|\theta)$ is called the **likelihood function**. A widely used estimator is the **maximum likelihood estimator** (MLE).

$$\hat{\theta}_{\mathrm{MLE}} = \arg\max_{\theta \in \Theta} \mathcal{L}(\theta|D). \tag{8.47}$$

Regardless of the estimator used, there are fundamental limits on the precision achievable for a given statistical model. This limit can be characterized by the **Fisher information** (FI), which measures how much information the observed data carries about the unknown parameter. Intuitively, it quantifies the sensitivity of the probability distribution to changes in the parameter. If the distribution changes rapidly with θ, it is easier to distinguish nearby values of θ, leading to higher precision.

Define the **score function** $S(\theta|\nu) = \frac{\partial}{\partial\theta} \log(\mathbb{P}(\nu|\theta))$. We first notice that the expectation value of the score function is zero:

$$\begin{aligned} \mathbb{E}_{\nu|\theta}[S(\theta|\nu)] &= \sum_{\nu \in \Sigma} \mathbb{P}(\nu|\theta) \frac{\partial_\theta \mathbb{P}(\nu|\theta)}{\mathbb{P}(\nu|\theta)} = \sum_{\nu \in \Sigma} \partial_\theta \mathbb{P}(\nu|\theta) \\ &= \partial_\theta \sum_{\nu \in \Sigma} \mathbb{P}(\nu|\theta) = \partial_\theta(1) = 0. \end{aligned} \tag{8.48}$$

The FI for a single sample is defined as the variance of the score function:

$$I_F(\theta) := \mathbb{V}(S(\theta|\nu)) = \mathbb{E}_{\nu|\theta}[S(\theta|\nu)^2] = \sum_{\nu \in \Sigma} \mathbb{P}(\nu|\theta) \left(\frac{\partial}{\partial\theta} \log\left(\mathbb{P}(\nu|\theta)\right) \right)^2. \tag{8.49}$$

For N independent samples with $D = (\nu_1, \ldots, \nu_N)$, the score function for the joint distribution is

$$S(\theta|D) = \sum_{i=1}^N S(\theta|\nu_i). \tag{8.50}$$

Since the samples are independent and the single-sample score has mean zero, the total Fisher information is additive:

$$I_F^{(N)}(\theta) = \mathbb{V}(S(\theta|D)) = \sum_{i=1}^{N} \mathbb{V}(S(\theta|\nu_i)) = NI_F(\theta). \tag{8.51}$$

An estimator $\hat{\theta}$ is called an **unbiased estimator** of θ if its expectation value equals the true value of the parameter for all $\theta \in \Theta$:

$$\mathbb{E}_{D|\theta}[\hat{\theta}] = \sum_{D \in \Sigma^N} \hat{\theta}(D)\mathbb{P}(D|\theta) = \theta, \quad \forall \theta \in \Theta. \tag{8.52}$$

Unbiasedness implies that the estimator does not systematically over- or underestimate the parameter.

The **Cramér-Rao bound** (CRB) is a fundamental result in parameter estimation that provides the minimum variance achievable by any unbiased estimator for a given statistical experiment.

THEOREM 8.12 (Cramér-Rao bound). *The variance of any unbiased estimator $\hat{\theta}$ of θ using N independent samples satisfies:*

$$\mathbb{V}(\hat{\theta}) \geq \frac{1}{I_F^{(N)}(\theta)} = \frac{1}{NI_F(\theta)}. \tag{8.53}$$

PROOF. Let D be the observed data from N independent samples. Since $\hat{\theta}$ is an unbiased estimator, we have $\mathbb{E}_{D|\theta}[\hat{\theta}] = \theta$. We examine the covariance between $\hat{\theta}$ and the score function $S(\theta|D)$. Since $\mathbb{E}[S(\theta|D)] = 0$,

$$\mathrm{Cov}(\hat{\theta}, S(\theta|D)) = \mathbb{E}_{D|\theta}[(\hat{\theta} - \theta)S(\theta|D)] = \mathbb{E}_{D|\theta}[\hat{\theta}S(\theta|D)]. \tag{8.54}$$

We evaluate this expectation similarly to how we evaluated the expectation of the score:

$$\begin{aligned} \mathbb{E}_{D|\theta}[\hat{\theta}S(\theta|D)] &= \sum_D \hat{\theta}(D) \frac{\partial_\theta \mathbb{P}(D|\theta)}{\mathbb{P}(D|\theta)} \mathbb{P}(D|\theta) \\ &= \partial_\theta \sum_D \hat{\theta}(D)\mathbb{P}(D|\theta) = \partial_\theta \mathbb{E}_{D|\theta}[\hat{\theta}] = \partial_\theta(\theta) = 1. \end{aligned} \tag{8.55}$$

By the Cauchy-Schwarz inequality for covariance, $(\mathrm{Cov}(X,Y))^2 \leq \mathbb{V}(X)\mathbb{V}(Y)$. Applying this to $\hat{\theta}$ and $S(\theta|D)$:

$$1^2 \leq \mathbb{V}(\hat{\theta})\mathbb{V}(S(\theta|D)) = \mathbb{V}(\hat{\theta})I_F^{(N)}(\theta). \tag{8.56}$$

Rearranging gives the Cramér-Rao bound: $\mathbb{V}(\hat{\theta}) \geq 1/I_F^{(N)}(\theta)$. □

An unbiased estimator $\hat{\theta}$ is an **efficient estimator** if its variance achieves the Cramér-Rao bound. A sequence of estimators $\{\hat{\theta}_N\}_{N\geq 1}$ is said to be **asymptotically efficient** if, as the sample size $N \to \infty$, the estimator is asymptotically unbiased and its variance approaches the Cramér-Rao lower bound. For instance, the MLE is an asymptotically efficient estimator [LC98].

Example 8.13 (Estimating success probability of a Bernoulli trial)**.** Consider estimating the success probability $p \in (0,1)$ of a Bernoulli trial (e.g., a coin flip or a noisy qubit measurement), where

the outcomes are 1 (success) and 0 (failure). The probabilities are $\mathbb{P}(1|p) = p$ and $\mathbb{P}(0|p) = 1 - p$. The derivatives of the log-probabilities (the scores) are:

$$\begin{aligned} \frac{\partial}{\partial p} \log \mathbb{P}(1|p) &= \frac{1}{p}, \\ \frac{\partial}{\partial p} \log \mathbb{P}(0|p) &= \frac{-1}{1-p}. \end{aligned} \tag{8.57}$$

The Fisher information for a single trial is:

$$\begin{aligned} I_F(p) &= p \left(\frac{1}{p}\right)^2 + (1-p) \left(\frac{-1}{1-p}\right)^2 \\ &= \frac{1}{p} + \frac{1}{1-p} = \frac{1}{p(1-p)}. \end{aligned} \tag{8.58}$$

The Cramér-Rao bound states that for N trials, the variance of any unbiased estimator $\hat{p}$ is bounded by $\mathbb{V}(\hat{p}) \geq p(1-p)/N$. The standard sample mean estimator (the fraction of successes) is unbiased and achieves this bound; it is therefore an efficient estimator. ◇

The Cramér–Rao bound provides insight into how increasing the Fisher information of an experiment can reduce the lower bound on the variance of any unbiased estimator. However, the Cramér–Rao bound concerns only the variance and does not describe the probability of large deviations of an estimator from the true parameter. In contrast, concentration inequalities provide non-asymptotic upper bounds on the probability that an estimator (not necessarily unbiased) deviates significantly from its expectation. Together, these results offer a more comprehensive characterization of estimator performance: the Cramér–Rao bound identifies the minimal achievable variance for unbiased estimators, while concentration inequalities quantify the likelihood of deviations beyond the variance scale.

8.5. Example: Estimating decoherence time

We study the following family of quantum channels parameterized by an experimental time t and an unknown decoherence time T_2. This channel acts on a state $|+\rangle\langle+|$:

$$\Lambda_{t,T_2} : |+\rangle\langle+| \mapsto |+\rangle\langle+|(e^{-t/T_2}) + \frac{I}{2}(1 - e^{-t/T_2}). \tag{8.59}$$

Here $I/2$ is the maximally mixed state, so what this channel represents is an exponential decay over time of an initially pure quantum state $|+\rangle\langle+|$ into the maximally mixed state (which can be interpreted as a uniform classical probability distribution over $\{0, 1\}$).

Our goal is to find the experimental time t that maximizes the Fisher information with respect to the parameter T_2. From a circuit of the form

$$|0\rangle \text{ — } \boxed{\text{H}} \text{ — } \boxed{\Lambda_{t,T_2}} \text{ — } \boxed{\text{H}} \text{ — } \boxed{\phantom{\text{H}}} \tag{8.60}$$

where above we slightly abuse the quantum circuit language to extend to the case, namely, the operations are quantum channels rather than unitary transformations. We see that the probability of measuring 0 for this experiment is

$$\mathbb{P}(0|T_2) = \mathrm{Tr}(|+\rangle\langle+|\Lambda_{t,T_2}(|+\rangle\langle+|)) = e^{-t/T_2} + \frac{1 - e^{-t/T_2}}{2} = \frac{1 + e^{-t/T_2}}{2}. \tag{8.61}$$

Let us then assume that we perform a single copy of this experiment (corresponding to $N = 1$ in Theorem 8.12) and measure 0. We then have that if we were to perform an experiment with time t then

$$\begin{aligned}\frac{\partial}{\partial T_2}\log(\mathbb{P}(0|T_2)) &= \frac{2}{1+e^{-t/T_2}}\left(\frac{\partial}{\partial T_2}\left(\frac{1+e^{-t/T_2}}{2}\right)\right)\\ &= \frac{te^{-t/T_2}}{T_2^2(1+e^{-t/T_2})}.\end{aligned} \tag{8.62}$$

Thus,

$$\left(\frac{\partial}{\partial T_2}\log(\mathbb{P}(0|T_2))\right)^2\mathbb{P}(0|T_2) = \frac{t^2e^{-2t/T_2}}{2T_2^4(1+e^{-t/T_2})}. \tag{8.63}$$

A similar calculation reveals

$$\left(\frac{\partial}{\partial T_2}\log(\mathbb{P}(1|T_2))\right)^2\mathbb{P}(1|T_2) = \frac{t^2e^{-2t/T_2}}{2T_2^4(1-e^{-t/T_2})}. \tag{8.64}$$

Note that from a Taylor series expansion of the denominator we can see that the latter probability is not singular as $t \to 0$.

As the set of measurement outcomes here is the discrete set $\{0, 1\}$ the Fisher information given by Theorem 8.12 becomes the following simple sum,

$$\begin{aligned}I_F(T_2) &= \left(\frac{\partial}{\partial T_2}\log(\mathbb{P}(0|T_2))\right)^2\mathbb{P}(0|T_2) + \left(\frac{\partial}{\partial T_2}\log(\mathbb{P}(1|T_2))\right)^2\mathbb{P}(1|T_2)\\ &= \frac{t^2}{T_2^4}\left(\frac{1}{e^{2t/T_2}-1}\right).\end{aligned} \tag{8.65}$$

We see from this that the Fisher information for T_2 has two competing tendencies: the numerator in Eq. (8.65) increases polynomially with t, whereas the denominator increases exponentially with t. Thus we expect to find a tradeoff between the two.

We can find the optimal value of the experimental time t by differentiation. Writing $x = t/T_2$, maximizing $I_F(T_2)$ is equivalent to maximizing $x^2/(e^{2x}-1)$, whose derivative vanishes when $e^{2x}(1-x) = 1$. Besides the trivial stationary point $x = 0$, the positive solution is

$$t = \left(1 + \frac{1}{2}\mathrm{LambertW}(-2e^{-2})\right)T_2 \approx 0.797T_2. \tag{8.66}$$

Substituting this value into $I_F(T_2)$ then yields that the optimal Fisher information is

$$I_F^{\mathrm{opt}}(T_2) \approx \frac{0.162}{T_2^2}. \tag{8.67}$$

Then the Cramér-Rao bound shows that the variance of any unbiased estimator of T_2 from a single experiment of this form satisfies

$$\mathbb{V}(\hat{T}_2) \gtrsim 6.18T_2^2. \tag{8.68}$$

This shows that the relative uncertainty of the decoherence time stays fixed as $T_2 \to \infty$, because the standard deviation of any unbiased estimator of $\hat{T}_2$ scales at least linearly with T_2.

8.6. Quantum Cramér-Rao bound

The Cramér-Rao bound (Theorem 8.12) gives a lower bound on the variance of any unbiased estimator for a fixed statistical experiment. In the quantum setting, the statistical model is generated by measuring a parameterized quantum state $\rho(\theta)$, and the choice of measurement is itself part of the problem. Quantum metrology asks how well θ can be estimated when one optimizes over all physically admissible measurements, possibly using ancillary systems and entanglement. This leads to the **quantum Cramér-Rao bound** (QCRB) [BC94]. A full treatment requires the quantum Fisher information [PG11], which upper bounds the classical Fisher information obtainable from any measurement strategy and therefore determines the ultimate precision allowed by quantum mechanics [ZPDK10, BWB01, BHW13].

A quantum measurement is described by a positive operator-valued measure (POVM), which is a set of positive semidefinite operators $\{E_\nu\}_{\nu\in\Sigma}$ such that $\sum_\nu E_\nu = I$. The probability of obtaining outcome ν when measuring $\rho(\theta)$ is given by the Born rule:

$$\mathbb{P}(\nu|\theta) = \mathrm{Tr}(\rho(\theta)E_\nu). \tag{8.69}$$

The (classical) Fisher information $I_F(\theta;\{E_\nu\})$ associated with this measurement is:

$$I_F(\theta;\{E_\nu\}) = \sum_{\nu\in\Sigma} \mathbb{P}(\nu|\theta)\left(\frac{\partial \log \mathbb{P}(\nu|\theta)}{\partial\theta}\right)^2 = \sum_{\nu\in\Sigma}\frac{1}{\mathbb{P}(\nu|\theta)}\left(\frac{\partial\mathbb{P}(\nu|\theta)}{\partial\theta}\right)^2. \tag{8.70}$$

The central idea of the QCRB is to maximize the classical Fisher information over all possible quantum measurements.

Definition 8.14 (Quantum Fisher Information)**.** *Let $\rho(\theta)$ be a parameterized family of density operators. The **quantum Fisher information** (QFI), denoted $\mathcal{F}_Q(\theta)$, is defined as the supremum of the classical Fisher information over all possible POVMs $\{E_\nu\}$:*

$$\mathcal{F}_Q(\theta) := \sup_{\{E_\nu\}} I_F(\theta;\{E_\nu\}). \tag{8.71}$$

The QFI quantifies the intrinsic information content about θ encoded in the state $\rho(\theta)$, independent of the measurement strategy. By definition, $\mathcal{F}_Q(\theta) \geq I_F(\theta;\{E_\nu\})$.

An explicit formula for the QFI can be derived using the **symmetric logarithmic derivative** (SLD). It can be viewed as the quantum analogue of the classical score function. The SLD, denoted by L_θ, is a Hermitian operator implicitly defined by the following Lyapunov equation:

$$\frac{\partial\rho(\theta)}{\partial\theta} = \frac{1}{2}\left(L_\theta\rho(\theta) + \rho(\theta)L_\theta\right). \tag{8.72}$$

The QFI can be elegantly expressed in terms of the SLD.

THEOREM 8.15 (QFI formula via SLD). *The quantum fisher information $\mathcal{F}_Q(\theta)$ for a parameterized state $\rho(\theta)$ is given by the expectation value of the square of the SLD operator:*

$$\mathcal{F}_Q(\theta) = \mathrm{Tr}(\rho(\theta)L_\theta^2). \tag{8.73}$$

Furthermore, the supremum in Eq. (8.71) *is attained by performing a projective measurement onto the eigenbasis of the SLD operator L_θ.*

PROOF. We begin by relating the derivative of the probabilities to the SLD. Using Eq. (8.72) and the properties of the trace:

$$\begin{aligned}\frac{\partial \mathbb{P}(\nu|\theta)}{\partial\theta} &= \operatorname{Tr}\left(\frac{\partial\rho}{\partial\theta}E_\nu\right) = \operatorname{Tr}\left(\frac{1}{2}(L_\theta\rho + \rho L_\theta)E_\nu\right)\\ &= \frac{1}{2}(\operatorname{Tr}(L_\theta\rho E_\nu) + \operatorname{Tr}(\rho L_\theta E_\nu)).\end{aligned} \tag{8.74}$$

Since ρ, L_θ, E_ν are Hermitian, $\operatorname{Tr}(L_\theta\rho E_\nu) = (\operatorname{Tr}(E_\nu\rho L_\theta))^*$. By the cyclic property, $\operatorname{Tr}(E_\nu\rho L_\theta) = \operatorname{Tr}(\rho L_\theta E_\nu)$. Thus, the two terms in the sum are complex conjugates of each other, yielding:

$$\frac{\partial \mathbb{P}(\nu|\theta)}{\partial\theta} = \operatorname{Re}(\operatorname{Tr}(\rho L_\theta E_\nu)). \tag{8.75}$$

Substituting this into the classical Fisher information formula and using the inequality $(\operatorname{Re}(z))^2 \leq |z|^2$:

$$I_F(\theta;\{E_\nu\}) = \sum_\nu \frac{(\operatorname{Re}(\operatorname{Tr}(\rho L_\theta E_\nu)))^2}{\operatorname{Tr}(\rho E_\nu)} \leq \sum_\nu \frac{|\operatorname{Tr}(\rho L_\theta E_\nu)|^2}{\operatorname{Tr}(\rho E_\nu)}. \tag{8.76}$$

We now apply the Cauchy-Schwarz inequality for the Hilbert-Schmidt inner product, $|\operatorname{Tr}(A^\dagger B)|^2 \leq \operatorname{Tr}(A^\dagger A)\operatorname{Tr}(B^\dagger B)$. We define operators $A_\nu = \sqrt{E_\nu}\sqrt{\rho}$ and $B_\nu = \sqrt{E_\nu}L_\theta\sqrt{\rho}$. Note that $\sqrt{E_\nu}$ and $\sqrt{\rho}$ are Hermitian. We have $\operatorname{Tr}(A_\nu^\dagger A_\nu) = \operatorname{Tr}(\sqrt{\rho}E_\nu\sqrt{\rho}) = \operatorname{Tr}(\rho E_\nu)$. The cross term is $\operatorname{Tr}(A_\nu^\dagger B_\nu) = \operatorname{Tr}(\sqrt{\rho}E_\nu L_\theta\sqrt{\rho}) = \operatorname{Tr}(\rho L_\theta E_\nu)$. The remaining term is $\operatorname{Tr}(B_\nu^\dagger B_\nu) = \operatorname{Tr}(\sqrt{\rho}L_\theta E_\nu L_\theta\sqrt{\rho}) = \operatorname{Tr}(\rho L_\theta E_\nu L_\theta)$. The Cauchy-Schwarz inequality yields:

$$|\operatorname{Tr}(\rho L_\theta E_\nu)|^2 \leq \operatorname{Tr}(\rho E_\nu)\cdot\operatorname{Tr}(\rho L_\theta E_\nu L_\theta). \tag{8.77}$$

Substituting this back into Eq. (8.76):

$$I_F(\theta;\{E_\nu\}) \leq \sum_\nu \operatorname{Tr}(\rho L_\theta E_\nu L_\theta) = \operatorname{Tr}\left(\rho L_\theta\left(\sum_\nu E_\nu\right)L_\theta\right). \tag{8.78}$$

Using the completeness relation $\sum_\nu E_\nu = I$, we obtain $I_F(\theta;\{E_\nu\}) \leq \operatorname{Tr}(\rho L_\theta^2)$. This implies $\mathcal{F}_Q(\theta) \leq \operatorname{Tr}(\rho L_\theta^2)$.

To show that this bound is attainable, consider the projective measurement defined by the eigenbasis of L_θ. Let $L_\theta = \sum_k \lambda_k \Pi_k$. Choosing $E_k = \Pi_k$, we have $\mathbb{P}(k|\theta) = \operatorname{Tr}(\rho\Pi_k)$. Since $L_\theta\Pi_k = \lambda_k\Pi_k$, the derivative formula above gives

$$\frac{\partial \mathbb{P}(k|\theta)}{\partial\theta} = \operatorname{Re}(\operatorname{Tr}(\rho L_\theta\Pi_k)) = \lambda_k\operatorname{Tr}(\rho\Pi_k). \tag{8.79}$$

Therefore,

$$I_F(\theta;\{\Pi_k\}) = \sum_k \frac{(\lambda_k\operatorname{Tr}(\rho\Pi_k))^2}{\operatorname{Tr}(\rho\Pi_k)} = \sum_k \lambda_k^2\operatorname{Tr}(\rho\Pi_k) = \operatorname{Tr}(\rho L_\theta^2). \tag{8.80}$$

Thus, the maximum is attained, and $\mathcal{F}_Q(\theta) = \operatorname{Tr}(\rho L_\theta^2)$. □

The calculation of the QFI simplifies significantly for pure states.

Proposition 8.16 (QFI for pure states)**.** *Let $\rho(\theta) = |\psi(\theta)\rangle\langle\psi(\theta)|$, and write $|\partial_\theta\psi\rangle = \frac{\partial}{\partial\theta}|\psi(\theta)\rangle$. Then*

$$\mathcal{F}_Q(\theta) = 4\left(\langle\partial_\theta\psi|\partial_\theta\psi\rangle - |\langle\psi|\partial_\theta\psi\rangle|^2\right). \tag{8.81}$$

PROOF. Differentiate $\rho(\theta) = |\psi(\theta)\rangle\langle\psi(\theta)|$ to obtain

$$\frac{\partial \rho(\theta)}{\partial \theta} = |\partial_\theta \psi\rangle\langle\psi| + |\psi\rangle\langle\partial_\theta \psi|. \tag{8.82}$$

Since $\langle\psi|\psi\rangle = 1$, differentiating the normalization condition gives

$$\langle\partial_\theta \psi|\psi\rangle + \langle\psi|\partial_\theta \psi\rangle = 0. \tag{8.83}$$

Therefore the operator

$$L_\theta := 2\left(|\partial_\theta \psi\rangle\langle\psi| + |\psi\rangle\langle\partial_\theta \psi|\right) \tag{8.84}$$

is Hermitian and satisfies the SLD equation Eq. (8.72). Indeed,

$$\begin{aligned} \frac{1}{2}\left(L_\theta \rho + \rho L_\theta\right) &= |\partial_\theta \psi\rangle\langle\psi| + |\psi\rangle\langle\partial_\theta \psi| \\ &\quad + \left(\langle\partial_\theta \psi|\psi\rangle + \langle\psi|\partial_\theta \psi\rangle\right)|\psi\rangle\langle\psi| \\ &= |\partial_\theta \psi\rangle\langle\psi| + |\psi\rangle\langle\partial_\theta \psi| \end{aligned} \tag{8.85}$$

by Eq. (8.83).

By Theorem 8.15 and Eq. (8.83), we have

$$\begin{aligned} \mathcal{F}_Q(\theta) &= \|L_\theta |\psi\rangle\|^2 \\ &= 4\,\||\partial_\theta \psi\rangle + \langle\partial_\theta \psi|\psi\rangle\,|\psi\rangle\|^2 \\ &= 4\left(\langle\partial_\theta \psi|\partial_\theta \psi\rangle - |\,\langle\psi|\partial_\theta \psi\rangle\,|^2\right), \end{aligned} \tag{8.86}$$

This proves Eq. (8.81). □

We can now state the result of quantum parameter estimation, which provides the lower bound on the variance of any locally unbiased estimator that is independent of the measurement strategy.

THEOREM 8.17 (Quantum Cramér-Rao bound). *Let $\rho(\theta)$ be a parameterized family of quantum states, and let $\mathcal{F}_Q(\theta)$ be the corresponding quantum Fisher information. Suppose we have access to N independent and identical copies of the state, $\rho(\theta)^{\otimes N}$. The variance of any locally unbiased estimator $\hat{\theta}$ derived from measurements on these states is bounded by*

$$\mathbb{V}(\hat{\theta}) \geq \frac{1}{N\mathcal{F}_Q(\theta)}. \tag{8.87}$$

PROOF. This follows from the classical Cramér-Rao bound and the definition of the QFI. For any measurement strategy $\{E_D\}$ on the joint state $\rho(\theta)^{\otimes N}$ (where D denotes the measurement outcome) and any estimator $\hat{\theta}(D)$ that is locally unbiased at θ, the classical CRB gives:

$$\mathbb{V}(\hat{\theta}) \geq \frac{1}{I_F(\theta; \{E_D\})}. \tag{8.88}$$

By definition, the QFI for the N copies, $\mathcal{F}_Q^{(N)}(\theta)$, is the supremum of $I_F(\theta; \{E_D\})$ over all measurements. Thus,

$$\mathbb{V}(\hat{\theta}) \geq \frac{1}{\mathcal{F}_Q^{(N)}(\theta)}. \tag{8.89}$$

To complete the proof, we must show the additivity of the QFI for independent systems, i.e., $\mathcal{F}_Q^{(N)}(\theta) = N\mathcal{F}_Q(\theta)$. The SLD for the composite system $\rho(\theta)^{\otimes N}$ is

$$L_{\text{tot}} = \sum_{i=1}^{N} L^{(i)}, \tag{8.90}$$

where $L^{(i)} = I^{\otimes(i-1)} \otimes L_\theta \otimes I^{\otimes(N-i)}$. The QFI is then $\mathcal{F}_Q^{(N)}(\theta) = \text{Tr}(\rho^{\otimes N} L_{\text{tot}}^2)$.

$$L_{\text{tot}}^2 = \sum_i (L^{(i)})^2 + \sum_{i \neq j} L^{(i)} L^{(j)}. \tag{8.91}$$

We observe that the expectation value of the SLD is zero. From the SLD definition (Eq. (8.72)), taking the trace yields:

$$\text{Tr}\left(\frac{\partial \rho}{\partial \theta}\right) = \text{Tr}\left(\frac{1}{2}(L_\theta \rho + \rho L_\theta)\right) = \text{Tr}(\rho L_\theta). \tag{8.92}$$

Furthermore, $\text{Tr}(\partial_\theta \rho) = \partial_\theta \,\text{Tr}(\rho) = \partial_\theta(1) = 0$. Thus, $\text{Tr}(\rho L_\theta) = 0$. For $i \neq j$, the expectation of the cross terms factorizes and vanishes: $\text{Tr}(\rho^{\otimes N} L^{(i)} L^{(j)}) = \text{Tr}(\rho L_\theta)\,\text{Tr}(\rho L_\theta) = 0$. The remaining terms yield the additivity:

$$\mathcal{F}_Q^{(N)}(\theta) = \sum_{i=1}^{N} \text{Tr}(\rho^{\otimes N} (L^{(i)})^2) = \sum_{i=1}^{N} \text{Tr}(\rho L_\theta^2) = N\mathcal{F}_Q(\theta). \tag{8.93}$$

Substituting this into the bound yields the QCRB. □

The QCRB establishes the fundamental limit of precision achievable in quantum metrology. For N experiments and any specific measurement $\{E_\nu\}$, we have:

$$\mathbb{V}(\hat{\theta}) \geq \frac{1}{N I_F(\theta; \{E_\nu\})} \geq \frac{1}{N\mathcal{F}_Q(\theta)}. \tag{8.94}$$

An optimal measurement strategy is one that saturates the inequality $I_F(\theta; \{E_\nu\}) \leq \mathcal{F}_Q(\theta)$ at the parameter value under consideration.

Example 8.18 (Single qubit phase estimation)**.** Consider the task of estimating an unknown phase θ encoded in the single-qubit state

$$|\psi(\theta)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\theta}|1\rangle). \tag{8.95}$$

We first determine the ultimate precision limit using the QFI formula for pure states (Eq. (8.81)). The derivative of the state vector is $|\partial_\theta \psi\rangle = \frac{i}{\sqrt{2}} e^{i\theta}|1\rangle$. We compute the necessary inner products:

$$\begin{aligned} \langle \partial_\theta \psi | \partial_\theta \psi \rangle &= \left(\frac{-i}{\sqrt{2}} e^{-i\theta}\langle 1|\right)\left(\frac{i}{\sqrt{2}} e^{i\theta}|1\rangle\right) = \frac{1}{2}, \\ \langle \psi | \partial_\theta \psi \rangle &= \left(\frac{1}{\sqrt{2}}(\langle 0| + e^{-i\theta}\langle 1|)\right)\left(\frac{i}{\sqrt{2}} e^{i\theta}|1\rangle\right) = \frac{i}{2}. \end{aligned} \tag{8.96}$$

The QFI is then

$$\mathcal{F}_Q(\theta) = 4\left(\frac{1}{2} - \left|\frac{i}{2}\right|^2\right) = 4\left(\frac{1}{2} - \frac{1}{4}\right) = 1. \tag{8.97}$$

The QCRB implies that the variance of any locally unbiased estimator based on N copies is bounded by $\mathbb{V}(\hat{\theta}) \geq 1/N$.

Now, let us analyze specific measurement strategies.

Suppose we measure in the computational basis, $\{E_0 = |0\rangle\langle 0|, E_1 = |1\rangle\langle 1|\}$. The outcome probabilities are $\mathbb{P}(0|\theta) = \mathbb{P}(1|\theta) = 1/2$. Since the probabilities are independent of θ, the classical Fisher information $I_F(\theta; Z) = 0$.

Now we measure in the X-basis, $\{E_+ = |+\rangle\langle +|, E_- = |-\rangle\langle -|\}$. The probability of the $+$ outcome is

$$\begin{aligned} \mathbb{P}(+|\theta) = |\langle +|\psi(\theta)\rangle|^2 &= \left| \frac{1}{\sqrt{2}}(\langle 0| + \langle 1|) \frac{1}{\sqrt{2}}(|0\rangle + e^{i\theta}|1\rangle) \right|^2 \\ &= \frac{1}{4}|1 + e^{i\theta}|^2 = \frac{1}{2}(1 + \cos\theta). \end{aligned} \tag{8.98}$$

Similarly, $\mathbb{P}(-|\theta) = \frac{1}{2}(1 - \cos\theta)$. The derivative is $\partial_\theta \mathbb{P}(+|\theta) = -\frac{1}{2}\sin\theta$. The classical Fisher information is

$$\begin{aligned} I_F(\theta; X) &= \frac{(-\frac{1}{2}\sin\theta)^2}{\frac{1}{2}(1 + \cos\theta)} + \frac{(\frac{1}{2}\sin\theta)^2}{\frac{1}{2}(1 - \cos\theta)} \\ &= \frac{1}{2}\sin^2\theta \left(\frac{1}{1 + \cos\theta} + \frac{1}{1 - \cos\theta} \right) \\ &= \frac{1}{2}\sin^2\theta \left(\frac{(1 - \cos\theta) + (1 + \cos\theta)}{1 - \cos^2\theta} \right) = 1. \end{aligned} \tag{8.99}$$

In this case, $I_F(\theta; X) = \mathcal{F}_Q(\theta) = 1$. This confirms that the X-basis measurement is an optimal strategy for estimating the phase θ encoded in this specific state. ◇

The QCRB is a cornerstone of quantum metrology, providing the theoretical foundation for understanding how quantum resources, such as entanglement, can enhance measurement precision beyond classical limits. This framework allows us to rigorously quantify the advantage of quantum strategies, leading to concepts such as the Heisenberg limit, which we will explore further in the context of phase estimation in Chapter 16.

Notes and further reading

For concentration inequalities and related nonasymptotic methods, see [BLM13]. In quantum settings, one important application of parameter estimation is Hamiltonian learning, where measurement data are used to estimate parameters of many-body systems. Classical shadows provide a compact representation of the quantum state from which many Pauli expectation values can be estimated in polynomial classical time [HKP20, HTFS23, HKT24, CW25]. Bayesian approaches to Hamiltonian learning and likelihood-based inference for experiments that are classically hard to simulate were developed in [GFWC12, WGFC14, WPS$^+$17, EHF19]. Related statistical ideas also appear in quantum computing verification and validation, including randomized benchmarking for average gate fidelities [DCEL09, MGE11] and more detailed reconstruction methods such as quantum process tomography and gate set tomography [NGR$^+$21].

Quantum hypothesis testing addresses the corresponding problem when one optimizes over measurements on quantum states rather than working only with a fixed classical output distribution. Quantum Stein's lemma gives asymptotic bounds on hypothesis-testing errors in terms of quantum relative entropy [BP10, ON02]. These topics belong more broadly to quantum information

theory, which studies the storage, transformation, and processing of information in quantum systems; see [Wat18, Wil13] for treatments that also cover entanglement theory and quantum channel capacities.

Part III

Algorithm

CHAPTER 9

Block encoding

This chapter introduces block encoding as an input model for matrix problems on a quantum computer. The basic difficulty is that many tasks in scientific computation are naturally phrased in terms of non-unitary linear maps, whereas the native operations available to quantum hardware are unitary. Block encoding addresses this mismatch by representing a target matrix A (up to a subnormalization factor and a prescribed error tolerance) as a submatrix block of a larger unitary U_A, so that applying U_A and post-selecting on ancilla qubits effectively applies A to a state.

The possibility of constructing an efficiently implementable U_A depends strongly on the structure of A and on the assumed access model. For a dense matrix without additional structure, any reasonable input model is typically prohibitive, since the input description may itself require exponential resources. We therefore focus on a few concrete settings in which block encodings can be constructed efficiently under suitable oracle access assumptions.

The true power of block encoding does not come directly from the ability to represent arbitrary matrices within blocks of a larger unitary. Rather, it stems from the ability to compose block encodings to block encode more complicated matrices and functions of matrices. We then describe how block encodings can be combined to obtain encodings of matrix additions and multiplications, while tracking the corresponding subnormalization factors and errors. Linear combinations of unitaries provide a flexible mechanism for such constructions. In this way, block encoding serves as an interface between matrix-oriented problem statements and unitary circuit realizations used throughout subsequent chapters.

9.1. Block encoding

The simplest example of block encoding is the following: assume we can find a $(n+1)$-qubit unitary matrix $U_A \in \mathrm{U}(2N)$ (where $N = 2^n$) such that

$$U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix}$$

where $*$ means that the corresponding matrix entries are irrelevant, then for any n-qubit quantum state $|b\rangle$, we can consider the state

$$|0, b\rangle = |0\rangle |b\rangle = \begin{pmatrix} b \\ 0 \end{pmatrix}, \tag{9.1}$$

and

$$U_A |0, b\rangle = \begin{pmatrix} Ab \\ * \end{pmatrix} =: |0\rangle A |b\rangle + |\perp\rangle . \tag{9.2}$$

Here the (unnormalized) state $|\perp\rangle$ can be written as $|1\rangle|\psi\rangle$ for some (unnormalized) state $|\psi\rangle$ that is irrelevant to the computation of $A|b\rangle$. In particular, it satisfies the orthogonality relation.

$$(|0\rangle\langle 0| \otimes I_N)|\perp\rangle = 0. \tag{9.3}$$

In order to obtain $A|b\rangle$, we measure the ancilla qubit and postselect on the outcome 0. This can be summarized into the following quantum circuit:

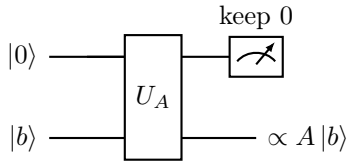


FIGURE 9.1. Circuit for block encoding of A using one ancilla qubit. By measuring the ancilla qubit and postselecting on the outcome 0, the state in the system register is a normalized state proportional to $A|b\rangle$.

Note that the output state is normalized after the measurement takes place. The success probability of obtaining 0 from the measurement can be computed as

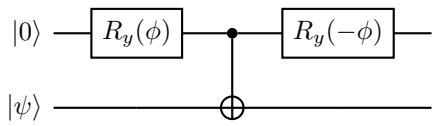
$$p(0) = \|A|b\rangle\|^2 = \langle b|A^\dagger A|b\rangle\,. \tag{9.4}$$

So the missing information of the norm $\|A|b\rangle\|$ can be recovered via the success probability $p(0)$ if needed. We find that the success probability is only determined by $A, |b\rangle$, and is independent of other irrelevant components of U_A.

Example 9.1. Consider the 2×2 matrix

$$A = \frac{3}{4}I + \frac{1}{4}X = \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{pmatrix}. \tag{9.5}$$

Consider the following circuit ($\phi = \frac{1}{3}\pi$)



Here

$$R_y(\theta) := \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix} = e^{-i\theta Y/2} \tag{9.6}$$

is the Y-rotation matrix. One may directly verify that U_A is an exact block encoding of A using one ancilla qubit. ◇

Note that we may not need to restrict the matrix U_A to be an $(n+1)$-qubit matrix. If we can find any $(n+m)$-qubit unitary matrix U_A so that

$$U_A = \begin{pmatrix} A & * & \cdots & * \\ * & * & \cdots & * \\ \vdots & & \vdots & \\ * & * & \cdots & * \end{pmatrix} \tag{9.7}$$

Here each $*$ stands for an n-qubit matrix, and there are 2^m block rows / columns in U_A. Using the partial application of operators in Definition 2.25, the relation above can be written compactly using the braket notation as

$$A = \langle 0^m | U_A | 0^m \rangle . \tag{9.8}$$

Exercise 9.1. Given a unitary matrix U and any submatrix block A, prove that $\|A\| \leq 1$.

In order to find such a block encoding U_A, Exercise 9.1 shows that a necessary condition for the existence of U_A is that $\|A\| \leq 1$. However, if we can find sufficiently large α and U_A so that

$$A/\alpha = \langle 0^m | U_A | 0^m \rangle . \tag{9.9}$$

By measuring the m ancilla qubits and postselecting on the outcome 0^m, we still obtain the normalized state $\frac{A|b\rangle}{\|A|b\rangle\|}$. The number α is hidden in the success probability:

$$p(0^m) = \frac{1}{\alpha^2} \|A|b\rangle\|^2 = \frac{1}{\alpha^2} \langle b|A^\dagger A|b\rangle . \tag{9.10}$$

So if α is chosen to be too large, the probability of obtaining all 0's from the measurement can be vanishingly small.

Finally, it can be difficult to find U_A to block encode A exactly. This is not a problem, since it is sufficient if we can find U_A to block encode A up to some error ϵ. We are now ready to give the definition of block encoding in Definition 9.2.

Definition 9.2 (Block encoding). *Given an n-qubit matrix A, if we can find $\alpha, \epsilon \in \mathbb{R}_+$, and an $(m+n)$-qubit unitary matrix U_A so that*

$$\|A - \alpha \langle 0^m | U_A | 0^m \rangle\| \leq \epsilon, \tag{9.11}$$

then U_A is called an (α, m, ϵ)-block-encoding of A. When the block encoding is exact with $\epsilon = 0$, U_A is called an (α, m)-block-encoding of A. The set of all (α, m, ϵ)-block-encodings of A is denoted by $\mathrm{BE}_{\alpha,m}(A, \epsilon)$. The parameter α is referred to as the block encoding factor, or the subnormalization factor.

When discussing block encodings, we often ignore certain errors such as the error in the finite precision number representation. We define a shorthand notation $\mathrm{BE}_{\alpha,m}(A) = \mathrm{BE}_{\alpha,m}(A, 0)$. Assume we know each matrix element of the n-qubit matrix A_{ij}, and we are given an $(n+m)$-qubit unitary U_A. In order to verify that $U_A \in \mathrm{BE}_{1,m}(A)$, we only need to verify that

$$\langle 0^m, i | U_A | 0^m, j \rangle = A_{ij}, \tag{9.12}$$

and U_A applied to any vector $|0^m, b\rangle$ can be obtained via the superposition principle.

Therefore we may first evaluate the state $U_A |0^m, j\rangle$, perform an inner product with $|0^m, i\rangle$, and verify the resulting inner product is A_{ij}. We will also use the following technique frequently. Assume $U_A = U_B U_C$, and then

$$\langle 0^m, i | U_A | 0^m, j \rangle = \langle 0^m, i | U_B U_C | 0^m, j \rangle = (U_B^\dagger |0^m, i\rangle)^\dagger (U_C |0^m, j\rangle). \tag{9.13}$$

So we can evaluate the states $U_B^\dagger |0^m, i\rangle, U_C |0^m, j\rangle$ independently, and then verify the inner product is A_{ij}. Such a calculation amounts to running the circuit Fig. 9.2, and if the ancilla qubits are measured to be 0^m, the system qubits return the normalized state $\sum_i A_{ij} |i\rangle / \|\sum_i A_{ij} |i\rangle\|$.

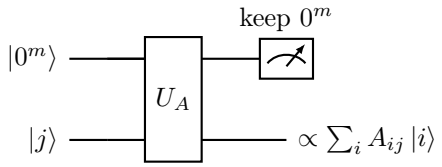


FIGURE 9.2. Circuit for general block encoding of A.

Example 9.3. For any n-qubit matrix A with $\|A\| \leq 1$ with singular value decomposition $A = W\Sigma V^\dagger$, all singular values in the diagonal matrix Σ are in $[0, 1]$. Then we may construct an $(n+1)$-qubit unitary matrix ($N = 2^n$)

$$\begin{aligned} U_A :=& \begin{pmatrix} W & 0 \\ 0 & I_N \end{pmatrix} \begin{pmatrix} \Sigma & \sqrt{I_N - \Sigma^2} \\ \sqrt{I_N - \Sigma^2} & -\Sigma \end{pmatrix} \begin{pmatrix} V^\dagger & 0 \\ 0 & I_N \end{pmatrix} \\ =& \begin{pmatrix} A & W\sqrt{I_N - \Sigma^2} \\ \sqrt{I_N - \Sigma^2} V^\dagger & -\Sigma \end{pmatrix} \end{aligned} \tag{9.14}$$

which is a $(1, 1)$-block-encoding of A. ◇

Example 9.3 shows that in principle, any matrix A with $\|A\| \leq 1$ can be accessed via a $(1, 1, 0)$-block-encoding. However, this construction does not state how to construct A using simple one and two qubit gates.

Example 9.4 (Random circuit block encoded matrix)**.** How can we construct a pseudo-random non-unitary matrix on a quantum computer? A naive approach would be to generate a dense pseudo-random matrix A classically and then encode it into a quantum circuit. However, this is highly inefficient in practice, particularly for large matrices, due to the exponential overhead in loading dense classical data into a quantum system.

Instead, we seek to work with matrices that are inherently easy to generate within a quantum circuit model. This motivates the **random circuit based block-encoded matrix** (RACBEM) model. Rather than first constructing a matrix A and then searching for a block-encoding unitary U_A, the RACBEM model reverses the thought process: we begin by constructing a unitary U_A that is easy to implement on a quantum computer, typically using random quantum circuits, and then extract A as a subblock of U_A. This provides a practical and scalable way to generate structured pseudo-random non-unitary matrices compatible with quantum algorithm design. Similar to the LINPACK benchmark, which is used to rank classical supercomputers in the TOP500 list by solving $Ax = b$ for pseudorandom matrices A, such block-encoded pseudorandom matrices can serve as a useful tool for benchmarking scientific computing applications on quantum computers. ◇

9.2. Linear combination of unitaries

The **linear combination of unitaries** (LCU) is an important quantum primitive, which allows quantum algorithms to be implemented as a superposition of unitary matrices rather than

attempting to find a single unitary that accomplishes a desired task. This often simplifies the design and analysis of quantum algorithms. LCU can also be viewed as a special way for constructing block encoding. Combined with a technique called qubitization, which will be discussed in detail in Chapter 10, LCU can be used to implement a large class of matrix functions (eigenvalue transformations) and generalized matrix functions (singular value transformations).

Let $T = \sum_{i=0}^{K-1} \alpha_i U_i$ be a linear combination of unitary matrices U_i. For simplicity let $K = 2^a$. Then

$$U_{\mathrm{SEL}} := \sum_{i\in[K]} |i\rangle\langle i| \otimes U_i, \tag{9.15}$$

implements the selection of U_i conditioned on the value of the a-qubit ancilla register (also called the control register). U_{SEL} is called a **select oracle**.

If all linear combination coefficients $\alpha_i \geq 0$, we can let V_{PREP} be a unitary operation satisfying

$$V_{\mathrm{PREP}} |0^a\rangle = \frac{1}{\sqrt{\|\alpha\|_1}} \sum_{i\in[K]} \sqrt{\alpha_i} |i\rangle , \tag{9.16}$$

which is called a **prepare oracle**. The 1-norm of the coefficients is given by

$$\|\alpha\|_1 = \sum_i |\alpha_i| . \tag{9.17}$$

In matrix form,

$$V_{\mathrm{PREP}} = \frac{1}{\sqrt{\|\alpha\|_1}} \begin{pmatrix} \sqrt{\alpha_0} & * & \cdots & * \\ \vdots & * & \ddots & \vdots \\ \sqrt{\alpha_{K-1}} & * & \cdots & * \end{pmatrix}. \tag{9.18}$$

where the first column is $V_{\mathrm{PREP}} |0^a\rangle$, and all other columns are orthogonal to it. Then

$$V_{\mathrm{PREP}}^\dagger = \frac{1}{\sqrt{\|\alpha\|_1}} \begin{pmatrix} \sqrt{\alpha_0} & \cdots & \sqrt{\alpha_{K-1}} \\ * & \cdots & * \\ \vdots & \ddots & \vdots \\ * & \cdots & * \end{pmatrix}. \tag{9.19}$$

More generally, we can arbitrarily decompose $\alpha_i = \beta_i \gamma_i$, so that

$$V_{\mathrm{PREP}} = \frac{1}{\|\beta\|_2} \begin{pmatrix} \beta_0 & * & \cdots & * \\ \vdots & * & \ddots & \vdots \\ \beta_{K-1} & * & \cdots & * \end{pmatrix}, \quad \widetilde{V}_{\mathrm{PREP}} = \frac{1}{\|\gamma\|_2} \begin{pmatrix} \gamma_0 & \cdots & \gamma_{K-1} \\ * & \cdots & * \\ \vdots & \ddots & \vdots \\ * & \cdots & * \end{pmatrix} \tag{9.20}$$

are unitaries and can be efficiently implemented. When $\alpha_i \geq 0$, we can choose $\beta_i = \gamma_i = \sqrt{\alpha_i}$ which gives $\widetilde{V}_{\mathrm{PREP}} = V_{\mathrm{PREP}}^\dagger$. Then T can be implemented using the unitary given in Lemma 9.5.

Lemma 9.5 (Linear combination of unitaries)**.** *For*

$$T = \sum_{i=0}^{K-1} \alpha_i U_i, \quad \alpha_i = \beta_i \gamma_i, \quad K = 2^a, \quad U_i \in \mathrm{U}(2^n), \tag{9.21}$$

let $U_{\mathrm{SEL}}, V_{\mathrm{PREP}}, \widetilde{V}_{\mathrm{PREP}}$ *be given in Eqs.* (9.15) *and* (9.20)*, respectively. Define*

$$W = (\widetilde{V}_{\mathrm{PREP}} \otimes I_n) U_{\mathrm{SEL}} (V_{\mathrm{PREP}} \otimes I_n) \tag{9.22}$$

as implemented in Fig. 9.3. Then $W \in \mathrm{BE}_{\|\beta\|_2\|\gamma\|_2,a}(T)$. *The smallest subnormalization factor is obtained by setting*

$$|\beta_i| = |\gamma_i| = \sqrt{|\alpha_i|}, \quad i \in [K], \tag{9.23}$$

and $W \in \mathrm{BE}_{\|\alpha\|_1,a}(T)$.

Proof. For any n-qubit state $|\psi\rangle$,

$$U_{\mathrm{SEL}}(V_{\mathrm{PREP}} \otimes I_n) |0^a\rangle |\psi\rangle = U_{\mathrm{SEL}} \frac{1}{\|\beta\|_2} \sum_i \beta_i |i\rangle |\psi\rangle = \frac{1}{\|\beta\|_2} \sum_i \beta_i |i\rangle U_i |\psi\rangle . \tag{9.24}$$

Let the state $|\widetilde{\perp}\rangle$ collect all the states marked by $*$ orthogonal to $|0^a\rangle$, and use $\beta_i\gamma_i = \alpha_i$,

$$(\widetilde{V}_{\mathrm{PREP}}\otimes I_n)U_{\mathrm{SEL}}(V_{\mathrm{PREP}}\otimes I_n) |0^a\rangle |\psi\rangle = \frac{1}{\|\beta\|_2 \|\gamma\|_2} |0^a\rangle \sum_i \alpha_i U_i |\psi\rangle + |\widetilde{\perp}\rangle = \frac{1}{\|\beta\|_2 \|\gamma\|_2} |0^a\rangle T |\psi\rangle + |\widetilde{\perp}\rangle . \tag{9.25}$$

Use Cauchy-Schwarz

$$\|\alpha\|_1 = \sum_i |\alpha_i| = \sum_i |\beta_i\gamma_i| \le \|\beta\|_2 \|\gamma\|_2 , \tag{9.26}$$

we find that the optimal prepare oracle should satisfy $|\beta_i| = |\gamma_i| = \sqrt{|\alpha_i|}, \forall i$. □

The LCU Lemma states that the number of ancilla qubits needed only depends logarithmically on K, the number of terms in the linear combination. Hence it is possible to implement the linear combination of a very large number of terms efficiently. From a practical perspective, the select and prepare oracles use multi-qubit controls, and may be difficult to implement themselves. Furthermore, if the select and prepare oracles are implemented directly, the number of multi-qubit controls again depends linearly on K and is not desirable. Therefore an efficient implementation using LCU (in terms of the gate complexity) also requires additional structure in these oracles.

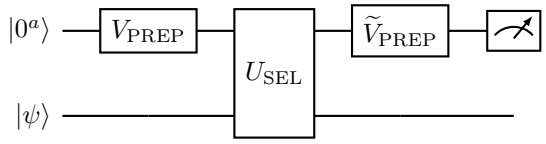


Figure 9.3. Circuit for linear combination of unitaries. When all coefficients are nonnegative, we may set $\widetilde{V}_{\mathrm{PREP}} = V_{\mathrm{PREP}}^\dagger$.

An important application of LCU is that if A, B can be accessed via their block encodings, then we can construct a block encoding of the matrix addition $A + B$.

Example 9.6 (Linear combination of two block encoded matrices)**.** Let U_A, U_B be two n-qubit unitaries, and we would like to construct a block encoding of $T = U_A + U_B$.

There are two terms in total, so one ancilla qubit is needed. The prepare oracle needs to implement

$$V_{\mathrm{PREP}} |0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \tag{9.27}$$

so this is the Hadamard gate. The circuit is given by Fig. 9.4, which constructs $W \in \mathrm{BE}_{2,1}(T)$.

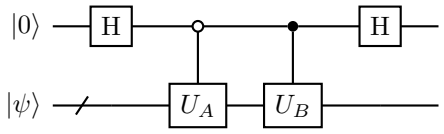


FIGURE 9.4. Circuit for linear combination of two unitaries.

◇

Exercise 9.2. Let A, B be two n-qubit matrices encoded by $U_A \in \mathrm{BE}_{1,m}(A), U_B \in \mathrm{BE}_{1,m}(B)$. Construct a circuit to block encode $C = A + B$. What about $U_A \in \mathrm{BE}_{\alpha_A,m}(A), U_B \in \mathrm{BE}_{\alpha_B,m}(B)$?

Exercise 9.3. Consider a system described by the linear combination $T = X + Y + 2Z$, where X, Y, Z are the Pauli matrices. Construct a select oracle U for this system, and describe how to use the LCU technique to construct a block encoding of T.

Example 9.7. Consider the following TFIM model with periodic boundary conditions ($Z_n = Z_0$), and $n = 2^{\mathfrak{n}}$,

$$\hat{H} = -\sum_{i\in[n]} Z_i Z_{i+1} - \sum_{i\in[n]} X_i. \tag{9.28}$$

In order to use LCU, we need $(\mathfrak{n}+1)$ ancilla qubits. In this case, the prepare oracle can be simply constructed from the Hadamard gate

$$V_{\mathrm{PREP}} = \mathrm{H}^{\otimes(\mathfrak{n}+1)}, \tag{9.29}$$

and the select oracle implements

$$U_{\mathrm{SEL}} = \sum_{i\in[n]} |i\rangle\langle i| \otimes (-Z_i Z_{i+1}) + \sum_{i\in[n]} |i+n\rangle\langle i+n| \otimes (-X_i). \tag{9.30}$$

The corresponding $W \in \mathrm{BE}_{2n,\mathfrak{n}+1}(\hat{H})$. ◇

Example 9.8 (Highly oscillatory integral)**.** Consider evaluating the matrix integral $\int_0^1 A(s)\,ds$, where $A(s) \in \mathbb{C}^{2^n\times 2^n}$, $A(0) = A(1)$ and $\sup_{s\in[0,1]} \|A(s)\| \le 1$. Given that the entries of $A(s)$ exhibit significant oscillations as a function of s, in general there is no known efficient method (classical or quantum) to compute this integral without using a sufficiently fine grid and numerical quadrature. For simplicity, we adopt a uniform grid defined by $\{s_k = \frac{k}{M}\}_{k=0}^{M}$, where M is sufficiently large, to implement the quadrature method.

$$\int_0^1 A(s)\,\mathrm{d}s = \frac{1}{M}\sum_{k=0}^{M-1} A(k/M) + E, \quad \|E\| \le \epsilon. \tag{9.31}$$

For each s, assume that $A(s)$ has a $(1, a, 0)$-block encoding denoted by $U_{A(s)}$, and the s-dependence can be implemented coherently using e.g., classical arithmetic operations. In a discretized setting, let $M = 2^m$, this means that the following select oracle defined on a register with $m + a + n$ qubits:

$$U_{\mathrm{SEL}} = \sum_{k=0}^{M-1} |k\rangle\langle k| \otimes U_{A(k/M)}, \tag{9.32}$$

which we assume can be efficiently implemented with cost $\mathrm{poly}(mn)$. The prepare oracle is simply the m-qubit Hadamard gate $\mathrm{H}^{\otimes m}$. Then the circuit $(\mathrm{H}^{\otimes m} \otimes I_{a+n}) U_{\mathrm{SEL}} (\mathrm{H}^{\otimes m} \otimes I_{a+n})$ is a $(1, a+m, \epsilon)$-block encoding of the matrix-valued integral $\int_0^1 A(s)\,\mathrm{d}s$. It uses m ancilla qubits, and the gate complexity is dominated by that of the select oracle and is $\mathrm{poly}(mn)$. This is an exponential improvement in the parameter M for constructing such a block encoding, compared to a direct classical quadrature implementation whose cost is at least linear in M. ◇

Example 9.9 (Fourier transformation and eigenvalue transformation)**.** With a subroutine performing Hamiltonian simulation, we can combine it with LCU to implement matrix functions expressed as a matrix Fourier series. Let H be an n-qubit Hermitian matrix. Consider $f(x) \in \mathbb{R}$ given by its Fourier expansion (up to a normalization factor)

$$f(x) = \int \hat{f}(k) e^{ikx}\,\mathrm{d}k, \tag{9.33}$$

and we are interested in computing the matrix function via numerical quadrature

$$f(H) = \int \hat{f}(k) e^{ikH}\,\mathrm{d}k \approx \Delta k \sum_{k \in \mathcal{K}} \hat{f}(k) e^{ikH}. \tag{9.34}$$

Here $\mathcal{K}$ is a uniform grid discretizing the interval $[-L, L]$ using $|\mathcal{K}| = 2^{\mathfrak{k}}$ grid points, and the grid spacing is $\Delta k = 2L/|\mathcal{K}|$. The prepare oracle is given by the coefficients $c_k = \Delta k \hat{f}(k)$, and the corresponding subnormalization factor is

$$\|c\|_1 = \sum_{k \in \mathcal{K}} \Delta k \left|\hat{f}(k)\right| \approx \int \left|\hat{f}(k)\right| \mathrm{d}k. \tag{9.35}$$

The select oracle is

$$U_{\mathrm{SELECT}} = \sum_{k \in \mathcal{K}} |k\rangle\langle k| \otimes e^{ikH}. \tag{9.36}$$

This can be efficiently implemented using the controlled matrix powers as in Fig. 16.3, where the basic unit is the short time Hamiltonian simulation $e^{i\Delta kH}$. This can be used to block encode a large class of matrix functions. ◇

9.3. Block encodings of matrix additions and multiplications

We now record basic composition rules for block encodings that will be used throughout the book.

The linear combination of unitaries (LCU) construction from Section 9.2 immediately yields a block encoding of a sum of block-encoded matrices. For simplicity, we state the result for $M = 2^m$ summands.

Proposition 9.10 (Sum of M block-encoded matrices)**.** *Let $M = 2^m$ and let $A_0, \ldots, A_{M-1}$ be matrices of the same dimension. Assume that for each $j \in [M]$ we are given a block encoding*

$$U_{A_j} \in \mathrm{BE}_{\alpha_j, a}(A_j, \epsilon_j), \qquad \alpha_j \geq 0. \tag{9.37}$$

Set $\gamma := \sum_{j=0}^{M-1} \alpha_j > 0$. Let $U_{\mathrm{SEL}} := \sum_{j \in [M]} |j\rangle\langle j| \otimes U_{A_j}$ be the select oracle acting on an m-qubit control register, the a-qubit ancilla register, and the system register. Let V_{PREP} be any unitary on

the m-qubit control register satisfying

$$V_{\mathrm{PREP}}\,|0^m\rangle = \frac{1}{\sqrt{\gamma}} \sum_{j=0}^{M-1} \sqrt{\alpha_j}\,|j\rangle\,. \tag{9.38}$$

Define

$$W := (V_{\mathrm{PREP}}^{\dagger} \otimes I)\, U_{\mathrm{SEL}}\, (V_{\mathrm{PREP}} \otimes I). \tag{9.39}$$

Then

$$W \in \mathrm{BE}_{\gamma,a+m}\left(\sum_{j=0}^{M-1} A_j,\ \sum_{j=0}^{M-1} \epsilon_j \right). \tag{9.40}$$

Proof. Write $B_j := \langle 0^a | U_{A_j} | 0^a \rangle$, so that $\|A_j - \alpha_j B_j\| \le \epsilon_j$ and $\|B_j\| \le 1$. By direct computation of the $(|0^m, 0^a\rangle)$ block,

$$\langle 0^m, 0^a | W | 0^m, 0^a \rangle = \sum_{j=0}^{M-1} \frac{\alpha_j}{\gamma}\, B_j. \tag{9.41}$$

Therefore

$$\left\| \sum_{j=0}^{M-1} A_j - \gamma\, \langle 0^m, 0^a | W | 0^m, 0^a \rangle \right\| \le \sum_{j=0}^{M-1} \|A_j - \alpha_j B_j\| \le \sum_{j=0}^{M-1} \epsilon_j, \tag{9.42}$$

which is the claimed block-encoding statement. □

Example 9.11 (Multiplication of block encoded matrices)**.** If A, B are given by their block encodings $U_A \in \mathrm{BE}_{\alpha,a}(A), U_B \in \mathrm{BE}_{\beta,b}(B)$, then the product AB can also be block encoded (see Fig. 9.5), which uses $a+b$ ancilla qubits. This is because $AB/(\alpha\beta) = \langle 0^{a+b} | (U_A \otimes I_b)(I_a \otimes U_B) | 0^{a+b} \rangle$. Hence $(U_A \otimes I_b)(I_a \otimes U_B) \in \mathrm{BE}_{\alpha\beta,a+b}(AB)$.

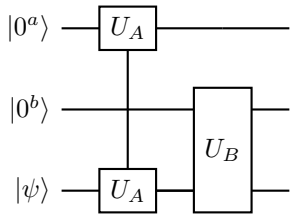


Figure 9.5. Quantum circuit for block encoding the product of matrices using $a + b$ ancilla qubits.

◇

We next record a simple (though not always ancilla-optimal) rule for block encoding a product.

Proposition 9.12 (Product of M block-encoded matrices)**.** *Let $A_0, \dots, A_{M-1}$ be matrices with compatible dimensions. Assume that for each $j \in [M]$ we are given*

$$U_{A_j} \in \mathrm{BE}_{\alpha_j, a_j}(A_j, \epsilon_j). \tag{9.43}$$

Let U be the unitary obtained by applying $U_{A_0}, U_{A_1}, \dots, U_{A_{M-1}}$ sequentially on disjoint ancilla registers (of sizes $a_0, \dots, a_{M-1}$) and a common system register. Then

$$U \in \mathrm{BE}_{\prod_{j=0}^{M-1}\alpha_j,\, \sum_{j=0}^{M-1} a_j}\Big(A_{M-1}\cdots A_0,\ \prod_{j=0}^{M-1}(\alpha_j+\epsilon_j) - \prod_{j=0}^{M-1}\alpha_j\Big). \tag{9.44}$$

Proof. For each j, define $B_j := \langle 0^{a_j}|U_{A_j}|0^{a_j}\rangle$ so that $\|A_j - \alpha_j B_j\| \le \epsilon_j$ and $\|B_j\| \le 1$. Since the ancilla registers are disjoint, we have

$$\langle 0^{a_0+\cdots+a_{M-1}}|U|0^{a_0+\cdots+a_{M-1}}\rangle = B_{M-1}\cdots B_0. \tag{9.45}$$

It remains to bound

$$\left\| A_{M-1}\cdots A_0 - \Big(\prod_{j=0}^{M-1}\alpha_j\Big) B_{M-1}\cdots B_0 \right\|. \tag{9.46}$$

We prove by induction on M the inequality

$$\left\| \prod_{j=0}^{M-1} A_j - \prod_{j=0}^{M-1}(\alpha_j B_j) \right\| \le \prod_{j=0}^{M-1}(\alpha_j+\epsilon_j) - \prod_{j=0}^{M-1}\alpha_j. \tag{9.47}$$

The case $M = 1$ is immediate. For the induction step, write $P := \prod_{j=0}^{M-2} A_j$ and $\widetilde{P} := \prod_{j=0}^{M-2}(\alpha_j B_j)$. Then

$$\begin{aligned} \left\| A_{M-1}P - (\alpha_{M-1}B_{M-1})\widetilde{P} \right\| &\le \|(A_{M-1} - \alpha_{M-1}B_{M-1})P\| + \left\| \alpha_{M-1}B_{M-1}(P-\widetilde{P}) \right\| \\ &\le \epsilon_{M-1}\|P\| + \alpha_{M-1}\left\| P - \widetilde{P} \right\|. \end{aligned} \tag{9.48}$$

Using $\|A_j\| \le \alpha_j + \epsilon_j$ (by $\|A_j\| \le \|A_j - \alpha_j B_j\| + \alpha_j \|B_j\|$), we have $\|P\| \le \prod_{j=0}^{M-2}(\alpha_j+\epsilon_j)$. Applying the induction hypothesis to $\left\|P - \widetilde{P}\right\|$ yields

$$\begin{aligned} \left\| A_{M-1}P - (\alpha_{M-1}B_{M-1})\widetilde{P} \right\| &\le \epsilon_{M-1}\prod_{j=0}^{M-2}(\alpha_j+\epsilon_j) + \alpha_{M-1}\Big(\prod_{j=0}^{M-2}(\alpha_j+\epsilon_j) - \prod_{j=0}^{M-2}\alpha_j\Big) \\ &= \prod_{j=0}^{M-1}(\alpha_j+\epsilon_j) - \prod_{j=0}^{M-1}\alpha_j, \end{aligned} \tag{9.49}$$

completing the induction. □

The procedure in Example 9.11 is not the most efficient way for block encoding the product of matrices. In Example 11.9, we have demonstrated that using deferred measurement, we only need one extra ancilla qubit to record whether the ancilla register is in the all 0 state. Specifically, assume $a = b$ for simplicity; Fig. 9.6 is a schematic circuit (the control denotes a check of the ancilla register being in $|0^a\rangle$) that constructs a unitary in $\mathrm{BE}_{\alpha\beta, a+1}(AB)$.

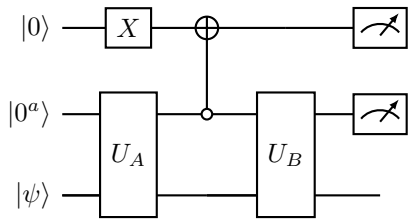


FIGURE 9.6. Quantum circuit for block encoding the product of matrices using $a+1$ ancilla qubits (assuming $a=b$).

Following this strategy, when multiplying L matrices A_i each given by $U_{A_i} \in \mathrm{BE}_{\alpha_i,a}(A_i)$, we can introduce $L-1$ ancilla qubits to obtain a unitary in $\mathrm{BE}_{\prod_{i=1}^{L}\alpha_i,a+L-1}(A_L\cdots A_1)$. Even more efficiently, using the compression gadget in Example 11.10, the number of ancilla qubits can be reduced to $a+\lceil\log_2(L+1)\rceil$.

Note that the matrix power A^L is a special case of multiplying L matrices. However, the method in Example 9.11 for encoding A^L can be highly inefficient. To see this, consider a matrix A with spectral radius

$$\rho(A) = \max\{\,|\lambda| \mid \lambda \in \mathrm{Spec}(A)\,\}, \tag{9.50}$$

where $\mathrm{Spec}(A)$ denotes the set of eigenvalues of A. Suppose that $\rho(A)<1$. Then there exists a constant C such that $\sup_{L\in\mathbb{N}}\left\|A^L\right\| \le C$. However, it is still possible that $\|A\|>1$, which means that the block encoding subnormalization factor of A must satisfy $\alpha \ge \|A\| > 1$. As a result, the subnormalization factor for encoding A^L using the method in Example 9.11 would scale as α^L, growing exponentially with L. This discrepancy in computing matrix powers is closely related to the challenges of solving linear differential equations. This is a topic that will be discussed in Chapter 20.

9.4. Example: implementing generalized measurements

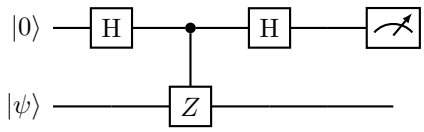
One of the most important applications of linear combinations of unitaries stems from the fact that LCU gives a straightforward method to implement a generalized measurement (or POVM).

Recall from Section 2.3 that a POVM is given by a set of positive semidefinite operators $\{P_i \succeq 0\}$ that sum to the identity, $\sum_i P_i = I$. Each P_i does not need to be a projector nor orthogonal to the others. For a density operator ρ, outcome i is observed with probability $\mathrm{Tr}[P_i\rho]$. Further, the quantum state upon measuring outcome i is updated according to

$$\rho \mapsto \frac{\sqrt{P_i}\rho\sqrt{P_i}}{\mathrm{Tr}[P_i\rho]}. \tag{9.51}$$

We will see that LCU provides a recipe for implementing all such measurements. First, let us consider an example of implementing a projective measurement in the computational basis.

Example 9.13. Measurement in the computational basis is a special case of a POVM wherein $P_0 = |0\rangle\langle 0| = (I+Z)/2$ and $P_1 = |1\rangle\langle 1| = (I-Z)/2$.



We can see that this corresponds to an LCU circuit with PREP = H and SELECT = $|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes Z$. Thus from Lemma 9.5 we have that

$$\begin{aligned} |\psi\rangle &\mapsto |0\rangle \otimes |0\rangle, \quad \text{with probability } \langle\psi| P_0 |\psi\rangle = |\langle 0|\psi\rangle|^2, \\ |\psi\rangle &\mapsto |1\rangle \otimes |1\rangle, \quad \text{with probability } \langle\psi| P_1 |\psi\rangle = |\langle 1|\psi\rangle|^2. \end{aligned} \tag{9.52}$$

Thus we can see that this circuit can be used to perform a computational basis measurement. Similarly any projective measurement on a single qubit can be carried out by applying a unitary transformation on Z. While this circuit may seem at first glance useless, as we could just as easily measure the bottom qubit to get the same result, it actually is used in photonic non-demolition experiments wherein a direct measurement would absorb the photon of interest. ◇

The above example shows that we can perform conventional measurements with block encodings, but not all important tasks can be naturally expressed as ordinary (or projective) measurements. We demonstrate this in the following example.

Example 9.14. Let us assume that we have two (potentially non-orthogonal) normalized states $|\psi\rangle$ and $|\phi\rangle$ and we are promised that the unknown state is one of these two. Since the states need not be orthogonal, they cannot be perfectly distinguished in a single shot.

Here is a POVM for state discrimination with two conclusive outcomes and one inconclusive outcome. Let $c := \langle\psi|\phi\rangle$ and assume $|c| < 1$. Define

$$|\psi_\perp\rangle := \frac{|\phi\rangle - c\,|\psi\rangle}{\sqrt{1-|c|^2}}, \qquad |\phi_\perp\rangle := \frac{|\psi\rangle - c^*\,|\phi\rangle}{\sqrt{1-|c|^2}}, \tag{9.53}$$

which satisfy $\langle\psi|\psi_\perp\rangle = 0$ and $\langle\phi|\phi_\perp\rangle = 0$. Then one valid choice of POVM elements is

$$\begin{aligned} P_\psi &= \tfrac{1}{1+|c|}\,|\phi_\perp\rangle\langle\phi_\perp|, \\ P_\phi &= \tfrac{1}{1+|c|}\,|\psi_\perp\rangle\langle\psi_\perp|, \\ P_? &= I - P_\psi - P_\phi. \end{aligned} \tag{9.54}$$

One checks that $P_\psi, P_\phi, P_? \succeq 0$ and $P_\psi + P_\phi + P_? = I$. Moreover, the conclusive outcomes are unambiguous in the sense that $\langle\phi| P_\psi |\phi\rangle = 0$ and $\langle\psi| P_\phi |\psi\rangle = 0$. The post-measurement update is given by Eq. (9.51). ◇

In Section 2.3, we discussed how POVMs can be related to projective measurements in a higher-dimensional space via Naimark's dilation. Here we give a different view on this dilation by expressing it as a block encoding in a higher-dimensional space.

Lemma 9.15. *Let $P = \{P_i : i \in [2^m]\}$ be a POVM. Assume that for each $i \in [2^m]$ we are given a unitary*

$$U_i \in \mathrm{BE}_{\beta,a}(\sqrt{P_i}) \tag{9.55}$$

with the same ancilla size a and the same block-encoding factor $\beta > 0$. For example, this is the case if each $\sqrt{P_i}$ has a linear-combination-of-unitaries decomposition with coefficient 1-norm at most β, by Lemma 9.5. Define the controlled unitary

$$W = \sum_{i \in [2^m]} |i\rangle\langle i| \otimes U_i. \tag{9.56}$$

Then a measurement of the POVM can be implemented with failure probability at most δ using

$$\mathcal{O}(\beta 2^{m/2} \log(1/\delta)) \tag{9.57}$$

queries to W and $W^\dagger$.

Proof. Let the output register be $\mathcal{H}_{\text{out}} \cong \mathbb{C}^{2^m}$, let the ancilla register for the block encoding be $\mathcal{H}_{\text{anc}} \cong \mathbb{C}^{2^a}$, and let the system register be $\mathcal{H}_{\text{sys}}$. Consider the uniform superposition

$$|u\rangle := \frac{1}{\sqrt{2^m}} \sum_{i \in [2^m]} |i\rangle \in \mathcal{H}_{\text{out}}. \tag{9.58}$$

For a pure input state $|\psi\rangle \in \mathcal{H}_{\text{sys}}$, we start from

$$|u\rangle\, |0^a\rangle\, |\psi\rangle\,. \tag{9.59}$$

Since $U_i \in \mathrm{BE}_{\beta,a}(\sqrt{P_i})$, for each i we have

$$U_i\, |0^a\rangle\, |\psi\rangle = \frac{1}{\beta}\, |0^a\rangle\, \sqrt{P_i}\, |\psi\rangle + |\perp_i\rangle\,, \tag{9.60}$$

where $(\langle 0^a| \otimes I)\, |\perp_i\rangle = 0$. Therefore

$$W\, |u\rangle\, |0^a\rangle\, |\psi\rangle = \frac{1}{\beta\sqrt{2^m}} \sum_{i \in [2^m]} |i\rangle\, |0^a\rangle\, \sqrt{P_i}\, |\psi\rangle + |\perp\rangle\,, \tag{9.61}$$

where again $(I \otimes \langle 0^a| \otimes I)\, |\perp\rangle = 0$.

We now measure the ancilla register and postselect on the outcome 0^a. The success probability is

$$\mathbb{P}(\text{succ}) = \frac{1}{\beta^2 2^m} \sum_{i \in [2^m]} \left\| \sqrt{P_i}\, |\psi\rangle \right\|^2 = \frac{1}{\beta^2 2^m} \sum_{i \in [2^m]} \langle\psi|\, P_i\, |\psi\rangle = \frac{1}{\beta^2 2^m}, \tag{9.62}$$

where we used $\sum_i P_i = I$. Conditioned on success, the output and system registers are in the state

$$\sum_{i \in [2^m]} |i\rangle \otimes \sqrt{P_i}\, |\psi\rangle\,. \tag{9.63}$$

This state is normalized because

$$\sum_{i \in [2^m]} \left\| \sqrt{P_i}\, |\psi\rangle \right\|^2 = \sum_{i \in [2^m]} \langle\psi|\, P_i\, |\psi\rangle = 1. \tag{9.64}$$

Measuring the output register now yields outcome i with probability

$$\mathbb{P}(i \mid \text{succ}) = \left\| \sqrt{P_i}\, |\psi\rangle \right\|^2 = \langle\psi|\, P_i\, |\psi\rangle\,, \tag{9.65}$$

and the post-measurement system state is

$$\frac{\sqrt{P_i}\, |\psi\rangle}{\sqrt{\langle\psi|\, P_i\, |\psi\rangle}}, \tag{9.66}$$

which is the usual pure-state version of the update rule in Eq. (9.51). The mixed-state formula follows by linearity.

Finally, amplitude amplification raises the success probability to a constant using

$$\mathcal{O}\left(\frac{1}{\sqrt{\mathbb{P}(\text{succ})}}\log(1/\delta)\right) = \mathcal{O}(\beta 2^{m/2}\log(1/\delta)) \tag{9.67}$$

queries to W and $W^\dagger$, which proves the claimed complexity.

□

9.5. Example: Quantum error correction as block encoding

9.6. Query models for matrix entries

Throughout the discussion we assume A is an n-qubit, square matrix, and the max norm of A (see Definition 2.45) satisfies $\|A\|_{\max} < 1$.

To query the entries of a matrix, one of the most convenient form is to encode the information of the matrix as the amplitude of a known vector, e.g.,

$$O_A|0\rangle|i\rangle|j\rangle = \left(A_{ij}|0\rangle + \sqrt{1-|A_{ij}|^2}|1\rangle\right)|i\rangle|j\rangle\,. \tag{9.68}$$

In other words, given $i, j \in [N]$, O_A performs a controlled rotation (controlling on i, j) on the ancilla qubit, which encodes the information in terms of amplitude of $|0\rangle$. We refer to Eq. (9.68) as the **amplitude oracle**.

Example 9.16 (Construction of amplitude oracle)**.** Assume $\|A\|_{\max} < 1$ and $A_{ij} \in \mathbb{R}$ for all i, j, and that we have access to a **bit oracle**

$$\widetilde{O}_A|0^{d'}\rangle|i\rangle|j\rangle = |\widetilde{A}_{ij}\rangle|i\rangle|j\rangle\,. \tag{9.69}$$

Here $\widetilde{A}_{ij}$ is a d'-bit fixed point representation of A_{ij}, and the value of $\widetilde{A}_{ij}$ is either computed on-the-fly with a quantum computer, or obtained through an external database using e.g., QRAM in Definition 5.6. Using the classical arithmetic operations (see Section 5.4), we can first convert this oracle into an oracle

$$O'_A|0^d\rangle|i\rangle|j\rangle = |\widetilde{\theta}_{ij}\rangle|i\rangle|j\rangle\,, \tag{9.70}$$

where $0 \le \widetilde{\theta}_{ij} < 1$, and $\widetilde{\theta}_{ij}$ is a d-bit representation of $\theta_{ij} = \arccos(A_{ij})/\pi$, and with some abuse of notation we redefine $\widetilde{A}_{ij} = \cos(\pi\widetilde{\theta}_{ij})$. This step may require some additional work registers not shown here.

Now using the controlled rotation in Proposition 5.7 and Fig. 5.3, the information of $\widetilde{\theta}_{ij}$ can now be transferred to the amplitude of the ancilla qubit. We should then perform uncomputation and free the work register storing such intermediate information $\widetilde{\theta}_{ij}$. The procedure is as follows

$$\begin{aligned}
|0\rangle \underbrace{|0^d\rangle}_{\text{work register}} |i\rangle|j\rangle &\xrightarrow{I_1\otimes O'_A} |0\rangle|\widetilde{\theta}_{ij}\rangle|i\rangle|j\rangle \\
&\xrightarrow{\text{CR}} \left(\widetilde{A}_{ij}|0\rangle + \sqrt{1-\left|\widetilde{A}_{ij}\right|^2}|1\rangle\right)|\widetilde{\theta}_{ij}\rangle|i\rangle|j\rangle \\
&\xrightarrow{I_1\otimes(O'_A)^{-1}} \left(\widetilde{A}_{ij}|0\rangle + \sqrt{1-\left|\widetilde{A}_{ij}\right|^2}|1\rangle\right)|0^d\rangle|i\rangle|j\rangle
\end{aligned} \tag{9.71}$$

After the uncomputation, the d-bit working register can be discarded, and we obtain the desired amplitude oracle of the input matrix A. ◇

Exercise 9.4. Construct a query oracle O_A similar to that in Eq. (9.71), when $A_{ij} \in \mathbb{C}$ with $\|A\|_{\max} < 1$.

9.7. Block encoding of s-sparse matrices

Example 9.17 (Block encoding of a diagonal matrix)**.** As a special case, let us consider the block encoding of a diagonal matrix, which is also a 1-sparse matrix. Since the row and column indices are the same, we may simplify the oracle Eq. (9.68) into

$$O_A |0\rangle |i\rangle = \left(A_{ii} |0\rangle + \sqrt{1 - |A_{ii}|^2} |1\rangle \right) |i\rangle . \tag{9.72}$$

Let $U_A = O_A$. Direct calculation shows that for any $i, j \in [N]$,

$$\langle 0| \langle i| U_A |0\rangle |j\rangle = A_{ii} \delta_{ij}. \tag{9.73}$$

This proves that $U_A \in \mathrm{BE}_{1,1}(A)$, i.e., U_A is a $(1,1)$-block-encoding of the diagonal matrix A. ◇

Example 9.18 (General 1-sparse matrices)**.** In a 1-sparse matrices, there is only one nonzero entry in each row and each column of the matrix. This means that for each $j \in [N]$, there is a unique $c(j) \in [N]$ such that $A_{c(j),j} \neq 0$, and the mapping c is a permutation. Assume that there exists a unitary O_c satisfying that

$$O_c |j\rangle = |c(j)\rangle , \quad O_c^\dagger |c(j)\rangle = |j\rangle . \tag{9.74}$$

The implementation of O_c may require the usage of some work registers that are omitted here.

We assume the matrix entry $A_{c(j),j}$ can be queried via

$$O_A |0\rangle |j\rangle = \left(A_{c(j),j} |0\rangle + \sqrt{1 - \left|A_{c(j),j}\right|^2} |1\rangle \right) |j\rangle . \tag{9.75}$$

Now we construct $U_A = (I \otimes O_c) O_A$, and compute the matrix element

$$\langle 0| \langle i| U_A |0\rangle |j\rangle = \langle 0| \langle i| \left(A_{c(j),j} |0\rangle + \sqrt{1 - \left|A_{c(j),j}\right|^2} |1\rangle \right) |c(j)\rangle = A_{c(j),j} \delta_{i,c(j)}. \tag{9.76}$$

This proves that $U_A \in \mathrm{BE}_{1,1}(A)$. ◇

For a general s-sparse matrix, we have $\|A\| \leq s \|A\|_{\max}$ according to Lemma 2.46, and the explicit construction of a block encoding below requires us to choose the subnormalization factor to be $\alpha = s \|A\|_{\max}$. Without loss of generality, we may assume each row and each column has exactly s designated entries by padding with zeros. For simplicity, let $s = 2^{\mathfrak{s}}$. Also we assume $\|A\|_{\max} = 1$ and will set $\alpha = s$.

Let us consider the construction of a block encoding for an s-sparse matrix by decomposing A into a sum of 1-sparse matrices. View the sparsity pattern of A as a bipartite graph with left vertices labeled by row indices and right vertices labeled by column indices, where an edge (i, j) is present if $A_{ij} \neq 0$. After padding with zero entries so that each row and each column has exactly s incident edges, the resulting bipartite graph is s-regular. By König's line-coloring theorem (see e.g., [Die25, Proposition 5.3.1]), the edges of an s-regular bipartite graph can be decomposed into s disjoint perfect matchings. Fix such a decomposition and index the matchings by $\ell \in [s]$. For each ℓ and each column j, let $c(j, \ell)$ denote the unique row index matched to j in the ℓ-th matching. Then, for each fixed ℓ, the mapping $j \mapsto c(j, \ell)$ is a permutation of $[N]$.

For each $\ell \in [s]$, define $A^{(\ell)}$ by setting $A^{(\ell)}_{c(j,\ell),j} = A_{c(j,\ell),j}$ and all other entries of $A^{(\ell)}$ to zero. Then each $A^{(\ell)}$ is 1-sparse, and

$$A = \sum_{\ell \in [s]} A^{(\ell)}. \tag{9.77}$$

According to Example 9.18, we may access each permutation $j \mapsto c(j,\ell)$ via a unitary oracle. Packaging all ℓ together, we assume access to a unitary O_c such that

$$O_c \left|\ell\right\rangle \left|j\right\rangle = \left|\ell\right\rangle \left|c(j,\ell)\right\rangle. \tag{9.78}$$

Similarly, we assume that the normalized matrix entries can be queried via

$$O_A \left|0\right\rangle \left|\ell\right\rangle \left|j\right\rangle = \left(A_{c(j,\ell),j} \left|0\right\rangle + \sqrt{1 - \left|A_{c(j,\ell),j}\right|^2} \left|1\right\rangle \right) \left|\ell\right\rangle \left|j\right\rangle. \tag{9.79}$$

We then define $D = \mathrm{H}^{\otimes \mathfrak{s}}$ (the $\mathfrak{s}$-qubit Hadamard transform) satisfying

$$D \left|0^{\mathfrak{s}}\right\rangle = \frac{1}{\sqrt{s}} \sum_{\ell \in [s]} \left|\ell\right\rangle. \tag{9.80}$$

With these ingredients, the circuit in Fig. 9.7 can be interpreted as an LCU-type construction over $\{A^{(\ell)}\}_{\ell \in [s]}$, yielding a block encoding with subnormalization factor $\alpha = s$.

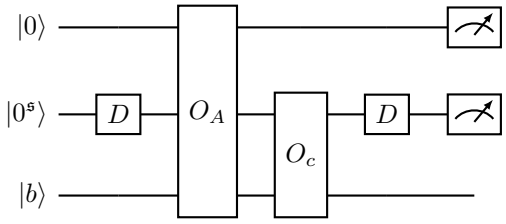


FIGURE 9.7. Quantum circuit for block encoding a s-sparse matrix using linear combination of unitaries. The measurement means that to obtain a state $\propto A\left|b\right\rangle$, the ancilla register should all return the value 0.

We now show that the circuit in Fig. 9.7 defines a unitary $U_A \in \mathrm{BE}_{s,\mathfrak{s}+1}(A)$ by direct calculation.

Proposition 9.19. *The circuit in Fig. 9.7 defines* $U_A \in \mathrm{BE}_{s,\mathfrak{s}+1}(A)$.

PROOF. We may write

$$U_A = (I \otimes D \otimes I)(I \otimes O_c) O_A (I \otimes D \otimes I). \tag{9.81}$$

In order to compute the inner product $\langle 0|\langle 0^{\mathfrak{s}}|\langle i|U_A|0\rangle|0^{\mathfrak{s}}\rangle|j\rangle$, we apply D, O_A, O_c to $|0\rangle|0^{\mathfrak{s}}\rangle|j\rangle$ successively as

$$\begin{aligned}
|0\rangle|0^{\mathfrak{s}}\rangle|j\rangle &\xrightarrow{D} \frac{1}{\sqrt{s}}\sum_{\ell\in[s]}|0\rangle|\ell\rangle|j\rangle \\
&\xrightarrow{O_A} \frac{1}{\sqrt{s}}\sum_{\ell\in[s]}\left(A_{c(j,\ell),j}|0\rangle + \sqrt{1-\left|A_{c(j,\ell),j}\right|^2}|1\rangle\right)|\ell\rangle|j\rangle \\
&\xrightarrow{O_c} \frac{1}{\sqrt{s}}\sum_{\ell\in[s]}\left(A_{c(j,\ell),j}|0\rangle + \sqrt{1-\left|A_{c(j,\ell),j}\right|^2}|1\rangle\right)|\ell\rangle|c(j,\ell)\rangle\,.
\end{aligned} \tag{9.82}$$

Instead of multiplying the leftmost factor $I\otimes D\otimes I$ to the last line, we apply it to $|0\rangle|0^{\mathfrak{s}}\rangle|i\rangle$ first to obtain (note that D is Hermitian)

$$|0\rangle|0^{\mathfrak{s}}\rangle|i\rangle \xrightarrow{D} \frac{1}{\sqrt{s}}\sum_{\ell'\in[s]}|0\rangle|\ell'\rangle|i\rangle\,. \tag{9.83}$$

Finally, taking the inner product yields

$$\langle 0|\langle 0^{\mathfrak{s}}|\langle i|U_A|0\rangle|0^{\mathfrak{s}}\rangle|j\rangle = \frac{1}{s}\sum_{\ell}A_{c(j,\ell),j}\delta_{i,c(j,\ell)} = \frac{1}{s}A_{ij}. \tag{9.84}$$

□

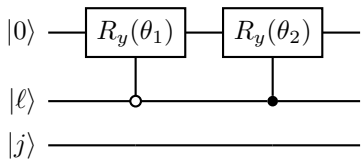
Example 9.20. Let us use the circuit in Fig. 9.7 to construct a block encoding of

$$A = \begin{bmatrix}\alpha_1 & \alpha_2\\ \alpha_2 & \alpha_1\end{bmatrix}, \quad 0\le\alpha_i\le 1, \quad i=1,2. \tag{9.85}$$

This matrix satisfies $\|A\|_{\max} = 1$, and can be viewed as a 2-sparse matrix. We can simply use CNOT as the O_c circuit by examining the truth table

ℓ	j		ℓ	$c(j,\ell)$
0	0		0	0
0	1	$\to$	0	1
1	0		1	1
1	1		1	0

Meanwhile O_A can be implemented using controlled $R_y(\theta_i), \theta_i = 2\arccos(\alpha_i), i=1,2$.



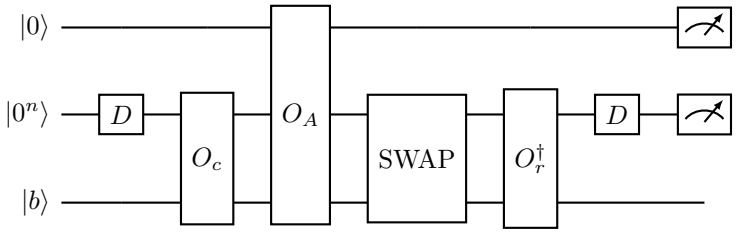


FIGURE 9.8. Quantum circuit for block encoding of general sparse matrices. The measurement means that to obtain a state $\propto A|b\rangle$, the ancilla register should all return the value 0.

For example, when $\alpha_1 = 1, \alpha_2 = 0.5$, The resulting matrix is

$$U_A = \begin{pmatrix} 0.500 & 0.250 & 0.500 & -0.250 & 0.0 & -0.433 & 0.0 & 0.433 \\ 0.250 & 0.500 & -0.250 & 0.500 & -0.433 & 0.0 & 0.433 & 0.0 \\ 0.500 & -0.250 & 0.500 & 0.250 & 0.0 & 0.433 & 0.0 & -0.433 \\ -0.250 & 0.500 & 0.250 & 0.500 & 0.433 & 0.0 & -0.433 & 0.0 \\ 0.0 & 0.433 & 0.0 & -0.433 & 0.500 & 0.250 & 0.500 & -0.250 \\ 0.433 & 0.0 & -0.433 & 0.0 & 0.250 & 0.500 & -0.250 & 0.500 \\ 0.0 & -0.433 & 0.0 & 0.433 & 0.500 & -0.250 & 0.500 & 0.250 \\ -0.433 & 0.0 & 0.433 & 0.0 & -0.250 & 0.500 & 0.250 & 0.500 \end{pmatrix}. \tag{9.86}$$

This is a $(2,2)$-block-encoding of A. ◇

Example 9.21 (Banded matrix)**.** A banded matrix of bandwidth s can be defined to have the sparsity pattern

$$c(j,\ell) = j + \ell - \ell_0 \pmod N, \tag{9.87}$$

for some shift $\ell_0 \in \mathbb{Z}$. The O_c circuit in Eq. (9.78) can be constructed using an adder circuit to perform the addition operation. ◇

Let us consider a different input model to construct the block encoding of a general s-sparse matrices. We assume access to the following two $(2n)$-qubit oracles

$$\begin{aligned} O_r|\ell\rangle|i\rangle &= |r(i,\ell)\rangle|i\rangle, \\ O_c|\ell\rangle|j\rangle &= |c(j,\ell)\rangle|j\rangle. \end{aligned} \tag{9.88}$$

Here $r(i,\ell), c(j,\ell)$ gives the ℓ-th nonzero entry in the i-th row and j-th column, respectively. It should be noted that although the index $\ell \in [s]$, we should expand it into an n-qubit state (e.g. let ℓ take the last $\mathfrak{s}$ qubits of the n-qubit register following the binary representation of integers).

We assume that the matrix entries are queried using the following oracle using controlled rotations

$$O_A|0\rangle|i\rangle|j\rangle = \left(A_{ij}|0\rangle + \sqrt{1-|A_{ij}|^2}|1\rangle\right)|i\rangle|j\rangle, \tag{9.89}$$

where the rotation is controlled by both row and column indices. However, if $A_{ij} = 0$ for some i, j, the rotation can be arbitrary, as there will be no contribution due to the usage of O_r, O_c.

Proposition 9.22. *Fig. 9.8 defines* $U_A \in \mathrm{BE}_{s,n+1}(A)$.

PROOF. We apply the first four gate sets to the source state

$$\begin{aligned} &|0\rangle |0^n\rangle |j\rangle \\ \xrightarrow{D,O_c,O_A} &\frac{1}{\sqrt{s}} \sum_{\ell\in[s]} \left(A_{c(j,\ell),j} |0\rangle + \sqrt{1-\left|A_{c(j,\ell),j}\right|^2} |1\rangle \right) |c(j,\ell)\rangle |j\rangle \\ \xrightarrow{\text{SWAP}} &\frac{1}{\sqrt{s}} \sum_{\ell\in[s]} \left(A_{c(j,\ell),j} |0\rangle + \sqrt{1-\left|A_{c(j,\ell),j}\right|^2} |1\rangle \right) |j\rangle |c(j,\ell)\rangle . \end{aligned} \tag{9.90}$$

We then apply D and O_r to the target state

$$|0\rangle |0^n\rangle |i\rangle \xrightarrow{D,O_r} \frac{1}{\sqrt{s}} \sum_{\ell'\in[s]} |0\rangle |r(i,\ell')\rangle |i\rangle . \tag{9.91}$$

Then the inner product gives

$$\begin{aligned} \langle 0| \langle 0^n| \langle i| U_A |0\rangle |0^n\rangle |j\rangle =& \frac{1}{s} \sum_{\ell,\ell'} A_{c(j,\ell),j} \delta_{i,c(j,\ell)} \delta_{r(i,\ell'),j} \\ =& \frac{1}{s} \sum_{\ell} A_{c(j,\ell),j} \delta_{i,c(j,\ell)} = \frac{1}{s} A_{ij}. \end{aligned} \tag{9.92}$$

If $A_{ij} \neq 0$, then there exists a unique ℓ such that $i = c(j,\ell)$ and a unique ℓ' such that $j = r(i,\ell')$; if $A_{ij} = 0$, then the same computation gives $\langle 0| \langle 0^n| \langle i| U_A |0\rangle |0^n\rangle |j\rangle = 0$. □

9.8. Hermitian block encoding

So far we have considered general s-sparse matrices. Note that if A is a Hermitian matrix, its (α, m, ϵ)-block-encoding U_A does not need to be Hermitian. Even if $\epsilon = 0$, we only have that the upper-left n-qubit block of U_A is Hermitian. For instance, even the block encoding of a Hermitian, diagonal matrix in Example 9.17 may not be Hermitian. On the other hand, there are cases when $U_A = U_A^\dagger$ is a Hermitian matrix, and hence the definition:

Definition 9.23 (Hermitian block encoding)**.** *Let U_A be an (α, m, ϵ)-block-encoding of A. If U_A is also Hermitian, then it is called an (α, m, ϵ)-Hermitian-block-encoding of A. When $\epsilon = 0$, it is called an (α, m)-Hermitian-block-encoding. The set of all (α, m, ϵ)-Hermitian-block-encodings of A is denoted by $\mathrm{HBE}_{\alpha,m}(A, \epsilon)$, and we define $\mathrm{HBE}_{\alpha,m}(A) = \mathrm{HBE}_{\alpha,m}(A, 0)$.*

The Hermitian block encoding provides the simplest scenario of the qubitization process in Section 10.2.1.

Next we consider the Hermitian block encoding of an s-sparse Hermitian matrix. Since A is Hermitian, we only need one oracle to query the location of the nonzero entries

$$O_c |\ell\rangle |j\rangle = |c(j,\ell)\rangle |j\rangle . \tag{9.93}$$

Here $c(j,\ell)$ gives the ℓ-th nonzero entry in the j-th column. It can also be interpreted as the ℓ-th nonzero entry in the j-th row. Again the first register needs to be interpreted as an n-qubit register. The operator D is the same as in **??**.

Unlike all discussions before, we introduce two control qubits, and a quantum state in the computational basis takes the form $|a\rangle |i\rangle |b\rangle |j\rangle$, where $a, b \in \{0,1\}, i, j \in [N]$. In other words, we

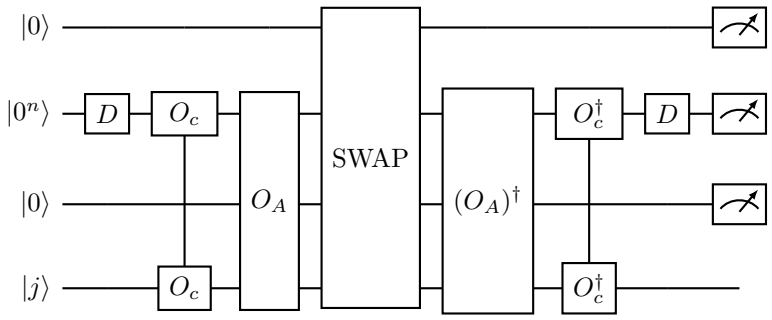


FIGURE 9.9. Quantum circuit for Hermitian block encoding of a general Hermitian matrix

may view $|a\rangle|i\rangle$ as the first register, and $|b\rangle|j\rangle$ as the second register. The $(n+1)$-qubit SWAP gate is defined as

$$\mathrm{SWAP}\,|a\rangle|i\rangle|b\rangle|j\rangle = |b\rangle|j\rangle|a\rangle|i\rangle\,. \tag{9.94}$$

To query matrix entries, we need access to the square root of A_{ij} as (note that act on the second single-qubit register)

$$O_A\,|i\rangle|0\rangle|j\rangle = |i\rangle\left(\sqrt{A_{ij}}\,|0\rangle + \sqrt{1-|A_{ij}|}\,|1\rangle\right)|j\rangle\,. \tag{9.95}$$

Throughout we assume $\|A\|_{\max} \le 1$, so that the right-hand side is normalized. The square root operation is well defined if $A_{ij} \ge 0$ for all entries. If A has negative (or complex) entries, we first write $A_{ij} = |A_{ij}|\,e^{i\theta_{ij}}, \theta_{ij} \in [0, 2\pi)$, and the square root is uniquely defined as $\sqrt{A_{ij}} = \sqrt{|A_{ij}|}e^{i\theta_{ij}/2}$.

Proposition 9.24. *Fig. 9.9 defines* $U_A \in \mathrm{HBE}_{s,n+2}(A)$.

PROOF. Apply the first four gate sets to the source state gives

$$\begin{aligned}
&|0\rangle|0^n\rangle|0\rangle|j\rangle \xrightarrow{D}\xrightarrow{O_c}\\
&\xrightarrow{O_A}\frac{1}{\sqrt{s}}\sum_{\ell\in[s]}|0\rangle|c(j,\ell)\rangle\left(\sqrt{A_{c(j,\ell),j}}\,|0\rangle + \sqrt{1-\left|A_{c(j,\ell),j}\right|}\,|1\rangle\right)|j\rangle\\
&\xrightarrow{\mathrm{SWAP}}\frac{1}{\sqrt{s}}\sum_{\ell\in[s]}\left(\sqrt{A_{c(j,\ell),j}}\,|0\rangle + \sqrt{1-\left|A_{c(j,\ell),j}\right|}\,|1\rangle\right)|j\rangle|0\rangle|c(j,\ell)\rangle
\end{aligned} \tag{9.96}$$

Apply the last three gate sets to the target state

$$\begin{aligned}
&|0\rangle|0^n\rangle|0\rangle|i\rangle \xrightarrow{D}\xrightarrow{O_c}\\
&\xrightarrow{O_A}\frac{1}{\sqrt{s}}\sum_{\ell'\in[s]}|0\rangle|c(i,\ell')\rangle\left(\sqrt{A_{c(i,\ell'),i}}\,|0\rangle + \sqrt{1-\left|A_{c(i,\ell'),i}\right|}\,|1\rangle\right)|i\rangle
\end{aligned} \tag{9.97}$$

Finally, take the inner product as

$$\begin{aligned}&\langle 0|\langle 0^n|\langle 0|\langle i|U_A|0\rangle|0^n\rangle|0\rangle|j\rangle\\ =&\frac{1}{s}\sum_{\ell,\ell'}\sqrt{A_{c(j,\ell),j}}\sqrt{A^*_{c(i,\ell'),i}}\delta_{i,c(j,\ell)}\delta_{c(i,\ell'),j}\\ =&\frac{1}{s}\sqrt{A_{ij}}\sqrt{A^*_{ji}}=\frac{1}{s}\big(\sqrt{A_{ij}}\big)^2=\frac{1}{s}A_{ij}.\end{aligned}\tag{9.98}$$

In this equality, we have used that A is Hermitian: $A_{ij}=A^*_{ji}$, and there exists a unique ℓ such that $i=c(j,\ell)$, as well as a unique ℓ' such that $j=c(i,\ell')$ when A_{ij} is nonzero. □

Exercise 9.5. Let $A\in\mathbb{C}^{N\times N}$ ($N=2^n$) be a Hermitian matrix with entries on the complex unit circle $A_{ij}=e^{i\theta_{ij}}$, $\theta_{ij}\in[0,2\pi)$, which can be accessed via a $2n$ qubit unitary $V\in\mathbb{C}^{N^2\times N^2}$ such that

$$V|0^n\rangle|j\rangle=\frac{1}{\sqrt{N}}\sum_{i\in[N]}e^{i\theta_{ij}/2}|i\rangle|j\rangle,\quad j\in[N].$$

Use V to implement a block encoding U of A with n ancilla qubits. What is the subnormalization factor α for this block encoding?

9.9. Block encoding beyond the computational basis

So far we have assumed that a matrix $A\in\mathbb{C}^{N\times N}$ is accessed through the upper left $N\times N$ block of a unitary $U_A\in\mathrm{U}(MN)$ in the computational basis with $M=2^m$, i.e., via the projector $\Pi_{0^m}:=|0^m\rangle\langle 0^m|\otimes I$ on m ancillas. However, the notion of block encoding is more general: one may encode a (possibly rectangular) matrix $A\in\mathbb{C}^{N'\times N}$ between two subspaces of the ambient space.

Choose an orthonormal basis of $\mathbb{C}^{MN}$ expressed in terms of the columns of a unitary $\Xi\in\mathrm{U}(MN)$ as

$$\mathcal{B}=\{|\varphi_0\rangle,\dots,|\varphi_{N-1}\rangle,|v_N\rangle,\dots,|v_{MN-1}\rangle\},\tag{9.99}$$

where the vectors $|\varphi_0\rangle,\dots,|\varphi_{N-1}\rangle$ are the first N columns of Ξ and span the range of a projector Π (equivalently, $\Pi=\sum_{j=0}^{N-1}|\varphi_j\rangle\langle\varphi_j|$). Similarly, choose another orthonormal basis of $\mathbb{C}^{MN}$ expressed in terms of the columns of another unitary $\Xi'\in\mathrm{U}(MN)$ as

$$\mathcal{B}'=\{|\psi_0\rangle,\dots,|\psi_{N'-1}\rangle,|w_{N'}\rangle,\dots,|w_{MN-1}\rangle\},\tag{9.100}$$

where the vectors $|\psi_0\rangle,\dots,|\psi_{N'-1}\rangle$ are the first N' columns of Ξ' and span the range of a projector Π' (equivalently, $\Pi'=\sum_{i=0}^{N'-1}|\psi_i\rangle\langle\psi_i|$). We naturally assume $N'\le MN$.

Now fix two projectors Π,Π' of rank N and N', where $\{|\varphi_j\rangle\}_{j\in[N]}$ is an orthonormal basis for range(Π), and $\{|\psi_i\rangle\}_{i\in[N']}$ is an orthonormal basis for range(Π'). Let $\mathscr{U}_A\in\mathrm{U}(MN)$ be a unitary with

$$\Pi'\mathscr{U}_A\Pi=\sum_{i\in[N'],\,j\in[N]}|\psi_i\rangle A_{ij}\langle\varphi_j|.\tag{9.101}$$

This is the same block-encoding idea as in the computational basis, except that the input and output subspaces are no longer required to be computational-basis subspaces.

To relate this formulation to the usual block matrix picture, set

$$U_A:=(\Xi')^\dagger\mathscr{U}_A\Xi.\tag{9.102}$$

Then U_A is the matrix representation of $\mathscr{U}_A$ with respect to the bases $\mathcal{B}, \mathcal{B}'$, and

$$[\mathscr{U}_A]_{\mathcal{B}}^{\mathcal{B}'} = U_A = \begin{pmatrix} A & * \\ * & * \end{pmatrix}. \tag{9.103}$$

The preceding discussion was exact. In applications we also allow a subnormalization factor and approximation error, as in Definition 9.2, but now relative to the chosen subspaces.

Definition 9.25. *Let $A \in \mathbb{C}^{N' \times N}$. Fix $\alpha, \epsilon \in \mathbb{R}_+$, and an ambient $(m+n)$-qubit space of dimension MN. Let Π, Π' be orthogonal projectors on $\mathbb{C}^{MN}$ with $\operatorname{rank}(\Pi) = N$ and $\operatorname{rank}(\Pi') = N'$. Choose unitaries $\Xi, \Xi' \in \mathrm{U}(MN)$ whose first N and N' columns form orthonormal bases for $\operatorname{range}(\Pi)$ and $\operatorname{range}(\Pi')$, respectively, as in Eqs. (9.99) and (9.100). Let $\Xi_N \in \mathbb{C}^{MN \times N}$ and $(\Xi')_{N'} \in \mathbb{C}^{MN \times N'}$ denote the matrices consisting of these first N and N' columns. Given a unitary $\mathscr{U}_A \in \mathrm{U}(MN)$, define the induced block*

$$\widetilde{A} := ((\Xi')_{N'})^\dagger \, \mathscr{U}_A \, \Xi_N \in \mathbb{C}^{N' \times N}. \tag{9.104}$$

We say that $\mathscr{U}_A$ is an (α, m, ϵ)-block-encoding of A with respect to (Π, Π') if

$$\left\| A - \alpha \widetilde{A} \right\| \leq \epsilon. \tag{9.105}$$

In the special case $\Pi = \Pi' = \Pi_{0^m}$ and $N' = N$, this reduces to the usual computational-basis definition.

Notes and further reading

The mathematical idea underlying block encodings is a form of unitary dilation: linear maps that are not themselves unitary can often be realized as a sub-block of a larger unitary acting on an extended space. In quantum information, this viewpoint is closely related to dilation theorems for completely positive maps. In quantum algorithms, the block-encoding terminology (together with explicit bookkeeping of the subnormalization factor and approximation error) was systematized as part of the modern polynomial-transformation framework; see [GSLW19].

The linear combination of unitaries (LCU) primitive used here originates in the Hamiltonian simulation algorithm [CW12, BCC$^+$14]. In particular, the sparse-matrix block-encoding constructions in this chapter are closely aligned with the query models developed for sparse Hamiltonian simulation (see, e.g., [BACS07]) and with the block-encoding-based linear-systems framework (see, e.g., [CKS17], which can be directly connected to the quantum circuit for Hermitian block encoding in Fig. 9.9). The connection between block encodings and quantum walks is mediated by the fact that many walk operators are themselves natural block encodings; see Szegedy's quantization of Markov chains [Sze04] for an early and influential formulation, which will be discussed in detail in Chapter 17. The RACBEM input model for pseudorandom nonunitary matrices was introduced in [DL21]. The quantum circuit in Fig. 9.8 is essentially the construction in [GSLW18, Lemma 48], which gives a $(s, n+3)$-block-encoding. The construction in Fig. 9.8 slightly simplifies the procedure and saves two extra qubits (used to mark whether $\ell \geq s$).

CHAPTER 10

Qubitization

Block encodings provide a unified interface for accessing matrices within quantum circuits, but simply iterating the encoding unitary is often insufficient to transform the underlying matrix. For example, if a block encoding U_A is Hermitian, its powers merely alternate between U_A and the identity. While this can be addressed by extending the block encoding to encode multiple powers of the matrix A, doing so requires breaking apart the abstraction of the block encoding and also requires adding additional qubits to address this issue. Qubitization addresses this limitation by constructing a unitary iterate whose action preserves two-dimensional subspaces associated with the eigenstructure of the encoded matrix. Within these subspaces, the iterate acts as a rotation, so that its powers implement Chebyshev polynomial transformations of the spectrum.

In this chapter, we progressively introduce the construction of qubitization, starting with Hermitian matrices encoded by Hermitian block encodings, then extending to general matrices. We demonstrate that the qubitization iterate naturally implements the singular value transformation using Chebyshev polynomials. We then show that the iterate can be interpreted using the cosine–sine decomposition in linear algebra. Finally, we discuss generalizing the concept of qubitization to apply beyond the computational basis.

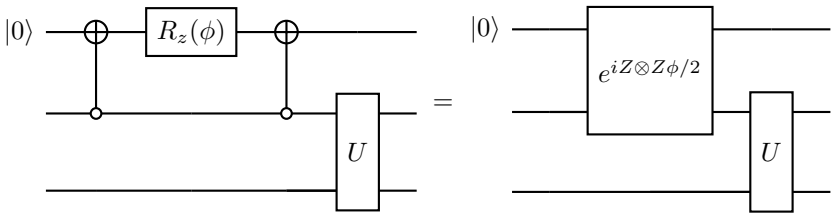
Qubitization was first proposed by Low and Chuang in [LC19] to improve on existing work by Childs [Chi10a]. This improvement led to the first quantum algorithm with optimal scaling with time and error tolerance. The core concepts behind qubitization, however, predate the invention of the name and now are viewed as a core design primitive for quantum algorithms that enables and simplifies spectral transformation for block encodings.

The logic behind qubitization is analogous to that used in Chapter 4 wherein we reduced the problem of performing a rotation in a two dimensional space to the problem of rotating a qubit. The logic behind qubitization is precisely the same: we entangle a system with a qubit space in order to manipulate the eigenvalues of the input. As an example of the logic behind qubitization, let us consider the following example. Let

$$U = \begin{bmatrix} Z & 0 \\ 0 & I \end{bmatrix} \tag{10.1}$$

which is nothing more than a zero-controlled Z gate controlled. We would like to transform the Z matrix contained in the first block. We can achieve this through the following circuit identities

(10.2)



If we trace over the top-most ancillary qubit, then we see that the circuit is equivalent to

$$\begin{bmatrix} -ie^{iZ(\phi/2+\pi/2)} & 0 \\ 0 & I \end{bmatrix} \tag{10.3}$$

This shows two interesting facts from this construction. First, by entangling the qubit space and the block encoding space we can apply single qubit rotations to affect the block encoding. Second, rotating the first qubit in this circuit serves to transform the eigenvalues of the block encoding. This is the core insight behind qubitization.

Our aim in this chapter is to build on this insight to generalize this insight to use rotations to manipulate the eigenvalues of generic block encoded matrices. This will not only directly lead to improved methods for simulation, as noted by Low and Chuang [LC19], but also will set the stage for our discussion of the quantum singular value transformation in Chapter 12 which is one of the most potent algorithmic design primitives yet discovered in quantum computing.

10.1. Eigenvalue transformations and singular value transformations

Consider a Hermitian matrix $A \in \mathbb{C}^{N\times N}$. Then A has the eigenvalue decomposition

$$A = V\Lambda V^\dagger. \tag{10.4}$$

Here $\Lambda = \mathrm{diag}(\{\lambda_i\})$ is a diagonal matrix, and $\lambda_0 \leq \cdots \leq \lambda_{N-1}$. Let the scalar function f be well defined on all λ_i's. We first recall the definition of matrix function restricted to Hermitian matrices.

Definition 10.1 (Matrix function of Hermitian matrices, or eigenvalue transformation)**.** *Let $A \in \mathbb{C}^{N\times N}$ be a Hermitian matrix with eigenvalue decomposition Eq.* (10.4)*. Let $f : \mathbb{R} \to \mathbb{C}$ be a scalar function such that $f(\lambda_i)$ is defined for all $i \in [N]$. The matrix function, or eigenvalue transformation of A is defined as*

$$f(A) := Vf(\Lambda)V^\dagger, \tag{10.5}$$

where

$$f(\Lambda) = \mathrm{diag}\left(f(\lambda_0), f(\lambda_1), \ldots, f(\lambda_{N-1})\right). \tag{10.6}$$

For any square matrix $A \in \mathbb{C}^{N\times N}$, the singular value decomposition (SVD) of A reads

$$A = W\Sigma V^\dagger, \tag{10.7}$$

or equivalently

$$A|v_i\rangle = \sigma_i |w_i\rangle, \quad A^\dagger |w_i\rangle = \sigma_i |v_i\rangle, \quad \sigma_i \geq 0, \quad i \in [N]. \tag{10.8}$$

The columns of W, V are called the left and right singular vectors of A, respectively. When A is given by its block encoding $U_A \in \mathrm{BE}_{1,m}(A)$, the singular values of A are in $[0, 1]$.

We may apply a function $f(\cdot)$ on its singular values and define generalized matrix functions below. Unlike matrix functions of Hermitian matrices, we can define three types of generalized matrix functions depending on how we choose the left and right singular vectors.

Definition 10.2 (Generalized matrix functions)**.** *Given $A \in \mathbb{C}^{N\times N}$ with singular value decomposition Eq.* (10.7)*, and let $f : \mathbb{R}_+ \to \mathbb{C}$ be a scalar function such that $f(\sigma_i)$ is defined for all $i \in [N]$. The* ***balanced generalized matrix function*** *is defined as*

$$f^\diamond(A) := Wf(\Sigma)V^\dagger, \tag{10.9}$$

where

$$f(\Sigma) = \mathrm{diag}\left(f(\sigma_0), f(\sigma_1), \ldots, f(\sigma_{N-1})\right). \tag{10.10}$$

*The **left generalized matrix function** and **right generalized matrix function** are defined in terms of the left and right singular vectors respectively as*

$$f^{\triangleleft}(A) := Wf(\Sigma)W^\dagger, \quad f^{\triangleright}(A) := Vf(\Sigma)V^\dagger. \tag{10.11}$$

Proposition 10.3. *The following relations hold:*

$$f^{\diamond}(A^\dagger) = (f^{\diamond}(A))^\dagger, \quad f^{\triangleright}(A) = f^{\triangleleft}(A^\dagger), \tag{10.12}$$

and

$$f^{\triangleright}(A) = f^{\diamond}(\sqrt{A^\dagger A}) = f(\sqrt{A^\dagger A}), \quad f^{\triangleleft}(A) = f^{\diamond}(\sqrt{AA^\dagger}) = f(\sqrt{AA^\dagger}). \tag{10.13}$$

Proof. Just note that $A^\dagger A = V\Sigma^2 V^\dagger$, we have $\sqrt{A^\dagger A} = V\Sigma V^\dagger$. So the eigenvalue and singular value decomposition coincide for both $\sqrt{A^\dagger A}$ and $\sqrt{AA^\dagger}$. □

For technical reasons that will become clear later, the definition of singular value transformation in quantum algorithms depends on the parity of f.

Definition 10.4 (Singular value transformation for functions with definite parity)**.** *Given $A \in \mathbb{C}^{N\times N}$ with singular value decomposition Eq. (10.7), let $f : \mathbb{R} \to \mathbb{C}$ be a scalar function such that $f(\pm\sigma_i)$ is defined for all $i \in [N]$. The **singular value transformation** of A is defined as*

$$f^{\mathrm{SV}}(A) = \begin{cases} f^{\diamond}(A), & f \text{ is odd}, \\ f^{\triangleright}(A), & f \text{ is even}. \end{cases} \tag{10.14}$$

We are often interested in a polynomial f. For a scalar x, the set of all real polynomials of finite degree forms the **real polynomial ring**, denoted by $\mathbb{R}[x]$. Similarly, the set of all complex polynomials of finite degree forms the **complex polynomial ring**, denoted by $\mathbb{C}[x]$.

When A is a Hermitian matrix and $A \succeq 0$, its eigenvalue decomposition and singular value decomposition coincide, so are its eigenvalue and singular value transformations of A.

When A is an indefinite Hermitian matrix, its eigenvalue decomposition is $A = VDV^\dagger$, and its singular value decomposition can be written as $A = W\Sigma V^\dagger$ with $W = V\,\mathrm{sign}(D), \Sigma = |D|$.

(1) If f is an odd function, then

$$f^{\mathrm{SV}}(A) = f^{\diamond}(A) = Wf(\Sigma)V^\dagger = Vf(\mathrm{sign}(D)\Sigma)V^\dagger = Vf(D)V^\dagger = f(A). \tag{10.15}$$

(2) If f is an even function, then

$$f^{\mathrm{SV}}(A) = f^{\triangleright}(A) = Vf(\Sigma)V^\dagger = Vf(D)V^\dagger = f(A). \tag{10.16}$$

Therefore as long as f has definite parity, the eigenvalue and singular value transformation of a Hermitian matrix A are the same.

For a general matrix $A \in \mathbb{C}^{N\times N}$, we can define a dilated Hermitian matrix using one ancilla qubit:

$$\widetilde{A} = \begin{bmatrix} 0 & A^\dagger \\ A & 0 \end{bmatrix}. \tag{10.17}$$

When A is given by its block encoding $U_A \in \mathrm{BE}_{1,m}(A)$, the dilated Hermitian matrix $\widetilde{A}$ can be obtained with one ancilla qubit through $U_{\widetilde{A}} = |0\rangle\langle 1| \otimes U_A^\dagger + |1\rangle\langle 0| \otimes U_A$, i.e., $U_{\widetilde{A}} \in \mathrm{BE}_{1,m}(\widetilde{A})$. Note that this requires the controlled version of $U_A, U_A^\dagger$.

From the SVD in Eq. (10.8), we can construct

$$|z_i^{\pm}\rangle = \frac{1}{\sqrt{2}}(|0\rangle\,|v_i\rangle \pm |1\rangle\,|w_i\rangle). \tag{10.18}$$

Direct calculation shows

$$\widetilde{A}\,|z_i^{\pm}\rangle = \pm\sigma_i\,|z_i^{\pm}\rangle\,, \tag{10.19}$$

i.e., $\{|z_i^{\pm}\rangle\}$ are all the eigenvectors of $\widetilde{A}$.

For an arbitrary polynomial $f \in \mathbb{C}[x]$, the matrix function $f(\widetilde{A})$ takes the form

$$\begin{aligned} f(\widetilde{A}) &= \sum_i |z_i^+\rangle\, f(\sigma_i)\, \langle z_i^+| + |z_i^-\rangle\, f(-\sigma_i)\, \langle z_i^-| \\ &= \sum_i \begin{pmatrix} |v_i\rangle\, f_{\rm even}(\sigma_i)\, \langle v_i| & |v_i\rangle\, f_{\rm odd}(\sigma_i)\, \langle w_i| \\ |w_i\rangle\, f_{\rm odd}(\sigma_i)\, \langle v_i| & |w_i\rangle\, f_{\rm even}(\sigma_i)\, \langle w_i| \end{pmatrix} \\ &= \begin{pmatrix} f_{\rm even}^{\triangleright}(A) & f_{\rm odd}^{\diamond}(A^\dagger) \\ f_{\rm odd}^{\diamond}(A) & f_{\rm even}^{\triangleleft}(A) \end{pmatrix}. \end{aligned} \tag{10.20}$$

Here

$$f_{\rm even}(x) = \frac{1}{2}(f(x) + f(-x)), \quad f_{\rm odd}(x) = \frac{1}{2}(f(x) - f(-x)). \tag{10.21}$$

Therefore applying the eigenvalue transformation of a dilated matrix $\widetilde{A}$ automatically implements singular value transformation of A using polynomials of even and odd parities.

In particular, if f is an even function, then

$$f(\widetilde{A})\,|0\rangle\,|\psi\rangle = |0\rangle\, f^{\triangleright}(A)\,|\psi\rangle\,. \tag{10.22}$$

In other words, by measuring the ancilla qubit we obtain 0 with certainty, and the state in the system register is $f_{\rm even}^{\triangleright}(A)\,|\psi\rangle$. Similarly, if f is odd, then

$$f(\widetilde{A})\,|0\rangle\,|\psi\rangle = |1\rangle\, f^{\diamond}(A)\,|\psi\rangle\,, \tag{10.23}$$

i.e., by measuring the ancilla qubit we obtain the output 1 with certainty.

In summary, when the function of interest is of definite parity, the singular value transformation and the eigenvalue transformation applied to a dilated Hermitian matrix are two sides of the same coin.

On the other hand, not all eigenvalue transformations can be expressed as singular value transformations. Consider the matrix power A^k as an example. Assume that A is a general non-Hermitian matrix that can be diagonalized as $A = VDV^{-1}$ and has the singular value decomposition $A = W\Sigma V^\dagger$. The matrix power is then given by $A^k = VD^kV^{-1}$. However, this expression cannot be directly written using the singular value decomposition. To see this, consider the case where $k = 2$. The squared matrix is $A^2 = (W\Sigma V^\dagger)(W\Sigma V^\dagger) = W\Sigma V^\dagger W\Sigma V^\dagger$. Here, the unitary matrix product $V^\dagger W$ does not generally have a simple expression, preventing a straightforward formulation of A^k in terms of singular values.

Many other matrix functions, such as matrix exponential e^A, matrix logarithm $\log A$ etc, cannot be expressed using singular value transformations either for general matrices. One notable exception is the matrix inverse: if A is invertible and $A = W\Sigma V^\dagger$, then $A^{-1} = V\Sigma^{-1}W^\dagger$. Since $f(x) = x^{-1}$ is odd, we find that $f^{\rm SV}(A^\dagger) = f^{\diamond}(A^\dagger) = A^{-1}$. Indeed, this will be the basis for using the quantum singular value transformation for computing matrix inverses.

10.2. Qubitization of Hermitian matrices and Chebyshev eigenvalue transformation

Let $A \in \mathbb{C}^{N\times N}$ be a Hermitian matrix with eigenvalue decomposition Eq. (10.4) with $\|A\| \leq 1$. The matrix Chebyshev polynomial $T_k(A)$ is a matrix function defined by the Chebyshev polynomial of the first kind:

$$T_k(x) = \cos(k \arccos(x)), \quad x \in [-1, 1], \quad k \in \mathbb{N}. \tag{10.24}$$

Qubitization provides an explicit quantum circuit to implement eigenvalue transformation with Chebyshev polynomials.

10.2.1. Qubitization of Hermitian matrices with Hermitian block encoding. We first introduce some heuristic idea behind qubitization. For any $-1 \leq \lambda \leq 1$, we can consider a 2×2 rotation matrix,

$$O(\lambda) = \begin{pmatrix} \lambda & -\sqrt{1-\lambda^2} \\ \sqrt{1-\lambda^2} & \lambda \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{10.25}$$

where we have performed the change of variable $\lambda = \cos\theta$ with $0 \leq \theta \leq \pi$.

Now direct computation shows

$$O^k(\lambda) = \begin{pmatrix} \cos(k\theta) & -\sin(k\theta) \\ \sin(k\theta) & \cos(k\theta) \end{pmatrix}. \tag{10.26}$$

Using the definition of Chebyshev polynomials (of first and second kinds, respectively)

$$T_k(\lambda) = \cos(k\theta) = \cos(k \arccos\lambda), \quad U_{k-1}(\lambda) = \frac{\sin(k\theta)}{\sin\theta} = \frac{\sin(k \arccos\lambda)}{\sqrt{1-\lambda^2}}, \tag{10.27}$$

we have

$$O^k(\lambda) = \begin{pmatrix} T_k(\lambda) & -\sqrt{1-\lambda^2}U_{k-1}(\lambda) \\ \sqrt{1-\lambda^2}U_{k-1}(\lambda) & T_k(\lambda) \end{pmatrix}. \tag{10.28}$$

Note that if we can somehow replace λ by A, we immediately obtain a $(1,1)$-block-encoding for the Chebyshev polynomial $T_k(A)$! This is precisely what qubitization aims at achieving, though there are some small twists.

In the simplest scenario, we assume that $U_A \in \mathrm{HBE}_{1,m}(A)$. Start from the spectral decomposition

$$A = \sum_i \lambda_i |v_i\rangle\langle v_i|, \tag{10.29}$$

we have that for each eigenstate $|v_i\rangle$ we can express the action of the unitary U_A as

$$U_A |0^m\rangle |v_i\rangle = |0^m\rangle A |v_i\rangle + |\widetilde{\perp}_i\rangle = \lambda_i |0^m\rangle |v_i\rangle + |\widetilde{\perp}_i\rangle . \tag{10.30}$$

Here $|\widetilde{\perp}_i\rangle$ is an unnormalized state that is orthogonal to all states of the form $|0^m\rangle |\psi\rangle$, i.e.,

$$\Pi|\widetilde{\perp}_i\rangle = 0. \tag{10.31}$$

where

$$\Pi = |0^m\rangle\langle 0^m| \otimes I \tag{10.32}$$

is a projection operator.

Since the right hand side of Eq. (10.30) is a normalized state, we may also write

$$|\widetilde{\perp}_i\rangle = \sqrt{1-\lambda_i^2}\, |\perp_i\rangle , \tag{10.33}$$

where $|\perp_i\rangle$ is a normalized state.

Now if $\lambda_i = \pm 1$, then $\mathcal{H}_i = \text{span}\{|0^m\rangle |v_i\rangle\}$ is already an invariant subspace of U_A, and $|\perp_i\rangle$ can be any state. Otherwise, use the fact that $U_A = U_A^\dagger$, we can apply U_A again to both sides of Eq. (10.30) and obtain

$$U_A |\perp_i\rangle = \sqrt{1-\lambda_i^2}\, |0^m\rangle |v_i\rangle - \lambda_i |\perp_i\rangle . \tag{10.34}$$

Therefore $\mathcal{H}_i = \text{span}\{|0^m\rangle |v_i\rangle , |\perp_i\rangle\}$ is an invariant subspace of U_A. Furthermore, the matrix representation of U_A with respect to the basis $\mathcal{B}_i = \{|0^m\rangle |v_i\rangle , |\perp_i\rangle\}$ is

$$[U_A]_{\mathcal{B}_i} = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix}, \tag{10.35}$$

i.e., U_A restricted to $\mathcal{H}_i$ is a reflection operator. This also leads to the name "qubitization", which means that each eigenvector $|v_i\rangle$ is "qubitized" into a two-dimensional space $\mathcal{H}_i$.

In order to construct a block encoding for $T_k(A)$, we need to turn U_A into a rotation. For this note that $\mathcal{H}_i$ is also an invariant subspace for the projection operator $\Pi = |0^m\rangle\langle 0^m|$:

$$[\Pi]_{\mathcal{B}_i} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{10.36}$$

Similarly define $Z_\Pi = 2\Pi - I$, since

$$[Z_\Pi]_{\mathcal{B}_i} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{10.37}$$

Z_Π acts as a reflection operator restricted to each subspace $\mathcal{H}_i$. Then $\mathcal{H}_i$ is an invariant subspace for the following matrix called the **iterate**

$$O = U_A Z_\Pi \tag{10.38}$$

and

$$[O]_{\mathcal{B}_i} = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix} \tag{10.39}$$

is the desired rotation matrix. Therefore

$$[O^k]_{\mathcal{B}_i} = [(U_A Z_\Pi)^k]_{\mathcal{B}_i} = \begin{pmatrix} T_k(\lambda_i) & -\sqrt{1-\lambda_i^2} U_{k-1}(\lambda_i) \\ \sqrt{1-\lambda_i^2} U_{k-1}(\lambda_i) & T_k(\lambda_i) \end{pmatrix}. \tag{10.40}$$

Since $\{|0^m\rangle |v_i\rangle\}$ spans the range of Π, we have

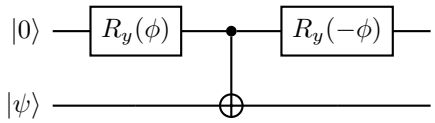
$$O^k = \begin{pmatrix} T_k(A) & * \\ * & * \end{pmatrix} \tag{10.41}$$

i.e., $O^k = (U_A Z_\Pi)^k$ is a $(1, m, 0)$-block-encoding of the Chebyshev polynomial $T_k(A)$.

Example 10.5. Recall the 2×2 Hermitian matrix in Example 9.1,

$$A = \frac{3}{4} I + \frac{1}{4} X = \begin{pmatrix} 0.75 & 0.25 \\ 0.25 & 0.75 \end{pmatrix}. \tag{10.42}$$

To illustrate the Hermitian-block-encoding setting of this subsection, we use the circuit from Example 9.1 with $\phi = \frac{\pi}{3}$:



This circuit implements the unitary

$$U_A = \begin{pmatrix} A & -\sqrt{I-A^2} \\ -\sqrt{I-A^2} & \frac{1}{4}I + \frac{3}{4}X \end{pmatrix} \in \mathrm{HBE}_{1,1}(A). \tag{10.43}$$

In this example,

$$\sqrt{I-A^2} = \frac{\sqrt{3}}{4}(I-X), \qquad I - 2A^2 = -\frac{1}{4}I - \frac{3}{4}X. \tag{10.44}$$

Since $m = 1$, we have $Z_\Pi = Z \otimes I$. The qubitization iterate is $O = U_A Z_\Pi$. Let us verify for $k = 2$. First,

$$O = U_A Z_\Pi = \begin{pmatrix} A & -\sqrt{I-A^2} \\ -\sqrt{I-A^2} & \frac{1}{4}I + \frac{3}{4}X \end{pmatrix} \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \begin{pmatrix} A & \sqrt{I-A^2} \\ -\sqrt{I-A^2} & -\frac{1}{4}I - \frac{3}{4}X \end{pmatrix}.$$

This particular matrix satisfies a number of identities such as $2A\sqrt{I-A^2} = \sqrt{I-A^2}$. Direct calculation shows

$$O^2 = \begin{pmatrix} 2A^2 - I & 2A\sqrt{I-A^2} \\ -2A\sqrt{I-A^2} & 2A^2 - I \end{pmatrix}.$$

The top-left block of O^2 is

$$T_2(A) = 2A^2 - I = \frac{1}{4}I + \frac{3}{4}X = \begin{pmatrix} 0.25 & 0.75 \\ 0.75 & 0.25 \end{pmatrix}.$$

$\diamond$

In order to implement Z_Π, note that if $m = 1$, then Z_Π is just the Pauli Z gate. When $m > 1$, the circuit in Fig. 10.1 maps $|1\rangle|b\rangle$ to $|1\rangle|b\rangle$ if $b = 0^m$, and to $-|1\rangle|b\rangle$ if $b \neq 0^m$. So this precisely implements Z_Π where the signal qubit $|1\rangle$ is used as a work register. We may also discard the signal qubit, and resulting unitary is denoted by Z_Π.

Therefore the circuit in Fig. 10.1 implements the operator O. Repeating the circuit k times gives a $(1, m)$-block-encoding of $T_k(A)$.

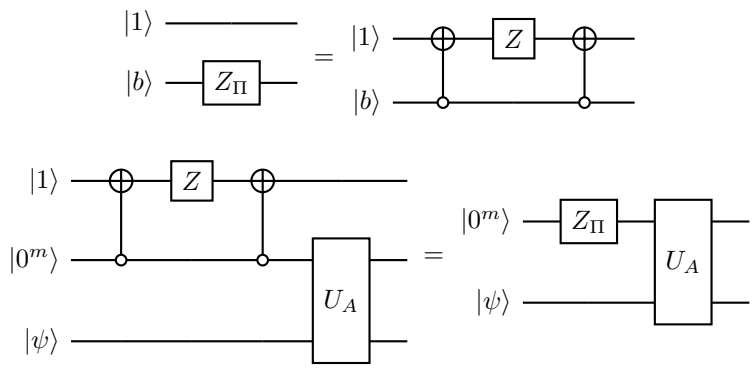


FIGURE 10.1. Circuit implementing one step of qubitization with a Hermitian block encoding of a Hermitian matrix. Here $U_A \in \mathrm{HBE}_{1,m}(A)$.

10.2.2. Qubitization of Hermitian matrices with general block encoding. In Section 10.2.1 we assume that $U_A = U_A^\dagger$ to block encode a Hermitian matrix A. For instance, s-sparse Hermitian matrices, such Hermitian block encodings can be constructed following the construction in Fig. 9.9. However, this can come at the expense of requiring additional structures and oracles. In general, the block encoding of a Hermitian matrix may not be Hermitian itself. In this section we demonstrate that the strategy of qubitization can be modified to accommodate general block encodings.

Again start from the eigendecomposition Eq. (10.29), we apply U_A to $|0^m\rangle|v_i\rangle$ and obtain

$$U_A|0^m\rangle|v_i\rangle = \lambda_i|0^m\rangle|v_i\rangle + \sqrt{1-\lambda_i^2}\,|\perp_i'\rangle, \tag{10.45}$$

where $|\perp_i'\rangle$ is a normalized state satisfying $\Pi|\perp_i'\rangle = 0$.

Since U_A block-encodes a Hermitian matrix A, we have

$$U_A^\dagger = \begin{pmatrix} A & * \\ * & * \end{pmatrix}, \tag{10.46}$$

which implies that there exists another normalized state $|\perp_i\rangle$ satisfying $\Pi|\perp_i\rangle = 0$ and

$$U_A^\dagger|0^m\rangle|v_i\rangle = \lambda_i|0^m\rangle|v_i\rangle + \sqrt{1-\lambda_i^2}\,|\perp_i\rangle. \tag{10.47}$$

Now apply U_A to both sides of Eq. (10.47), we obtain

$$|0^m\rangle|v_i\rangle = \lambda_i^2|0^m\rangle|v_i\rangle + \lambda_i\sqrt{1-\lambda_i^2}\,|\perp_i'\rangle + \sqrt{1-\lambda_i^2}U_A|\perp_i\rangle, \tag{10.48}$$

which gives

$$U_A|\perp_i\rangle = \sqrt{1-\lambda_i^2}\,|0^m\rangle|v_i\rangle - \lambda_i|\perp_i'\rangle. \tag{10.49}$$

Define

$$\mathcal{B}_i = \{|0^m\rangle|v_i\rangle, |\perp_i\rangle\}, \quad \mathcal{B}_i' = \{|0^m\rangle|v_i\rangle, |\perp_i'\rangle\}, \tag{10.50}$$

and the associated two-dimensional subspaces $\mathcal{H}_i = \operatorname{span}\mathcal{B}_i, \mathcal{H}_i' = \operatorname{span}\mathcal{B}_i'$, we find that U_A maps $\mathcal{H}_i$ to $\mathcal{H}_i'$. Correspondingly $U_A^\dagger$ maps $\mathcal{H}_i'$ to $\mathcal{H}_i$.

Then Eqs. (10.45) and (10.49) give the matrix representation

$$[U_A]^{\mathcal{B}_i'}_{\mathcal{B}_i} = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix}. \tag{10.51}$$

Similar calculation shows that

$$[U_A^\dagger]^{\mathcal{B}_i}_{\mathcal{B}_i'} = \begin{pmatrix} \lambda_i & \sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & -\lambda_i \end{pmatrix}. \tag{10.52}$$

Meanwhile both $\mathcal{H}_i$ and $\mathcal{H}_i'$ are the invariant subspaces of the projector Π, with matrix representation

$$[\Pi]_{\mathcal{B}_i} = [\Pi]_{\mathcal{B}_i'} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{10.53}$$

Therefore

$$[Z_\Pi]_{\mathcal{B}_i} = [Z_\Pi]_{\mathcal{B}_i'} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{10.54}$$

Hence $\mathcal{H}_i$ is an invariant subspace of $\widetilde{O} = U_A^\dagger Z_\Pi U_A Z_\Pi$, with matrix representation

$$[\widetilde{O}]_{\mathcal{B}_i} = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix}^2. \tag{10.55}$$

Repeating k times, we have

$$\begin{aligned} [\widetilde{O}^k]_{\mathcal{B}_i} =& (U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix}^{2k} \\ =& \begin{pmatrix} T_{2k}(\lambda_i) & -\sqrt{1-\lambda_i^2}U_{2k-1}(\lambda_i) \\ \sqrt{1-\lambda_i^2}U_{2k-1}(\lambda_i) & T_{2k}(\lambda_i) \end{pmatrix}. \end{aligned} \tag{10.56}$$

Since any vector $|0^m\rangle|\psi\rangle$ can be expanded in terms of the eigenvectors $|0^m\rangle|v_i\rangle$, we have

$$(U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \begin{pmatrix} T_{2k}(A) & * \\ * & * \end{pmatrix}. \tag{10.57}$$

Therefore if we would like to construct an **even** order Chebyshev polynomial $T_{2k}(A)$, the circuit $(U_A^\dagger Z_\Pi U_A Z_\Pi)^k$ straightforwardly gives a $(1,m)$-block-encoding.

In order to construct the block-encoding of an **odd** polynomial $T_{2k+1}(A)$, we note that

$$[U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k]^{\mathcal{B}_i'}_{\mathcal{B}_i} = \begin{pmatrix} T_{2k+1}(\lambda_i) & -\sqrt{1-\lambda_i^2}U_{2k}(\lambda_i) \\ \sqrt{1-\lambda_i^2}U_{2k}(\lambda_i) & T_{2k+1}(\lambda_i) \end{pmatrix}. \tag{10.58}$$

Using the fact that $\mathcal{B}_i, \mathcal{B}_i'$ share the common basis $|0^m\rangle|v_i\rangle$, we still have the block-encoding

$$U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \begin{pmatrix} T_{2k+1}(A) & * \\ * & * \end{pmatrix}. \tag{10.59}$$

Therefore $U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k$ is a $(1,m)$-block-encoding of $T_{2k+1}(A)$.

In summary, the block-encoding of $T_l(A)$ is given by applying $U_A Z_\Pi$ and $U_A^\dagger Z_\Pi$ alternately. If $l = 2k$, then there are exactly k such pairs. Otherwise if $l = 2k+1$, then there is an extra $U_A Z_\Pi$. The effect is to map each eigenvector $|0^m\rangle|v_i\rangle$ back and forth between the two-dimensional subspaces $\mathcal{H}_i$ and $\mathcal{H}_i'$. We summarize these results into the following proposition.

Proposition 10.6 (Chebyshev eigenvalue transformation)**.** *Let $A \in \mathbb{C}^{N\times N}$ be an n-qubit Hermitian matrix given by its block encoding $U_A \in \mathrm{BE}_{1,m}(A)$. Let $Z_\Pi = (2|0^m\rangle\langle 0^m| - I)\otimes I$. Then*

$$(U_A^\dagger Z_\Pi U_A Z_\Pi)^k \in \mathrm{BE}_{1,m}(T_{2k}(A)), \quad U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k \in \mathrm{BE}_{1,m}(T_{2k+1}(A)), \quad k \in \mathbb{N}. \tag{10.60}$$

10.3. Qubitization of general matrices and Chebyshev singular value transformation

In Section 10.2.2 we have observed that when A is a Hermitian matrix, the qubitization procedure introduces two different subspaces $\mathcal{H}_i$ and $\mathcal{H}_i'$ associated with each eigenvector $|v_i\rangle$. In particular, U_A maps $\mathcal{H}_i$ to $\mathcal{H}_i'$, and $U_A^\dagger$ maps $\mathcal{H}_i'$ to $\mathcal{H}_i$. Furthermore, both $\mathcal{H}_i$ and $\mathcal{H}_i'$ are the invariant subspaces of the projection operator Π. Therefore $\mathcal{H}_i$ is an invariant subspace of $U_A^\dagger f(\Pi) U_A$ for any function f.

For a general matrix A, the eigenvalues of A may not be on the real line. In fact, A may not be diagonalizable. Here we illustrate that the correct generalization for a general matrix A is singular value transformation defined as a generalized matrix function. The procedure below almost entirely parallels that of Section 10.2.2.

Starting from the SVD in Eq. (10.8), we apply U_A to $|0^m\rangle|v_i\rangle$ and obtain

$$U_A|0^m\rangle|v_i\rangle = \sigma_i|0^m\rangle|w_i\rangle + \sqrt{1-\sigma_i^2}\,|\perp_i'\rangle, \tag{10.61}$$

where $|\perp_i'\rangle$ is a normalized state satisfying $\Pi|\perp_i'\rangle = 0$.

Since U_A block encodes a matrix A, we have

$$U_A^\dagger = \begin{pmatrix} A^\dagger & * \\ * & * \end{pmatrix}, \tag{10.62}$$

which implies that there exists another normalized state $|\perp_i\rangle$ satisfying $\Pi|\perp_i\rangle = 0$ and

$$U_A^\dagger|0^m\rangle|w_i\rangle = \sigma_i|0^m\rangle|v_i\rangle + \sqrt{1-\sigma_i^2}\,|\perp_i\rangle. \tag{10.63}$$

Applying U_A to both sides of Eq. (10.63), we obtain

$$|0^m\rangle|w_i\rangle = \sigma_i^2|0^m\rangle|w_i\rangle + \sigma_i\sqrt{1-\sigma_i^2}\,|\perp_i'\rangle + \sqrt{1-\sigma_i^2}U_A|\perp_i\rangle, \tag{10.64}$$

which gives

$$U_A|\perp_i\rangle = \sqrt{1-\sigma_i^2}\,|0^m\rangle|w_i\rangle - \sigma_i|\perp_i'\rangle. \tag{10.65}$$

Define

$$\mathcal{B}_i = \{|0^m\rangle|v_i\rangle, |\perp_i\rangle\}, \quad \mathcal{B}_i' = \{|0^m\rangle|w_i\rangle, |\perp_i'\rangle\}, \tag{10.66}$$

and the associated two-dimensional subspaces $\mathcal{H}_i = \operatorname{span}\mathcal{B}_i, \mathcal{H}_i' = \operatorname{span}\mathcal{B}_i'$, we find that U_A maps $\mathcal{H}_i$ to $\mathcal{H}_i'$. Correspondingly $U_A^\dagger$ maps $\mathcal{H}_i'$ to $\mathcal{H}_i$.

Then Eqs. (10.61) and (10.65) give the matrix representation

$$[U_A]_{\mathcal{B}_i}^{\mathcal{B}_i'} = \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix}. \tag{10.67}$$

Similar calculation shows that

$$[U_A^\dagger]_{\mathcal{B}_i'}^{\mathcal{B}_i} = \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix}. \tag{10.68}$$

Meanwhile both $\mathcal{H}_i$ and $\mathcal{H}_i'$ are the invariant subspaces of the projector Π, with matrix representation

$$[\Pi]_{\mathcal{B}_i} = [\Pi]_{\mathcal{B}_i'} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{10.69}$$

Therefore

$$[Z_\Pi]_{\mathcal{B}_i} = [Z_\Pi]_{\mathcal{B}_i'} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{10.70}$$

Hence $\mathcal{H}_i$ is an invariant subspace of $\widetilde{O} = U_A^\dagger Z_\Pi U_A Z_\Pi$, with matrix representation

$$[\widetilde{O}]_{\mathcal{B}_i} = \begin{pmatrix} \sigma_i & -\sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & \sigma_i \end{pmatrix}^2. \tag{10.71}$$

The quantum circuit for each $\widetilde{O}$ is

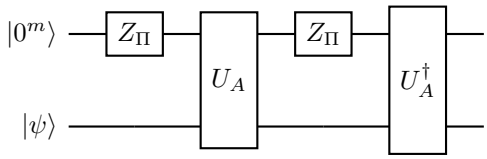


FIGURE 10.2. Circuit implementing one step of qubitization. This block encodes $T_2^{(SV)}(A)$. Here $U_A \in \mathrm{BE}_{1,m}(A)$. Note that the implementation of Z_Π requires a working qubit.

Repeating k times, we have

$$\begin{aligned} [\widetilde{O}^k]_{\mathcal{B}_i} =& (U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \begin{pmatrix} \sigma_i & -\sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & \sigma_i \end{pmatrix}^{2k} \\ =& \begin{pmatrix} T_{2k}(\sigma_i) & -\sqrt{1-\sigma_i^2} U_{2k-1}(\sigma_i) \\ \sqrt{1-\sigma_i^2} U_{2k-1}(\sigma_i) & T_{2k}(\sigma_i) \end{pmatrix}. \end{aligned} \tag{10.72}$$

In other words,

$$\widetilde{O}^k = \begin{pmatrix} \sum_i v_i T_{2k}(\sigma_i) v_i^\dagger & * \\ * & * \end{pmatrix} = \begin{pmatrix} T_{2k}^{\triangleright}(A) & * \\ * & * \end{pmatrix}. \tag{10.73}$$

Therefore, the circuit $(U_A^\dagger Z_\Pi U_A Z_\Pi)^k$ yields a $(1,m)$-block-encoding of $T_{2k}^{\triangleright}(A)$.

Similarly,

$$[U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k]_{\mathcal{B}_i}^{\mathcal{B}_i'} = \begin{pmatrix} T_{2k+1}(\sigma_i) & -\sqrt{1-\sigma_i^2} U_{2k}(\sigma_i) \\ \sqrt{1-\sigma_i^2} U_{2k}(\sigma_i) & T_{2k+1}(\sigma_i) \end{pmatrix}. \tag{10.74}$$

In other words,

$$U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \begin{pmatrix} \sum_i w_i T_{2k+1}(\sigma_i) v_i^\dagger & * \\ * & * \end{pmatrix} = \begin{pmatrix} T_{2k+1}^{\diamond}(A) & * \\ * & * \end{pmatrix}. \tag{10.75}$$

Therefore, the circuit $U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k$ yields a $(1,m)$-block-encoding of $T_{2k+1}^{\diamond}(A)$.

Proposition 10.7 (Chebyshev singular value transformation)**.** *Let $A \in \mathbb{C}^{N\times N}$ be an n-qubit Hermitian matrix given by its block encoding $U_A \in \mathrm{BE}_{1,m}(A)$. Let $Z_\Pi = (2|0^m\rangle\langle 0^m| - I_m)\otimes I_n$. Then*

$$(U_A^\dagger Z_\Pi U_A Z_\Pi)^k \in \mathrm{BE}_{1,m}(T_{2k}^{\mathrm{SV}}(A)), \quad U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k \in \mathrm{BE}_{1,m}(T_{2k+1}^{\mathrm{SV}}(A)), \quad k\in\mathbb{N}. \tag{10.76}$$

Example 10.8. Consider the 2×2 nilpotent matrix

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{10.77}$$

Its singular value decomposition $A = W\Sigma V^\dagger$ is given by

$$W = I, \quad \Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad V = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{10.78}$$

Note that $T_2^{\triangleright}(A) = VT_2(\Sigma)V^\dagger = X\,\mathrm{diag}(1,-1)X = \mathrm{diag}(-1,1)$.

A $(1,1)$-block-encoding of A can be constructed as

$$U_A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{10.79}$$

Here the basis order is $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. The qubitization iterate $\widetilde{O} = U_A^\dagger Z_\Pi U_A Z_\Pi$ can be computed directly. With $Z_\Pi = Z\otimes I = \mathrm{diag}(1,1,-1,-1)$, we have

$$\widetilde{O} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{10.80}$$

The top-left block is $\mathrm{diag}(-1,1)$, which matches $T_2^{\triangleright}(A)$. ◇

10.4. Cosine–sine decomposition and qubitization

The fact that an arbitrarily large block encoding matrix U_A can be partially block diagonalized into N subblocks of size 2×2 may seem a rather peculiar algebraic structure. In this section we use the **cosine–sine (CS) decomposition** to provide a unified perspective of qubitization. Qubitization stems from the fact that all involved transformations act on direct sums of irreducible two-dimensional subspaces. The CS decomposition makes this observation manifest and further provides a representation for the unitary where these rotations can be expressed as a block matrix wherein the sub-blocks play an analogous role to cosine and sine functions.

THEOREM 10.9 (Cosine–sine decomposition of a unitary matrix). *Let $q \geq p$ and $U \in \mathbb{C}^{(p+q)\times(p+q)}$ be any unitary matrix. There exists a decomposition*

$$U = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix} \begin{pmatrix} C & S & 0 \\ S & -C & 0 \\ 0 & 0 & I_{q-p} \end{pmatrix} \begin{pmatrix} V_1^\dagger & 0 \\ 0 & V_2^\dagger \end{pmatrix}. \tag{10.81}$$

Here, $W_1, V_1 \in \mathbb{C}^{p\times p}$, $W_2, V_2 \in \mathbb{C}^{q\times q}$ are unitary matrices and $C = \mathrm{diag}(c_1,\ldots,c_p)$, $S = \mathrm{diag}(s_1,\ldots,s_p)$ are real, non-negative diagonal matrices so that $C^2 + S^2 = I_p$.

PROOF. Let

$$U = \begin{pmatrix} U_{00} & U_{01} \\ U_{10} & U_{11} \end{pmatrix}, \tag{10.82}$$

where $U_{00} \in \mathbb{C}^{p\times p}$ and $U_{11} \in \mathbb{C}^{q\times q}$. The proof proceeds by considering singular value decompositions of each of the block matrices in the unitary. Using the SVD, U_{00} can be expressed for some unitary V_1 and $W_1^\dagger$ as

$$U_{00} = W_1 C V_1^\dagger. \tag{10.83}$$

As U_{00} is embedded in a unitary, we must have that its singular values C are in $[0, 1]$.

Next, consider the QR decomposition

$$U_{10} V_1 = W_2 R \tag{10.84}$$

for a unitary matrix $W_2 \in \mathbb{C}^{q\times q}$ and an upper triangular matrix $R \in \mathbb{C}^{q\times p}$ with non-negative diagonal elements. Using a similar argument we can see that there exists a unitary matrix $V_2 \in \mathbb{C}^{q\times q}$ and a lower triangular matrix $L \in \mathbb{C}^{p\times q}$ with non-negative diagonal elements such that

$$W_1^\dagger U_{01} = L V_2^\dagger. \tag{10.85}$$

This shows that we can write

$$U = \begin{pmatrix} W_1 & 0 \\ 0 & W_2 \end{pmatrix} \begin{pmatrix} C & L \\ R & W_2^\dagger U_{11} V_2 \end{pmatrix} \begin{pmatrix} V_1^\dagger & 0 \\ 0 & V_2^\dagger \end{pmatrix}. \tag{10.86}$$

Now let us argue about the structure of R, L. From the fact that the rows and columns of any unitary matrix must be orthonormal, and that R is upper triangular,

$$R = \begin{pmatrix} S \\ 0 \end{pmatrix}, \quad C^2 + S^2 = I_p. \tag{10.87}$$

By the same argument we have

$$L = \begin{pmatrix} S & 0 \end{pmatrix}, \quad C^2 + S^2 = I_p. \tag{10.88}$$

In other words, $R = L^\dagger$. Continuing the same reasoning,

$$W_2^\dagger U_{11} V_2 = \begin{pmatrix} -C & 0 \\ 0 & U_{22} \end{pmatrix}, \tag{10.89}$$

for some unitary U_{22}. If we absorb this unitary U_{22} into either W_2 or V_2, we obtain the desired factorization in Eq. (10.81). □

Given $U_A \in \mathrm{BE}_{1,m}(A)$ for an n-qubit matrix $A = W\Sigma V^\dagger$, Theorem 10.9 implies that there exists $W', V' \in \mathbb{C}^{N(M-1)\times N(M-1)}$ so that

$$U_A = \begin{pmatrix} W & 0 \\ 0 & W' \end{pmatrix} \begin{pmatrix} \Sigma & S & 0 \\ S & -\Sigma & 0 \\ 0 & 0 & I_{(M-2)N} \end{pmatrix} \begin{pmatrix} V^\dagger & 0 \\ 0 & V'^\dagger \end{pmatrix}. \tag{10.90}$$

Here, $S = \sqrt{I - \Sigma^2}$ is the supplementary diagonal matrix. For notation brevity, the large unitary matrices are denoted as

$$\widetilde{W} := \begin{pmatrix} W & 0 \\ 0 & W' \end{pmatrix}, \quad \widetilde{V} := \begin{pmatrix} V & 0 \\ 0 & V' \end{pmatrix}. \tag{10.91}$$

The matrix in the middle exhibits a special structure. Let $\mathscr{P}$ be a permutation matrix of size $2N \times 2N$ that permutes rows $\{0, 1 \ldots, N-1, N, \ldots, 2N-1\}$ to $\{0, N, 1, N+1, \ldots, N-1, 2N-1\}$. Then we may verify

$$\mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix} \mathscr{P}^\dagger = \begin{pmatrix} \Sigma & S \\ S & -\Sigma \end{pmatrix}. \tag{10.92}$$

In other words,

$$\begin{pmatrix} \Sigma & S & 0 \\ S & -\Sigma & 0 \\ 0 & 0 & I_{(M-2)N} \end{pmatrix} = \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix} \mathscr{P}^\dagger \right\} \bigoplus I_{(M-2)N} \tag{10.93}$$

is expressed as a direct sum of 2-by-2 blocks and an identity matrix. This is exactly the matrix representation used by qubitization as in Eq. (10.67).

THEOREM 10.10 (Qubitization from cosine–sine decomposition). *For any n-qubit matrix A encoded by $U_A \in \mathrm{BE}_{1,m}(A)$, there exists $(m+n)$-qubit unitary matrices $\widetilde{W}, \widetilde{V}$ and an $(n+1)$-qubit permutation matrix $\mathscr{P}$, such that*

$$U_A = \widetilde{W} \begin{pmatrix} \Sigma & S & 0 \\ S & -\Sigma & 0 \\ 0 & 0 & I_{(M-2)N} \end{pmatrix} \widetilde{V}^\dagger = \widetilde{W} \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix} \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{V}^\dagger, \tag{10.94}$$

and

$$U_A^\dagger = \widetilde{V} \begin{pmatrix} \Sigma & S & 0 \\ S & -\Sigma & 0 \\ 0 & 0 & I_{(M-2)N} \end{pmatrix} \widetilde{W}^\dagger = \widetilde{V} \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix} \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{W}^\dagger. \tag{10.95}$$

Following the same decomposition, Z_Π can be decomposed as

$$Z_\Pi = \left\{ \mathscr{P} \left(\bigoplus_{i\in[N]} Z \right) \mathscr{P}^\dagger \right\} \bigoplus (-I)_{(M-2)N}. \tag{10.96}$$

Thanks to the block diagonal structure, Z_Π commutes with $\widetilde{V}, \widetilde{W}$. So the definition of Z_Π does not explicitly refer to either $\widetilde{W}$ or $\widetilde{V}$. This would not be true if Z were replaced by Pauli X or Y matrices, and this is the key reason allowing us to choose a convenient phase matrix as in **??**. Also use the fact that $\mathscr{P}^\dagger \mathscr{P} = I$ for a permutation matrix, we have

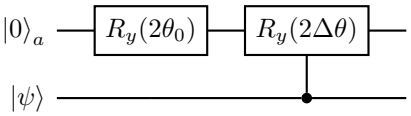
$$(U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \widetilde{V} \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} T_{2k}(\sigma_i) & -\sqrt{1-\sigma_i^2} U_{2k-1}(\sigma_i) \\ \sqrt{1-\sigma_i^2} U_{2k-1}(\sigma_i) & T_{2k}(\sigma_i) \end{pmatrix} \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{V}^\dagger. \tag{10.97}$$

Similarly

$$U_A Z_\Pi (U_A^\dagger Z_\Pi U_A Z_\Pi)^k = \widetilde{W} \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} T_{2k+1}(\sigma_i) & -\sqrt{1-\sigma_i^2} U_{2k}(\sigma_i) \\ \sqrt{1-\sigma_i^2} U_{2k}(\sigma_i) & T_{2k+1}(\sigma_i) \end{pmatrix} \mathscr{P}^\dagger \bigoplus (-I)_{(M-2)N} \right\} \widetilde{V}^\dagger. \tag{10.98}$$

This result shows that we can decompose an arbitrary unitary into a direct sum of cosine or sine matrices that, in effect, carry out two dimensional rotations.

Example 10.11. Consider a single-qubit Hermitian matrix $A = \mathrm{diag}(0.8, 0.6)$ encoded using one ancilla qubit ($m = 1$). The singular values are $\sigma_0 = 0.8$ and $\sigma_1 = 0.6$, which are distinct. The corresponding complementary values are $s_0 = \sqrt{1 - 0.8^2} = 0.6$ and $s_1 = \sqrt{1 - 0.6^2} = 0.8$. We can implement a block encoding U_A using a controlled rotation circuit on the ancilla, controlled by the system qubit:



where $\theta_0 = \arccos(0.8)$ and $\Delta\theta = \arccos(0.6) - \arccos(0.8)$. The unitary U_A takes the form

$$U_A = \begin{pmatrix} 0.8 & 0 & -0.6 & 0 \\ 0 & 0.6 & 0 & -0.8 \\ 0.6 & 0 & 0.8 & 0 \\ 0 & 0.8 & 0 & 0.6 \end{pmatrix}.$$

Here, the top-left block is precisely A. The qubitization iterate $O = U_A Z_\Pi$, with $Z_\Pi = Z \otimes I$, flips the sign of the columns where the ancilla is $|1\rangle$:

$$O = U_A(Z \otimes I) = \begin{pmatrix} 0.8 & 0 & 0.6 & 0 \\ 0 & 0.6 & 0 & 0.8 \\ 0.6 & 0 & -0.8 & 0 \\ 0 & 0.8 & 0 & -0.6 \end{pmatrix}.$$

Applying the permutation $\mathscr{P}$ that reorders the basis to group by system index $\{|0\rangle_a |0\rangle, |1\rangle_a |0\rangle, |0\rangle_a |1\rangle, |1\rangle_a |1\rangle\}$ yields a block diagonal matrix:

$$\mathscr{P} O \mathscr{P}^\dagger = \begin{pmatrix} 0.8 & 0.6 \\ 0.6 & -0.8 \end{pmatrix} \bigoplus \begin{pmatrix} 0.6 & 0.8 \\ 0.8 & -0.6 \end{pmatrix}.$$

Thus the 4×4 operator decouples into two independent 2×2 reflections, each acting on the subspace associated with a singular vector. ◇

10.5. Linear combination of unitaries and qubitization

Let $f \in \mathbb{R}[x]$ be a polynomial of definite parity. For simplicity, assume f is an even polynomial of degree $2(K-1)$ and set $K = 2^a$. Let us combine LCU and qubitization to construct the block encoding of:

$$f^{\mathrm{SV}}(A) = \sum_{k \in [K]} \alpha_k T_{2k}^{\mathrm{SV}}(A). \tag{10.99}$$

Here A is given by its block encoding $U_A \in \mathrm{BE}_{1,m}(A)$. Due to the connection between eigenvalue and singular value transformation in Section 10.1, when A is Hermitian this becomes an eigenvalue transformation $f(A)$.

Using qubitization (Proposition 10.7), we have constructed $U_{2k} \in \mathrm{BE}_{1,m}(T_{2k}^{\mathrm{SV}}(A))$. The select oracle is given by

$$U_{\mathrm{SEL}} := \sum_{k \in [K]} |k\rangle\langle k| \otimes U_{2k}. \tag{10.100}$$

The problem with a direct implementation of the select oracle via multi-qubit controls is that the complexity is very high. The circuit U_{2k} to block encode $T_{2k}^{\mathrm{SV}}(A)$ makes $2k$ queries to U_A. Therefore

the total number of queries to construct the select oracle is $\mathcal{O}(K^2)$. This is highly inefficient: the circuit blocks $\widetilde{O} = U_A^\dagger Z_\Pi U_A Z_\Pi$ in each U_{2k} are implemented independently and not reused.

An efficient implementation of the select oracle makes use of a binary representation $k = (k_a \cdots k_0)$. Then direct calculation shows that the circuit in Fig. 10.3 correctly implements U_{SEL}. The total number of queries to U_A is $2(1 + 2 + \cdots + 2^{a-1}) = 2^{a+1} - 2 = 2K - 2$. This is equal to the query complexity for block encoding a single term $T_{2K-2}(A)$.

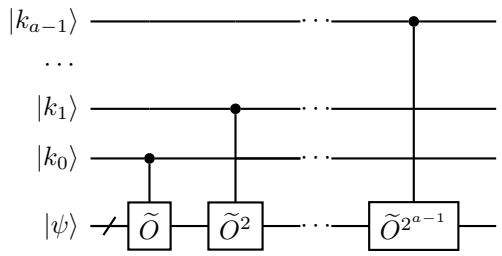


FIGURE 10.3. Circuit for select oracle for even matrix Chebyshev polynomials up to order $2^{a+1} - 2$. Here $\widetilde{O} = U_A^\dagger Z_\Pi U_A Z_\Pi$.

We also assume the availability of the prepare oracle

$$V_{\mathrm{PREP}} |0^a\rangle = \frac{1}{\|\beta\|_2} \sum_{k\in[K]} \beta_k |k\rangle, \quad \widetilde{V}_{\mathrm{PREP}} |0^a\rangle = \frac{1}{\|\gamma\|_2} \sum_{k\in[K]} \gamma_k |k\rangle \tag{10.101}$$

with β_i, γ_i described by Lemma 9.5. Then using LCU, we obtain a $(\|\alpha\|_1, m + a)$-block-encoding of $f^{\mathrm{SV}}(A)$. The gate complexity is

$$(2K - 2) \times \mathrm{gate}(U_A) + \mathrm{gate}(V_{\mathrm{PREP}}) + \mathrm{gate}(\widetilde{V}_{\mathrm{PREP}}). \tag{10.102}$$

Note that the gate complexity depends on the cost for the implementation of the prepare oracle, which may involve QRAM. The construction of the LCU for an odd polynomial is similar.

Exercise 10.1. Construct the circuit for efficient implementation of the select oracle

$$U = \sum_{k\in[K]} |k\rangle\langle k| \otimes U_{2k+1}. \tag{10.103}$$

THEOREM 10.12 (LCU based singular value transformation for polynomials of definite parity). *Let $A \in \mathbb{C}^{N\times N}$ be encoded by its $(1, m)$-block-encoding U_A. For a polynomial $f(x) \in \mathbb{C}[x]$ with degree d of parity $(d \mod 2)$*

$$f(x) = \sum_{k=0}^{d} \alpha_k T_k(x), \tag{10.104}$$

we can implement a $(\|\alpha\|_1, m + a)$-block encoding of the singular value transformation $f^{\mathrm{SV}}(A)$. It uses $a = \mathcal{O}(\log_2 d)$ additional ancilla qubits, and queries $U_A, U_A^\dagger$ for $\mathcal{O}(d)$ times.

If A is a Hermitian matrix, we may construct an eigenvalue transformation $f(A)$ for a general polynomial f. Note that

$$f_{\text{even}}(x) = \frac{1}{2}(f(x) + f(-x)), \quad f_{\text{odd}}(x) = \frac{1}{2}(f(x) - f(-x)), \tag{10.105}$$

we can implement a block encoding of $f_{\text{even}}(A)$ and $f_{\text{odd}}(A)$, respectively. Then we use one more ancilla qubit to implement a block encoding of $f_{\text{even}}(A) + f_{\text{odd}}(A) = f(A)$; this multiplies the subnormalization factor by 2.

10.6. Qubitization beyond the computational basis

Assume that $A \in \mathbb{C}^{N' \times N}$ is given via a subspace block-encoding as in Section 9.9 and Definition 9.25, i.e., by a unitary $\mathscr{U}_A \in \mathrm{U}(MN)$ and projectors Π, Π' with $\operatorname{rank}(\Pi) = N$ and $\operatorname{rank}(\Pi') = N'$. Define the associated reflections

$$Z_\Pi = 2\Pi - I, \qquad Z_{\Pi'} = 2\Pi' - I. \tag{10.106}$$

The qubitization iterate, defined as a product of reflections, is

$$\mathscr{U}_A^\dagger Z_{\Pi'} \mathscr{U}_A Z_\Pi. \tag{10.107}$$

When $N' = N$, this reduces to the usual qubitization iterate under a change of basis. When $N' \neq N$, the same iterate remains well defined and admits the same CS-decomposition-based analysis; this is the natural setting for QSVT with a basis change in Section 13.3.

Example 10.13. Let $m = n = 1$, so $M = N = 2$ and $MN = 4$, and take $\mathscr{U}_A = I \in \mathrm{U}(4)$. Fix

$$\Pi = |0\rangle\langle 0| \otimes I, \tag{10.108}$$

so that $Z_\Pi = 2\Pi - I = Z \otimes I$. Let $\theta \in (0, \pi/2)$ and define the real rotation

$$R(\theta) := \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \in \mathrm{U}(2). \tag{10.109}$$

Set $\Xi := I$ and $\Xi' := R(\theta) \otimes I$, and define $\Pi' := \Xi' \Pi (\Xi')^\dagger$. Then $Z_{\Pi'} = \Xi' Z_\Pi (\Xi')^\dagger$.

With respect to the bases $\{|00\rangle, |01\rangle\}$ for $\operatorname{range}(\Pi)$ and $\{\Xi'|00\rangle, \Xi'|01\rangle\}$ for $\operatorname{range}(\Pi')$, the encoded matrix is the overlap matrix

$$A_{ij} = \langle \psi_i | \varphi_j \rangle, \qquad |\varphi_j\rangle := |0j\rangle, \ |\psi_i\rangle := \Xi'|0i\rangle, \tag{10.110}$$

and a direct computation gives $A = \cos\theta\, I_2$.

The qubitization step (the product of reflections) is

$$\mathscr{U}_A^\dagger Z_{\Pi'} \mathscr{U}_A Z_\Pi = Z_{\Pi'} Z_\Pi = (R(\theta) Z R(\theta)^\dagger Z) \otimes I = R(2\theta) \otimes I. \tag{10.111}$$

Hence the iterate has eigenvalues $e^{\pm 2i\theta}$ (each with multiplicity 2), and the corresponding eigenphases $\pm 2\theta$ determine the singular value $\cos\theta$ of A. ◇

Notes and references

Background on generalized matrix functions can be found in [HBI73, ABF16], which correspond to the "balanced" generalized matrix function $f^\diamond(A)$, i.e., singular value transformation for odd functions.

The cosine–sine (CS) decomposition provides an algebraic explanation for the qubitization structure by making the underlying direct-sum decomposition into 2×2 blocks explicit; see [Don23, TT24]. The same two-dimensional reduction principle also appears as Jordan's lemma: the product

of two reflections acts as a rotation on an invariant two-dimensional subspace [Jor75], and this perspective is closely related to product decompositions in quantum signal processing [Haa19].

The viewpoint of block-encoding and qubitization beyond the computational basis connects directly to Grover's search algorithm, amplitude amplification, and Szegedy's quantum walk. The Chebyshev expansion combined with LCU already yields arbitrary polynomial singular value transformations (for functions of definite parity), but it uses an additional control register to implement the required linear combination with a logarithmic overhead. A more direct and elegant alternative is quantum signal processing and quantum singular value transformation, which implement polynomial transformations via a structured SU(2) recursion, with further connections to nonlinear Fourier analysis on SU(2) [AMT24, ALM$^+$26].

CHAPTER 11

Amplitude amplification based algorithms

Amplitude amplification is one of the most significant tools at the disposal of a quantum algorithm designer. The central idea behind these methods is that the amplitude (or probability) of a desired portion of a quantum state can be rotated between the success and failure branches of a quantum algorithm. Relative to statistical sampling, this quantum approach is fully unitary and requires quadratically fewer operations. This leads to quadratic advantages for sampling algorithms involving statistical sampling, such as Monte-Carlo integration, machine learning applications such as Boltzmann machine training and nearest neighbor classification. Further, any problem in NP can more generally be quadratically accelerated relative to a brute force classical approach and further much of our understanding of the limitations of quantum algorithms stems from amplitude amplification and in turn its earliest incarnation: the celebrated Grover search algorithm.

Grover's algorithm was one of the earliest quantum algorithms to demonstrate a provable speedup in the oracle model: while any classical strategy requires $\Theta(N)$ queries in the worst case, Grover succeeds with $\mathcal{O}(\sqrt{N})$ oracle queries. More importantly, its analysis isolates a mechanism that recurs throughout quantum algorithms: a small success probability can be encoded as an eigenphase of a two-dimensional rotation, and repeated two-reflection steps coherently drive that phase so that the success probability becomes bounded below by a constant. This abstraction leads to amplitude amplification, and further to oblivious amplitude amplification, where one reconstructs a target unitary using only a block encoding and reflections on ancillas, without access to the input state.

The common thread running through amplitude amplification algorithms (sometimes called Grover-type algorithms) in this chapter is that they admit an interpretation as Chebyshev polynomial transformations as seen in qubitization. In this viewpoint, iterating a fixed two-reflection unitary implements a Chebyshev polynomial on an underlying singular value, and "amplification" becomes the task of choosing a polynomial that maps the relevant parameter to ± 1. We also prove a matching lower bound that shows the limits of any such polynomial-based amplification strategy.

11.1. Unstructured search problem and Grover's algorithm

The simplest example of the amplitude amplification paradigm for algorithmic design is Grover's problem. This problem can be thought of as the following. Assume we have $N = 2^n$ boxes, and we are given the promise that only one of the boxes contains an orange, and each of the remaining boxes contains an apple. The goal is to find the box that contains the orange.

Mathematically, given a Boolean function $f : \{0,1\}^n \to \{0,1\}$ as either a bit oracle or a phase oracle and the promise that there exists a unique marked state x_0 such that $f(x_0) = 1$, we would like to find x_0. This is called an **unstructured search problem**. Classically, there is no simpler method than opening $(N-1)$ boxes in the worst case to determine x_0. This fact is demonstrated in the following proposition.

Proposition 11.1. *Let $f : \{0,1\}^n \to \{0,1\}$ be a function such that there exists a marked element x^* such that $f(x) = 1$ if and only if $x = x^*$. No unbiased classical algorithm exists that can identify x^* with probability greater than $1/2$ using fewer than $2^n - 1$ queries to f in the worst case scenario.*

PROOF. Let us assume, seeking a contradiction, that there exists an algorithm that can identify the marked element x^* using at most $2^n - 2$ queries in the worst case scenario. If the algorithm requires fewer than $2^n - 2$ queries then we can pad the list of queries that we make to size $2^n - 2$ as we know that because there is only one marked element any subsequent queries will have $f(x) = 0$ if x is not the marked element. Thus without loss of generality we can assume that precisely $2^n - 2$ queries are always used to find the marked element.

If our algorithm makes precisely $2^n - 2$ queries to identify the marked value of x^*. We can then denote the particular values used in the input to the oracle to be $x_1, \ldots, x_{2^n-2}$. This means that even if $x^* \notin \{x_1, \ldots, x_{2^n-2}\}$ then x^* must be uniquely identifiable by these values. There are two values of x not in the set of inputs and let us denote these as x^* and x'. As we are interested in an algorithm that can decide between these hypotheses in the worst case scenario, let us assume that the marked element happens to be one of these two values. Now we can see that if x' is the marked element then we would have that $f(x_1) = f(x_2) = \cdots = f(x_{2^n-2}) = 0$. Similarly, if x^* were the marked element then our evidence is exactly the same: $f(x_1) = f(x_2) = \cdots = f(x_{2^n-2}) = 0$. Thus if the algorithm returns an estimate $x = x^*$ with probability greater than $1/2$ then the estimator must be biased towards x^* because the evidence observed from both queries is equally likely from both possibilities. Thus by contradiction, the number of queries needed to identify x^* with probability greater than $1/2$ must be greater than or equal to $2^n - 1$. □

The above argument shows that it is not possible for a classical computer to solve the search problem, with high probability, using a number of queries to the boxes that is less than linear in the number of boxes for the search problem.

At first glance, it may seem that quantum algorithms may not be able to provide an advantage for the search problem due to the fact that each query made to the oracle in a classical setting provides nearly negligible information about the marked element. In fact, this was the intuition behind the pioneering work of Boyer et al [BBHT98] which initially sought to show that quantum computers cannot provide a substantial advantage for searching in terms of the queries made to V_f. This intuition though proved misleading. Their attempts to prove query lower bounds on the decision version of the search problem, wherein the user must decide if there are one or zero marked elements such that $f(x) = 1$, showed that at least $\Omega(\sqrt{2^n})$ queries to $f(x)$ are needed to identify the marked element. Any algorithm that can find the marked x, if it exists, can be used to determine if a marked element is present. Thus we can reduce from the decision search problem to see that $\Omega(\sqrt{2^n})$ queries are needed to identify the marked element as well (which can also be seen because the decision search problem is equivalent to computing the OR function of the bits held for $f(x)$ in the oracle, which requires $\Omega(\sqrt{N})$ queries from **??**). This opens up the possibility that a quadratic separation is possible.

Grover's algorithm settled any doubt about whether a quantum advantage exists for the search problem by revealing that $\mathcal{O}(\sqrt{N})$ queries are needed to find the marked element with high probability. This, combined with the aforementioned lower bound suggests that the optimal quantum scaling for search is $\Theta(\sqrt{2^n})$, which constitutes a quadratic advantage over the best possible classical algorithms. It uses the natural quantum generalization of the classical oracle for the marking function f, namely the unitary bit oracle

$$V_f |x, y\rangle = |x, y \oplus f(x)\rangle, \quad x \in \{0,1\}^n, y \in \{0,1\}, \tag{11.1}$$

Algorithm 11.1 Grover's Algorithm for the case of 1 marked element

Require: Oracle V_f marking solutions, search space size $N = 2^n$ and assume that there is precisely one marked element x^* such that $f(x^*) = 1$
Ensure: A solution x such that $f(x) = 1$ (with high probability)
1: Initialize $|\psi\rangle \leftarrow |0\rangle^{\otimes n} |1\rangle$
2: Apply Hadamard transform to each qubit: $|\psi\rangle \leftarrow \mathrm{H}^{\otimes n+1} |\psi\rangle = |+\rangle^{\otimes n} |-\rangle$
3: Set $\theta \leftarrow 2 \arcsin(1/\sqrt{N})$
4: **for** $k = 1$ to $\left\lfloor \frac{\pi}{2\theta} - \frac{1}{2} \right\rfloor$ **do**
5: Apply oracle: $|\psi\rangle \leftarrow V_f |\psi\rangle$
6: Apply diffusion operator: $|\psi\rangle \leftarrow ((2|\psi_0\rangle\langle\psi_0| - I) \otimes I) |\psi\rangle$
7: **end for**
8: Measure $|\psi\rangle$ to obtain x
9: **return** x

Grover's algorithm, given in Algorithm 11.1, converts this bit oracle into a phase oracle by phase kickback and then repeatedly applies a pair of reflections. This can find x^* using $\mathcal{O}(\sqrt{N})$ queries.

The origin of the quadratic speedup can be summarized as follows: while classical probabilistic algorithms work with probability densities, quantum algorithms work with wavefunction amplitudes, of which the square gives the probability densities. This means that a rotation through an angle θ in Hilbert space will lead to a growth in probability of $\mathcal{O}(\theta^2)$ in probability. This allows us to attain, through Born's rule, a quadratic advantage over classical computing. The following claim can be made specifically about Grover's algorithm.

THEOREM 11.2 (Quantum search). *Assume $f : \{0,1\}^n \mapsto \{0,1\}$ is a Boolean function such that there exists a unique $x^* \in \{0,1\}^n$ such that $f(x^*) = 1$. Then Algorithm 11.1 uses $\mathcal{O}(\sqrt{N})$ queries to V_f and returns x^* with probability at least $1 - 4/N$. Consequently, by combining Grover's algorithm with classical verification, one obtains success probability greater than $2/3$ using $\mathcal{O}(\sqrt{N})$ queries.*

PROOF. The algorithm starts from a uniform superposition of all states as the initial state

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{x \in [N]} |x\rangle . \tag{11.2}$$

This state can be prepared using Hadamard gates as

$$|\psi_0\rangle = \mathrm{H}^{\otimes n} |0^n\rangle . \tag{11.3}$$

Let $x_0 = x^*$ denote the unique marked string. We would like to **amplify** the desired amplitude corresponding to $|x_0\rangle$ from $1/\sqrt{N}$ to $\sqrt{p} = \Omega(1)$.

The first step of Grover's algorithm is to turn the bit oracle given in Eqn. (11.1) into a phase oracle that returns a phase of -1 for each marked element. The simplest way to achieve this is to use the fact that $X |-\rangle = - |-\rangle$ to see that a bit oracle with output on $|-\rangle$ will provide a sign flip, which is precisely the choice made in the second step of Algorithm 11.1. More specifically, note that for any $x \in \{0,1\}^n$,

$$V_f |x, -\rangle = \frac{1}{\sqrt{2}} (|x, f(x)\rangle - |x, 1 \oplus f(x)\rangle) = (-1)^{f(x)} |x, -\rangle . \tag{11.4}$$

Any quantum state $|\psi\rangle$ can be decomposed as

$$|\psi\rangle = \alpha\,|x_0\rangle + \beta\,|\varphi\rangle\,, \tag{11.5}$$

where $|\varphi\rangle$ is a unit vector orthogonal to $|x_0\rangle$, i.e., $\langle\varphi|x_0\rangle = 0$. We have

$$V_f\,|\psi\rangle \otimes |-\rangle = (-\alpha\,|x_0\rangle + \beta\,|\varphi\rangle) \otimes |-\rangle\,. \tag{11.6}$$

Here the minus sign is gained through the phase kickback. Discarding the $|-\rangle$ which is unchanged by applying V_f, we obtain an n-qubit unitary

$$R_{x_0}(\alpha\,|x_0\rangle + \beta\,|\varphi\rangle) = -\alpha\,|x_0\rangle + \beta\,|\varphi\rangle\,. \tag{11.7}$$

Therefore R_{x_0} is a reflection operator across the hyperplane orthogonal to $|x_0\rangle$ as

$$R_{x_0} = I - 2\,|x_0\rangle\,\langle x_0|\,. \tag{11.8}$$

The Grover iterate can then be expressed as

$$G = (2|\psi_0\rangle\langle\psi_0| - I)(I - 2|x_0\rangle\langle x_0|). \tag{11.9}$$

As the Grover iterate is a product of two reflections it can be seen from Jordan's lemma that this creates a rotation in the two-dimensional space spanned by $|\psi_0\rangle$ and $|x_0\rangle$. In effect the Grover iterate solves the search problem by rotating the initial state toward the target state. To make this explicit, we verify that G acts as a rotation within this space. The geometric picture is in fact even clearer in Fig. 11.1, and the same argument appear many times throughout the text including in amplitude amplification, qubitization, and quantum walks.

To see that G acts as a two-dimensional rotation on this space, let us begin by hypothesizing that G has an invariant subspace of the form $\mathrm{span}(|\psi_0\rangle\,, G\,|\psi_0\rangle)$. We now verify this. First note that this basis for the subspace is not necessarily orthonormal. We can orthogonalize it using Gram-Schmidt orthogonalization, which allows us to define an orthogonal state $|\psi_0^\perp\rangle$ via

$$|\psi_0^\perp\rangle = \frac{G\,|\psi_0\rangle - |\psi_0\rangle\,\langle\psi_0|\,G\,|\psi_0\rangle}{\sqrt{1 - |\,\langle\psi_0|\,G\,|\psi_0\rangle\,|^2}}. \tag{11.10}$$

We can then express the sub-matrix of G inside this space as

$$[G]_{\psi_0,\psi_0^\perp} = \begin{bmatrix} \langle\psi_0|\,G\,|\psi_0\rangle & \langle\psi_0|\,G\,|\psi_0^\perp\rangle \\ \langle\psi_0^\perp|\,G\,|\psi_0\rangle & \langle\psi_0^\perp|\,G\,|\psi_0^\perp\rangle \end{bmatrix}. \tag{11.11}$$

We can now proceed to compute the matrix elements of the submatrix. Specifically,

$$\begin{aligned} \langle\psi_0|\,G\,|\psi_0\rangle &= \langle\psi_0|\,(2|\psi_0\rangle\langle\psi_0| - I)(I - 2|x_0\rangle\langle x_0|)\,|\psi_0\rangle \\ &= 1 - 2|\,\langle\psi_0|x^*\rangle\,|^2 \\ &:= 1 - 2\sin^2(\theta/2) = \cos(\theta) \end{aligned} \tag{11.12}$$

where $\theta = 2\arcsin(\langle\psi_0|x_0\rangle) = 2\arcsin(1/\sqrt{N})$ is the rotation angle that the Grover iterate applies within this space.

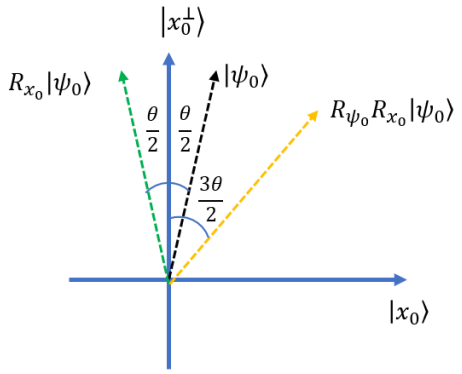


FIGURE 11.1. Geometric interpretation of one Grover iteration.

Similarly, we see that the second matrix element in the first row can be written as

$$\begin{aligned}
\langle\psi_0|\, G\, |\psi_0^\perp\rangle &= \frac{\langle\psi_0|\, G^2\, |\psi_0\rangle - |\,\langle\psi_0|\, G\, |\psi_0\rangle\,|^2}{\sin(\theta)} \\
&= \frac{\langle\psi_0|\,(2|\psi_0\rangle\langle\psi_0| - I)(I - 2|x_0\rangle\langle x_0|)(2|\psi_0\rangle\langle\psi_0| - I)(I - 2|x_0\rangle\langle x_0|)\,|\psi_0\rangle - \cos^2(\theta)}{\sin(\theta)} \\
&= \frac{1 - 8\cos^2(\theta/2) + 8\cos^4(\theta/2) - \cos^2(\theta)}{\sin(\theta)} \\
&= -\sin(\theta) \qquad (11.13)
\end{aligned}$$

Repeating this reasoning to the two remaining elements yields the matrix

$$[G]_{\psi_0,\psi_0^\perp} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \equiv e^{-iY\theta}. \qquad (11.14)$$

As this submatrix is unitary and G is unitary, there cannot be any other non-zero matrix elements in the corresponding rows and columns of the full matrix. This proves that the dynamics is confined to this two-dimensional invariant subspace.

To express the state in terms of the marked and unmarked directions, define

$$|x_0^\perp\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \neq x_0} |x\rangle\,. \qquad (11.15)$$

Then

$$|\psi_0\rangle = \sin(\theta/2)\,|x_0\rangle + \cos(\theta/2)\,|x_0^\perp\rangle\,, \qquad (11.16)$$

and a direct computation gives

$$G\,|x_0\rangle = \cos(\theta)\,|x_0\rangle - \sin(\theta)\,|x_0^\perp\rangle\,, \qquad G\,|x_0^\perp\rangle = \sin(\theta)\,|x_0\rangle + \cos(\theta)\,|x_0^\perp\rangle\,. \qquad (11.17)$$

Thus G acts as a rotation by angle θ on $\mathrm{span}(|x_0\rangle\,, |x_0^\perp\rangle)$.

Applying the Grover operator k times, we obtain from the fact that $\left(e^{-i\theta Y}\right)^k = e^{-ik\theta Y}$

$$G^k\,|\psi_0\rangle = \sin((2k+1)\theta/2)\,|x_0\rangle + \cos((2k+1)\theta/2)\,|x_0^\perp\rangle\,. \qquad (11.18)$$

For the choice $k = \left\lfloor \frac{\pi}{2\theta} - \frac{1}{2} \right\rfloor$, we have $(2k+1)\theta/2 \leq \pi/2$ and

$$\frac{(2k+1)\theta}{2} \geq \frac{\pi}{2} - \theta. \tag{11.19}$$

Therefore the probability of failure satisfies

$$\begin{aligned} \mathbb{P}(fail) &= \cos^2((2k+1)\theta/2) \\ &\leq \cos^2\left(\frac{\pi}{2} - \theta\right) \\ &= \sin^2(\theta) \\ &= 4\sin^2(\theta/2)\cos^2(\theta/2) \\ &\leq 4\sin^2(\theta/2) = \frac{4}{N}. \end{aligned} \tag{11.20}$$

In practice, $\sqrt{N}\pi/4$ may not be an integer, and we may not have $\sin((2k+1)\theta/2) \approx 1$. As mentioned in Theorem 11.2, this can lead to a probability of failure as large as $4/N$. This means that Grover's algorithm may fail, although the probability of such failures is small compared to the cost. In particular, as the output of Grover's algorithm can be classically checked using the marking function $f(x)$ we can see if a failure happened and then try again. The number of trials needed before a success is achieved is then geometrically distributed with a success probability of at least $\mathbb{P}(succ) \geq 1 - 4/N$. Using the fact that the mean number of such trials is $1/\mathbb{P}(succ)$ and each trial requires $\mathcal{O}(\sqrt{N})$ queries to V_f it follows that the expected query complexity of the search algorithm is

$$\mathcal{O}\left(\frac{\sqrt{N}}{\mathbb{P}(succ)}\right) = \mathcal{O}\left(\frac{\sqrt{N}}{1 - 4/N}\right) = \mathcal{O}\left(\sqrt{N} + \frac{4}{\sqrt{N}}\right) = \mathcal{O}(\sqrt{N}). \tag{11.21}$$

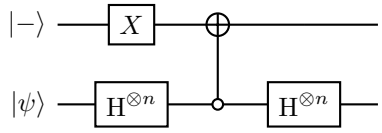
Thus if the expected number of iterations needed in order to find a success is $\mathcal{O}(\sqrt{N})$ it follows from Markov's inequality that with probability greater than $2/3$ we will also only require $\mathcal{O}(\sqrt{N})$ queries to the marking oracle to find the marked state, which proves our claim. □

Interestingly, even if we do not know how to check x_0, statistical amplification as in Example 8.6 implies that applying the majority voting can also robustly produce x_0 with probability of failure δ using $\mathcal{O}(\log(1/\delta))$ repetition of the circuit provided that the probability of success is greater than $1/2$.

To draw the quantum circuit of Grover's algorithm, we need an implementation of R_{ψ_0}. Note that

$$R_{\psi_0} = \mathrm{H}^{\otimes n}(2\left|0^n\right\rangle\left\langle 0^n\right| - I)\,\mathrm{H}^{\otimes n}. \tag{11.22}$$

This can be implemented via the following circuit using one ancilla qubit:



Here the controlled-NOT gate is an n-qubit controlled-X gate, and is only active if the system qubits are in the 0^n state. Discarding the signal qubit, we obtain an implementation of R_{ψ_0}. Since the signal qubit $|-\rangle$ only changes up to a sign, it can be reused for both R_{ψ_0} and R_{x_0}.

Exercise 11.1. Construct a circuit to show that the reflector R_{ψ_0} can also be implemented without using any ancilla qubits.

The reasoning behind Grover's search for a single marked state can be generalized straight forwardly to M marked states as we will see below. The primary difference is that the number of Grover iterations that are needed to achieve a marked state are, as expected, reduced if there are more potential marked states that we can measure. However, as with the previous discussion, the number of marked states needs to be known in order for a **direct** application of the reasoning behind Grover's algorithm to work in this setting. We discuss this situation in the following example.

Example 11.3 (Generalization of Grover's algorithm to multiple marked states)**.** Suppose that there are $M \geq 1$ marked states among $N = 2^n$ basis states, i.e., $f(x) = 1$ for M values of $x \in \{0,1\}^n$ and $f(x) = 0$ otherwise. As in the single-marked case, it is convenient to collect the marked subspace into a single normalized state

$$|w\rangle = \frac{1}{\sqrt{M}} \sum_{x:f(x)=1} |x\rangle \,, \tag{11.23}$$

and similarly the (normalized) superposition of unmarked states

$$|w^\perp\rangle = \frac{1}{\sqrt{N-M}} \sum_{x:f(x)=0} |x\rangle \,. \tag{11.24}$$

Then the uniform superposition can be written as

$$|\psi_0\rangle = \sqrt{\frac{M}{N}}\,|w\rangle + \sqrt{\frac{N-M}{N}}\,|w^\perp\rangle = \sin(\theta/2)\,|w\rangle + \cos(\theta/2)\,|w^\perp\rangle \,, \tag{11.25}$$

where $\sin(\theta/2) = \sqrt{M/N}$.

Using phase kickback, the phase oracle implements the reflection

$$R_w\,|x\rangle = (-1)^{f(x)}\,|x\rangle \,. \tag{11.26}$$

Restricted to the invariant subspace $\mathrm{span}\{|w\rangle\,, |w^\perp\rangle\}$, this operator acts as $R_w = I - 2|w\rangle\langle w|$. As before, we choose

$$R_{\psi_0} = -(I - 2|\psi_0\rangle\langle\psi_0|) = 2|\psi_0\rangle\langle\psi_0| - I, \tag{11.27}$$

Let $\mathcal{B} = \{|w\rangle\,, |w^\perp\rangle\}$. The same calculation as above shows that the Grover iterate $G = R_{\psi_0} R_w$ satisfies

$$G^k\,|\psi_0\rangle = \sin\Big(\frac{(2k+1)\theta}{2}\Big)\,|w\rangle + \cos\Big(\frac{(2k+1)\theta}{2}\Big)\,|w^\perp\rangle \,. \tag{11.28}$$

Thus, the success probability of measuring a marked state equals $\sin^2\big(\frac{(2k+1)\theta}{2}\big)$. Choosing $k \approx \frac{\pi}{2\theta} - \frac{1}{2} \approx \frac{\pi}{4}\sqrt{\frac{N}{M}}$ makes this probability bounded below by a constant. ⋄

Example 11.4 (Grover's algorithm as Chebyshev singular value transformation)**.** Let us view Grover's algorithm from the perspective of qubitization beyond the computational basis as in Section 10.6. Let $|x_0\rangle$ be the marked state, and $|\psi_0\rangle$ be the uniform superposition of states. We define an orthonormal basis set $\mathcal{B} = \{|\psi_0\rangle\,, |v_1\rangle\,, \ldots, |v_{N-1}\rangle\}$, where all states $|v_i\rangle$ are orthogonal to $|\psi_0\rangle$. Similarly define an orthonormal basis set $\mathcal{B}' = \{|x_0\rangle\,, |w_1\rangle\,, \ldots, |w_{N-1}\rangle\}$, where all states

$|w_i\rangle$ are orthogonal to $|x_0\rangle$. Then the matrix of reflection operator R_{ψ_0} with respect to $\mathcal{B}, \mathcal{B}'$ is (let $a = 1/\sqrt{N} = \sin(\theta/2)$)

$$[R_{\psi_0}]_{\mathcal{B}}^{\mathcal{B}'} = \begin{pmatrix} a & * \\ * & * \end{pmatrix}, \tag{11.29}$$

Therefore $\mathscr{U}_A = R_{\psi_0}$ serves as the block encoding of a 1×1 scalar $A = a = 1/\sqrt{N}$. The projectors $\Pi = |\psi_0\rangle\langle\psi_0|$ and $\Pi' = |x_0\rangle\langle x_0|$ are implicitly defined via the provided reflection operator $Z_\Pi = R_{\psi_0}, Z_{\Pi'} = -R_{x_0}$, respectively. This also means $\mathscr{U}_A Z_\Pi = R_{\psi_0}^2 = I$.

The qubitization invoking $\mathscr{U}_A$ for $(2k+1)$ times gives

$$\Pi' \mathscr{U}_A Z_\Pi (\mathscr{U}_A^\dagger Z_{\Pi'} \mathscr{U}_A Z_\Pi)^k \Pi = \Pi'(R_{\psi_0}(-R_{x_0}))^k \Pi = T_{2k+1}(a)|x_0\rangle\langle\psi_0| = (-1)^k \sin\left(\frac{(2k+1)\theta}{2}\right)|x_0\rangle\langle\psi_0|. \tag{11.30}$$

Here we have used the fact that $T_{2k+1}(a) = (-1)^k \sin((2k+1)\arcsin(a))$ for $a \in [0,1]$. Letting $\sin((2k+1)\theta/2) \approx 1$, we recover the same query complexity as Grover's algorithm. Note that $\mathscr{U}_A^\dagger Z_{\Pi'} \mathscr{U}_A Z_\Pi = R_{\psi_0}(-R_{x_0}) = -G$, this procedure differs from the original Grover's algorithm just by a global phase factor $(-1)^k$. ◇

11.2. Amplitude amplification

The idea behind Grover's algorithm is not restricted to the problem of unstructured search. It can be extended beyond this setting to a broader concept that is called **amplitude amplification** (AA) [BHMT02], which is used ubiquitously as a subroutine to achieve quadratic speedups. Further, amplitude amplification has also proven invaluable as a technique for converting information stored in an amplitude to information stored in a phase. This is the key insight behind amplitude estimation, which allows us to learn a probability quadratically faster than statistical sampling allows.

Just as Grover's problem has one, or multiple, marked states we assume for amplitude amplification that there is a set of states that we consider to be "good", and assume in our context that our algorithm is successful if any of the states in the good space is found. For example, for Grover's problem the good states correspond to the marked states. A more complicated example is given below involving binary satisfiability.

Example 11.5. Amplitude amplification can be naturally applied to any problem in the complexity class NP. This is because a solution to any "yes"-instance of a decision problem in NP can be verified in polynomial time through given an appropriate witness. For example we can consider the case of 3-SAT which is an NP-complete problem, which means that all problems in the complexity class NP can be solved by an oracle that solves any instance of 3-SAT. Specifically, the 3-SAT problem is specified by a list of literals $x_1, \ldots, x_n$ and a conjuncative normal form formula of the formula. ◇

Grover's algorithm in fact exists as a special case of a larger algorithmic design paradigm known as amplitude amplification. Amplitude amplification follows the exact same structure as Grover's search but instead of marking a set of bit strings, amplitude amplification marks instead a subspace of valid states. Amplitude amplification can then be used to rotate probability between states in this "good" subspace and the "bad" subspace which is its compliment.

Amplitude amplification involves a decomposition of the Hilbert space into two subspaces which we define by the projector Π_{good} and its compliment $I - \Pi_{\text{good}} = \Pi_{\text{bad}}$ (where recall that a projector

is a Hermitian operator that squares to itself).

$$|\psi_0\rangle = (\Pi_{\text{good}} + \Pi_{\text{bad}})\,|\psi_0\rangle = \sqrt{p}\,|\psi_{\text{good}}\rangle + \sqrt{1-p}\,|\psi_{\text{bad}}\rangle\,, \tag{11.31}$$

where $p = \mathbb{P}(\text{good})1$. Here $|\psi_{\text{good}}\rangle$ and $|\psi_{\text{bad}}\rangle$ are orthonormal. We do not have direct access to $|\psi_{\text{good}}\rangle$, but would like to obtain a state that has a large overlap with $|\psi_{\text{good}}\rangle$. Amplitude amplification gives a way of providing a quadratic advantage for such problems and as a result is used ubiquitously in quantum algorithms in place of statistical sampling or brute force searches.

The following proposition gives our main claims about the performance of amplitude amplification. This result actually subsumes Grover's algorithm, but as we will see the slightly more abstract definition of amplitude amplification will make some applications more obvious.

Proposition 11.6 (Amplitude Amplification)**.** *Let $\Pi_{\text{good}} \in L(\mathbb{C}^N)$ be a projection operator (i.e. $\Pi_{\text{good}}^2 = \Pi_{\text{good}}$), further let $R_{\psi_0} \in L(\mathbb{C}^N)$ be a reflection operator such that $R_{\psi_0} = 2|\psi_0\rangle\langle\psi_0| - I$ for initial state $|\psi_0\rangle \in \mathbb{C}^N$, and assume that we are provided oracles (and their inverses) $R_{\text{good}} := I - 2\Pi_{\text{good}}$ and $U_{\psi_0} : |0\rangle \mapsto |\psi_0\rangle$. Define $p := \langle\psi_0|\,\Pi_{\text{good}}\,|\psi_0\rangle$ and $\theta \in [0,\pi]$ by $\sqrt{p} = \sin(\theta/2)$. Let $W = R_{\psi_0}R_{\text{good}}$. Then the following properties hold:*

1. *For any integer $k \geq 0$, $|\Pi_{\text{good}}W^k\,|\psi_0\rangle\,| = \sin((2k+1)\theta/2)$.*
2. *The dynamics of $|\psi_0\rangle$ within the subspace $\operatorname{span}(|\psi_0\rangle, |\psi_0^\perp\rangle)$ takes the form*

$$[W]_{\psi_0,\psi_0^\perp} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

   where $|\psi_0^\perp\rangle = \cos(\theta/2)\,|\psi_{\text{good}}\rangle - \sin(\theta/2)\,|\psi_{\text{bad}}\rangle$.
3. *The eigenvectors of $[W]_{\psi_0,\psi_0^\perp}$ are $(|\psi_0\rangle + i\,|\psi_0^\perp\rangle)/\sqrt{2}$ and $(|\psi_0\rangle - i\,|\psi_0^\perp\rangle)/\sqrt{2}$. The corresponding eigenvalues are $e^{-i\theta}$ and $e^{i\theta}$, respectively, where $\theta = 2\arcsin\big(\sqrt{\langle\psi_0|\,\Pi_{\text{good}}\,|\psi_0\rangle}\big)$.*

Proof. Let

$$|\psi_{\text{good}}\rangle = \frac{\Pi_{\text{good}}\,|\psi_0\rangle}{\sqrt{p}}, \qquad |\psi_{\text{bad}}\rangle = \frac{(I - \Pi_{\text{good}})\,|\psi_0\rangle}{\sqrt{1-p}}. \tag{11.32}$$

Then

$$|\psi_0\rangle = \sin(\theta/2)\,|\psi_{\text{good}}\rangle + \cos(\theta/2)\,|\psi_{\text{bad}}\rangle\,, \tag{11.33}$$

and the orthogonal vector

$$|\psi_0^\perp\rangle = \cos(\theta/2)\,|\psi_{\text{good}}\rangle - \sin(\theta/2)\,|\psi_{\text{bad}}\rangle \tag{11.34}$$

spans the same two-dimensional subspace.

Since $R_{\text{good}} = I - 2\Pi_{\text{good}}$, we have

$$R_{\text{good}}\,|\psi_{\text{good}}\rangle = -\,|\psi_{\text{good}}\rangle\,, \qquad R_{\text{good}}\,|\psi_{\text{bad}}\rangle = |\psi_{\text{bad}}\rangle\,. \tag{11.35}$$

Also, $R_{\psi_0}\,|\psi_0\rangle = |\psi_0\rangle$ and $R_{\psi_0}\,|\psi_0^\perp\rangle = -\,|\psi_0^\perp\rangle$. Therefore

$$W\,|\psi_0\rangle = \cos(\theta)\,|\psi_0\rangle + \sin(\theta)\,|\psi_0^\perp\rangle\,, \tag{11.36}$$

and

$$W\,|\psi_0^\perp\rangle = -\sin(\theta)\,|\psi_0\rangle + \cos(\theta)\,|\psi_0^\perp\rangle\,. \tag{11.37}$$

Hence

$$[W]_{\psi_0,\psi_0^\perp} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} = e^{-iY\theta}. \tag{11.38}$$

This proves the second item. The third item now follows from the eigenvectors of Y.

Raising the rotation matrix to the kth power gives

$$W^k |\psi_0\rangle = \cos(k\theta) |\psi_0\rangle + \sin(k\theta) |\psi_0^\perp\rangle . \tag{11.39}$$

Since

$$\Pi_{\text{good}} |\psi_0\rangle = \sin(\theta/2) |\psi_{\text{good}}\rangle , \qquad \Pi_{\text{good}} |\psi_0^\perp\rangle = \cos(\theta/2) |\psi_{\text{good}}\rangle , \tag{11.40}$$

we obtain

$$\Pi_{\text{good}} W^k |\psi_0\rangle = (\cos(k\theta)\sin(\theta/2) + \sin(k\theta)\cos(\theta/2)) |\psi_{\text{good}}\rangle . \tag{11.41}$$

Using $\sin(a+b) = \sin(a)\cos(b) + \cos(a)\sin(b)$, this becomes

$$\Pi_{\text{good}} W^k |\psi_0\rangle = \sin((2k+1)\theta/2) |\psi_{\text{good}}\rangle , \tag{11.42}$$

which proves the first item. □

Example 11.7 (Reflection with respect to signal qubits)**.** One common scenario is that the implementation of U_{ψ_0} requires m ancilla qubits (also called signal qubits), i.e.,

$$U_{\psi_0} |0^m\rangle |0^n\rangle = \sqrt{p} |0^m\rangle |\psi\rangle + \sqrt{1-p} |\perp\rangle , \tag{11.43}$$

where $|\perp\rangle$ is some orthogonal state satisfying

$$(\Pi \otimes I) |\perp\rangle = 0, \quad \Pi = |0^m\rangle\langle 0^m|. \tag{11.44}$$

Therefore

$$|\psi_{\text{good}}\rangle = |0^m\rangle |\psi\rangle , \quad |\psi_{\text{bad}}\rangle = |\perp\rangle . \tag{11.45}$$

This setting is special since the "good" state can be verified by measuring the ancilla qubits after applying U_{ψ_0} in Eq. (11.43), and post-select the outcome 0^m. In particular, the expected number of measurements needed to obtain $|\psi_{\text{good}}\rangle$ is $1/p$.

In order to employ the amplitude amplification procedure, we first note that the reflection operator can be simplified as

$$R_{\text{good}} = (I - 2|0^m\rangle\langle 0^m|) \otimes I. \tag{11.46}$$

This is because $|\psi_{\text{good}}\rangle$ can be entirely identified by measuring the ancilla qubits. Meanwhile

$$R_{\psi_0} = U_{\psi_0}(2|0^{m+n}\rangle\langle 0^{m+n}| - I)U_{\psi_0}^\dagger. \tag{11.47}$$

Let $G = R_{\psi_0} R_{\text{good}}$. For a suitable integer $k = \mathcal{O}(1/\sqrt{p})$, applying G^k to $U_{\psi_0} |0^{m+n}\rangle$ yields a state with constant overlap with $|\psi_{\text{good}}\rangle$. This achieves the desired quadratic speedup. ◇

Corollary 11.8. *Under the assumptions of Proposition 11.6 let us further assume that we are provided with the true value of p and that we have access to controlled oracle $cR_{\text{good}} = |1\rangle\langle 1| \otimes R_{\text{good}} + |0\rangle\langle 0| \otimes I$ then there exists a quantum algorithm that can yield a state of the form $|0\rangle |\psi_{\text{good}}\rangle$ such that $\Pi_{\text{good}} |\psi_{\text{good}}\rangle = |\psi_{\text{good}}\rangle$ that uses $\mathcal{O}(1/\sqrt{p})$ queries to controlled R_{good}.*

Proof. Let

$$k^* := \left\lceil \frac{\pi}{4 \arcsin(\sqrt{p})} - \frac{1}{2} \right\rceil , \tag{11.48}$$

and define

$$p^* := \sin^2\left(\frac{\pi}{2(2k^*+1)}\right) . \tag{11.49}$$

By construction $p^* \leq p$, and if $\theta^* = 2\arcsin(\sqrt{p^*})$ then $\theta^* = \pi/(2k^*+1)$.

Introduce one ancilla qubit and let B be any single-qubit unitary satisfying

$$B|0\rangle = \sqrt{1-p^*/p}\,|0\rangle + \sqrt{p^*/p}\,|1\rangle\,. \tag{11.50}$$

Define

$$U' := (B \otimes U_{\psi_0}), \qquad \Pi'_{\text{good}} := |1\rangle\langle 1| \otimes \Pi_{\text{good}}, \tag{11.51}$$

and let

$$|\psi'_0\rangle := U'|0\rangle|0\rangle\,. \tag{11.52}$$

Then

$$\Pi'_{\text{good}}|\psi'_0\rangle = \sqrt{p^*}\,|1\rangle|\psi_{\text{good}}\rangle\,, \tag{11.53}$$

so the new success probability is exactly p^*.

Now apply Proposition 11.6 to the pair $(|\psi'_0\rangle, \Pi'_{\text{good}})$. Since $\theta^* = \pi/(2k^*+1)$, after k^* iterations the success amplitude becomes

$$\sin\left(\frac{(2k^*+1)\theta^*}{2}\right) = \sin(\pi/2) = 1. \tag{11.54}$$

Therefore the resulting state lies in the image of Π'_{good}, hence it has the form $|1\rangle|\psi_{\text{good}}\rangle$ for some $|\psi_{\text{good}}\rangle$ satisfying $\Pi_{\text{good}}|\psi_{\text{good}}\rangle = |\psi_{\text{good}}\rangle$. Applying X to the ancilla yields $|0\rangle|\psi_{\text{good}}\rangle$.

It remains to count queries. The reflection about the good space is

$$I - 2\Pi'_{\text{good}} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes (I - 2\Pi_{\text{good}}) = cR_{\text{good}}, \tag{11.55}$$

so each amplitude-amplification step uses one query to controlled R_{good}. Since $k^* = \mathcal{O}(1/\sqrt{p})$, the total number of controlled queries is $\mathcal{O}(1/\sqrt{p})$.

□

This shows that we can use amplitude amplification to rotate the state deterministically to a good state, if we know the success probability before starting. This is significant because in some applications, such as Grover's problem, we often know the success probability apriori. We also know it for problems such as preparing the state $\frac{1}{\sqrt{L}}\sum_{j=0}^{L-1}|j\rangle$ from $(\mathrm{H}|0\rangle)^{\otimes\lceil\log_2(L)\rceil}$. However, it is important to note that doing so also requires that we have access to a controllable (and invertible) version of our oracles. This is often, in practice, a very reasonable assumption but is important to consider in settings such as in learning theory wherein the assumptions made by models such as the quantum PAC model of learning implicitly forbid the use of these oracles [ADW17].

A major potential issue with amplitude amplification, and Grover's search as an application, is that the success probability needs to be known to understand how many applications of the amplitude amplification operator in order to achieve a high probability of success. The standard approach used in most modern algorithms is a concept known as fixed point amplitude amplification wherein the quantum singular value transformation is used to transform the eigenvalues of the walk operator, and in turn the rotation angles, to ensure that the transformed rotation is ϵ-close to 100% success. This will be discussed in detail in Section 13.1.

The older, and simpler approach for solving this problem involves statistical sampling and involves choosing a number of applications of W that is uniformly drawn from the interval $[1, 2^m - 1]$ for an integer value of m. If you find a success, then we can verify this using R_{good} via the Hadamard test circuit. In the event that we fail, then we increase m by one and repeat the process. If $2^m\theta > 2\pi$

then the process effectively samples from random angles in the unit circle. The average value of $\cos^2(\theta)$ in this regime is

$$\frac{1}{2\pi}\int_0^{2\pi}\cos^2(\theta)d\theta = 1/2, \tag{11.56}$$

and so we expect that in such cases the success probability is at least a constant in this regime. The number of repetitions needed for this procedure before a success is observed is geometrically distributed and has a mean of a constant. Thus the cost will be with high probability a cost times the cost of achieving $2^m\theta \approx 2\pi$, which is $\mathcal{O}(1/\sqrt{p})$. Details of this argument can be found in [NC00].

11.3. Applications of Amplitude Amplification

We will now provide some examples of how amplitude amplification can be used to solve particular problems. These examples represent just a small fraction of the scope of amplitude amplification as an algorithmic design primative.

Example 11.9. Consider an algorithm that incorporates multiple intermediate measurements, where success is determined by measuring all ancilla qubits to yield 0. One example is the multiplication of block encodings in Section 9.3. Let the probability of success at the i-th stage (conditioned on the previous stages being successful) be denoted as p_i. Therefore, the cumulative probability of achieving all 0s across stages is $p = p_1 \times \cdots \times p_L$, and the number of repetitions needed for success is $\mathcal{O}(1/p)$. By the principle of deferred measurement, one can transform this into a coherent process by using $L-1$ additional ancilla qubits. This enables the construction of a reflection operator acting on the L signal qubits. Applying amplitude amplification then reduces the number of repetitions to $\mathcal{O}(1/\sqrt{p})$.

◇

Example 11.10 (Compression gadget)**.** Fig. 11.2 uses $L-1$ ancilla qubits to coherently implement an algorithm that incorporates multiple intermediate measurements. It turns out that the number of ancilla qubits can be significantly reduced to $\mathcal{O}(\log L)$.

To do this we introduce a counter register to count how many intermediate measurements are successful. This counter register contains $m = \lceil \log_2(L+1) \rceil$ qubits, so it represents integers modulo $M := 2^m$. We introduce a unitary operator ADD on this register defined as

$$\mathrm{ADD}\,|c\rangle = |(c+1) \bmod M\rangle\,. \tag{11.57}$$

This operator can be implemented as a classical arithmetic circuit, and performs addition modulo M. Correspondingly $\mathrm{ADD}^\dagger$ performs subtraction. We first add L to the counter register, subtract by 1 each time a measurement result is successful. In the end, if all steps are successful the counter register will be in the state $|0^m\rangle$. The circuit construction for the above coherent procedure is described in Fig. 11.3. Then we may apply amplitude amplification to enhance the success probability using $\mathcal{O}(1/\sqrt{p})$ repetitions of the coherent circuit.

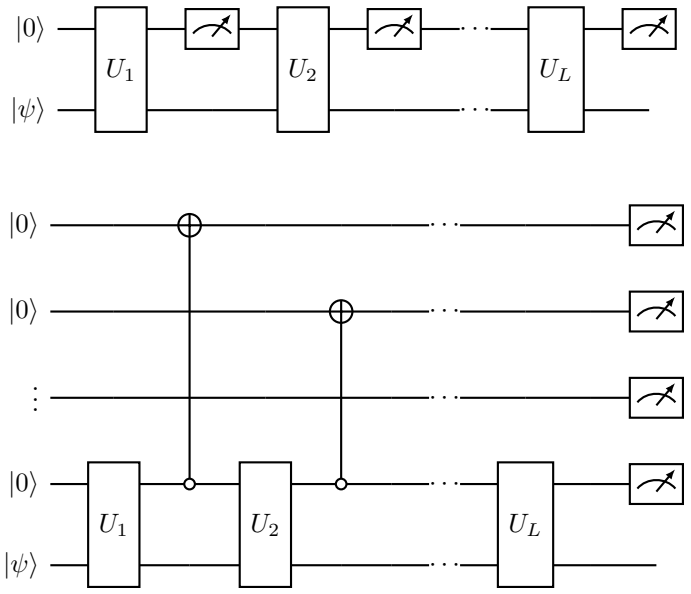


FIGURE 11.2. Using deferred measurement to coherently implement an algorithm that incorporates multiple intermediate measurements. This allows us to use the amplitude amplification procedure to reduce the number of repetitions.

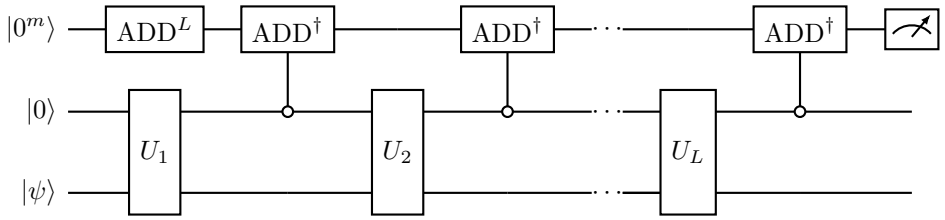


FIGURE 11.3. Circuit for compression gadget to coherently implement an algorithm that incorporates multiple intermediate measurements. The counter register, containing $m = \lceil \log_2(L+1) \rceil$ qubits, is used for keeping track of whether each measurement is successful. The ADD circuit implements addition by 1 modulo the smallest power of 2 that is larger than or equal to $L+1$.

◇

11.4. Oblivious amplitude amplification

Oblivious amplitude amplification is perhaps one of the most important techniques yet invented for use in block encodings. A major challenge with block encodings is that the normalization constant of the block encoding often severely limits the success probability. Specifically, if we have

a unitary V that provides a block-encoding of a matrix A with normalization constant γ then

$$V = \begin{bmatrix} A/\gamma & \cdot \\ \cdot & \cdot \end{bmatrix} \tag{11.58}$$

We then have from Lemma 9.5 that the probability of successfully applying A to a state $|\psi\rangle$ is

$$\mathbb{P}(A|\psi) := \frac{\langle\psi| A^\dagger A |\psi\rangle}{\gamma^2}. \tag{11.59}$$

Amplitude amplification can be used to boost the success probability of this procedure to near-unity; however, doing so requires reflections about the marked subspace and the initial state $V|0\rangle|\psi\rangle$. If the algorithm only requires a single application of the block encoding then the success probability will not be problematic. In applications though such as simulation, we will see, that many timesteps will need to be combined in order to boost the success probability so a value that is near unity at reasonable cost. As such a reflection is about **the initial state** $V|0\rangle|\psi\rangle$, the algorithm would at subsequent time steps need to revert back to the initial state to perform the reflection. This eliminates the benefit of the hard work used to reach the current time step and in turn makes this process of inversion impractical if multiple time steps are used in the algorithm.

One aspect that further makes the inversion challenging is that in general, we learn something about $|\psi\rangle$ upon successfully applying A to the state. In particular, let us consider two states $|\psi\rangle$ and $|\phi\rangle$. Let us assume that the block encoding was successfully applied. In this case, we have that the likelihood ratio between the two hypotheses is

$$\frac{\mathbb{P}(A|\psi)}{\mathbb{P}(A|\phi)} = \frac{\langle\psi| A^\dagger A |\psi\rangle}{\langle\phi| A^\dagger A |\phi\rangle} \tag{11.60}$$

Thus the likelihood ratio will, for generic states, vary wildly between zero and infinity. This means that a hypothesis test can be performed to distinguish between two potential hypotheses for the state based simply on whether the projection occurred. Thus any unitary process that seeks to chain together a sequence of applications of block encodings will run into issues surrounding the fact that success or failure of the protocol provides information about the state and in turn faces limitations from state distinguishability limits in quantum mechanics.

Oblivious amplitude amplification provides a way to skip this problem by removing the need to reflect about the initial state and instead reflect about a subspace that contains the initial state. The key idea behind oblivious amplitude amplification is to focus only on settings wherein no information is gleaned about $|\psi\rangle$ from the success or failure of a block encoding. A sufficient condition for this holding is that A is unitary in which case we have that

$$\frac{\mathbb{P}(A|\psi)}{\mathbb{P}(A|\phi)} = 1 \tag{11.61}$$

which implies that no distinguishing information can be provided from such experiments about whether the state is $|\psi\rangle$ or $|\phi\rangle$.

The initial example that motivated this technique in [BCK15] was Hamiltonian simulation using linear combination of unitaries wherein

$$(\langle 0| \otimes I)V(|0\rangle \otimes I) = \frac{A}{\alpha} \approx \frac{e^{-iHt}}{\alpha}. \tag{11.62}$$

In this case, the success probability of applying this unitary shrinks for every time step that this operator is applied. Specifically, the probability of the algorithm working in 1 step is $1/\alpha^2$. If we wished to apply two timesteps with this then the probability would be $1/\alpha^4$ and so on. We would

like to fight this exponentially shrinking probability using amplitude amplification, but the method requires a reflection about the **initial state**. As we do not know what the value of $e^{-iHt}|\psi_0\rangle$ is in general for initial state $|\psi_0\rangle$ in Hamiltonian simulation problems, this feat would require that we unroll time evolutions to reconstruct intermediate times so we can perform the reflection. This process, while possible, leads to exponential overheads that impede the viability of the approach in general. Oblivious amplitude amplification provides a way to rectify this problem by reflecting about the good space (in this case $I - 2|0\rangle\langle 0|$) and a subspace that the initial state for a given timestep was contained in (in this case this reflection $(V(1 - 2|0\rangle\langle 0| \otimes I)V^\dagger)$).

Amplitude amplification is stated in slightly more general language than this specific Hamiltonian simulation example above wherein there is a notion of a good space and a bad space. Below we provide a definition that adopts this language to describe amplitude amplification with respect to these spaces and in turn introduce the oblivious amplitude amplification walk operator.

Definition 11.11. *Let $Z_{\Pi_{\text{good}}} = I - 2\Pi_{\text{good}}$ for $\Pi_{\text{good}} \in L(\mathbb{C}^{2^a})$ a projection operator of rank r that projects onto a space that we consider to be "good". Let $V \in U(2^{n+a})$ and $U \in U(2^n)$ be unitary matrices, and suppose that the projector Π_{good} flags a $(\alpha, a, 0)$ block encoding of the unitary U within V, meaning that for all $|\psi_{\text{good}}\rangle$ such that $\Pi_{\text{good}}|\psi_{\text{good}}\rangle = |\psi_{\text{good}}\rangle$,*

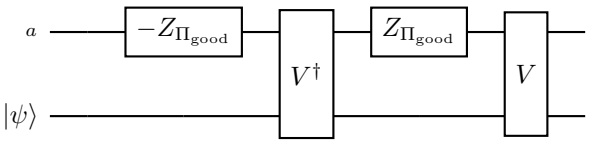
$$(\langle\psi_{\text{good}}| \otimes I)V(|\psi_{\text{good}}\rangle \otimes I) = \frac{U}{\alpha}$$

The oblivious amplitude amplification walk operator is then defined to be the operator

$$W = -V(Z_{\Pi_{\text{good}}} \otimes I)V^\dagger(Z_{\Pi_{\text{good}}} \otimes I),$$

acting on $\mathbb{C}^{2^a} \otimes \mathbb{C}^{2^n}$, which is represented by

$W :=$



The walk operator, W, defined above plays exactly the same role as the walk operator for amplitude amplification. However, a key assumption as mentioned before is the fact that the operator provides no information about the specific subspace that it acts on and further the reflections used are not about the initial state but rather are reflections about the good space and the $V(Z_{\Pi_{\text{good}}} \otimes I)V^\dagger$ in place of the initial reflection.

Lemma 11.12 (Oblivious Amplitude Amplification)**.** *Let V be an $(\alpha, m, 0)$ block encoding of a unitary U flagged by a projector Π_{good} as given in Definition 11.11. Then the oblivious amplitude amplification walk operator W satisfies for any $|\psi_{\text{good}}\rangle$ such that $\Pi_{\text{good}}|\psi_{\text{good}}\rangle = |\psi_{\text{good}}\rangle$*

$$(\langle\psi_{\text{good}}| \otimes I)W^k V(|\psi_{\text{good}}\rangle \otimes I) = U\sin((2k+1)\arcsin(1/\alpha))$$

using $2k+1$ applications of V and $2k$ applications of $Z_{\Pi_{\text{good}}}$.

Proof. Proof follows similarly to the proof of ordinary amplitude amplification. Let us assume that for any $|\psi_{\text{good}}\rangle$ that is in the image of the projector Π_{good} the dynamics lies within a two-dimensional space spanned by $|\psi_{\text{good}}\rangle|\lambda\rangle$ and $|\psi_\perp\rangle$ such that $U|\lambda\rangle = e^{i\lambda}|\lambda\rangle$ and

$$|\psi_\perp\rangle = \frac{W|\psi_{\text{good}}\rangle|\lambda\rangle - |\psi_{\text{good}}\rangle|\lambda\rangle\langle\psi_{\text{good}}|\langle\lambda|W|\psi_{\text{good}}\rangle|\lambda\rangle}{\|W|\psi_{\text{good}}\rangle|\lambda\rangle - |\psi_{\text{good}}\rangle|\lambda\rangle\langle\psi_{\text{good}}|\langle\lambda|W|\psi_{\text{good}}\rangle|\lambda\rangle\|} \tag{11.63}$$

Next evaluating the matrix element $\langle\psi_{\text{good}}|\langle\lambda|W|\psi_{\text{good}}\rangle|\lambda\rangle$

$$\begin{aligned}\langle\psi_{\text{good}}|\langle\lambda|W|\psi_{\text{good}}\rangle|\lambda\rangle &= -\langle\psi_{\text{good}}|\langle\lambda|V(Z_{\Pi_{\text{good}}}\otimes I)V^\dagger(Z_{\Pi_{\text{good}}}\otimes I)|\psi_{\text{good}}\rangle|\lambda\rangle \\ &= \langle\psi_{\text{good}}|\langle\lambda|V(Z_{\Pi_{\text{good}}}\otimes I)V^\dagger|\psi_{\text{good}}\rangle|\lambda\rangle \end{aligned} \tag{11.64}$$

Next we have that for orthogonal state $|\psi'_\perp\rangle$

$$V^\dagger|\psi_{\text{good}}\rangle|\lambda\rangle = \frac{e^{-i\lambda}}{\alpha}|\psi_{\text{good}}\rangle|\lambda\rangle + \sqrt{1-\frac{1}{\alpha^2}}|\psi'_\perp\rangle \tag{11.65}$$

Thus if we define $\sin(\theta) = 1/\alpha$, which we can always do for real θ because $\alpha \geq 1$ by convention.

$$\langle\psi_{\text{good}}|\langle\lambda|V(Z_{\Pi_{\text{good}}}\otimes I)V^\dagger|\psi_{\text{good}}\rangle|\lambda\rangle = 1-\frac{2}{\alpha^2} = 1-2\sin^2(\theta) = \cos(2\theta). \tag{11.66}$$

Note that here the eigenvalues of U cancel in this application because of unitarity. If U were not unitary then this would not hold and the matrix element would not follow.

Next we can use this matrix element to see that

$$|\psi_\perp\rangle = \frac{W|\psi_{\text{good}}\rangle|\lambda\rangle - |\psi_{\text{good}}\rangle|\lambda\rangle\cos(2\theta)}{\sqrt{1-\cos^2(2\theta)}} \tag{11.67}$$

Thus we can express

$$\langle\psi_\perp|W|\psi_{\text{good}}\rangle|\lambda\rangle = \frac{1}{\sin(2\theta)}\Big(1-\cos(2\theta)\langle\psi_{\text{good}}|\langle\lambda|W|\psi_{\text{good}}\rangle|\lambda\rangle\Big) = \sin(2\theta). \tag{11.68}$$

Repeating the same procedure for the remaining matrix elements we see that

$$[W]_{\psi_{\text{good}},\psi_\perp} = \begin{bmatrix}\cos(2\theta) & -\sin(2\theta)\\ \sin(2\theta) & \cos(2\theta)\end{bmatrix} \tag{11.69}$$

which shows that W keeps this irreducible two-dimensional space invariant because the submatrix is unitary and thus all other matrix elements in the corresponding rows/columns of W must be zero. Thus using the fact that $W \equiv e^{-2i\theta Y}$ within this irreducible subspace it then follows that $W^k \equiv e^{-i2k\theta Y}$ within the space. This in turn is the same as saying that

$$\left[W^k\right]_{\psi_{\text{good}},\psi_\perp} = \begin{bmatrix}\cos(2k\theta) & -\sin(2k\theta)\\ \sin(2k\theta) & \cos(2k\theta)\end{bmatrix} \tag{11.70}$$

Since V block encodes U with normalization constant α we can always write

$$V|\psi_{\text{good}}\rangle|\lambda\rangle = \sin(\theta)e^{i\lambda}|\psi_{\text{good}}\rangle|\lambda\rangle + \cos(\theta)|\phi_\perp\rangle, \tag{11.71}$$

for some orthogonal state $|\phi_\perp\rangle$. Thus we must have that

$$\begin{aligned}\langle\psi_{\text{good}}|\langle\lambda|W^kV|\psi_{\text{good}}\rangle|\lambda\rangle &= \cos(2k\theta)\langle\psi_{\text{good}}|\langle\lambda|V|\psi_{\text{good}}\rangle|\lambda\rangle - \sin(2k\theta)\langle\psi_\perp|V|\psi_{\text{good}}\rangle|\lambda\rangle \\ &= \cos(2k\theta)\sin(\theta)e^{i\lambda} - \sin(2k\theta)\langle\psi_\perp|V|\psi_{\text{good}}\rangle|\lambda\rangle \end{aligned} \tag{11.72}$$

Now

$$\begin{aligned}
\langle\psi_\perp| V |\psi_{\text{good}}\rangle |\lambda\rangle &= \frac{1}{\sin(2\theta)}\Big(\langle\psi_{\text{good}}| \langle\lambda| W^\dagger V |\psi_{\text{good}}\rangle |\lambda\rangle - \cos(2\theta) \langle\psi_{\text{good}}| \langle\lambda| V |\psi_{\text{good}}\rangle |\lambda\rangle \Big) \\
&= \frac{1}{\sin(2\theta)}\Big(\langle\psi_{\text{good}}| \langle\lambda| W^\dagger V |\psi_{\text{good}}\rangle |\lambda\rangle - \cos(2\theta)\sin(\theta)e^{i\lambda} \Big) \\
&= \frac{1}{\sin(2\theta)}\Big(- \langle\psi_{\text{good}}| \langle\lambda| (Z_{\Pi_{\text{good}}} \otimes I) V (Z_{\Pi_{\text{good}}} \otimes I) |\psi_{\text{good}}\rangle |\lambda\rangle - \cos(2\theta)\sin(\theta)e^{i\lambda} \Big) \\
&= \frac{1}{\sin(2\theta)}\Big(- \langle\psi_{\text{good}}| \langle\lambda| V |\psi_{\text{good}}\rangle |\lambda\rangle - \cos(2\theta)\sin(\theta)e^{i\lambda} \Big) \\
&= \frac{1}{\sin(2\theta)}\Big(- \sin(\theta)e^{i\lambda} - \cos(2\theta)\sin(\theta)e^{i\lambda} \Big) \\
&= -e^{i\lambda}\cot(\theta)\sin(\theta) = -\cos(\theta)e^{i\lambda} \qquad (11.73)
\end{aligned}$$

Therefore substituting this into our expression and using standard trigonometric identities yields

$$\begin{aligned}
\langle\psi_{\text{good}}| \langle\lambda| W^k V |\psi_{\text{good}}\rangle |\lambda\rangle &= (\cos(2k\theta)\sin(\theta) + \sin(2k\theta)\cos(\theta))e^{i\lambda} \\
&= \sin((2k+1)\theta)e^{i\lambda} = \sin((2k+1)\arcsin(1/\alpha))e^{i\lambda}. \qquad (11.74)
\end{aligned}$$

We therefore have that for any eigenvector of the unitary operator U, $|\lambda\rangle$, and any integer k

$$(\langle\psi_{\text{good}}| \otimes I) W^k V (|\psi_{\text{good}}\rangle \otimes I) |\lambda\rangle = U |\lambda\rangle \sin((2k+1)\arcsin(1/\alpha)). \qquad (11.75)$$

Finally because U is unitary, it has a complete orthonormal eigenbasis. That is to say for any $|\psi\rangle \in \mathbb{C}^{2^n}$, there exist $\{a_j : j = 0 \dots 2^n - 1\}$ such that

$$|\psi\rangle = \sum_j a_j |\lambda_j\rangle . \qquad (11.76)$$

. Further we have that

$$\begin{aligned}
(\langle\psi_{\text{good}}| \otimes I) W^k V (|\psi_{\text{good}}\rangle \otimes I) |\psi\rangle &= \sum_j a_j (\langle\psi_{\text{good}}| \otimes I) W^k V (|\psi_{\text{good}}\rangle \otimes I) |\lambda_j\rangle \\
&= \sum_j a_j U |\lambda_j\rangle \sin((2k+1)\arcsin(1/\alpha)) \\
&= U |\psi\rangle \sin((2k+1)\arcsin(1/\alpha)). \qquad (11.77)
\end{aligned}$$

Thus by linearity oblivious amplitude amplification produces the desired block encoding for any input state, which verifies our lemma. □

The above result shows an important generalization of amplitude amplification wherein we do not need to reflect about the initial state of the algorithm but instead can reflect about a subspace that marks success to apply a block encoding if the desired block encoded matrix is unitary. A limitation of the above claim, however, is that the result does not directly hold if the block encoded matrix is only approximately unitary. The results of Chapter 3 can then be used to show that we do not actually need the result to be precisely unitary for the result to work. This statement of the result is known is robust oblivious amplitude amplification [BCK15]

Corollary 11.13 (Robust Oblivious Amplitude Amplification)**.** *Let $\tilde{V}$ be an $(\alpha, m, 0)$ block encoding of a matrix $\tilde{U} \in \mathbb{C}^{2^n}$ flagged by a projector Π_{good} as given in Definition 11.11 such that there exists $U \in U(2^n)$ with $\|U - \tilde{U}\| \leq \delta$. We then have that the oblivious amplitude amplification walk operator for $\tilde{U}$, $\tilde{W}$, satisfies*

$$\left\| (\langle \psi_{\text{good}}| \otimes I)\tilde{W}^k \tilde{V} (|\psi_{\text{good}}\rangle \otimes I) - \tilde{U} \sin((2k+1)\arcsin(1/\alpha)) \right\| \in \mathcal{O}(k\delta)$$

Proof of this result is left as an exercise.

Exercise 11.2. Provide a proof of Corollary 11.13 using the techniques contained in 3 to perturb the block encodings given above. Refrain from following the direct proof in this exercise given in [BCK15] that directly proves the result from first principles and instead show that the result follows from perturbative arguments.

Exercise 11.3. Let us assume that a hypothetical algorithm existed for performing oblivious amplitude amplification that will yield after $O(k)$ queries to a fundamental unitary a block encoding $U \sin((2k+1)\arcsin(1/\alpha))$ for a non-unitary U.

a) Provide a query efficient quantum algorithm that can prepare for any k-local positive semi-definite Hamiltonian that is efficiently row-computable, H, a zero-error block encoding of state e^{-H} using the proposed amplitude amplification scheme.
b) Show that the existence of this hypothetical amplitude amplification algorithm would imply that $\mathsf{QMA} \subseteq \mathsf{BQP}$

The astute reader may notice that the circuit given in Definition 11.11 for oblivious amplitude amplification looks, up to a global phase, equivalent to the circuits used for qubitization discussed in Chapter 10. This suggests that the analysis of qubitization can be alternatively used to understand how oblivious amplitude amplification works.

The key insight behind our argument is that if the matrix that we block encode is unitary then we can perform a polynomial transformation of the unitary within the space using qubitization to block encode the unitary within a matrix and then transform the block encoding constant of U by rotating it closer to 1. This rotation can be achieved by stems from the relationship between Chebyshev polynomials and trigonometric functions which will ultimately allow us to perform rotations within the two-dimensional block matrix.

Specifically, assume that we have access to a block encoding $V \in \text{BE}_{\gamma,a}(U)$, where $U \in \text{U}(N)$. Then V serves as a $(1, a)$-block encoding of $A = U/\gamma$. When V is applied to a state vector $|\psi\rangle$, the postselected vector is $U|\psi\rangle/\gamma$. If we would like to apply amplitude amplification to boost the success probability, it requires access to a reflection operator with respect to the initial state $|\psi\rangle$. However, since U is unitary, we can achieve this reconstruction without relying on the initial state. This means U can be reconstructed only using multiple applications of V and $V^\dagger$. An advantage of this way of thinking relative to the more traditional argument given above is that it obviates the need to focus on the dynamics of eigenvectors within the two-dimensional space. We then state the result as an application of qubitization below.

Proposition 11.14. *Let $V \in \text{BE}_{\gamma,a}(U)$ for unitary $U \in U(N)$ and $\gamma \geq 1$. Then if we let W be the walk operator of Definition 11.11 corresponding to this choice of V. We then have that for any $k \geq 0$ $W^k V$, as depicted in Fig. 11.4, implements a block encoding of the form*

$$W^k V = \begin{bmatrix} (-1)^k T_{2k+1}(1/\gamma)U & \cdot \\ \cdot & \cdot \end{bmatrix} \tag{11.78}$$

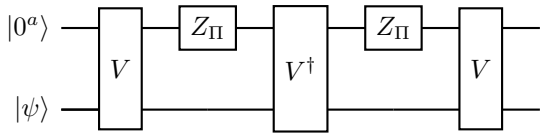


FIGURE 11.4. Circuit for implementing the oblivious amplitude amplification with $V \in \mathrm{BE}_{2,a}(U)$ for a unitary matrix U. This implements $T_3^\diamond(U/2) = -U$.

and specifically if $\gamma^{-1} = \sin\left(\frac{\pi}{2(2k'+1)}\right)$ *for non-negative integer* k' *then*

$$W^{k'}V = \begin{bmatrix} U & 0 \\ 0 & \cdot \end{bmatrix}$$

PROOF. The key observations are (1) the set of singular values of A is a single point $\{\gamma^{-1}\}$, and (2) for any unitary matrix, $U(U^\dagger U) = U$. In particular, the singular value transformation of A using any odd polynomial f satisfies

$$f^\diamond(A) = f(\gamma^{-1})U. \tag{11.79}$$

If we can choose an odd polynomial such that $f(\gamma^{-1}) = \pm 1$, then $f^\diamond(U/\gamma) = \pm U$. This process only uses reflections with respect to the a ancilla qubits used to block encode A, and is oblivious with respect to the initial state.

Next, let us consider applying $f^\diamond = T_{2k+1}$. The Chebyshev polynomial T_{2k+1} is, for $k \in \mathbb{N}$, an odd polynomial function and thus $T_{2k+1}(U/\gamma) = T_{2k+1}(\gamma^{-1})U$ as argued above. We have already shown in Proposition 10.6 that $W^k V$ implements a transformation of the form

$$W^k V = \begin{bmatrix} (-1)^k T_{2k+1}(U/\gamma) & \cdot \\ \cdot & \cdot \end{bmatrix} = \begin{bmatrix} (-1)^k T_{2k+1}(1/\gamma)U & \cdot \\ \cdot & \cdot \end{bmatrix} \tag{11.80}$$

Thus the transformation implements the Chebyshev polynomial transform on $1/\gamma$ as claimed.

Now let us look at the success probability claim. Consider the case $\gamma = 2$ first. Note that the third order Chebyshev polynomial $T_3(x) = 4x^3 - 3x$ satisfies $T_3(\frac{1}{2}) = -1$. So up to a phase we only need to implement $T_3^\diamond(U/\gamma)$, which can be performed using qubitization without invoking LCU, see Fig. 11.4.

What about a more general γ? Fig. 11.5 plots the polynomials and choice of γ^{-1} for $T_{2k+1}(x)$ for $k = 1, 2, 3$ and we can see a pattern from this data that at specific values of $x = 1/\gamma$ the transformation maps to an multiplicative factor of ± 1 for the block encoding. In particular, when $k = 1$, we have $\gamma^{-1} = \sin\frac{\pi}{6} = \frac{1}{2}$ which coincides with the $\gamma = 2$ case considered previously. We can find these special (γ, k) pairs by focusing on odd polynomials, and using the fact that $T_{2k+1}(x) = \cos((2k+1)\arccos(x))$, if γ satisfies, for some $k' \in \mathbb{N}$,

$$\gamma^{-1} = \sin\frac{\pi}{2(2k+1)}. \tag{11.81}$$

Then

$$T_{2k+1}(\gamma^{-1}) = \cos\left((2k+1)\arccos(\gamma^{-1})\right) = \cos\left((2k+1)\left(\frac{\pi}{2} - \frac{\pi}{2(2k+1)}\right)\right) = \cos(k\pi) = (-1)^k. \tag{11.82}$$

Therefore oblivious amplitude amplification can be achieved using qubitization, which implements $(-1)^k T^{\diamond}_{2k+1}(U/\gamma) = U$. This uses $k+1$ queries to V and k queries to $V^\dagger$. □

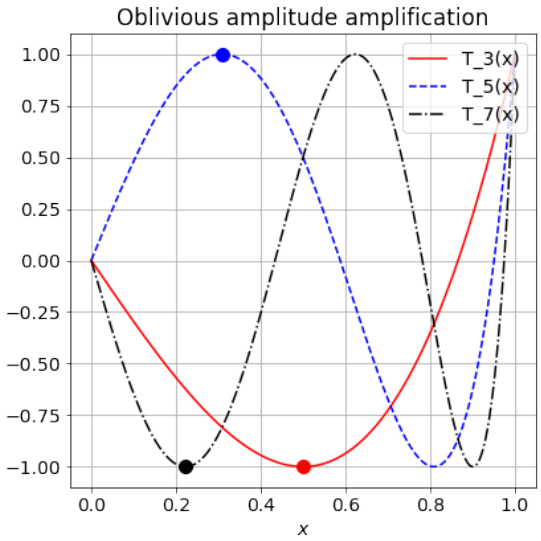


FIGURE 11.5. Chebyshev polynomials (lines) and associated choice of $\gamma^{-1} = \sin(\pi/(2(2k+1)))$ for integer k (filled dots) used for oblivious amplitude amplification.

Notes and further reading

Grover's algorithm [Gro96] achieves a quadratic speedup in query complexity for searching unsorted databases in the black-box model. However, the implications for gate complexity are more nuanced: whether a speedup in query complexity translates into an overall gate-level advantage depends on the cost of implementing the oracle, as well as on the overhead of state preparation and reflection operations. This dependence is model-specific and often function-dependent. A universally recognized instance where Grover-type search yields a clear asymptotic advantage in gate complexity over the best classical approach has not been established so far.

The lower bound in **??** is a hybrid argument showing that $\Omega(\sqrt{N})$ queries are necessary, matching Grover's $\mathcal{O}(\sqrt{N})$ upper bound up to constants. Alternative lower-bound techniques include the polynomial method [BBC+01], which relates query complexity to the degree of a polynomial representing (or approximating) the acceptance probability and connects, for symmetric functions, to classical approximation theory such as [Pat92]. The adversary method provides another approach and admits several equivalent formulations; see [SS04, HLS07].

CHAPTER 12

Quantum signal processing

The linear combination of unitaries and qubitization allow us to express a wide range of matrix computation tasks as matrix polynomial transformations on quantum computers. However, these constructions can incur nontrivial circuit costs, particularly in implementing the prepare and select oracles. Quantum signal processing (QSP) and quantum singular value transformation (QSVT) provide an alternative route by realizing polynomial transformations through a structured product of SU(2) rotations specified by a sequence of phases.

This chapter introduces the QSP part, i.e., a structured product of SU(2) rotations. Along with the representation power of QSP for target polynomials, there are two associated computational tasks. First, given a QSP-admissible target polynomial, one must synthesize the corresponding phase factors. Second, when the goal is to approximate a function on a subinterval of $[0, 1]$, one must design a polynomial that both approximates the target and satisfies the admissibility constraints required by QSP. We describe simple numerical procedures addressing these tasks, including a fixed-point iteration algorithm for finding phase factors, and a convex-optimization approach for constructing near-optimal admissible polynomials. We also illustrate the connection between QSP and the nonlinear Fourier transform on SU(2), and generalization of QSP beyond representing polynomial functions.

12.1. Quantum signal processing

Let $x \in [-1, 1]$ be a scalar with a one-qubit Hermitian block encoding

$$U(x) = \begin{pmatrix} x & \sqrt{1-x^2} \\ \sqrt{1-x^2} & -x \end{pmatrix}. \tag{12.1}$$

Then

$$O(x) = U(x)Z = \begin{pmatrix} x & -\sqrt{1-x^2} \\ \sqrt{1-x^2} & x \end{pmatrix} \tag{12.2}$$

is a rotation matrix.

Consider the following parameterized expression:

$$U_\Phi(x) = e^{i\phi_0 Z} O(x) e^{i\phi_1 Z} O(x) \cdots e^{i\phi_{d-1} Z} O(x) e^{i\phi_d Z}. \tag{12.3}$$

By setting $\phi_0 = \cdots = \phi_d = 0$, we immediately obtain the block encoding of the Chebyshev polynomial $T_d(x)$. The representation power of this formulation is characterized by Theorem 12.1, which is based on slight modification of [GSLW19, Theorem 4]. In the following discussion, even functions have parity 0 and odd functions have parity 1.

THEOREM 12.1 (Quantum signal processing). *There exists a set of* ***phase factors*** $\Phi := (\phi_0, \cdots, \phi_d) \in \mathbb{R}^{d+1}$ *such that*

$$U_\Phi(x) = e^{i\phi_0 Z} \prod_{j=1}^{d} \left[O(x) e^{i\phi_j Z} \right] = \begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ \overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix}, \tag{12.4}$$

if and only if $P, Q \in \mathbb{C}[x]$ *satisfy*

(1) $\deg(P) \le d, \deg(Q) \le d-1$,
(2) P *has parity* $d \bmod 2$ *and* Q *has parity* $d-1 \bmod 2$, *and*
(3) $|P(x)|^2 + (1-x^2)|Q(x)|^2 = 1$ *for all* $x \in [-1,1]$.

Here $\deg Q = -1$ *means* $Q = 0$.

PROOF OF THEOREM 12.1. This theorem is proved by direct computation.

$\Rightarrow$:

Since both $e^{i\phi Z}$ and $O(x)$ are unitary, the matrix $U_\Phi(x)$ is always a unitary matrix, which (together with the structure in Eq. (12.4)) immediately implies the condition (3). Below we only need to verify the conditions (1), (2).

When $d = 0$, $U_\Phi(x) = e^{i\phi_0 Z}$, which gives $P(x) = e^{i\phi_0}$ and $Q = 0$, satisfying all three conditions. For induction, suppose $U_{(\phi_0,\cdots,\phi_{d-1})}(x)$ takes the form in Eq. (12.4) with degree $d-1$, then for any $\phi \in \mathbb{R}$, we have

$$\begin{aligned} U_{(\phi_0,\cdots,\phi_{d-1},\phi)}(x) &= \begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ \overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix} \begin{pmatrix} x & -\sqrt{1-x^2} \\ \sqrt{1-x^2} & x \end{pmatrix} \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix} \\ &= \begin{pmatrix} xP(x) - (1-x^2)Q(x) & -\sqrt{1-x^2}(P(x) + xQ(x)) \\ \sqrt{1-x^2}(\overline{P(x)} + x\overline{Q(x)}) & x\overline{P(x)} - (1-x^2)\overline{Q(x)} \end{pmatrix} \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix} \\ &= \begin{pmatrix} e^{i\phi}(xP(x) - (1-x^2)Q(x)) & -e^{-i\phi}\sqrt{1-x^2}(P(x) + xQ(x)) \\ e^{i\phi}\sqrt{1-x^2}(\overline{P(x)} + x\overline{Q(x)}) & e^{-i\phi}(x\overline{P(x)} - (1-x^2)\overline{Q(x)}) \end{pmatrix}. \end{aligned} \tag{12.5}$$

Therefore $U_{(\phi_0,\cdots,\phi_{d-1},\phi)}(x)$ satisfies conditions (1),(2).

$\Leftarrow$:

When $d = 0$, the only possibility is $P(x) = e^{i\phi_0}$ and $Q = 0$, which satisfies Eq. (12.4).

For $d > 0$, when d is even we may first consider the special case $\deg P = 0$, i.e., $P(x) = e^{i\phi_0}$ and $Q = 0$. In this case, note that

$$O^{-1}(x) = O(x)^\dagger = \begin{pmatrix} x & \sqrt{1-x^2} \\ -\sqrt{1-x^2} & x \end{pmatrix} = e^{-i\frac{\pi}{2}Z} O(x) e^{+i\frac{\pi}{2}Z}, \tag{12.6}$$

we may set $\phi_j = (-1)^j \frac{\pi}{2}$, $j = 1, \ldots, d$, and

$$e^{i\phi_0 Z} \prod_{j=1}^{d} \left[O(x) e^{i\phi_j Z} \right] = e^{i\phi_0 Z} \prod_{k=1}^{\frac{d}{2}} \left[O(x) e^{-i\frac{\pi}{2}Z} O(x) e^{+i\frac{\pi}{2}Z} \right] = e^{i\phi_0 Z} \prod_{k=1}^{\frac{d}{2}} \left[O(x) O(x)^\dagger \right] = e^{i\phi_0 Z}. \tag{12.7}$$

Thus the statement holds.

Now given P, Q satisfying conditions (1)–(3), with $\deg P = \ell > 0$, and $\ell \equiv d \pmod 2$. Then $\deg(|P(x)|^2) = 2\ell > 0$, and according to the condition (3) we must have $\deg(Q) = \ell - 1$. Let P, Q

be expanded as

$$P(x) = \sum_{k=0}^{\ell} \alpha_k x^k, \quad Q(x) = \sum_{k=0}^{\ell-1} \beta_k x^k, \tag{12.8}$$

then the leading term of $|P(x)|^2 + (1-x^2)|Q(x)|^2$ is

$$|\alpha_\ell|^2 x^{2\ell} - x^2 |\beta_{\ell-1}|^2 x^{2\ell-2} = (|\alpha_\ell|^2 - |\beta_{\ell-1}|^2) x^{2\ell} = 0, \tag{12.9}$$

which implies $|\alpha_\ell| = |\beta_{\ell-1}|$, and $\alpha_\ell/\beta_{\ell-1}$ is a complex phase.

For any $\phi \in \mathbb{R}$, we have

$$\begin{aligned}
&\begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ \overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix} e^{-i\phi Z} O(x)^\dagger \\
=&\begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ \overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix} \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} x & \sqrt{1-x^2} \\ -\sqrt{1-x^2} & x \end{pmatrix} \\
=&\begin{pmatrix} e^{-i\phi}xP(x) + (1-x^2)Q(x)e^{i\phi} & -\sqrt{1-x^2}(-e^{-i\phi}P(x) + xQ(x)e^{i\phi}) \\ \sqrt{1-x^2}(-e^{i\phi}\overline{P(x)} + x\overline{Q(x)}e^{-i\phi}) & e^{i\phi}x\overline{P(x)} + (1-x^2)\overline{Q(x)}e^{-i\phi} \end{pmatrix} \\
=:&\begin{pmatrix} \widetilde{P}(x) & -\widetilde{Q}(x)\sqrt{1-x^2} \\ \overline{\widetilde{Q}(x)}\sqrt{1-x^2} & \overline{\widetilde{P}(x)} \end{pmatrix}.
\end{aligned} \tag{12.10}$$

It may appear that $\deg \widetilde{P} = \ell + 1$. However, by properly choosing ϕ we may obtain $\deg \widetilde{P} = \ell - 1$. Let $e^{2i\phi} = \alpha_\ell/\beta_{\ell-1}$. Then the coefficient of the $x^{\ell+1}$ term in $\widetilde{P}$ is

$$e^{-i\phi}\alpha_\ell - e^{i\phi}\beta_{\ell-1} = 0. \tag{12.11}$$

Similarly, the coefficient of the x^ℓ term in $\widetilde{Q}$ is

$$-e^{-i\phi}\alpha_\ell + e^{i\phi}\beta_{\ell-1} = 0. \tag{12.12}$$

The coefficient of the x^ℓ term in $\widetilde{P}$, and the coefficient of the $x^{\ell-1}$ term in $\widetilde{Q}$ are both 0 by the parity condition. So we have

(1) $\deg(\widetilde{P}) \le \ell - 1 \le d - 1, \deg(\widetilde{Q}) \le \ell - 2 \le d - 2$,
(2) $\widetilde{P}$ has parity $d - 1 \bmod 2$ and $\widetilde{Q}$ has parity $d - 2 \bmod 2$, and
(3) $|\widetilde{P}(x)|^2 + (1-x^2)|\widetilde{Q}(x)|^2 = 1, \forall x \in [-1, 1]$.

Here the condition (3) is automatically satisfied due to unitarity. The induction follows until $\ell = 0$, and apply the argument in Eq. (12.7) to represent the remaining constant phase factor if needed. □

Note that the normalization condition (3) in Theorem 12.1 imposes very strong constraints on the coefficients of $P, Q \in \mathbb{C}[x]$. If we are only interested in QSP for real polynomials, the conditions can be significantly relaxed. The following result is a variant of [GSLW19, Corollary 5].

THEOREM 12.2 (Quantum signal processing for real polynomials of definite parity). *Given a real polynomial $F(x) \in \mathbb{R}[x]$ of degree $d > 0$ satisfying*

(1) *F has parity $d \bmod 2$,*
(2) *$|F(x)| \le 1$ for all $x \in [-1, 1]$,*

then there exists polynomials $P(x), Q(x) \in \mathbb{C}[x]$ with $F = \operatorname{Im} P$ and a set of phase factors $\Phi := (\phi_0, \cdots, \phi_d) \in \mathbb{R}^{d+1}$ such that the QSP representation Eq. (12.4) holds.

Compared to Theorem 12.1, the conditions in Theorem 12.2 are much easier to satisfy: given any polynomial $F(x) \in \mathbb{R}[x]$ satisfying condition (1) on parity, we can always scale F to satisfy the condition (2) on its magnitude. Also note that

$$\mathrm{Re}[U_\Phi(x)]_{1,1} = \mathrm{Im}[e^{i\frac{\pi}{4}Z} U_\Phi(x) e^{i\frac{\pi}{4}Z}]_{1,1}. \tag{12.13}$$

Thus $\mathrm{Re}\, P(x) = \mathrm{Re}[U_\Phi(x)]_{1,1}$ can be recovered from the imaginary part by adding $\frac{\pi}{4}$ to both ϕ_0 and ϕ_d. Consequently, the conclusion of Theorem 12.2 also holds if we replace $F = \mathrm{Im}\, P$ by $F = \mathrm{Re}\, P$.

12.2. Symmetric quantum signal processing

There are multiple equivalent ways of stating the QSP parameterization commonly seen in the literature. Let us refer to the convention used in Theorem 12.1 as the **O-convention**, i.e.,

$$U_\Phi(x) = e^{i\phi_0 Z} \prod_{j=1}^{d} \left[O(x) e^{i\phi_j Z} \right], \quad O(x) = \begin{pmatrix} x & -\sqrt{1-x^2} \\ \sqrt{1-x^2} & x \end{pmatrix}. \tag{12.14}$$

We may also use the X-rotation

$$W(x) = e^{-i\frac{\pi}{4}Z} O(x) e^{+i\frac{\pi}{4}Z} = \begin{pmatrix} x & i\sqrt{1-x^2} \\ i\sqrt{1-x^2} & x \end{pmatrix} = e^{i \arccos(x) X}, \tag{12.15}$$

and express the QSP parameterization as

$$U_{\Phi W}(x) = e^{i\phi_0^W Z} \prod_{j=1}^{d} \left[W(x) e^{i\phi_j^W Z} \right] = \begin{pmatrix} P(x) & iQ(x)\sqrt{1-x^2} \\ i\overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix}. \tag{12.16}$$

This is referred to as the **W-convention**. There is a simple relation connecting between the phase factors using the O and W

$$\phi_j = \begin{cases} \phi_0^W - \frac{\pi}{4}, & j = 0, \\ \phi_j^W, & j = 1, \dots, d-1, \\ \phi_d^W + \frac{\pi}{4}, & j = d. \end{cases} \tag{12.17}$$

If we are interested in a real polynomial $F(x) \in \mathbb{R}[x]$ of degree d, due to the parity constraint, F can be expanded in the Chebyshev basis as

$$F(x) = \begin{cases} \sum_{j=0}^{\widetilde{d}-1} c_j T_{2j}(x), & F \text{ is even}, \\ \sum_{j=0}^{\widetilde{d}-1} c_j T_{2j+1}(x), & F \text{ is odd}. \end{cases} \tag{12.18}$$

Here $\widetilde{d} = \lceil \frac{d+1}{2} \rceil$, and $c = (c_0, c_1, \dots, c_{\widetilde{d}-1}) \in \mathbb{R}^{\widetilde{d}}$ is the Chebyshev coefficient vector. Thus the number of effective degrees of freedom in F is only $\widetilde{d}$. How to reconcile this with the $d+1$ degrees of freedom in the phase factors?

The QSP sequence in the W-convention offers a clue to this question. Since W is a complex symmetric matrix, i.e., $W = W^\top$, from Eq. (12.16) we have

$$U_{\Phi W}^\top(x) = e^{i\phi_d^W Z} \prod_{j=1}^{d} \left[W(x) e^{i\phi_{d-j}^W Z} \right], \tag{12.19}$$

i.e., the transpose of $U_{\Phi W}(x)$ can be obtained by reversing the order of the phase factors. In QSP applications we often do not care about Q, so if we choose Q to be a real polynomial, then the

matrix $U_{\Phi w}(x)$ is complex symmetric, i.e., $U_{\Phi w}(x) = U_{\Phi w}(x)^\top$. This means that the phase factors may also be chosen symmetrically:

$$\phi_j^W = \phi_{d-j}^W, \quad \forall j = 0, 1, \cdots, d. \tag{12.20}$$

With the symmetry condition, the number of effective degrees of freedom in phase factors is equal to $\widetilde{d} = \lceil \frac{d+1}{2} \rceil$, and matches that in F.

Example 12.3. Consider the all-zero phase factors in the W-convention $\Phi^W = (0, \ldots, 0) \in \mathbb{R}^{d+1}$. Direct calculation shows the upper-left entry of $U_{\Phi w}(x)$ is the Chebyshev polynomial $P(x) = T_d(x)$. The corresponding O-convention is $\Phi = (-\pi/4, 0, \ldots, 0, \pi/4)$. Now let $\Phi^W = (\pi/4, 0, \ldots, 0, \pi/4) \in \mathbb{R}^{d+1}$. The upper-left entry of $U_{\Phi w}(x)$ becomes $P(x) = iT_d(x)$. The corresponding O-convention is $\Phi = (0, 0, \ldots, 0, \pi/2)$. ◇

Example 12.4. A linear combination of Chebyshev polynomials $F(x) = 0.2T_1(x) + 0.4T_3(x)$ can be encoded using phase factors $\Phi^W = (1.3622, -0.1132, -0.1132, 1.3622)$, so that $F(x) = \mathrm{Im}[U_{\Phi w}(x)]_{1,1}$. ◇

The results below guarantee that, under the assumption that Q is a real polynomial, the symmetry restriction is without loss of generality and yields a unique phase vector in a canonical domain.

THEOREM 12.5 (Existence and uniqueness of symmetric phase factors, W-convention). *Consider any $P \in \mathbb{C}[x]$ and $Q \in \mathbb{R}[x]$ satisfying the following conditions.*

1. $\deg(P) = d$ *and* $\deg(Q) = d - 1$.
2. P *has parity* $(d \bmod 2)$ *and* Q *has parity* $(d - 1 \bmod 2)$.
3. $|P(x)|^2 + (1 - x^2)|Q(x)|^2 = 1$ *for all* $x \in [-1, 1]$.
4. *If* d *is odd, then the leading coefficient of* Q *is positive.*

Then there exists a ***unique*** *set of symmetric phase factors*

$$\Phi^W := (\phi_0^W, \phi_1^W, \cdots, \phi_d^W) \in D_d, \tag{12.21}$$

where Φ^W *is symmetric in the sense of Eq.* (12.20) *and*

$$D_d := \begin{cases} [-\frac{\pi}{2}, \frac{\pi}{2})^{\frac{d}{2}} \times [-\pi, \pi) \times [-\frac{\pi}{2}, \frac{\pi}{2})^{\frac{d}{2}}, & d \text{ is even}, \\ [-\frac{\pi}{2}, \frac{\pi}{2})^{d+1}, & d \text{ is odd}, \end{cases} \tag{12.22}$$

such that

$$U_{\Phi w}(x) = e^{i\phi_0^W Z} \prod_{j=1}^{d} \left[W(x) e^{i\phi_j^W Z} \right] = \begin{pmatrix} P(x) & iQ(x)\sqrt{1-x^2} \\ iQ(x)\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix}. \tag{12.23}$$

For real polynomials, the symmetric version of the theorem that is parallel to Theorem 12.2 is as follows.

Corollary 12.6 (Symmetric quantum signal processing for real polynomials, W-convention)**.** *Given a real polynomial* $F(x) \in \mathbb{R}[x]$ *of degree* d *satisfying*

1. F *has parity* $d \bmod 2$,
2. $|F(x)| \leq 1$ *for all* $x \in [-1, 1]$,

then there exists polynomials $G(x), Q(x) \in \mathbb{R}[x]$ *and a set of symmetric phase factors* $\Phi^W := (\phi_0^W, \phi_1^W, \cdots, \phi_d^W) \in \mathbb{R}^{d+1}$ *satisfying Eq.* (12.20) *such that the following QSP representation holds:*

$$U_{\Phi^W}(x) = e^{i\phi_0^W Z} \prod_{j=1}^{d} \left[W(x) e^{i\phi_j^W Z} \right] = \begin{pmatrix} G(x) + iF(x) & iQ(x)\sqrt{1-x^2} \\ iQ(x)\sqrt{1-x^2} & G(x) - iF(x) \end{pmatrix}. \tag{12.24}$$

12.3. Fixed-point iteration algorithm for finding phase factors

According to Eq. (12.18), a target polynomial for quantum signal processing $F \in \mathbb{R}[x]$ of degree d only has $\widetilde{d} = \lceil \frac{d+1}{2} \rceil$ effective degrees of freedom characterized by the Chebyshev coefficient vector $c = (c_0, c_1, \ldots, c_{\widetilde{d}-1}) \in \mathbb{R}^{\widetilde{d}}$.

Given the discussion in Section 12.2, we focus on finding symmetric phase factors Φ^W for a target polynomial of definite parity. We can define the associated **reduced phase factors** as

$$\Phi^R = (\phi_0^R, \phi_1^R, \ldots, \phi_{\widetilde{d}-1}^R) := \begin{cases} (\frac{1}{2}\phi_{\widetilde{d}-1}^W, \phi_{\widetilde{d}}^W, \cdots, \phi_d^W), & d \text{ is even}, \\ (\phi_{\widetilde{d}}^W, \phi_{\widetilde{d}+1}^W, \cdots, \phi_d^W), & d \text{ is odd}. \end{cases} \tag{12.25}$$

Under the symmetry condition Eq. (12.20) (and the canonical domain in Theorem 12.5), Φ^R uniquely determines Φ^W. The reason why the reduced phase factors start from the middle is that the phase factors tend to be large in the middle and decay to zero towards the ends (see Fig. 12.1).

Let $\mathscr{F} : \mathbb{R}^{\widetilde{d}} \to \mathbb{R}^{\widetilde{d}}$ denote the mapping from reduced phase factors $\Phi^R \in \mathbb{R}^{\widetilde{d}}$ (equivalently, from the associated symmetric phase factors Φ^W) to the Chebyshev coefficient vector $c \in \mathbb{R}^{\widetilde{d}}$ of the target polynomial $F(x)$ defined by $F(x) = \mathrm{Im}[U_{\Phi^W}(x)]_{1,1}$. The problem of finding phase factors in QSP is to solve the inverse problem: given $c \in \mathbb{R}^{\widetilde{d}}$ such that the associated real polynomial $F(x)$ satisfies the norm constraint in Corollary 12.6, find Φ^R such that $\mathscr{F}(\Phi^R) = c$.

There are many algorithms for finding phase factors. Here we present perhaps the simplest algorithm, called the **fixed-point iteration algorithm** (FPI). We start from a trivial reduced phase factors

$$\Phi^{R,(0)} = (0, 0, \ldots, 0) \in \mathbb{R}^{\widetilde{d}}. \tag{12.26}$$

The findings of Example 12.3 can be stated as that

$$\mathscr{F}(\Phi^{R,(0)}) = \mathbf{0} \in \mathbb{R}^{\widetilde{d}}, \tag{12.27}$$

i.e., $\mathscr{F}$ maps $\Phi^{R,(0)}$ to the all zero Chebyshev coefficients. Furthermore, the factor $\frac{1}{2}$ in Eq. (12.25) ensures that the Jacobian matrix of $\mathscr{F}$ at $\Phi^{R,(0)}$ is the scaled identity matrix, i.e., $\nabla\mathscr{F}(\Phi^{R,(0)}) = 2I_{\widetilde{d}}$.

Then given $c \in \mathbb{R}^{\widetilde{d}}$, starting from $\Phi^{R,(0)}$, the FPI algorithm is given in Algorithm 12.1. Conceptually, it only involves one line:

$$\Phi^{R,(\ell+1)} = \Phi^{R,(\ell)} - \left(\nabla\mathscr{F}(\Phi^{R,(0)}) \right)^{-1} \left(\mathscr{F}\left(\Phi^{R,(\ell)}\right) - c \right) = \Phi^{R,(\ell)} - \frac{1}{2}\left(\mathscr{F}\left(\Phi^{R,(\ell)}\right) - c \right), \quad \ell \in \mathbb{N}. \tag{12.28}$$

Ref. [DLNW24a] proves that the FPI method converges exponentially to one solution (called the maximal solution) when $\|c\|_1 \leq 0.861$.

Example 12.7. Consider $F(x) = \frac{1}{2}\cos(10x)$. We can first approximate the function by an even polynomial $p(x)$ using Chebyshev interpolation, and then use the fixed-point iteration (FPI) algorithm in Algorithm 12.1 to find symmetric phase factors Φ^W such that $\mathrm{Im}[U_{\Phi^W}(x)]_{1,1} = p(x)$.

Algorithm 12.1 Fixed-point iteration algorithm for finding reduced phase factors for a real polynomial with definite parity

Input: Chebyshev-coefficient vector c of a target polynomial, and stopping criteria.
Initialize $\Phi^{R,(0)} = (0, \ldots, 0)$, $\ell = 0$.
while stopping criterion is not satisfied **do**
  Update $\Phi^{R,(\ell+1)} \leftarrow \Phi^{R,(\ell)} - \frac{1}{2}\left(\mathscr{F}\left(\Phi^{R,(\ell)}\right) - c\right)$;
  Set $\ell \leftarrow \ell + 1$.
end while
Output: Reduced phase factors Φ^R.

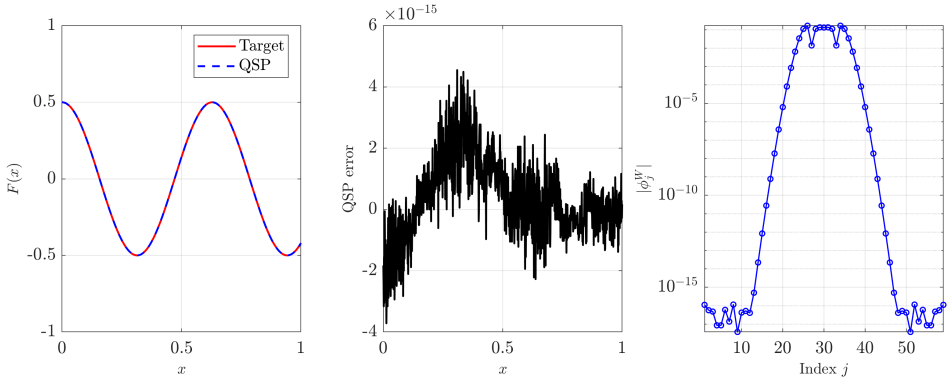


FIGURE 12.1. QSP representation of $F(x) = \frac{1}{2}\cos(10x)$ using an even polynomial $p(x)$ of degree 60. Left: the target function and the QSP representation of $p(x)$. Middle: Error between $p(x)$ and its QSP representation. Right: phase factors plotted on a log scale.

Fig. 12.1 shows one such polynomial of degree 60. The QSP error (defined as the difference between the QSP representation and $p(x)$) approaches machine precision. The phase factors are symmetric with respect to the center of the interval and decay rapidly away from the center.

◇

12.4. Convex optimization-based method for constructing approximate polynomials

The fixed-point iteration method in Section 12.3 converts a QSP-admissible target polynomial into a phase sequence. We now discuss a complementary task: how to construct, for a given function g, an approximately optimal polynomial F that both approximates g on a prescribed set and satisfies the QSP admissibility constraint $|F(x)| \leq 1$.

Many applications of QSP (and, more generally, QSVT) aim to approximate a real function $g(x)$ of definite parity on a set $\mathcal{I} \subseteq [0, 1]$. Fix a polynomial degree d and define $\widetilde{d} := \lceil \frac{d+1}{2} \rceil$. According to Eq. (12.18), a real polynomial $F \in \mathbb{R}[x]$ of degree at most d with parity $d \bmod 2$ is

specified by its Chebyshev coefficient vector $c = (c_0, c_1, \ldots, c_{\widetilde{d}-1}) \in \mathbb{R}^{\widetilde{d}}$ via

$$F(x) = \sum_{j=0}^{\widetilde{d}-1} A_j(x) c_j, \tag{12.29}$$

where

$$A_j(x) = \begin{cases} T_{2j}(x), & d \text{ is even}, \\ T_{2j+1}(x), & d \text{ is odd}. \end{cases} \tag{12.30}$$

Conceptually, the coefficient vector c can be obtained by solving the following min-max optimization problem,

$$\begin{aligned} \min_{c \in \mathbb{R}^{\widetilde{d}}} \quad & \max_{x \in \mathcal{I}} |F(x) - g(x)| \\ \text{s.t.} \quad & F(x) = \sum_{j=0}^{\widetilde{d}-1} A_j(x) c_j, \quad |F(x)| \le 1, \quad \forall x \in [0,1]. \end{aligned} \tag{12.31}$$

Since F has definite parity, the constraint $|F(x)| \le 1$ on $[0,1]$ is equivalent to the corresponding constraint on $[-1,1]$. The objective function is convex in c and the constraint is linear in c. So this is a convex optimization problem. In fact, after introducing a slack variable denoted by z, the optimization problem becomes

$$\begin{aligned} \min_{c \in \mathbb{R}^{\widetilde{d}}} \quad & z \\ \text{s.t.} \quad & F(x) = \sum_{j=0}^{\widetilde{d}-1} A_j(x) c_j, \quad \forall x \in [0,1], \\ & F(x) \le 1, \quad \forall x \in [0,1], \\ & -F(x) \le 1, \quad \forall x \in [0,1], \\ & F(x) - g(x) \le z, \quad \forall x \in \mathcal{I}, \\ & g(x) - F(x) \le z, \quad \forall x \in \mathcal{I}. \end{aligned} \tag{12.32}$$

This is a linear programming problem. After discretization, it can be efficiently solved on a classical computer using standard convex optimization solvers.

In practice, we discretize Eq. (12.31) as follows. Without loss of generality, $\mathcal{I}$ takes the form of a union of intervals $\bigcup_{\ell=1}^{L} [a_\ell, b_\ell]$ with $0 \le a_1 < b_1 < a_2 < b_2 < \cdots < a_L < b_L \le 1$. Let $\mathcal{K}_{\mathcal{I}}$ be a set of grid points in $\mathcal{I}$, and let $\mathcal{K}_{\overline{\mathcal{I}}}$ be a set of grid points in the complement $\overline{\mathcal{I}} := [0,1] \backslash \mathcal{I}$ (which may be empty if $\mathcal{I} = [0,1]$). Since the bound constraint is enforced only on a finite grid, we generally have

$$\max_{x \in [0,1]} |F(x)| \ge \max_{x \in \mathcal{K}_{\mathcal{I}} \cup \mathcal{K}_{\overline{\mathcal{I}}}} |F(x)| \,. \tag{12.33}$$

To avoid overshooting, we assume $|g(x)| \le 1 - \eta$ for all $x \in \mathcal{I}$ and enforce $|F(x)| \le 1 - \eta$ on $\mathcal{K}_{\mathcal{I}} \cup \mathcal{K}_{\overline{\mathcal{I}}}$.

The discretized min-max optimization problem becomes

$$\begin{aligned} &\min_{c\in\mathbb{R}^{\widetilde{d}}} \quad \max_{x\in\mathcal{K}_{\mathcal{I}}} |F(x)-g(x)| \\ &\text{s.t.} \quad F(x)=\sum_{j=0}^{\widetilde{d}-1} A_j(x)c_j, \quad |F(x)|\le 1-\eta, \quad \forall x\in\mathcal{K}_{\mathcal{I}}\cup\mathcal{K}_{\overline{\mathcal{I}}}. \end{aligned} \tag{12.34}$$

For instance, using the CVXPY software package [GB14, DB16], the optimization problem can be solved with a few lines. Here the matrix A_{ij} evaluates $A_j(x_i)$ for $x_i \in \mathcal{K}_{\mathcal{I}} \cup \mathcal{K}_{\overline{\mathcal{I}}}$, and `I` is an index set referring to the set of grid points in $\mathcal{K}_{\mathcal{I}}$.

```
c = cp.Variable(n_degree)
f = cp.Variable(n_grid)
objective = cp.Minimize(cp.norm(f[I] - g[I], inf))
constraints = [f == A @ c,  f >= -(1-eta), f <= (1-eta)]
problem = cp.Problem(objective, constraints)
problem.solve()
```

12.5. Examples of quantum signal processing

In this section we consider two examples illustrating the workflow above. They will be used in Section 13.4.

12.5.1. Approximate sign function. We would like to approximate the sign function $\mathrm{sgn}(x)$ on $[-1,-\delta]\cup[\delta,1]$ by an odd polynomial, while keeping $|p(x)|\le 1$ on $[-1,1]$. We may use the following analytic construction (see [LC17a, Corollary 6] and [GSLW18, Lemma 25]). The proof of Lemma 12.8 is constructive.

Lemma 12.8 (Polynomial approximation to the sign function $\mathrm{sgn}(x)$)**.** *For any $\delta\in(0,1]$ and $\epsilon\in(0,\frac{1}{2})$, there exists an odd polynomial $p\in\mathbb{R}[x]$ of degree $d=\mathcal{O}\big(\frac{1}{\delta}\log(1/\epsilon)\big)$ that satisfies*

$$\sup_{x\in[\delta,1]} |p(x)-\mathrm{sgn}(x)|\le\epsilon, \qquad \sup_{x\in[-1,1]}|p(x)|\le 1. \tag{12.35}$$

Proof sketch. We first use the error function $\mathrm{erf}(kx)$ with $k=\mathcal{O}\big(\delta^{-1}\sqrt{\log(1/\epsilon)}\big)$ to approximate $\mathrm{sgn}(x)$ on $[-1,-\delta]\cup[\delta,1]$ to precision ϵ. We then estimate the accuracy of the Chebyshev approximation to this error function and multiply by a scaling factor to satisfy the bound constraint. □

From the convex optimization viewpoint, we may seek an odd polynomial F that approximates

$$g(x)=1, \quad x\in\mathcal{I}=[\delta,1]. \tag{12.36}$$

Fig. 12.2 compares the approximation error for the task of sign function approximation with $\delta=0.2$. The L^∞ errors measured on $[\delta,1]$ are comparable between the polynomial approximation derived using an analytic formula (through the constructive proof of Lemma 12.8) with degree 51, and the polynomial approximation from the convex optimization method with degree 31. We find that the convex optimization method can achieve a smaller error with a lower polynomial degree, which is not surprising since the optimization method directly minimizes the approximation error.

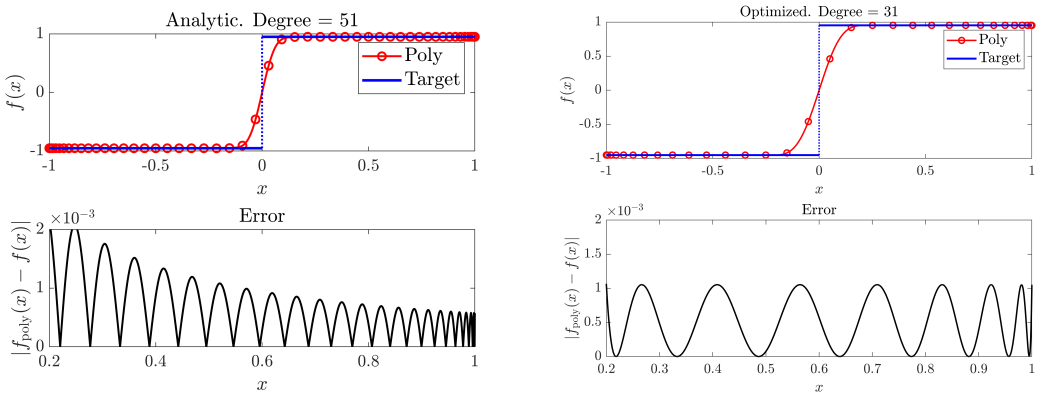


FIGURE 12.2. Comparison between polynomial approximations to the sign function on $[\delta, 1]$ using the analytic formula and convex optimization. Here $\delta = 0.2$.

12.5.2. Approximate truncated linear function. We consider an odd polynomial approximation to

$$g(x) = \alpha x, \quad x \in \mathcal{I} = [0, \alpha^{-1}]. \tag{12.37}$$

At first sight, this task seems trivial: the first-order polynomial $F(x) = \alpha x$ is odd and equals $g(x)$ exactly. However, αx violates the bound constraint on $[\alpha^{-1}, 1]$. It turns out that the polynomial must be more complicated in order to approximate a linear function as closely as possible on a subinterval, while satisfying the bound constraint on a larger interval. The proof of Lemma 12.9 is constructive, and we give a proof sketch here. We refer readers to [GSLW18, Lemma 29] and [LC17a, Corollary 8] for details.

Lemma 12.9 (Polynomial approximation to the truncated linear function)**.** *For any $\alpha \in (1, \infty)$, $\delta \in (0, 1]$, and $\epsilon \in (0, 1/(2\alpha))$, there exists an odd polynomial $p \in \mathbb{R}[x]$ of degree $d = \mathcal{O}\big(\frac{\alpha}{\delta} \log(\alpha/\epsilon)\big)$ such that*

$$\sup_{x \in [0, \alpha^{-1}]} |(1+\delta)p(x) - \alpha x| \le \epsilon, \qquad \sup_{x \in [-1,1]} |p(x)| \le 1. \tag{12.38}$$

PROOF SKETCH. Using Lemma 12.8, we can construct a real polynomial $q(x)$ that approximates $\operatorname{sgn}(x)$ away from a small neighborhood of the origin at scale $\alpha^{-1}\delta$. Then the **even** polynomial

$$r(x) = \frac{q(x + \alpha^{-1}(1+\delta/2)) + q(\alpha^{-1}(1+\delta/2) - x)}{2}, \tag{12.39}$$

approximates a rectangular function supported on an interval of length $\mathcal{O}(\alpha^{-1})$,

$$g_{\mathrm{R},\alpha,\delta}(x) = \begin{cases} 1, & x \in [-\alpha^{-1}(1+\delta/2), \alpha^{-1}(1+\delta/2)], \\ 0, & \text{otherwise}, \end{cases} \tag{12.40}$$

on $\mathcal{I} = [0, \alpha^{-1}] \cup [\alpha^{-1}(1+\delta), 1]$. The target precision is $\epsilon' := \epsilon/\alpha$, and the polynomial degree is $d = \mathcal{O}\big(\frac{\alpha}{\delta} \log(\alpha/\epsilon)\big)$. The desired polynomial is obtained by setting $p(x) = \frac{\alpha x}{1+\delta} r(x)$. Therefore $(1+\delta)p(x)$ approximates αx on $[0, \alpha^{-1}]$ to precision ϵ. To satisfy the bound constraint $\sup_{x \in [-1,1]} |p(x)| \le 1$, one may include an additional scaling (at the level of $1 + \mathcal{O}(\epsilon)$) to avoid overshooting. □

Fig. 12.3 compares the approximation error with $\alpha = 5, \delta = 0.05$. The L^∞ error measured on $[0, \alpha^{-1}]$ are comparable between the polynomial approximation derived using an analytic formula (through the constructive proof of Lemma 12.9) with degree 1001, and the polynomial approximation from the convex optimization method with degree 51. We find that the convex optimization method can achieve a smaller error with a much lower polynomial degree. Furthermore, we find the polynomial approximation from the convex optimization method is much more oscillatory on $[\alpha^{-1}, 1]$ than the one from the analytic formula, which is perfectly acceptable since the approximation error is only measured on $[0, \alpha^{-1}]$.

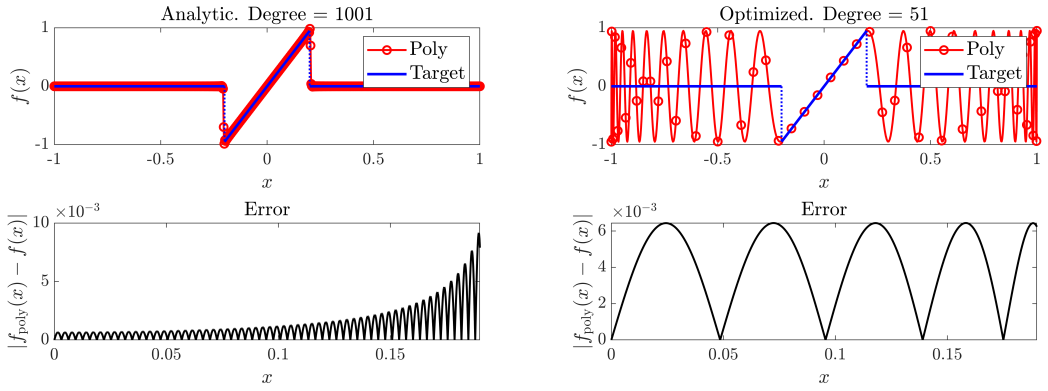


FIGURE 12.3. Comparison between polynomial approximations to x/a on $[0, a]$ using the analytic formula and convex optimization. Here $a = \alpha^{-1} = 0.2$, $\delta = 0.05$

This transformation has found great use in differential equations, wherein the ability to amplify the block encoding constant of a differential operator allows the exponentially decaying success probability of conventional LCU approaches to be boosted to near unit block encoding constants [FLT23].

12.6. Quantum signal processing and nonlinear Fourier transform on SU(2)

The key idea of QSP is that polynomial expressions, which are naturally built from addition and multiplication, can be represented through a structured product of matrices. This can be viewed as a special case of the **nonlinear Fourier transform** (NLFT), which replaces the addition operation in the linear Fourier transform with matrix multiplication.

In this section we introduce the NLFT on SU(2) in its simplest form. Given two integers $m < n$, let $\boldsymbol{\gamma} = (\gamma_m, \dots, \gamma_n)$ be a complex-valued sequence. Its entries are called the nonlinear Fourier coefficients. The nonlinear Fourier transform of $\boldsymbol{\gamma}$ is defined as a finite product of matrix-valued functions,

$$\widehat{\boldsymbol{\gamma}}(z) := \prod_{k=m}^{n} \left[\frac{1}{\sqrt{1 + |\gamma_k|^2}} \begin{pmatrix} 1 & \gamma_k z^k \\ -\overline{\gamma_k} z^{-k} & 1 \end{pmatrix} \right] = \begin{pmatrix} a(z) & b(z) \\ * & * \end{pmatrix}, \quad z \in \mathbb{C}. \tag{12.41}$$

The upper left entry $a(z)$ and upper right entry $b(z)$ are in general not polynomials but Laurent polynomials, i.e., they can contain both positive and negative powers of z.

Taking the determinant of the matrix factors appearing in Eq. (12.41), we see that the determinant of each factor, and hence also of $\widehat{\boldsymbol{\gamma}}(z)$, is 1 everywhere. Moreover, when z is restricted to the unit circle denoted by $\mathbb{T}$, the matrix factors are elements of SU(2), and thus so is $\widehat{\boldsymbol{\gamma}}(z)$.

When $\sum_{k=m}^{n} |\gamma_k|$ is small, the NLFT of $\boldsymbol{\gamma}$ can be approximated by its linear approximation,

$$\widehat{\boldsymbol{\gamma}}(z) \approx \begin{pmatrix} 1 & \sum_{k=m}^{n} \gamma_k z^k \\ -\sum_{k=m}^{n} \overline{\gamma_k} z^{-k} & 1 \end{pmatrix}. \tag{12.42}$$

Therefore, the standard Fourier series can be viewed as the leading order contribution to the upper-right entry of $\widehat{\boldsymbol{\gamma}}(z)$, where the coefficients γ_k are sufficiently small that higher-order terms in the product expansion can be neglected. When the coefficients γ_k are not small, the difference between the two quantities can become significant. The transformation from $\boldsymbol{\gamma}$ to $\widehat{\boldsymbol{\gamma}}$ is called the forward NLFT, and the mapping from $\widehat{\boldsymbol{\gamma}}$ back to $\boldsymbol{\gamma}$ is called the inverse NLFT.

Proposition 12.10 (Connection between QSP and NLFT)**.** *For any $d \in \mathbb{N}$ and $\Phi^W := (\phi_0^W, \phi_1^W, \cdots, \phi_d^W)$ in the W-convention with $\phi_k^W \in (-\pi/2, \pi/2)$, define the sequence $\boldsymbol{\gamma} = (\gamma_k)_{k=0}^d$ with $\gamma_k := \tan \phi_k^W$. Then for all $\theta \in [0, \pi]$ we have*

$$S\,\mathrm{H}\; U_{\Phi w}(\cos\theta)\; \mathrm{H}\, S^\dagger = \widehat{\boldsymbol{\gamma}}(e^{2i\theta}) \begin{pmatrix} e^{id\theta} & 0 \\ 0 & e^{-id\theta} \end{pmatrix}, \tag{12.43}$$

where $U_{\Phi w}$ is defined in Eq. (12.16) with $x = \cos\theta$, H is the Hadamard gate, and S is the phase gate.

Furthermore, $\mathrm{Im}[P(\cos\theta)] = \mathrm{Re}\big(b(e^{2i\theta})e^{-id\theta}\big)$*, where P is the upper-left entry of $U_{\Phi w}$ (as in Eq. (12.16)), and b is the upper-right entry of $\widehat{\boldsymbol{\gamma}}$ as in Eq. (12.41).*

Proof. Recall that $\mathrm{H}\,Z\,\mathrm{H} = X$ and $\mathrm{H}\,X\,\mathrm{H} = Z$. Set $x = \cos\theta$. Define $\widetilde{W}(x) := \mathrm{H}\,W(x)\,\mathrm{H}$. Since $\cos\theta = x$, we have

$$\widetilde{W}(x) = \mathrm{H}\,W(x)\,\mathrm{H} = \mathrm{H}\,e^{i\theta X}\,\mathrm{H} = e^{i\theta Z}. \tag{12.44}$$

Since S commutes with Z, it follows that $S\widetilde{W}(x)S^\dagger = \widetilde{W}(x)$. Together with the definition of γ_k, this implies

$$S\,\mathrm{H}\,e^{i\phi_k^W Z}\,\mathrm{H}\,S^\dagger = Se^{i\phi_k^W X}S^\dagger = e^{i\phi_k^W Y} = \frac{1}{\sqrt{1+|\gamma_k|^2}} \begin{pmatrix} 1 & \gamma_k \\ -\overline{\gamma_k} & 1 \end{pmatrix}, \;\; k = 0, \ldots, d. \tag{12.45}$$

Next, the left-hand sides of Eq. (12.43) equate to $S\,\mathrm{H}\,U_{\Phi w}(\cos\theta)\,\mathrm{H}\,S^\dagger$, which we can also express in the following ordered product form using Eqs. (12.44) and (12.45):

$$S\,\mathrm{H}\,U_{\Phi w}(\cos\theta)\,\mathrm{H}\,S^\dagger = \frac{1}{\sqrt{1+|\gamma_0|^2}} \begin{pmatrix} 1 & \gamma_0 \\ -\overline{\gamma_0} & 1 \end{pmatrix} \prod_{k=1}^{d} \left[e^{i\theta Z} \frac{1}{\sqrt{1+|\gamma_k|^2}} \begin{pmatrix} 1 & \gamma_k \\ -\overline{\gamma_k} & 1 \end{pmatrix} \right]. \tag{12.46}$$

Finally, notice the following identity, for any $t \in \mathbb{R}$:

$$\begin{pmatrix} e^{i\theta t} & 0 \\ 0 & e^{-i\theta t} \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ -\overline{\gamma_k} & 1 \end{pmatrix} = \begin{pmatrix} 1 & \gamma_k e^{2i\theta t} \\ -\overline{\gamma_k} e^{-2i\theta t} & 1 \end{pmatrix} \begin{pmatrix} e^{i\theta t} & 0 \\ 0 & e^{-i\theta t} \end{pmatrix}, \tag{12.47}$$

which allows us to simplify the right-hand side of Eq. (12.46) to obtain

$$S\,\mathrm{H}\,U_{\Phi w}(\cos\theta)\,\mathrm{H}\,S^\dagger = \left(\prod_{k=0}^{d}\left[\frac{1}{\sqrt{1+|\gamma_k|^2}}\begin{pmatrix}1 & \gamma_k e^{2ik\theta}\\ -\overline{\gamma_k}e^{-2ik\theta} & 1\end{pmatrix}\right]\right)\begin{pmatrix}e^{id\theta} & 0\\ 0 & e^{-id\theta}\end{pmatrix} \tag{12.48}$$
$$= \widetilde{\boldsymbol{\gamma}}(e^{2i\theta})\begin{pmatrix}e^{id\theta} & 0\\ 0 & e^{-id\theta}\end{pmatrix}.$$

This is exactly Eq. (12.43). Furthermore, writing $\sin\theta = \sqrt{1-x^2}$ and using Eq. (12.16), a direct computation gives

$$S\,\mathrm{H}\,U_{\Phi w}(\cos\theta)\,\mathrm{H}\,S^\dagger = \begin{pmatrix}* & \mathrm{Im}[P(\cos\theta)] - i\,\mathrm{Im}[Q(\cos\theta)]\sin\theta\\ * & *\end{pmatrix}. \tag{12.49}$$

While the right-hand side of Eq. (12.43) is

$$\begin{pmatrix}* & b(e^{2i\theta})e^{-id\theta}\\ * & *\end{pmatrix}.$$

By comparing the real part of the upper right element and using Eq. (12.49), we conclude that $\mathrm{Im}[P(\cos\theta)] = \mathrm{Re}\big(b(e^{2i\theta})e^{-id\theta}\big)$. □

Based on Proposition 12.10, we see that computing the phase factors can be reduced to an inverse NLFT problem. In particular, if we are interested in solving QSP phase factors for $F(x) = \mathrm{Im}[P(x)]$, one may seek an SU(2)-valued function $\widetilde{\boldsymbol{\gamma}}(z)$ on $\mathbb{T}$ whose upper-right entry $b(z)$ satisfies $F(\cos\theta) = \mathrm{Re}\big(b(e^{2i\theta})e^{-id\theta}\big)$, recover the nonlinear Fourier coefficients $\boldsymbol{\gamma}$ via the inverse NLFT, and then obtain the phase factors by $\phi_k^W = \arctan(\gamma_k)$.

12.7. Infinite quantum signal processing

So far the discussion of QSP has been focused on polynomial functions. The problem of **infinite quantum signal processing** (iQSP) asks whether the QSP representation can be extended to non-polynomial functions f through a product of countably many unitary matrices. NLFT provides a satisfactory answer to this question. For simplicity, we focus on the case of real-valued even functions defined on $[0,1]$.

The convention for the integral on the unit circle $\mathbb{T}$ is

$$\int_{\mathbb{T}} g := \frac{1}{2\pi}\int_0^{2\pi} g(e^{i\theta})\,\mathrm{d}\theta. \tag{12.50}$$

If a real-valued measurable even function $f : [0,1] \to \mathbb{R}$ can be expressed as

$$f(\cos\theta) = g(e^{i\theta}), \quad \forall\theta \in [0, 2\pi), \tag{12.51}$$

for some function g defined on $\mathbb{T}$, then the **Szegő norm** of f, denoted $\|f\|_{\mathbf{S}}$, can be defined as the L^2 norm of g on $\mathbb{T}$:

$$\int_{\mathbb{T}} |g|^2 := \frac{1}{2\pi}\int_0^{2\pi} |f(\cos\theta)|^2\,\mathrm{d}\theta = \frac{2}{\pi}\int_0^1 |f(x)|^2\,\frac{\mathrm{d}x}{\sqrt{1-x^2}} := \|f\|_{\mathbf{S}}^2\,. \tag{12.52}$$

A real-valued measurable even function $f : [0,1] \to [-1,1]$ is called a **Szegő function** if it satisfies the following Szegő-type condition:

$$\int_0^1 \log|1 - f(x)^2|\frac{\mathrm{d}x}{\sqrt{1-x^2}} > -\infty\,. \tag{12.53}$$

We use $\mathbf{S}$ to denote the set of all Szegő functions. Since $y \le -\log(1-y)$ for all $y \in [0,1)$, the Szegő condition in Eq. (12.53) implies that $\|f\|_{\mathbf{S}} < \infty$.

In standard L^2 theory of Fourier analysis, the Plancherel identity plays a fundamental role, namely for $f(x) = \sum_{k=0}^{\infty} c_k T_k(x)$, we have

$$\int_{-1}^{1} |f(x)|^2 \frac{\mathrm{d}x}{\sqrt{1-x^2}} = \pi |c_0|^2 + \frac{\pi}{2} \sum_{k=1}^{\infty} |c_k|^2 . \tag{12.54}$$

Let $\mathbf{P}$ denote the space of infinite sequences $\Phi = (\phi_k)_{k\in\mathbb{N}}$ with $\phi_k \in [-\pi/2, \pi/2]$. Given any $\Phi \in \mathbf{P}$ and $x \in [0,1]$, one can define a sequence of unitary matrices using the following recursive relation:

$$\begin{aligned} V_0(x,\Phi) &= e^{i\phi_0 Z} \\ V_d(x,\Phi) &= e^{i\phi_d Z} W(x) V_{d-1}(x,\Phi) W(x) e^{i\phi_d Z}. \end{aligned} \tag{12.55}$$

A direct check shows that this corresponds to symmetric phase factors Φ^W of the form

$$\Phi^W = (\phi_d, \phi_{d-1}, \ldots, \phi_1, \phi_0, \phi_1, \ldots, \phi_{d-1}, \phi_d) \in \mathbb{R}^{2d+1}, \tag{12.56}$$

such that $V_d(x,\Phi) = U_{\Phi^W}(x)$. So Φ can be viewed as the reduced phase factors in the infinite dimensional case. Let $P_d(x,\Phi) = [V_d(x,\Phi)]_{1,1}$. NLFT provides a L^2-theory for infinite QSP for all Szegő functions, together with a nonlinear generalization of the Plancherel identity [ALM+26, Theorem 1].

THEOREM 12.11. *For each $f \in \mathbf{S}$ satisfying $\|f\|_\infty < 1$, there exists a unique sequence $\Phi = (\phi_k)_{k\in\mathbb{N}} \in \mathbf{P}$ such that*

(a) $\operatorname{Im} P_d(\cdot,\Phi)$ *converges to f in the L^2 sense:*

$$\lim_{d\to\infty} \|\operatorname{Im} P_d(\cdot,\Phi) - f\|_{\mathbf{S}} = 0, \tag{12.57}$$

(b) *the following* ***nonlinear Plancherel identity*** *holds:*

$$-\frac{2}{\pi} \int_0^1 \log|1 - f(x)^2| \frac{\mathrm{d}x}{\sqrt{1-x^2}} = \sum_{k\in\mathbb{Z}} \log(1 + \tan^2 \phi_{|k|}). \tag{12.58}$$

Notes and further reading

Quantum signal processing (QSP) grew out of single-qubit composite gate design, where structured products of SU(2) rotations are used to synthesize prescribed response functions; see [LYC16]. The formulation was subsequently developed into a general primitive for implementing polynomial transformations, achieving optimal query complexity for Hamiltonian simulation [LC17b]. The extension from this scalar SU(2) representation to matrix singular value transformation, together with the block-encoding viewpoint and its algorithmic consequences, was established in [GSLW19]; see also reviews in [MRTC21, Lin25]. The symmetric choice of phase factors was first suggested in [DMWL21], and Theorem 12.5 and Corollary 12.6 were subsequently developed in [WDL22].

From the algorithmic perspective, the proof of [GSLW19, Corollary 5] gives a constructive synthesis for real polynomials by first computing complementary polynomials satisfying the constraints of Theorem 12.1, and then recovering phase factors via a recursive "layer stripping" procedure. As analyzed in [Haa19], layer stripping is numerically unstable in general and may require $\mathcal{O}(d \log(d/\epsilon))$ bits of working precision, where d is the degree and ϵ is the target approximation

error. Recent work has substantially improved the stability and practical performance of algorithms [CDG+20, DMWL21, Yin22, WDL22, DLNW24a, DLNW24b, BS24, AMT24, ALM+26, MW24, NY24, NSYL25]. The fixed-point iteration algorithm in Algorithm 12.1, together with many other numerical methods for finding phase factors, is implemented in QSPPACK[1]. We used QSPPACK throughout the book for QSP related examples.

Ref. [DLNW24a] provided the first infinite QSP construction. The connection between QSP and the SU(2) nonlinear Fourier transform (NLFT), as formalized in Proposition 12.10, was established in [AMT24]. Theorem 12.11 was first established in [AMT24] for Szegő" functions satisfying $\|f\|_\infty < \frac{1}{\sqrt{2}}$, and extended to all Szegő" functions in [ALM+26]. Furthermore, NLFT provides a unified description of QSP and its generalization, called generalized quantum signal processing [MW24].

[1] `https://qsppack.gitbook.io/qsppack/`

CHAPTER 13

Quantum singular value transformation

Quantum signal processing (QSP) provides a systematic way to implement scalar polynomial transformations by composing a sequence of single-qubit rotations with a fixed signal oracle. However, the ability to solely manipulate two-dimensional unitaries is, prima facie, a substantial limitation. Ideally we would like to be able to use the insights from quantum signal processing to provide methodologies for transforming a block encoding. That is to say, we would ideally like to perform a transformation of a positive-semidefinite matrix A that is of the form

$$\begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix} \mapsto \begin{bmatrix} P(A)/\alpha' & \cdot \\ \cdot & \cdot \end{bmatrix} \tag{13.1}$$

for an appropriately chosen set of normalization constants α, α' and operator valued polynomial P. With a technique like this, we could provide simple methods for simulating Hamiltonian dynamics on quantum computers, efficient methods for matrix inversion and much more.

The technique that was developed to solve this problem in its most general form is known as the quantum singular value transformation [GSLW18], and its impacts have become so broad in quantum algorithm design that it has been hailed as a grand unification of quantum algorithms [MRTC21].

The goal of performing transformations on block encoded matrices is also generalized through the quantum singular value transform by providing a method for transforming the singular values of a matrix decomposition. This allows analogous transformations to be carried out even in cases where A is not even a square matrix. Our goal here is to provide the general theory behind the quantum singular value transform and discuss the multitude of applications of this technique in later chapters.

We begin by deriving QSVT directly from the qubitization structure (see Section 10.1 for an intuitive introduction to singular value transforms in qubitization) given by the cosine–sine decomposition. We then discuss circuit-level refinements such as efficient controlled implementations and applications of QSVT including fixed-point amplitude amplification, uniform singular value amplification, and Gibbs state preparation via polynomial approximation and purification. We also use perturbation theory to explain the robustness of singular value transformations to approximate input oracles.

13.1. Derivation from cosine–sine decomposition

We begin with the cosine–sine decomposition form of qubitization (Theorem 10.10). For an n-qubit matrix A encoded by $U_A \in \mathrm{BE}_{1,m}(A)$, let $N = 2^n$ and $M = 2^m$. Then there exist $(m+n)$-qubit unitary matrices $\widetilde{W}, \widetilde{V}$, and an $(n+1)$-qubit permutation matrix $\mathscr{P}$ that permutes rows

$\{0, 1, \ldots, N-1, N, \ldots, 2N-1\}$ to $\{0, N, 1, N+1, \ldots, N-1, 2N-1\}$, such that

(13.2)
$$U_A = \widetilde{W} \begin{pmatrix} \Sigma & S & 0 \\ S & -\Sigma & 0 \\ 0 & 0 & I_{(M-2)N} \end{pmatrix} \widetilde{V}^\dagger = \widetilde{W} \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix} \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{V}^\dagger,$$

where $A = W\Sigma V^\dagger$ where Σ is the matrix of singular values of A and W and V are unitary matrices and S is the supplementary diagonal matrix $\sqrt{1-\Sigma^2}$ and

(13.3)
$$U_A^\dagger = \widetilde{V} \begin{pmatrix} \Sigma & S & 0 \\ S & -\Sigma & 0 \\ 0 & 0 & I_{(M-2)N} \end{pmatrix} \widetilde{W}^\dagger = \widetilde{V} \left\{ \mathscr{P} \bigoplus_{i\in[N]} \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix} \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{W}^\dagger.$$

Following the same decomposition, Z_Π can be written as

$$Z_\Pi = \left\{ \mathscr{P} \left(\bigoplus_{i\in[N]} Z \right) \mathscr{P}^\dagger \right\} \bigoplus (-I)_{(M-2)N}. \tag{13.4}$$

Each 2×2 block of $U_A \begin{pmatrix} \sigma_i & \sqrt{1-\sigma_i^2} \\ \sqrt{1-\sigma_i^2} & -\sigma_i \end{pmatrix}$ is a reflection; consequently, this block is exactly the same in both U_A and $U_A^\dagger$. This is essential to see that the adjoints used in the quantum singular value transformation retain the same action as quantum signal processing on this subspace.

Focusing our attention on this irreducible 2×2 block, let us use $U_\Phi(x)$ to denote the SU(2) matrix in the QSP representation (for instance, Eq. (12.4) in the O-convention) evaluated at $x \in [-1, 1]$:

$$U_\Phi(x) = e^{i\phi_0 Z} \prod_{j=1}^{d} \left[O(x) e^{i\phi_j Z} \right] = \begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ \overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix} \tag{13.5}$$

Here P is a complex polynomial of degree at most d with parity $d \bmod 2$. We would like to lift this scalar identity to a unitary (still denoted by U_Φ) that implements a block-encoding of the singular value transformation $P^{\mathrm{SV}}(A)$.

Assume first that d is even and consider the following circuit:

$$U_\Phi = e^{i\phi_0 Z_\Pi} \prod_{j=1}^{d/2} \left[(U_A^\dagger Z_\Pi) e^{i\phi_{2j-1} Z_\Pi} (U_A Z_\Pi) e^{i\phi_{2j} Z_\Pi} \right]. \tag{13.6}$$

Then

$$\begin{aligned} U_\Phi =& \widetilde{V} \left\{ \mathscr{P} \bigoplus_{i\in[N]} e^{i\phi_0 Z} \prod_{j=1}^{d} \left[O(\sigma_i) e^{i\phi_j Z} \right] \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{V}^\dagger \\ =& \widetilde{V} \left\{ \mathscr{P} \bigoplus_{i\in[N]} U_\Phi(\sigma_i) \mathscr{P}^\dagger \bigoplus I_{(M-2)N} \right\} \widetilde{V}^\dagger. \end{aligned} \tag{13.7}$$

Therefore U_Φ is a $(1, m+1)$-block-encoding of $P^{\triangleright}(A)$, where $P \in \mathbb{C}[x]$ is the polynomial appearing as the $(1,1)$ entry in Eq. (12.4). Since d is even, P is even, and hence $P^{\mathrm{SV}}(A) = P^{\triangleright}(A)$.

Similarly, when d is odd, consider the circuit:

$$U_\Phi = e^{i\phi_0 Z_\Pi}(U_A Z_\Pi e^{i\phi_1 Z_\Pi}) \prod_{j=1}^{(d-1)/2} \left[(U_A^\dagger Z_\Pi) e^{i\phi_{2j} Z_\Pi}(U_A Z_\Pi) e^{i\phi_{2j+1} Z_\Pi}\right]. \tag{13.8}$$

Then

$$\begin{aligned} U_\Phi =& \widetilde{W}\left\{\mathscr{P}\bigoplus_{i\in[N]} e^{i\phi_0 Z}\prod_{j=1}^{d}\left[O(\sigma_i)e^{i\phi_j Z}\right]\mathscr{P}^\dagger \bigoplus I_{(M-2)N}\right\}\widetilde{V}^\dagger \\ =& \widetilde{W}\left\{\mathscr{P}\bigoplus_{i\in[N]} U_\Phi(\sigma_i)\mathscr{P}^\dagger \bigoplus I_{(M-2)N}\right\}\widetilde{V}^\dagger. \end{aligned} \tag{13.9}$$

Therefore U_Φ is a $(1, m+1)$-block-encoding of $P^\diamond(A)$. Since d is odd, P is odd, and hence $P^{\mathrm{SV}}(A) = P^\diamond(A)$.

The unitaries in Eqs. (13.6) and (13.8) are called **quantum singular value transformation** (QSVT).

Note that these expressions involve interleaved factors of Z_Π and also require implementing $e^{i\phi Z_\Pi}$. Below we show that these can be implemented using multi-qubit controlled-NOT gates, single-qubit rotations, and a simple modification of the phase factors.

To implement $e^{i\phi Z_\Pi}$, we note that the circuit denoted by $\mathrm{CR}(\phi)$ in Fig. 13.1 maps $|0\rangle|0^m\rangle$ to $e^{i\phi}|0\rangle|0^m\rangle$, and maps $|0\rangle|b\rangle$ to $e^{-i\phi}|0\rangle|b\rangle$ for $b \neq 0^m$. The first (signal) qubit is returned to $|0\rangle$, so ignoring it, the induced operation on the m-qubit register is exactly $e^{i\phi Z_\Pi}$. Moreover, we do not need a separate implementation of Z_Π. Using $Z = -ie^{i\frac{\pi}{2}Z} = ie^{-i\frac{\pi}{2}Z}$, we have

$$Ze^{i\phi Z} = (-i)e^{i(\phi+\frac{\pi}{2})Z} = ie^{i(\phi-\frac{\pi}{2})Z}, \tag{13.10}$$

so by adding and subtracting $\pi/2$ to the phase factors in an alternating pattern we can absorb interleaved Z factors without introducing an additional global phase. This is particularly useful for controlled implementations of QSVT.

When d is even, let

$$\phi_j^C = \begin{cases} \phi_0, & j = 0, \\ \phi_j + \frac{\pi}{2}, & j \in \{1,\dots,d\} \text{ and } j \text{ is odd}, \\ \phi_j - \frac{\pi}{2}, & j \in \{1,\dots,d\} \text{ and } j \text{ is even}. \end{cases} \tag{13.11}$$

Then the overall global phase due to the resulting powers of i is canceled and

$$e^{i\phi_0^C Z}\prod_{j=1}^{d}\left[\begin{pmatrix} x & \sqrt{1-x^2} \\ \sqrt{1-x^2} & -x \end{pmatrix} e^{i\phi_j^C Z}\right] = e^{i\phi_0 Z}\prod_{j=1}^{d}\left[O(x)e^{i\phi_j Z}\right] = U_\Phi(x) = \begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ \overline{Q(x)}\sqrt{1-x^2} & \overline{P(x)} \end{pmatrix}. \tag{13.12}$$

When d is odd, we can choose

$$\phi_j^C = \begin{cases} \phi_0 - \frac{\pi}{2}, & j = 0, \\ \phi_j + \frac{\pi}{2}, & j \in \{1,\dots,d\} \text{ and } j \text{ is odd}, \\ \phi_j - \frac{\pi}{2}, & j \in \{1,\dots,d\} \text{ and } j \text{ is even}. \end{cases} \tag{13.13}$$

This cancels all the global phase factors, but there is an additional Z factor

(13.14)
$$e^{i\phi_0^C Z}\prod_{j=1}^{d}\left[\begin{pmatrix} x & \sqrt{1-x^2} \\ \sqrt{1-x^2} & -x \end{pmatrix} e^{i\phi_j^C Z}\right] = Ze^{i\phi_0 Z}\prod_{j=1}^{d}\left[O(x)e^{i\phi_j Z}\right] = ZU_\Phi(x) = \begin{pmatrix} P(x) & -Q(x)\sqrt{1-x^2} \\ -\overline{Q(x)}\sqrt{1-x^2} & -\overline{P(x)} \end{pmatrix}$$

Despite the additional Z factor in Eq. (13.14), both sides are block-encodings of the same polynomial $P(x)$ in the $(1,1)$ entry.

The phase factors $\Phi^C = (\phi_0^C, \cdots, \phi_d^C)$ are called the **C-convention** (or circuit convention) of phase factors associated with Φ (the O-convention). The modification rule can be summarized as follows.

(13.15)
$$\phi_j^C = \begin{cases} \phi_0 - \frac{\pi}{2}, & j = 0 \text{ and } d \text{ is odd}, \\ \phi_0, & j = 0 \text{ and } d \text{ is even}, \\ \phi_j + \frac{\pi}{2}, & j \in \{1, \ldots, d\} \text{ and } j \text{ is odd}, \\ \phi_j - \frac{\pi}{2}, & j \in \{1, \ldots, d\} \text{ and } j \text{ is even}. \end{cases}$$

The modification rule of phase factors starting from the W-convention is similar and is omitted here.

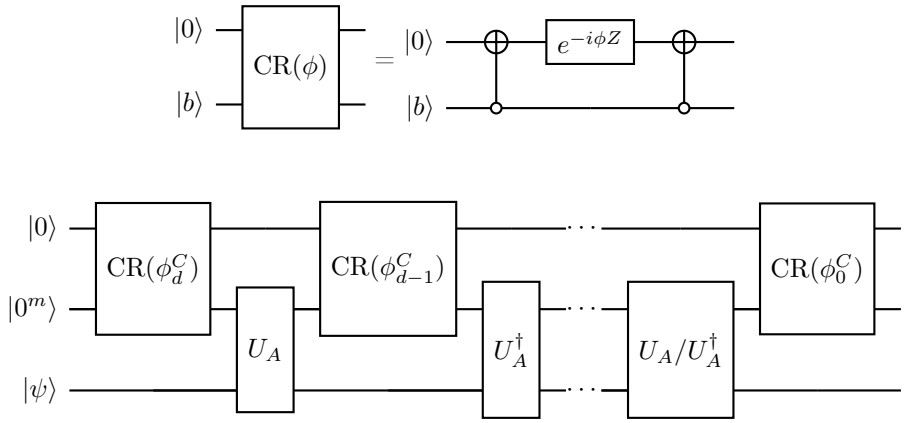


FIGURE 13.1. Circuit of quantum singular value transformation to construct $U_{P^{\mathrm{SV}}(A)} \in \mathrm{BE}_{1,m+1}(P^{\mathrm{SV}}(A))$, using $U_A \in \mathrm{BE}_{1,m}(A)$, and $U_A, U_A^\dagger$ are applied in an alternating order. The last gate is U_A when the degree d is odd, and is $U_A^\dagger$ if d is even. One possible way to express the phase factors $\{\phi_j^C\}$ in the circuit in terms of $\{\phi_j\}$ in Theorem 12.1 is given in Eq. (13.15).

THEOREM 13.1 (Quantum singular value transformation with complex polynomials of definite parity). *Let $A \in \mathbb{C}^{N\times N}$ be encoded by its $(1,m)$-block-encoding U_A. For a complex polynomial $P(x) \in \mathbb{C}[x]$ with degree d and parity given by $d \mod 2$ satisfying the conditions in Theorem 12.1, we can find a sequence of phase factors $\Phi \in \mathbb{R}^{d+1}$ according to Theorem 12.1, and a corresponding sequence of C-convention phase factors Φ^C according to Eq.* (13.15)*. With this sequence Φ^C, the circuit in Fig. 13.1 implements a $(1, m+1)$-block-encoding of $P^{\mathrm{SV}}(A)$, using $U_A, U_A^\dagger$, m-qubit controlled-NOT, and single-qubit rotation gates a total of $\mathcal{O}(d)$ times.*

13.2. Real polynomial singular value transformation

Instead of $P^{\mathrm{SV}}(A)$, in many applications we are only interested in a block-encoding of

$$F^{\mathrm{SV}}(A) = \frac{1}{2}(P^{\mathrm{SV}}(A) + \overline{P}^{\mathrm{SV}}(A)), \quad F(x) = \mathrm{Re}\, P(x). \tag{13.16}$$

This can be done by using Theorem 13.1 to construct a block-encoding of $P^{\mathrm{SV}}(A), \overline{P}^{\mathrm{SV}}(A)$, respectively, and use LCU with one ancilla qubit to construct the linear combination. However, due to the special structure of QSP, we demonstrate an elegant way to solve this problem without introducing any additional ancilla qubit.

Given $\Phi = (\phi_0, \cdots, \phi_d) \in \mathbb{R}^{d+1}$, define $-\Phi := (-\phi_0, \cdots, -\phi_d) \in \mathbb{R}^{d+1}$. Taking entrywise complex conjugation of $U_\Phi(x)$ in Eq. (12.4) gives

$$(U_\Phi(x))^* = U_{-\Phi}(x) = e^{-i\phi_0 Z}\prod_{j=1}^{d}\left[O(x)e^{-i\phi_j Z}\right] = \begin{pmatrix} \overline{P(x)} & -\overline{Q(x)}\sqrt{1-x^2} \\ Q(x)\sqrt{1-x^2} & P(x) \end{pmatrix}. \tag{13.17}$$

As a result, from qubitization, when d is even,

$$U_{-\Phi} = \widetilde{V}\left\{\mathscr{P}\bigoplus_{i\in[N]} U_{-\Phi}(\sigma_i)\mathscr{P}^\dagger \bigoplus I_{(M-2)N}\right\}\widetilde{V}^\dagger. \tag{13.18}$$

is a $(1, m+1)$-block-encoding of $\overline{P}^{\triangleright}(A)$ for an even polynomial P. From Eq. (13.11),

$$e^{-i\phi_0^C Z}\prod_{j=1}^{d}\left[\begin{pmatrix} x & \sqrt{1-x^2} \\ \sqrt{1-x^2} & -x \end{pmatrix} e^{-i\phi_j^C Z}\right] = e^{-i\phi_0 Z}\prod_{j=1}^{d}\left[O(x)e^{-i\phi_j Z}\right] = U_{-\Phi}(x). \tag{13.19}$$

Thus $U_{-\Phi}$ can be implemented by negating each phase factor ϕ_j^C.

When d is odd,

$$U_{-\Phi} = \widetilde{W}\left\{\mathscr{P}\bigoplus_{i\in[N]} U_{-\Phi}(\sigma_i)\mathscr{P}^\dagger \bigoplus I_{(M-2)N}\right\}\widetilde{V}^\dagger \tag{13.20}$$

is a $(1, m+1)$-block-encoding of $\overline{P}^{\diamond}(A)$ for an odd polynomial P. From Eq. (13.13),

$$e^{-i\phi_0^C Z}\prod_{j=1}^{d}\left[\begin{pmatrix} x & \sqrt{1-x^2} \\ \sqrt{1-x^2} & -x \end{pmatrix} e^{-i\phi_j^C Z}\right] = Ze^{-i\phi_0 Z}\prod_{j=1}^{d}\left[O(x)e^{-i\phi_j Z}\right] = ZU_{-\Phi}(x). \tag{13.21}$$

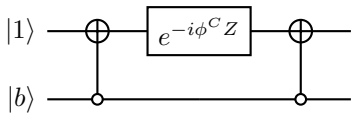
Thus negating each phase factor ϕ_j^C implements the unitary

$$\widetilde{W}\left\{\mathscr{P}\bigoplus_{i\in[N]} ZU_{-\Phi}(\sigma_i)\mathscr{P}^\dagger \bigoplus I_{(M-2)N}\right\}\widetilde{V}^\dagger \tag{13.22}$$

which is a block-encoding of $\overline{P}^{\diamond}(A)$ (the additional Z only affects other blocks).

In summary, it suffices to negate all phase factors in Φ^C. In order to implement $\mathrm{CR}(-\phi^C)$, we do not actually need to implement a new circuit. Instead we may simply initialize the signal qubit

in $|1\rangle$:



which outputs $e^{-i\phi^C}|1\rangle|0^m\rangle$ if $b = 0^m$, and $e^{i\phi^C}|1\rangle|b\rangle$ if $b \neq 0^m$. Equivalently, relative to the convention of $\mathrm{CR}(\phi^C)$, this realizes $\mathrm{CR}(-\phi^C)$. In other words, the circuits for $U_{\overline{P}^{\mathrm{SV}}(A)}$ and $U_{P^{\mathrm{SV}}(A)}$ are exactly the same except that the state of the signal qubit is changed from $|0\rangle$ to $|1\rangle$.

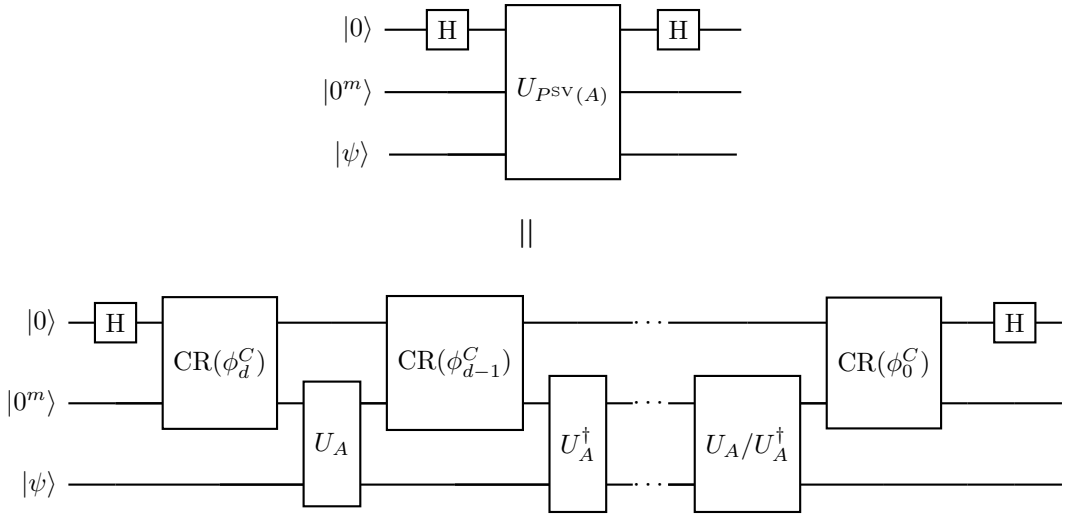


FIGURE 13.2. Circuit of quantum singular value transformation to construct $U_{F^{\mathrm{SV}}(A)} \in \mathrm{BE}_{1,m+1}(F^{\mathrm{SV}}(A))$, using $U_A \in \mathrm{BE}_{1,m}(A)$, and $U_A, U_A^\dagger$ are applied in an alternating order. Here $F(x) = \mathrm{Re}\, P(x)$. The last gate is U_A when the degree d is odd, and is $U_A^\dagger$ if d is even. One possible way to express the phase factors $\{\phi_j^C\}$ in the circuit in terms of $\{\phi_j\}$ in Theorem 12.1 is given in Eq. (13.15). Conceptually, this is a circuit using a linear combination of block-encodings for $P^{\mathrm{SV}}(A)$ and $\overline{P}^{\mathrm{SV}}(A)$.

Now we claim the circuit in Fig. 13.2 implements a block-encoding of $F^{\mathrm{SV}}(A)$ via a linear combination of unitaries. Direct calculation shows

$$
\begin{aligned}
& |0\rangle |0^m\rangle |\psi\rangle \\
\xrightarrow{\mathrm{H}\otimes I} & \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) |0^m\rangle |\psi\rangle \\
\xrightarrow{U_{P^{\mathrm{SV}}(A)}} & \frac{1}{\sqrt{2}} |0\rangle (|0^m\rangle P^{\mathrm{SV}}(A) |\psi\rangle + |\perp\rangle) + \frac{1}{\sqrt{2}} |1\rangle (|0^m\rangle \overline{P}^{\mathrm{SV}}(A) |\psi\rangle + |\perp'\rangle) \\
\xrightarrow{\mathrm{H}\otimes I} & |0\rangle \left(|0^m\rangle \frac{P^{\mathrm{SV}}(A) + \overline{P}^{\mathrm{SV}}(A)}{2} |\psi\rangle \right) + |1\rangle \left(|0^m\rangle \frac{P^{\mathrm{SV}}(A) - \overline{P}^{\mathrm{SV}}(A)}{2} |\psi\rangle \right) + |\widetilde{\perp}\rangle \\
= & |0\rangle |0^m\rangle F^{\mathrm{SV}}(A) |\psi\rangle + |\widetilde{\perp}\rangle
\end{aligned}
\tag{13.23}
$$

Here $|\perp\rangle, |\perp'\rangle$ are two $(m+n)$-qubit state orthogonal to any state $|0^m\rangle |x\rangle$, while $|\widetilde{\perp}\rangle$ is a $(m+n+1)$-qubit state orthogonal to any state of the form $|0\rangle |0^m\rangle |x\rangle$. In other words, upon measuring the $(m+1)$ ancilla qubits and obtaining $|0^{m+1}\rangle$, the corresponding (unnormalized) state in the system register is $F^{\mathrm{SV}}(A) |\psi\rangle = (\mathrm{Re}\, P)^{\mathrm{SV}}(A) |\psi\rangle$. As a byproduct, if we obtain $|1, 0^m\rangle$ in the ancilla register, then we obtain $i(\mathrm{Im}\, P)^{\mathrm{SV}}(A) |\psi\rangle$ in the system register.

Corollary 13.2 (Quantum singular value transformation with real polynomials of definite parity)**.** *Let $A \in \mathbb{C}^{N\times N}$ be encoded by its $(1,m)$-block-encoding U_A. For a real polynomial $F(x) \in \mathbb{R}[x]$ with degree d and parity given by $d \mod 2$ satisfying the conditions in Theorem 12.2, we can find a sequence of phase factors $\Phi \in \mathbb{R}^{d+1}$ according to Theorem 12.2, and a corresponding sequence of C-convention phase factors Φ^C according to Eq.* (13.15)*. With this sequence Φ^C, the circuit in Fig. 13.2 implements a $(1, m+1)$-block-encoding of $F^{\mathrm{SV}}(A)$, using $U_A, U_A^\dagger$, m-qubit controlled-NOT, and single-qubit rotations a total of $\mathcal{O}(d)$ times.*

Example 13.3 (Controlled implementation of the QSVT circuit)**.** When implementing a controlled QSVT circuit U_Φ, one possibility is to implement a controlled version of every gate. This means that d controlled applications of U_A or $U_A^\dagger$ are required.

Observe that (1) a controlled implementation of the controlled rotation $\mathrm{CR}(\phi^C)$ can be implemented by controlling the single-qubit rotation gate; (2) $U_A^\dagger U_A = I$. We find that when d is even, the controlled QSVT circuit can be implemented by controlled single-qubit rotations without any controlled U_A or $U_A^\dagger$. When d is odd, there is one extra U_A that cannot be cancelled, so a single controlled U_A is needed (see Fig. 13.3).

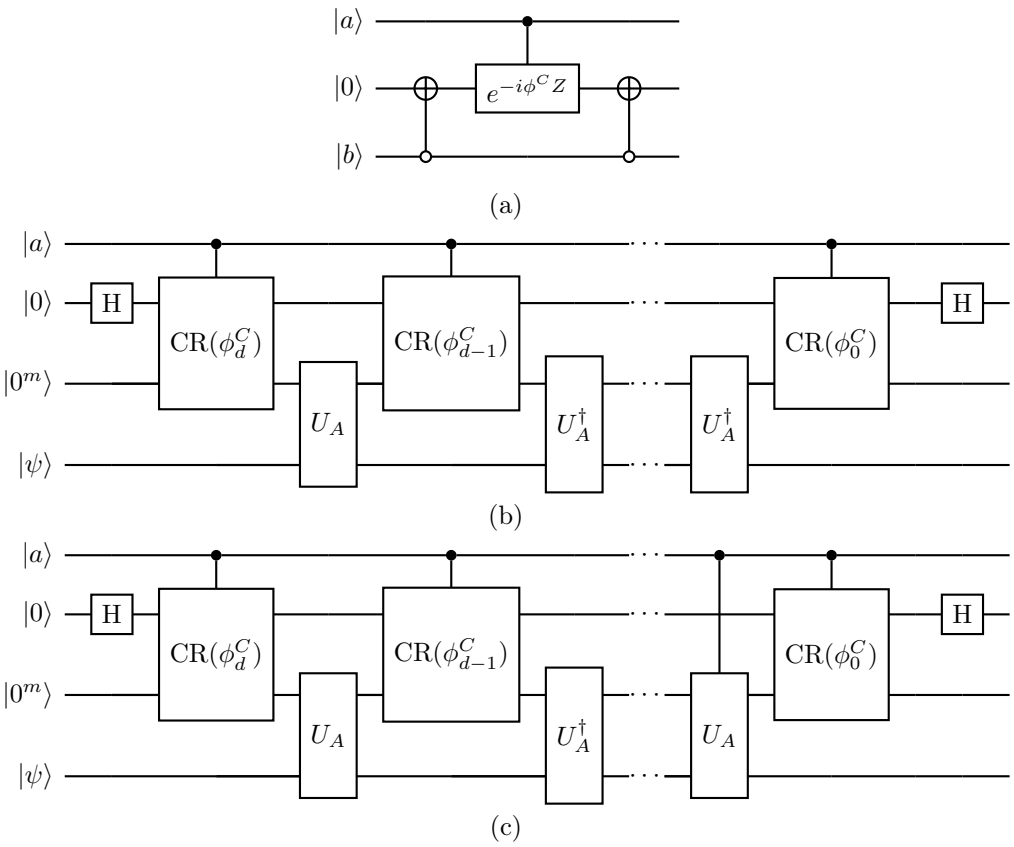


FIGURE 13.3. (a) Controlled implementation of the controlled rotation. (b) Circuit for controlled implementation of the QSVT circuit for even polynomial, which does not use controlled U_A or $U_A^\dagger$. (c) Circuit for controlled implementation of the QSVT circuit for odd polynomial, which uses the controlled U_A circuit once.

◇

For singular value transformations, we may extend the function of interest from $[0,1]$ to $[-1,1]$ as either an even or an odd function. In many applications, this choice is dictated by whether the final expression needs access to both left and right singular vectors, or only one of them. For eigenvalue transformations, there are additional degrees of freedom.

First, if the polynomial of interest $F(x) \in \mathbb{R}[x]$ does not have a definite parity, we can use the expression

$$F(x) = F_{\mathrm{even}}(x) + F_{\mathrm{odd}}(x), \tag{13.24}$$

where $F_{\mathrm{even}}(x) = \frac{1}{2}(F(x) + F(-x)), F_{\mathrm{odd}}(x) = \frac{1}{2}(F(x) - F(-x))$. If $|F(x)| \leq 1$ on $[-1,1]$, then $|F_{\mathrm{even}}(x)|, |F_{\mathrm{odd}}(x)| \leq 1$ on $[-1,1]$, and $F_{\mathrm{even}}(x)$ and $F_{\mathrm{odd}}(x)$ can each be constructed using QSVT in Corollary 13.2. Introducing another ancilla qubit and using the LCU technique, we obtain a

$(2, m+2)$-block-encoding of $F(A) = F_{\text{even}}(A) + F_{\text{odd}}(A)$. Note that unlike the case of the block-encoding of $(\operatorname{Re} P)(A)$, we lose a subnormalization factor of 2 here. Using the construction in Fig. 13.3, the implementation of the select oracle in LCU only requires a single controlled implementation of U_A when implementing a controlled block-encoding for $F_{\text{odd}}(A)$.

Following the same principle, suppose the polynomial of interest $F(x) \in \mathbb{C}[x]$ satisfies $|F(x)| \leq 1$ for all $x \in [-1, 1]$ (otherwise rescale F and account for the resulting subnormalization). We can write

$$F(x) = G(x) + iH(x) \tag{13.25}$$

with $G, H \in \mathbb{R}[x]$. Then $|G(x)| \leq 1$ and $|H(x)| \leq 1$ for all $x \in [-1, 1]$. If G, H have definite parity, then Corollary 13.2 gives $U_{G(A)} \in \mathrm{BE}_{1,m+1}(G(A)), U_{H(A)} \in \mathrm{BE}_{1,m+1}(H(A))$. Applying LCU, we obtain $U_{F(A)} \in \mathrm{BE}_{2,m+2}(F(A))$.

If G, H do not have definite parity, then by the argument above we can construct $U_{G(A)} \in \mathrm{BE}_{2,m+2}(G(A))$ and $U_{H(A)} \in \mathrm{BE}_{2,m+2}(H(A))$. Applying another round of LCU then yields $U_{F(A)} \in \mathrm{BE}_{4,m+3}(F(A))$.

13.3. Quantum singular value transformation beyond the computational basis

So far we have assumed that a matrix $A \in \mathbb{C}^{N \times N}$ is accessed through the upper left $N \times N$ block of a unitary $U_A \in \mathrm{U}(MN)$ in the computational basis, i.e., via the projector $\Pi_{0^m} := |0^m\rangle\langle 0^m| \otimes I$ on m ancillas with $M = 2^m$. As explained in Section 9.9 and Definition 9.25, the notion of block-encoding is more general: one may replace Π_{0^m} by other projectors, and one may also encode a rectangular matrix $A \in \mathbb{C}^{N' \times N}$ between two subspaces.

Fix projectors Π, Π' on $\mathbb{C}^{MN}$ with $\operatorname{rank}(\Pi) = N$ and $\operatorname{rank}(\Pi') =: N'$ and a unitary $\mathscr{U}_A \in \mathrm{U}(MN)$ such that $\mathscr{U}_A$ is a block-encoding of A with respect to (Π, Π'). Equivalently, choose unitaries $\Xi, \Xi' \in \mathrm{U}(MN)$ defining bases $\mathcal{B}, \mathcal{B}'$ as in Eqs. (9.99) and (9.100), so that the matrix representation $U_A := (\Xi')^\dagger \mathscr{U}_A \Xi$ has the block form in Eq. (9.103).

The projectors Π, Π' can be accessed through the reflection operators

$$Z_\Pi = 2\Pi - I, \qquad Z_{\Pi'} = 2\Pi' - I. \tag{13.26}$$

With these reflections, the qubitization iterate becomes $\mathscr{U}_A^\dagger Z_{\Pi'} \mathscr{U}_A Z_\Pi$, and the QSVT construction carries over verbatim.

Let $A = W\Sigma V^\dagger$ be a singular value decomposition of A (with Σ possibly rectangular), and let the expanded singular vectors $\widetilde{W}, \widetilde{V}$ be given by the CS decomposition in Eq. (10.91). If the polynomial degree d is even, define

$$\mathscr{U}_\Phi = e^{i\phi_0 Z_\Pi} \prod_{j=1}^{d/2} \left[(\mathscr{U}_A^\dagger Z_{\Pi'}) e^{i\phi_{2j-1} Z_{\Pi'}} (\mathscr{U}_A Z_\Pi) e^{i\phi_{2j} Z_\Pi} \right] \tag{13.27}$$

and if d is odd, define

$$\mathscr{U}_\Phi = e^{i\phi_0 Z_{\Pi'}} \mathscr{U}_A Z_\Pi \prod_{j=1}^{(d-1)/2} \left[(\mathscr{U}_A^\dagger Z_{\Pi'}) e^{i\phi_{2j-1} Z_{\Pi'}} (\mathscr{U}_A Z_\Pi) e^{i\phi_{2j} Z_\Pi} \right] \tag{13.28}$$

In a suitable orthonormal basis adapted to Π, Π' (equivalently, after the basis change described in Section 9.9), the unitary $\mathscr{U}_\Phi$ decomposes into a direct sum of 2×2 blocks $U_\Phi(\sigma_i)$ associated with the singular values σ_i of A, together with additional 1×1 blocks when $N' \neq N$.

Let us introduce the controlled rotation operator $\mathrm{CR}_\Pi(\phi)$ acting on an additional qubit and the $(n+m)$-qubit register, defined by

$$\mathrm{CR}_\Pi(\phi) := (\mathrm{C}_\Pi\,\mathrm{NOT})(e^{-i\phi Z}\otimes I)(\mathrm{C}_\Pi\,\mathrm{NOT}). \tag{13.29}$$

When the additional qubit is initialized in $|0\rangle$, the induced action on the $(n+m)$-qubit register is $e^{i\phi Z_\Pi}$. As discussed before, one may absorb the explicit reflections $Z_\Pi, Z_{\Pi'}$ into $\mathrm{CR}_\Pi, \mathrm{CR}_{\Pi'}$ by modifying the phase factors accordingly. To implement the rotation $\mathrm{CR}_\Pi(\phi)$ efficiently, we need access to

$$\begin{aligned}\mathrm{C}_\Pi\,\mathrm{NOT} :=& X\otimes\Pi + I_1\otimes(I-\Pi)\\ =& X\otimes\frac{I+Z_\Pi}{2} + I_1\otimes\frac{I-Z_\Pi}{2}\\ =& \frac{I_1+X}{2}\otimes I + \frac{X-I_1}{2}\otimes Z_\Pi\\ =& |+\rangle\langle+|\otimes I + |-\rangle\langle-|\otimes(-Z_\Pi)\\ =& (\mathrm{H}\otimes I)(|0\rangle\langle 0|\otimes I + |1\rangle\langle 1|\otimes(-Z_\Pi))(\mathrm{H}\otimes I).\end{aligned} \tag{13.30}$$

Therefore assuming access to Z_Π, the $\mathrm{C}_\Pi\,\mathrm{NOT}$ gate can be implemented using the circuit in Fig. 13.4.

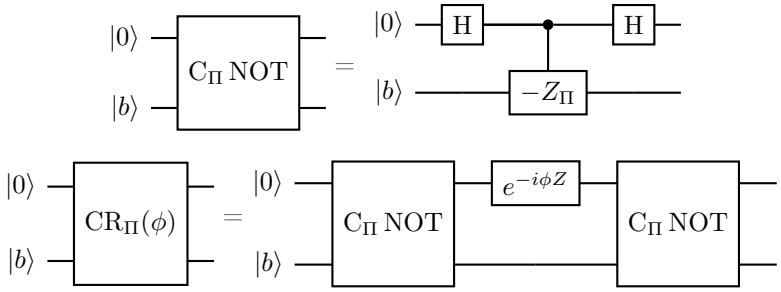


FIGURE 13.4. Circuit for implementing $\mathrm{C}_\Pi\,\mathrm{NOT}$ using a controlled reflection operator $-Z_\Pi$, and for $\mathrm{CR}_\Pi(\phi)$ that implements $e^{i\phi Z_\Pi}$ on the $(n+m)$-qubit register when the additional qubit is initialized in $|0\rangle$. The circuit can be further simplified using matrix identities.

This setup also covers the rectangular case $N' \neq N$. In summary, we obtain the following result.

Corollary 13.4 (Quantum singular value transformation with a basis change)**.** *Given a unitary $\mathscr{U}_A \in \mathrm{U}(MN)$ and two projectors Π, Π' on $\mathbb{C}^{MN}$ that can be accessed via reflection operators $Z_\Pi, Z_{\Pi'}$, with $\mathrm{rank}(\Pi) = N$ and $\mathrm{rank}(\Pi') =: N'$. Let $\mathcal{B}, \mathcal{B}'$ be orthonormal bases for $\mathrm{range}(\Pi)$ and $\mathrm{range}(\Pi')$, respectively. Then $[\mathscr{U}_A]^{\mathcal{B}'}_{\mathcal{B}}$ provides a $(1,m)$-block-encoding of A. Given a polynomial $F(x) \in \mathbb{R}[x]$ of degree d satisfying the conditions in Theorem 12.2, we can find a sequence of phase factors $\Phi \in \mathbb{R}^{d+1}$ according to Theorem 12.2, and a corresponding sequence of C-convention phase factors Φ^C according to Eq. (13.15). With this sequence Φ^C, we can implement a unitary $\mathscr{U}_\Phi$, so that when d is even, $[\mathscr{U}_\Phi]^{\mathcal{B}}_{\mathcal{B}}$ is a $(1,m+1)$-block-encoding of $F^{\triangleright}(A)$, and when d is odd, $[\mathscr{U}_\Phi]^{\mathcal{B}'}_{\mathcal{B}}$ is a $(1,m+1)$-block-encoding of $F^{\diamond}(A)$.*

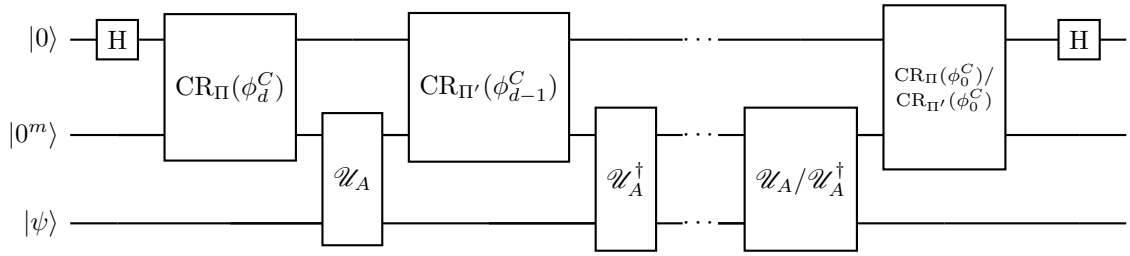


FIGURE 13.5. Circuit of quantum singular value transformation with real polynomials of definite parity and a basis change.

13.4. Example: Fixed-point amplitude amplification and uniform singular value amplification

Recall that Grover's search algorithm and amplitude amplification can overshoot the target state. This is not robust when the number of iterations is not chosen carefully. Moreover, for amplitude amplification the optimal iteration count depends on the initial overlap, which is typically unknown. Fixed-point amplitude amplification resolves these issues. Implemented via QSVT, it only requires a known lower bound on the overlap and avoids overshooting. The construction is closely related to oblivious amplitude amplification and singular value transformation.

Proposition 13.5 (**Fixed-point amplitude amplification**). *Let $\mathscr{U}_A$ be an n-qubit unitary and Π' be an n-qubit orthogonal projector with* $\mathrm{rank}(\Pi') \geq 1$ *such that*

$$\Pi' \mathscr{U}_A |\varphi_0\rangle = a |\psi\rangle, \quad a \geq \delta > 0. \tag{13.31}$$

Then there is a $(n+1)$-qubit unitary circuit $\mathscr{U}_\Phi$ such that

$$D_p(|0\rangle |\psi\rangle, \mathscr{U}_\Phi |0\rangle |\varphi_0\rangle) \leq \epsilon, \tag{13.32}$$

which uses $\mathscr{U}_A, \mathscr{U}_A^\dagger, \mathrm{C}_{\Pi'}\,\mathrm{NOT}, \mathrm{C}_{|\varphi_0\rangle\langle\varphi_0|}\,\mathrm{NOT}$ and single-qubit rotation gates $\mathcal{O}(\log(1/\epsilon)\delta^{-1})$ times. Here $D_p(\cdot,\cdot)$ is the global phase invariant distance between two state vectors.

PROOF. Let $N = 2^n$. Construct an orthonormal basis $\mathcal{B} = \{|\varphi_0\rangle, |v_1\rangle, \ldots, |v_{N-1}\rangle\}$, where each $|v_i\rangle$ is orthogonal to $|\varphi_0\rangle$. Similarly, let $\mathcal{B}' = \{|\psi\rangle, |w_1\rangle, \ldots, |w_{N-1}\rangle\}$ be an orthonormal basis, where each $|w_i\rangle$ is orthogonal to $|\psi\rangle$. Since $|\psi\rangle$ belongs to the range of Π',

$$\langle\psi|\mathscr{U}_A|\varphi_0\rangle = \langle\psi|\Pi'\mathscr{U}_A|\varphi_0\rangle = a, \tag{13.33}$$

i.e.,

$$[\mathscr{U}_A]_{\mathcal{B}}^{\mathcal{B}'} = \begin{pmatrix} a & * \\ * & * \end{pmatrix}. \tag{13.34}$$

Choose an odd real polynomial $F(x)$ satisfying

$$|F(x) - 1| \leq \epsilon^2/2, \quad \forall x \in [\delta, 1]. \tag{13.35}$$

In addition, to apply QSVT we require $|F(x)| \leq 1$ for all $x \in [-1, 1]$. Using Lemma 12.8, we can achieve this by approximating the sign function, and the polynomial degree is $\deg(F) = \mathcal{O}(\log(1/\epsilon)\delta^{-1})$. The corresponding QSVT circuit $\mathscr{U}_\Phi$ uses one ancilla qubit and implements a

block encoding of $F(a)|\psi\rangle\langle\varphi_0|$. The overlap between $|0\rangle|\psi\rangle$ and $\mathscr{U}_\Phi|0\rangle|\varphi_0\rangle$ is $|F(a)|$. According to Eq. (3.68), the global phase invariant distance is

$$D_p(\mathscr{U}_\Phi|0\rangle|\varphi_0\rangle, |0\rangle|\psi\rangle) = \sqrt{2(1-|F(a)|)} \leq \epsilon. \tag{13.36}$$

□

Example 13.6. Let us apply the fixed-point amplitude amplification to the unstructured search problem. Let $|x_0\rangle$ be the marked state, and let $|\psi_0\rangle$ be the uniform superposition. Let Π' be the projector onto $|x_0\rangle$. Then $\mathrm{C}_{\Pi'}\mathrm{NOT}$ and $\mathrm{C}_{|\psi_0\rangle\langle\psi_0|}\mathrm{NOT}$ are implemented by the reflection operators R_{x_0} and R_{ψ_0}, respectively. Furthermore,

$$\Pi' R_{\psi_0}|\psi_0\rangle = \frac{1}{\sqrt{N}}|x_0\rangle. \tag{13.37}$$

So we can take $\mathscr{U}_A = R_{\psi_0}$. By choosing an odd, real polynomial $F(x)$ satisfying

$$\left|F(1/\sqrt{N}) - 1\right| \leq \epsilon^2/2, \tag{13.38}$$

using $\deg(F) = \mathcal{O}(\log(1/\epsilon)\sqrt{N})$, we can find the marked state to precision ϵ. ◇

Next we discuss another application of QSVT. Recall that oblivious amplitude amplification is only applicable to block encodings of unitary matrices; a key simplification there is that the singular values are all equal to a single scalar, so one only needs to amplify that scalar. Now consider a general matrix $A \in \mathbb{C}^{N\times N}$ and a block encoding $U_A \in \mathrm{BE}_{\alpha,m}(A)$. Can we construct a new block encoding of A whose subnormalization factor is close to the optimal value $\|A\|$? This task is called uniform singular value amplification.

Proposition 13.7 (Uniform singular value amplification). *From a block encoding $U_A \in \mathrm{BE}_{\alpha,m}(A)$, for any $\delta \in (0,1], \epsilon \in (0, 1/(2\alpha)]$ and $\alpha > \|A\|$, we can construct a $U_\Phi \in \mathrm{BE}_{\|A\|(1+\delta),m+1}(A,\epsilon)$, using $\mathcal{O}\left(\frac{\alpha}{\delta\|A\|}\log\left(\frac{\alpha}{\|A\|\epsilon}\right)\right)$ applications of $U_A, U_A^\dagger$.*

Proof. Let $A = \sum_i \sigma_i |u_i\rangle\langle v_i|$ be a singular value decomposition, so $\sigma_i \in [0, \|A\|]$. The block encoding condition $U_A \in \mathrm{BE}_{\alpha,m}(A)$ means that, upon projecting the ancilla register onto $|0^m\rangle$, the induced operator is A/α. In particular, QSVT applied to U_A implements odd polynomial transformations of the singular values of A/α.

Define $\alpha' := \alpha/\|A\| > 1$. Then the singular values of A/α lie in $[0, \alpha'^{-1}]$. Choose

$$\epsilon' := \min\left\{\frac{\epsilon}{\|A\|}, \frac{1}{2\alpha'}\right\}. \tag{13.39}$$

By Lemma 12.9, there exists an odd polynomial $p \in \mathbb{R}[x]$ with

$$\sup_{x\in[0,\alpha'^{-1}]} |(1+\delta)p(x) - \alpha' x| \leq \epsilon', \qquad \sup_{x\in[-1,1]} |p(x)| \leq 1, \tag{13.40}$$

and degree $\deg(p) = \mathcal{O}\left(\frac{\alpha'}{\delta}\log\left(\frac{\alpha'}{\epsilon'}\right)\right) = \mathcal{O}\left(\frac{\alpha}{\delta\|A\|}\log\left(\frac{\alpha}{\|A\|\epsilon}\right)\right)$.

Applying QSVT with this polynomial produces a unitary $U_\Phi \in \mathrm{BE}_{1,m+1}(p^\diamond(A/\alpha))$. Moreover,

$$\begin{aligned} \|\|A\|(1+\delta)p^\diamond(A/\alpha) - A\| &= \left\|\sum_i \left(\|A\|(1+\delta)p\left(\frac{\sigma_i}{\alpha}\right) - \sigma_i\right)|u_i\rangle\langle v_i|\right\| \\ &\leq \|A\| \sup_{x\in[0,\alpha'^{-1}]} |(1+\delta)p(x) - \alpha' x| \leq \|A\|\epsilon' \leq \epsilon. \end{aligned} \tag{13.41}$$

Therefore $U_\Phi \in \mathrm{BE}_{\|A\|(1+\delta),m+1}(A,\epsilon)$. The number of applications of U_A and $U_A^\dagger$ is $\mathcal{O}(\deg(p))$, which gives the stated query complexity. □

13.5. Quantum Gibbs state preparation

Given a Hamiltonian $H \in \mathbb{C}^{N\times N}$ (without loss of generality we assume $H \succeq 0$), the **quantum Gibbs state** at inverse temperature $\beta = 1/T$ is defined as

$$\sigma_\beta = \frac{e^{-\beta H}}{Z_\beta}, \quad Z_\beta = \mathrm{Tr}\big[e^{-\beta H}\big]. \tag{13.42}$$

where Z_β is known as the **partition function**.

Quantum Gibbs states can be prepared using QSVT and a technique called **purification**. Consider the purified Gibbs state

$$|\sigma_\beta\rangle = \sqrt{\frac{N}{Z_\beta}}\big(I \otimes e^{-\beta H/2}\big)\left(\frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}|j\rangle\,|j\rangle\right), \tag{13.43}$$

which satisfies $\langle\sigma_\beta|\sigma_\beta\rangle = 1$, since $H \succeq 0$ implies $Z_\beta = \mathrm{Tr}[e^{-\beta H}] \le \mathrm{Tr}[I] = N$. The Gibbs state σ_β is then obtained by tracing out the first (ancillary) register:

$$\mathrm{Tr}_A[|\sigma_\beta\rangle\langle\sigma_\beta|] = \frac{1}{Z_\beta}e^{-\beta H/2}\left(\sum_{j=0}^{N-1}|j\rangle\langle j|\right)e^{-\beta H/2} = \frac{e^{-\beta H}}{Z_\beta} = \sigma_\beta. \tag{13.44}$$

Thus, it suffices to construct a block-encoding of $e^{-\beta H/2}$ and apply it to the maximally entangled state $\frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}|j\rangle\,|j\rangle$.

Since $f(x) = e^{-\beta x/2}$ is neither even nor odd, one way to use QSVT is to approximate its even and odd parts separately. This is problematic if one insists on a uniform approximation on a symmetric interval, since $f(-x) = e^{\beta x/2}$ grows exponentially with β. One may instead try to approximate f by an even function, but the symmetrized function $g(x) = e^{-\beta|x|/2}$ has a cusp at $x = 0$, and consequently the approximation error decays only polynomially with the degree.

We therefore assume a different access model, namely $V_H \in \mathrm{BE}_{1,m}(I - H/\alpha_H)$, where α_H is chosen so that $0 \preceq H \preceq \alpha_H I$. The spectrum of $I - H/\alpha_H$ is contained in $[0,1]$. Using the identity

$$e^{-\beta H/2} = e^{-\frac{\beta\alpha_H}{2}(I-(I-H/\alpha_H))}, \tag{13.45}$$

we can construct a block-encoding of $e^{-\beta H/2}$ using V_H. For polynomial approximations to $e^{-\gamma(1-x)}$ on $[-1,1]$, we have the following result from [GSLW18, Corollary 64].

Proposition 13.8. *Let $\gamma > 0$ and $\epsilon \in \big(0, \frac{1}{2}\big]$. Then there exists a real polynomial P with degree $\mathcal{O}\left(\sqrt{\max\left[\gamma, \log\left(\frac{1}{\epsilon}\right)\right]\log\left(\frac{1}{\epsilon}\right)}\right)$ such that*

$$\left\|e^{-\gamma(1-x)} - P(x)\right\|_{[-1,1]} \le \epsilon. \tag{13.46}$$

The polynomial in Proposition 13.8 does not have definite parity. Therefore we implement its even and odd parts using QSVT, and combine them to obtain a block-encoding of $e^{-\beta H/2}$ using

$\mathcal{O}\left(\sqrt{\beta\alpha_H}\log(1/\epsilon)\right)$ queries to V_H. Since

$$\left\|\left(I\otimes e^{-\beta H/2}\right)\left(\frac{1}{\sqrt{N}}\sum_{j=0}^{N-1}|j\rangle|j\rangle\right)\right\| = \sqrt{\frac{Z_\beta}{N}}, \tag{13.47}$$

amplitude amplification yields a total query complexity

$$\mathcal{O}\left(\sqrt{\frac{N}{Z_\beta}}\sqrt{\beta\alpha_H}\log^2(1/\epsilon)\right) \tag{13.48}$$

for preparing $|\sigma_\beta\rangle$.

Remark 13.9. The $\mathcal{O}(\sqrt{\beta})$ scaling (here $\gamma=\beta\alpha_H/2$) may seem surprising, given that $\sup_{x\in[0,1]}\left|\frac{\mathrm{d}}{\mathrm{d}x}e^{-\gamma(1-x)}\right| = \gamma$. This is because, after the transformation, the largest derivative occurs at the boundary $x=1$, while the Chebyshev polynomial $T_k(x)=\cos(k\arccos(x))$ varies rapidly near $x=1$. Specifically,

$$T_k'(1) = \lim_{\theta\to 0}\frac{k\sin(k\theta)}{\sin(\theta)} = k^2. \tag{13.49}$$

Thus, a polynomial of degree $\mathcal{O}(\sqrt{\beta})$ is sufficient to resolve the large derivative at the boundary.

It is worth noting that this $\mathcal{O}(\sqrt{\beta})$ dependence relies on having access to $V_H\in \mathrm{BE}_{1,m}(I-H/\alpha_H)$. If we only have access to $V_H\in\mathrm{BE}_{\eta,m}(I-H/\alpha_H)$ for some constant $\eta>1$, then rewriting

$$e^{-\beta H/2} = e^{-\frac{\beta\alpha_H\eta}{2}(I/\eta-(I-H/\alpha_H)/\eta)}. \tag{13.50}$$

shows that one is naturally led to the function $x\mapsto e^{-\gamma(\eta^{-1}-x)}$ (with $\gamma=\beta\alpha_H\eta/2$). This function exceeds 1 for $x>\eta^{-1}$, and therefore no polynomial bounded on $[-1,1]$ can approximate it uniformly on $[-1,1]$ to small additive error. In particular, Proposition 13.8 does not apply in this form. ⋄

13.6. Quantum eigenvalue transformation with Hamiltonian evolution oracles

Given the Hamiltonian evolution oracle $U=e^{-iH}$ with $0\preceq H\preceq\pi$ for simplicity. Can we construct a block encoding of a matrix function $f(H)$ using QSP? One possibility is to first construct a block encoding of H by implementing the matrix logarithm $H=i\log U$ using QSVT, followed by another layer of QSVT to implement $f(H)$. A Slightly simpler approach is to construct $\cos(H)=(e^{-iH}+e^{iH})/2$ using LCU and then apply QSVt to implement the arccosine and then compute $f(H)$ on the result. In both cases, the procedure of constructing a transformation of the generator of U is a complex multistage procedure. Here we show that this process can be made much simpler using a single layer of QSVT-like circuit with one ancilla qubit. This is called the **quantum eigenvalue transformation of unitary matrices** with real polynomials (QETU).

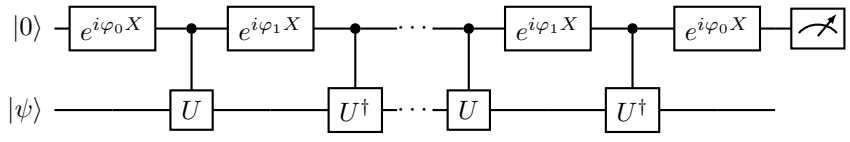


FIGURE 13.6. Circuit of quantum eigenvalue transformation of unitary matrices.

THEOREM 13.10 (Quantum eigenvalue transformation of unitary matrices). *Let $U = e^{-iH}$ with an n-qubit Hermitian matrix H. For any even real polynomial $F(x)$ of degree $2d$ satisfying $|F(x)| \leq 1, \forall x \in [-1,1]$, we can find a sequence of symmetric phase factors $\Phi := (\varphi_0, \varphi_1, \cdots, \varphi_1, \varphi_0) \in \mathbb{R}^{2d+1}$, such that the circuit in Fig. 13.6 denoted by $\mathcal{U}$ satisfies $(\langle 0| \otimes I_n)\mathcal{U}(|0\rangle \otimes I_n) = F\left(\cos \frac{H}{2}\right)$.*

Let the matrix function of interest be expressed as $f(H) = (f \circ g)(\cos \frac{H}{2})$, where $g(x) = 2\arccos(x)$. Therefore we can find an even polynomial approximation $F(x)$ so that

$$\sup_{x \in [\sigma_{\min}, \sigma_{\max}]} |(f \circ g)(x) - F(x)| \leq \epsilon. \tag{13.51}$$

Here $\sigma_{\min} = \cos \frac{\lambda_{\max}}{2}, \sigma_{\max} = \cos \frac{\lambda_{\min}}{2}$, respectively (note that $\cos(x/2)$ is a monotonically *decreasing* function on $[0, \pi]$). This ensures that the operator norm error satisfies

$$\|(\langle 0| \otimes I_n)\mathcal{U}(|0\rangle \otimes I_n) - f(H)\| \leq \epsilon. \tag{13.52}$$

Compared to the QSVT circuit for block encoding $f(H)$ with a real polynomial of definite parity, we find that instead of the Z rotation $e^{i\varphi Z}$, the circuit uses now the X rotation $e^{i\varphi X}$. For the proof of Theorem 13.10, we refer readers to [DLT22].

Exercise 13.1. Given access to a unitary $U = e^{-iH}$ where $\|H\| \leq \pi/2$. Use QSVT to design a quantum algorithm to approximately implement a block encoding of H, using controlled U and its inverses, as well as elementary quantum gates.

13.7. Perturbation theory of singular value transformations

So far we have assumed that $U \in \mathrm{BE}_{\alpha,m}(A)$ is an exact block encoding of A. Suppose instead that we can only implement $\widetilde{U} \in \mathrm{BE}_{\alpha,m}(\widetilde{A})$ with $\left\|\widetilde{A} - A\right\| \leq \epsilon$. In this setting we cannot directly invoke the linear error growth property in Proposition 3.21, because we do not have access to the exact block encoding matrix U and therefore cannot compute $\left\|U - \widetilde{U}\right\|$. It is therefore useful to develop a perturbation theory that directly controls $\left\|f^{\mathrm{SV}}(\widetilde{A}) - f^{\mathrm{SV}}(A)\right\|$ in terms of $\left\|\widetilde{A} - A\right\|$.

Definition 13.11. *Given a function $\omega : [0,\infty) \to [0,\infty)$ and an interval $I \subset \mathbb{R}$, a function $f : I \to \mathbb{C}$ admits ω as a modulus of continuity if*

$$|f(x) - f(y)| \leq \omega(|x - y|), \quad \forall x, y \in I. \tag{13.53}$$

Results from approximation theory [FN09] can be used to characterize the robustness of eigenvalue transformations of Hermitian matrices.

THEOREM 13.12. *Let $f : [-1,1] \to \mathbb{C}$ be a function that admits a modulus of continuity $\omega : [0,2] \to [0,\infty)$. Then for all Hermitian matrices $A, \widetilde{A} \in \mathbb{C}^{N \times N}$ such that $\|A\|, \left\|\widetilde{A}\right\| \leq 1$, we have*

$$\left\|f(A) - f(\widetilde{A})\right\| \leq 4\left[\ln\left(\frac{2}{\|A - \widetilde{A}\|} + 1\right) + 1\right]^2 \omega(\|A - \widetilde{A}\|). \tag{13.54}$$

At first sight, the logarithmic factor in Theorem 13.12 may seem to suggest a deterioration as $\left\|A - \widetilde{A}\right\|$ becomes small. This is misleading, because the modulus of continuity ω also vanishes as its argument tends to 0. Hence the overall bound still tends to 0 as $\left\|A - \widetilde{A}\right\| \to 0$. For instance, if f is Lipschitz continuous with constant L, then $\omega(\delta) = L\delta$, and Theorem 13.12 yields

$$\left\|f(A) - f(\widetilde{A})\right\| \leq 4L \left[\ln\left(\frac{2}{\left\|A - \widetilde{A}\right\|} + 1\right) + 1\right]^2 \left\|A - \widetilde{A}\right\|. \tag{13.55}$$

More generally, if f is Hölder continuous with exponent $\alpha \in (0, 1]$, then $\omega(\delta) = \mathcal{O}(\delta^\alpha)$, and asymptotically the error bound behaves like $\mathcal{O}\left(\left\|A - \widetilde{A}\right\|^\alpha \ln^2(1/\left\|A - \widetilde{A}\right\|)\right)$ as $\left\|A - \widetilde{A}\right\| \to 0$.

Using the connection between singular value transformation and eigenvalue transformation for dilated matrices from Section 10.1, we obtain the following perturbation result for singular value transformation.

Corollary 13.13. *Let $f : [-1, 1] \to \mathbb{C}$ be a function of definite parity that admits a modulus of continuity $\omega : [0, 2] \to [0, \infty)$. Then for all matrices $A, \widetilde{A} \in \mathbb{C}^{\tilde{N} \times N}$ such that $\|A\|, \left\|\widetilde{A}\right\| \leq 1$, we have*

$$\left\|f^{\mathrm{SV}}(A) - f^{\mathrm{SV}}(\widetilde{A})\right\| \leq 4 \left[\ln\left(\frac{2}{\|A - \widetilde{A}\|} + 1\right) + 1\right]^2 \omega(\|A - \widetilde{A}\|). \tag{13.56}$$

Proof. Define the Hermitian dilations

$$\mathcal{D}(A) := \begin{pmatrix} 0 & A^\dagger \\ A & 0 \end{pmatrix}, \qquad \mathcal{D}(\widetilde{A}) := \begin{pmatrix} 0 & \widetilde{A}^\dagger \\ \widetilde{A} & 0 \end{pmatrix}. \tag{13.57}$$

Since $\|A\|, \left\|\widetilde{A}\right\| \leq 1$, both $\mathcal{D}(A)$ and $\mathcal{D}(\widetilde{A})$ are Hermitian and have operator norm at most 1. Moreover,

$$\mathcal{D}(A) - \mathcal{D}(\widetilde{A}) = \begin{pmatrix} 0 & (A - \widetilde{A})^\dagger \\ A - \widetilde{A} & 0 \end{pmatrix}, \tag{13.58}$$

and hence

$$\left(\mathcal{D}(A) - \mathcal{D}(\widetilde{A})\right)^2 = \begin{pmatrix} (A - \widetilde{A})^\dagger (A - \widetilde{A}) & 0 \\ 0 & (A - \widetilde{A})(A - \widetilde{A})^\dagger \end{pmatrix}. \tag{13.59}$$

Therefore

$$\left\|\mathcal{D}(A) - \mathcal{D}(\widetilde{A})\right\| = \left\|A - \widetilde{A}\right\|. \tag{13.60}$$

By the dilation identity in Section 10.1, if f is even then

$$f(\mathcal{D}(A)) = \begin{pmatrix} f^{\triangleright}(A) & 0 \\ 0 & f^{\triangleleft}(A) \end{pmatrix}, \qquad f(\mathcal{D}(\widetilde{A})) = \begin{pmatrix} f^{\triangleright}(\widetilde{A}) & 0 \\ 0 & f^{\triangleleft}(\widetilde{A}) \end{pmatrix}. \tag{13.61}$$

Since $f^{\mathrm{SV}}(A) = f^{\triangleright}(A)$ and $f^{\mathrm{SV}}(\widetilde{A}) = f^{\triangleright}(\widetilde{A})$ in the even case, we obtain

$$\left\|f^{\mathrm{SV}}(A) - f^{\mathrm{SV}}(\widetilde{A})\right\| = \left\|f^{\triangleright}(A) - f^{\triangleright}(\widetilde{A})\right\| \leq \left\|f(\mathcal{D}(A)) - f(\mathcal{D}(\widetilde{A}))\right\|. \tag{13.62}$$

If f is odd, then

$$f(\mathcal{D}(A)) = \begin{pmatrix} 0 & f^\diamond(A^\dagger) \\ f^\diamond(A) & 0 \end{pmatrix}, \qquad f(\mathcal{D}(\widetilde{A})) = \begin{pmatrix} 0 & f^\diamond(\widetilde{A}^\dagger) \\ f^\diamond(\widetilde{A}) & 0 \end{pmatrix}. \tag{13.63}$$

Since $f^{\mathrm{SV}}(A) = f^\diamond(A)$ and $f^{\mathrm{SV}}(\widetilde{A}) = f^\diamond(\widetilde{A})$ in the odd case, together with

$$f^\diamond(A^\dagger) = (f^\diamond(A))^\dagger \tag{13.64}$$

we obtain

$$f(\mathcal{D}(A)) - f(\mathcal{D}(\widetilde{A})) = \begin{pmatrix} 0 & (f^{\mathrm{SV}}(A) - f^{\mathrm{SV}}(\widetilde{A}))^\dagger \\ f^{\mathrm{SV}}(A) - f^{\mathrm{SV}}(\widetilde{A}) & 0 \end{pmatrix}. \tag{13.65}$$

Therefore

$$\left\| f^{\mathrm{SV}}(A) - f^{\mathrm{SV}}(\widetilde{A}) \right\| = \left\| f(\mathcal{D}(A)) - f(\mathcal{D}(\widetilde{A})) \right\|. \tag{13.66}$$

Applying Theorem 13.12 to the Hermitian matrices $\mathcal{D}(A)$ and $\mathcal{D}(\widetilde{A})$ gives

$$\left\| f(\mathcal{D}(A)) - f(\mathcal{D}(\widetilde{A})) \right\| \leq 4 \left[\ln \left(\frac{2}{\left\| \mathcal{D}(A) - \mathcal{D}(\widetilde{A}) \right\|} + 1 \right) + 1 \right]^2 \omega\big(\left\| \mathcal{D}(A) - \mathcal{D}(\widetilde{A}) \right\| \big). \tag{13.67}$$

Substituting $\left\| \mathcal{D}(A) - \mathcal{D}(\widetilde{A}) \right\| = \left\| A - \widetilde{A} \right\|$ proves the claim. □

For specific problems this general bound is often not sharp. The next two examples show that for Hamiltonian simulation and oblivious amplitude amplification one can prove stronger bounds by direct arguments.

Example 13.14 (Perturbation analysis for Hamiltonian simulation)**.** Consider a block encoding $U_{\widetilde{H}} \in \mathrm{BE}_{1,m}(H, \epsilon)$. Then the Duhamel principle (Proposition 3.22) gives

$$\left\| e^{i\widetilde{H}} - e^{iH} \right\| = \left\| i \int_0^1 e^{iH(1-s)} (\widetilde{H} - H) e^{i\widetilde{H}s} \, \mathrm{d}s \right\| \leq \left\| \widetilde{H} - H \right\| \leq \epsilon. \tag{13.68}$$

This gives

$$\left\| \cos(\widetilde{H}) - \cos(H) \right\| = \left\| \frac{e^{i\widetilde{H}} + e^{-i\widetilde{H}}}{2} - \frac{e^{iH} + e^{-iH}}{2} \right\| \leq \frac{1}{2} \left\| e^{i\widetilde{H}} - e^{iH} \right\| + \frac{1}{2} \left\| e^{-i\widetilde{H}} - e^{-iH} \right\| \leq \epsilon. \tag{13.69}$$

Similarly

$$\left\| \sin(\widetilde{H}) - \sin(H) \right\| \leq \epsilon. \tag{13.70}$$

These bounds are independent of the polynomial degree used to approximate these functions. ◇

Example 13.15 (Refined perturbation analysis for oblivious amplitude amplification)**.** Let A be an approximate implementation of a unitary matrix U such that $\|A - U\| \leq \epsilon$. According to the oblivious amplitude amplification (see Section 11.4), if we choose

$$\gamma_k^{-1} = \sin \frac{\pi}{2(2k+1)}, \quad k \in \mathbb{N}_+, \tag{13.71}$$

then $T^{\diamond}_{2k+1}(U/\gamma_k) = (-1)^k U$. This means that if we have access to a block encoding $\mathcal{V} \in \mathrm{BE}_{\gamma_k,a}(A) = \mathrm{BE}_{\gamma_k,a}(U,\epsilon)$, then $T^{\diamond}_{2k+1}(A/\gamma_k)$ is an approximate implementation of $(-1)^k U$ using $k+1$ queries to $\mathcal{V}$ and k queries to $\mathcal{V}^\dagger$. We now bound the error $\big\|(-1)^k T^{\diamond}_{2k+1}(A/\gamma_k) - U\big\|$.

Let $A = W\Sigma V^\dagger$ be a singular value decomposition. The perturbation theorem for singular values (Theorem 7.10) states that $\|\Sigma - I\| \le \epsilon$. Hence $T^{\diamond}_{2k+1}(A/\gamma_k) = W T_{2k+1}(\Sigma/\gamma_k) V^\dagger$ is an approximate implementation of $(-1)^k W V^\dagger$. Note that the Chebyshev polynomial at γ_k^{-1} satisfies

$$T_{2k+1}(\gamma_k^{-1}) = (-1)^k, \quad T'_{2k+1}(\gamma_k^{-1}) = 0, \quad T''_{2k+1}(\gamma_k^{-1}) = (-1)^{k+1}\frac{(2k+1)^2}{1-\gamma_k^{-2}}. \tag{13.72}$$

By Taylor's theorem and the continuity of T''_{2k+1}, for each k there exists some $\epsilon_k > 0$ such that for any $|x-1| \le \epsilon \le \epsilon_k$,

(13.73)
$$\begin{aligned}\big|(-1)^k T_{2k+1}(x/\gamma_k) - 1\big| &= \big|T_{2k+1}(x/\gamma_k) - T_{2k+1}(\gamma_k^{-1})\big| \le 2\cdot\frac{1}{2}\cdot\big|T''_{2k+1}(\gamma_k^{-1})\big|\,\frac{\epsilon^2}{\gamma_k^2} = \frac{(2k+1)^2}{1-\gamma_k^{-2}}\cdot\frac{\epsilon^2}{\gamma_k^2} \\ &= \frac{(2k+1)^2\epsilon^2}{\gamma_k^2-1} = \left(\epsilon(2k+1)\tan\frac{\pi}{2(2k+1)}\right)^2 < \pi^2\epsilon^2.\end{aligned}$$

In the last inequality we used the fact that $a^{-1}\tan a < 2$ for any $a = \frac{\pi}{2(2k+1)} \in [0, \pi/6]$. Therefore

$$\big\|(-1)^k T^{\diamond}_{2k+1}(A/\gamma_k) - WV^\dagger\big\| \le \pi^2\epsilon^2. \tag{13.74}$$

Finally, if $\pi^2\epsilon < 1$, the triangle inequality gives
(13.75)
$$\big\|(-1)^k T^{\diamond}_{2k+1}(A/\gamma_k) - U\big\| \le \big\|(-1)^k T^{\diamond}_{2k+1}(A/\gamma_k) - WV^\dagger\big\| + \big\|WV^\dagger - W\Sigma V^\dagger\big\| + \big\|W\Sigma V^\dagger - U\big\| = 3\epsilon.$$

This bound is independent of the polynomial degree used in the construction. Fig. 13.7 confirms the validity of this error bound. This bound agrees with the refined analysis of oblivious amplitude amplification in [GSLW19, Theorem 15].

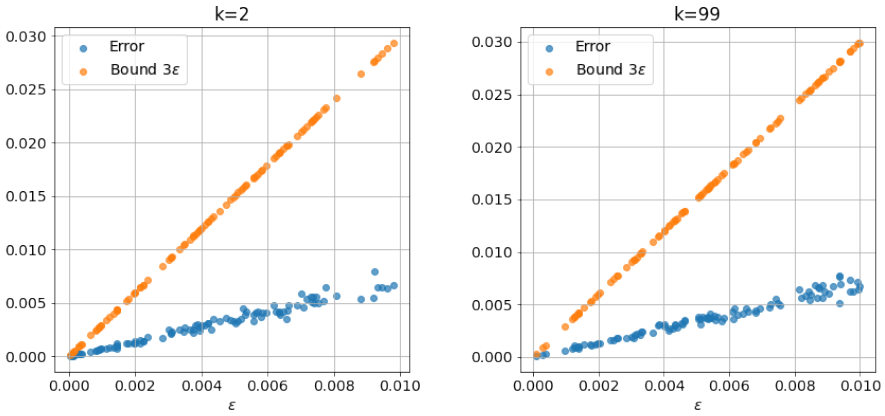


FIGURE 13.7. Error of oblivious amplitude amplification $\left\|(-1)^k T^{\diamond}_{2k+1}(A/\gamma_k) - U\right\|$ versus the error bound for 100 random matrices with $\|A - U\| = \epsilon$. Neither the computed error nor the error bound depends on k.

◇

Notes and further reading

Many applications of QSVT can be found in the seminal paper [GSLW19]. When the input is Hermitian, the connection between singular value and eigenvalue transformation (cf. Section 10.1) implies that the same circuits implement eigenvalue transformations of A; this special case is sometimes called quantum eigenvalue transformation (QET). Recent usage often reserves "eigenvalue processing/transformation" for settings beyond Hermitian inputs, such as eigenvalue transformations associated with nonunitary or more general matrix dynamics; see, e.g., [ALL23, LS26]. A generalization of the QETU algorithm is given by generalized quantum signal processing [MW24], which can also be interpreted using the nonlinear Fourier transform [AMT24].

The $\mathcal{O}(\sqrt{\beta})$ dependence discussed in Section 13.5 can also be achieved under alternative access models for H, such as access to $\sqrt{H}$ [CS17, ACNR22]. The Gibbs sampler based on linear combination of Hamiltonian simulation [ALL23, ACL26] (see also Section 20.4) applies to positive semidefinite Hamiltonians and requires only the ability to simulate the dynamics; its complexity is $\widetilde{\mathcal{O}}\left(\sqrt{\frac{N}{Z_\beta}}\beta\alpha_H \left(\log\left(\frac{1}{\epsilon}\right)\right)^{1/\gamma}\right)$ for any $\gamma \in (0,1)$. The factor $\sqrt{\frac{N}{Z_\beta}}$ becomes large at low temperature. This also means that efficient Gibbs preparation without additional structure is typically confined to sufficiently high-temperature regimes.

CHAPTER 14

Block encoding based Hamiltonian simulation

Simulation of one quantum Hamiltonian by another quantum system was also one of the motivations of Feynman's proposal for design of quantum computers [Fey82]. Hamiltonian simulation is the process of implementing the unitary operator $U(t) = e^{-itH}$, where H is the Hamiltonian of the system and t is the evolution time.

More generally, a quantum computer can be thought of as a quantum mechanical system wherein the system Hamiltonian is changed over time to implement the various gates that we wish to apply to our system. These control fields are actually not best modeled as a single fixed Hamiltonian, and instead is modeled by a time-dependent Hamiltonian. Such time-dependent Hamiltonians appear in a number of places. They are essential to understand the operations of quantum computers at a physical level and also are fundamental to approaches to understand adiabatic state preparation [WKAG09] and related adiabatic algorithms [FG98].

Our aim is to show how such quantum dynamics can be emulated on a quantum computer. We begin with simulation techniques for time-independent Hamiltonians. We then explain the time-ordering formalism for time-dependent Hamiltonians and then discuss how truncated Dyson series methods can be used to simulate the underlying dynamics. Finally we will use these results to present the interaction picture simulation method, which takes a time-independent Hamiltonian and transforms it into a related time-dependent Hamiltonian with the aim of reducing the computational complexity of quantum simulation.

14.1. Quantum signal processing and time-independent Hamiltonian simulation with optimal query complexity

Given a block encoding of a Hamiltonian H, the Hamiltonian simulation problem aims at constructing a block encoding of the unitary $U = e^{-iHt}$.

Since $e^{-iHt} = e^{-i(H/\alpha)(\alpha t)}$, the normalization factor α can be absorbed into the simulation time t, and we may assume $\alpha = 1$. If we start from a block encoding $U_{\widetilde{H}} \in \mathrm{BE}_{1,m}(\widetilde{H})$ with $\left\|\widetilde{H} - H\right\| \leq \epsilon'$, then the perturbation bound follows from Duhamel's formula (a.k.a. variation of constants):

$$\left\|e^{-i\widetilde{H}t} - e^{-iHt}\right\| = \left\|-i\int_0^t e^{-iH(t-s)}(\widetilde{H} - H)e^{-i\widetilde{H}s}\,\mathrm{d}s\right\| \leq \epsilon' t. \tag{14.1}$$

In order to approximate e^{-iHt} to precision ϵ, it is sufficient to choose $\epsilon' = \epsilon/(2t)$ and then approximate $e^{-i\widetilde{H}t}$ to precision $\epsilon/2$. Hence, without loss of generality, we assume the block encoding $U_H \in \mathrm{BE}_{1,m}(H)$ is error-free.

We use QSP/QSVT to construct a block encoding of $e^{-iHt} = \cos(Ht) - i\sin(Ht)$. Note that $\cos(tx)$ is real and even, whereas $\sin(tx)$ is real and odd. Accordingly, we construct block encodings for $\cos(Ht)$ and $\sin(Ht)$ separately using QSVT, and then combine them using LCU.

To implement this, we use the Fourier–Chebyshev series of the trigonometric functions on $[-1,1]$ (the Jacobi-Anger expansion):

$$\begin{aligned}\cos(tx) =& J_0(t) + 2\sum_{k=1}^{\infty}(-1)^k J_{2k}(t)T_{2k}(x),\\ \sin(tx) =& 2\sum_{k=0}^{\infty}(-1)^k J_{2k+1}(t)T_{2k+1}(x).\end{aligned} \tag{14.2}$$

Here $J_\nu(t)$ denotes Bessel functions of the first kind. This series converges very rapidly. We first prove a useful bound for the Lambert-W function.

Lemma 14.1. *Let $a > 0$ and $\epsilon \in (0, e^{-1})$, and set $L := \ln(1/\epsilon)$. Define*

$$K_*(a,\epsilon) := \frac{L}{W(L/a)}, \tag{14.3}$$

where W is the (principal branch of the) Lambert-W function. Then $K_*(a,\epsilon)$ is the unique positive solution of

$$\left(\frac{a}{K}\right)^K = \epsilon. \tag{14.4}$$

Moreover, $K_*(a,\epsilon)$ satisfies

$$K_*(a,\epsilon) = \mathcal{O}\left(a + \ln(1/\epsilon)\right). \tag{14.5}$$

There is also a more refined bound

$$K_*(a,\epsilon) = \mathcal{O}\left(a + \frac{\ln(1/\epsilon)}{\ln\left(e + \ln(1/\epsilon)/a\right)}\right). \tag{14.6}$$

Proof. Consider the function $f(K) := K\ln(K/a)$ for $K > a$. Since $f'(K) = \ln(K/a) + 1 > 0$, f is strictly increasing on (a,∞). The equation $(a/K)^K = \epsilon$ is equivalent to

$$f(K) = \ln(1/\epsilon) = L. \tag{14.7}$$

Writing $K = ay$ with $y > 1$ gives $ay\ln y = L$, or equivalently $y\ln y = L/a$. Setting $u := \ln y$ yields $ue^u = L/a$. Its solution defines the Lambert-W function as $u = W(L/a)$. Therefore

$$K = ay = ae^{W(L/a)} = \frac{L}{W(L/a)} = K_*(a,\epsilon). \tag{14.8}$$

The monotonicity of f implies that $K \geq K_*(a,\epsilon)$ is sufficient for $(a/K)^K \leq \epsilon$.

We first prove the crude bound Eq. (14.5). Take $K := a + L$. Using the inequality $\ln(1+x) \geq x/(1+x)$ for $x \geq 0$, we obtain

$$f(K) = K\ln\left(\frac{K}{a}\right) = (a+L)\ln\left(1+\frac{L}{a}\right) \geq (a+L)\cdot\frac{L/a}{1+L/a} = L. \tag{14.9}$$

Therefore $(a/K)^K = e^{-f(K)} \leq e^{-L} = \epsilon$, which implies $K_*(a,\epsilon) \leq a + L$.

To obtain the refined bound Eq. (14.6), we set $z := L/a$. If $z \leq 1$ (equivalently, $L \leq a$), then taking $K = 2a$ gives

$$\left(\frac{a}{K}\right)^K = \left(\frac{1}{2}\right)^{2a} = e^{-2a\ln 2} \leq e^{-a} \leq e^{-L} = \epsilon, \tag{14.10}$$

using $2\ln 2 > 1$. Hence $K = \mathcal{O}(a)$ suffices in this regime.

If $z \geq 1$, let $u := \frac{1}{2}\ln z \geq 0$. Since $e^u \geq u$ for $u \geq 0$, we have $\ln z = 2u \leq 2e^u = 2\sqrt{z}$, and therefore

$$ue^u = \tfrac{1}{2}(\ln z)\sqrt{z} \leq z. \tag{14.11}$$

By monotonicity of $w \mapsto we^w$ on $[0,\infty)$ and the defining relation $W(z)e^{W(z)} = z$, this implies $W(z) \geq u = (1/2)\ln z$. Consequently,

$$K_*(a,\epsilon) = \frac{L}{W(z)} \leq \frac{2L}{\ln z} = \mathcal{O}\left(\frac{\ln(1/\epsilon)}{\ln\left(e + \ln(1/\epsilon)/a\right)}\right). \tag{14.12}$$

Combining the two cases yields Eq. (14.6). □

Lemma 14.2 (Jacobi-Anger expansion)**.** *For any $t > 0$, $\epsilon \in (0, e^{-1})$, we can choose*

$$K = \Theta\left(t + \frac{\ln(1/\epsilon)}{\ln(e + \ln(1/\epsilon)/t)}\right) \tag{14.13}$$

such that

$$\sup_{x\in[-1,1]} \left|\cos(tx) - \left(J_0(t) + 2\sum_{k=1}^{K}(-1)^k J_{2k}(t)T_{2k}(x)\right)\right| \leq \epsilon, \tag{14.14}$$

and

$$\sup_{x\in[-1,1]} \left|\sin(tx) - 2\sum_{k=0}^{K}(-1)^k J_{2k+1}(t)T_{2k+1}(x)\right| \leq \epsilon. \tag{14.15}$$

Proof sketch. The Bessel function satisfies the tail bound

$$|J_m(t)| \leq \frac{1}{m!}\left|\frac{t}{2}\right|^m. \tag{14.16}$$

This means that the tail contribution is upper bounded by

$$2\sum_{k=2K+1}^{\infty}|J_k(t)| \leq 2\sum_{k=2K+1}^{\infty}\frac{1}{k!}\left|\frac{t}{2}\right|^k = \mathcal{O}\left(\frac{1}{(2K+1)!}\left(\frac{t}{2}\right)^{2K+1}e^{t/2}\right) = \mathcal{O}\left(\left(\frac{et}{2K+1}\right)^{2K+1}e^{t/2}\right). \tag{14.17}$$

In particular, one may view the choice of K as governed (up to constants) by a model inequality of the form $(a/K)^K \leq \epsilon$, whose solution involves the Lambert-W function (see Lemma 14.1). Applying the refined estimate Eq. (14.6) with $a = \Theta(t)$ yields Eq. (14.13). □

We now present the following algorithm for simulating time-independent Hamiltonians [LC17b], which matches the complexity lower bound for Hamiltonian simulation [BACS07] and thus achieves the optimal query complexity.

Theorem 14.3 (Time-independent Hamiltonian simulation with optimal query complexity). *From a block encoding $U_H \in \mathrm{BE}_{1,m}(H)$, for any $\epsilon \in (0,1), t > 0$, we can construct a unitary $U_\Phi \in \mathrm{BE}_{2(1+\epsilon),m+2}(e^{-iHt},\epsilon)$. It uses $\mathcal{O}\left(t + \frac{\ln(1/\epsilon)}{\ln(e+\ln(1/\epsilon)/t)}\right)$ applications of $U_H, U_H^\dagger$, and one application of controlled U_H.*

PROOF. Using Eq. (14.13), we choose K so that $\cos(tx)$ and $\sin(tx)$ are each approximated on $[-1,1]$ to precision $\epsilon/2$. Denote the resulting truncations by $C(x)$ and $S(x)$. Choose $\beta = 1+\epsilon$ so that $\left|\beta^{-1}C(x)\right| \leq 1$ and $\left|\beta^{-1}S(x)\right| \leq 1$ for all $x \in [-1,1]$. Moreover,

$$\max_{x\in[-1,1]} \left|(C(x) - iS(x)) - e^{-itx}\right| \leq \sqrt{\left(\frac{\epsilon}{2}\right)^2 + \left(\frac{\epsilon}{2}\right)^2} = \epsilon/\sqrt{2} < \epsilon. \tag{14.18}$$

Corollary 12.6 guarantees the existence of symmetric phase factors Φ_C, Φ_S that represent the polynomials $\beta^{-1}C(x)$ and $\beta^{-1}S(x)$, respectively. Using these phase factors, we obtain block encodings $U_C \in \mathrm{BE}_{\beta,m+1}(\cos(Ht), \epsilon/2)$ and $U_S \in \mathrm{BE}_{\beta,m+1}(\sin(Ht), \epsilon/2)$. Finally, we use one more ancilla qubit and LCU to combine U_C and U_S into the desired block encoding U_Φ. In the corresponding select oracle (see Fig. 13.3), $C(H)$ does not require any controlled-U_H, whereas $S(H)$ uses a controlled-U_H circuit once. □

Example 14.4. Fig. 14.1 shows the QSP representation error for approximating $\cos(tx)$ using $P_{\mathrm{Re}}(x) = C_d(x)$ with $t = 4\pi, \beta = 1.001, d = 24$. The approximation improves significantly with a larger degree $d = 50$ (see Fig. 14.2). The phase factors are obtained via QSPPACK. The results for the sine function are similar. ◇

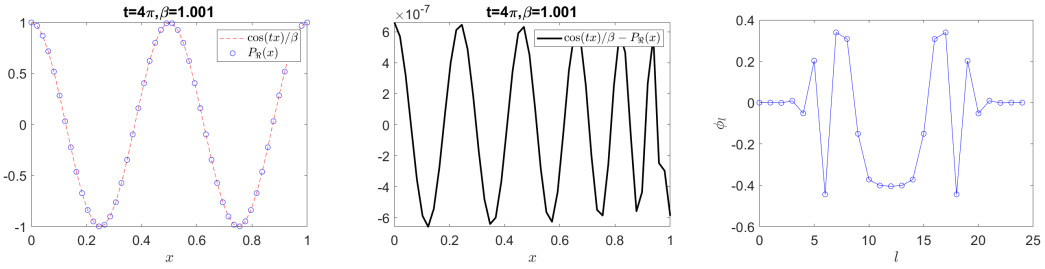


FIGURE 14.1. QSP representation of $\cos(tx)/\beta$ with $t = 4\pi, \beta = 1.001, d = 24$. The phase factors plotted remove a factor of $\pi/4$ on both ends (see **??**).

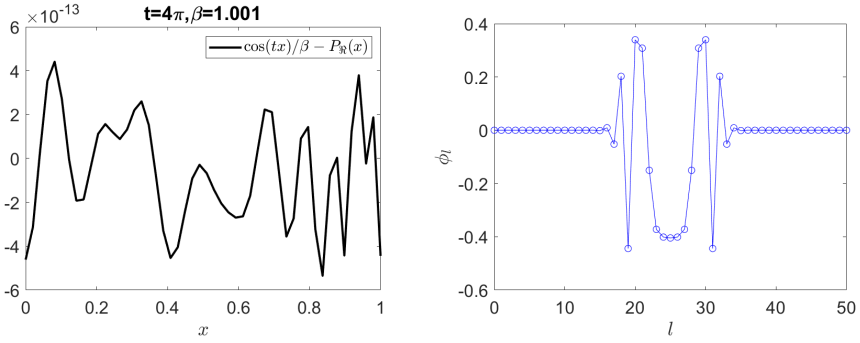


FIGURE 14.2. Error of the QSP representation of $\cos(tx)/\beta$ with $t = 4\pi, \beta = 1.001, d = 50$. The phase factors plotted remove a factor of $\pi/4$ on both ends (see **??**).

Example 14.5 (Oblivious amplitude amplification for Hamiltonian simulation)**.** In the Hamiltonian simulation problem, we use LCU to obtain $U_\Phi \in \mathrm{BE}_{2\beta,m+2}(e^{-iHt},\epsilon)$, where $\beta = 1+\epsilon$. Since

$$\left\|e^{-iHt} - 2\left\langle 0^{m+2}|U_\Phi|0^{m+2}\right\rangle\right\| \le \left\|e^{-iHt} - 2\beta\left\langle 0^{m+2}|U_\Phi|0^{m+2}\right\rangle\right\| + 2\epsilon\left\|U_\Phi\right\| \le 3\epsilon, \tag{14.19}$$

we also have $U_\Phi \in \mathrm{BE}_{2,m+2}(e^{-iHt},3\epsilon)$. According to the perturbation analysis of oblivious amplitude amplification in Example 13.15, we can use 2 uses of U_Φ and 1 use of $U_\Phi^\dagger$ to construct a block encoding $\mathfrak{U} \in \mathrm{BE}_{1,m+2}(e^{-iHt},9\epsilon)$. It uses 3 applications of controlled U_H.

If we would like to use the oblivious amplitude amplified Hamiltonian simulation as a subroutine and to simulate for an even longer period $T = Lt$ for some integer L, we can simply use $\mathfrak{U}^L$ and the error is bounded by $9\epsilon L$ using the linear error growth property. ⋄

14.2. Truncated Taylor series method

We now introduce an alternative approach for simulating time-independent Hamiltonians: the **truncated Taylor series method**, which predates the QSP-based methods. While it does not achieve optimal query complexity, it offers a very different perspective on Hamiltonian simulation. Moreover, it serves as a natural precursor to more advanced algorithms for time-dependent Hamiltonians, such as the truncated Dyson series method.

Assume $\|H\| \le 1$ for simplicity. For a short time Δt, the truncated Taylor method approximates the short-time evolution operator by truncating the Taylor series after order $K-1$:

$$e^{-iH\Delta t} \approx \sum_{k=0}^{K-1} \frac{(-iH\Delta t)^k}{k!}. \tag{14.20}$$

The choice of K will be specified later.

We first construct a sequence of unitary operations U_k that correspond to the terms $(-iH)^k$ using products of block encodings. Then we implement a select oracle

$$U_{\mathrm{SELECT}} = \sum_{k=0}^{K-1} |k\rangle\langle k| \otimes U_k. \tag{14.21}$$

We also assume access to a prepare oracle (and assume $\log_2 K$ is an integer for simplicity)

$$V_{\mathrm{PREP}}\,|0^{\log_2 K}\rangle = \frac{1}{\|c\|_1}\sum_{k=0}^{K-1}\sqrt{c_k}\,|k\rangle\,, \quad c_k = \frac{(\Delta t)^k}{k!}. \tag{14.22}$$

We choose $\Delta t = \ln 2$ so that the full Taylor series satisfies $\sum_{k=0}^{\infty}(\Delta t)^k/k! = e^{\Delta t} = 2$. For finite truncation order K, one has $\|c\|_1 \le 2$ and $|\|c\|_1 - 2|$ is controlled by the Taylor remainder. Then LCU implements a block encoding of $e^{-iH\Delta t}$ with normalization factor $\|c\|_1 \le 2$. After oblivious amplitude amplification, this yields a block encoding

$$W \in \mathrm{BE}_{1,a}(e^{-iH\Delta t},\epsilon'), \tag{14.23}$$

where $a = \mathcal{O}(\log_2 K + m)$, if U_{SELECT} is implemented using the compression gadget in Example 11.10.

For simulations over longer durations $t = L\Delta t$, we concatenate the segments:

$$e^{-iHt} \approx \left(\sum_{k=0}^{K-1}\frac{(-iH\Delta t)^k}{k!}\right)^L. \tag{14.24}$$

Each term in the Taylor series can be implemented using a block encoding, and their linear combination forms a block encoding of the approximated evolution operator. Using oblivious amplitude amplification and the fact that the target $e^{-iH\Delta t}$ is unitary, we have

$$\left\|(\langle 0^a| W |0^a\rangle)^L - e^{-iHL\Delta t}\right\| \leq L\epsilon'. \tag{14.25}$$

To approximate e^{-iHt} to precision ϵ, it is sufficient to choose $\epsilon' = \epsilon/L = \epsilon\Delta t/t$. The success probability satisfies $p \geq (1 - L\epsilon')^2$.

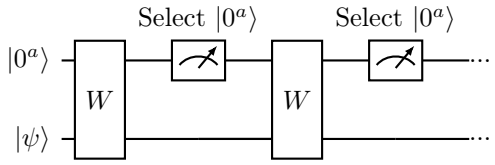


FIGURE 14.3. Circuit for simulating time-independent Hamiltonian evolution via the truncated Taylor series method.

Finally, we bound the remainder of the Taylor expansion.

$$\left\|\sum_{k=K}^{\infty} \frac{(-iH\Delta t)^k}{k!}\right\| \leq \frac{(\|H\|\,\Delta t)^K}{K!} e^{\|H\|\Delta t} \leq \left(\frac{e\,\|H\|\,\Delta t}{K}\right)^K e^{\|H\|\Delta t} \leq \epsilon'. \tag{14.26}$$

Here we use the relation

$$K^K \leq e^K K!, \tag{14.27}$$

and we may choose K using the refined estimate Eq. (14.6). Concretely, taking $a = e\,\|H\|\,\Delta t$ and replacing ϵ' by $\epsilon' e^{-\|H\|\Delta t}$ gives an inequality of the form $(a/K)^K \leq \epsilon' e^{-\|H\|\Delta t}$; since $a = \mathcal{O}(1)$ for $\Delta t = \ln 2$ and $\|H\| \leq 1$, Eq. (14.6) yields

$$K = \mathcal{O}\left(\frac{\log(1/\epsilon')}{\log\log(1/\epsilon')}\right) = \mathcal{O}\left(\frac{\log(t/\epsilon)}{\log\log(t/\epsilon)}\right). \tag{14.28}$$

The total query complexity to U_H is $\mathcal{O}\left(\frac{t\log(t/\epsilon)}{\log\log(t/\epsilon)}\right)$, and the number of ancilla qubits is $\mathcal{O}(m + \log\log(t/\epsilon))$.

14.3. Time-ordered operator exponentials

Let us first consider a simple time-dependent Hamiltonian $H(t) = (T-t)I + tX$, for which the Schrödinger equation reads

$$\partial_t |\psi(t)\rangle = -i((T-t)I + tX)|\psi(t)\rangle\,, \quad |\psi(0)\rangle = |\psi_0\rangle\,. \tag{14.29}$$

For some initial state $|\psi_0\rangle$, we can rewrite the problem as an operator differential equation for the time evolution operator $U(t)$ such that $U(t)|\psi_0\rangle = |\psi(t)\rangle$ for any t. The solution to the differential equation is

$$U(t) = e^{-i\int_0^t ((T-s)I + sX)\,\mathrm{d}s} = e^{-i(I(Tt - t^2/2) + t^2 X/2)}. \tag{14.30}$$

This can be verified by differentiating the right-hand side, using that $H(s)$ commutes with $H(s')$ for all s, s' in this example.

On the other hand, if we change the Hamiltonian to $H(t) = (T-t)Z + tX$, then

$$U(t) \neq e^{-i(Z(Tt-t^2/2)+t^2X/2)}. \tag{14.31}$$

The exponential of the integrated Hamiltonian does not solve the differential equation in this case because $H(t)$ fails to commute with itself at different times. Specifically, for $t \neq t'$ one has $\|[H(t), H(t')]\| \neq 0$ (assuming $T \neq 0$). This prevents us from differentiating $e^{-i\int_0^t H(s)\,\mathrm{d}s}$ by the usual chain rule.

This example illustrates that time dependence introduces genuinely new features. In particular, the time dependence of $H(t)$ need not be analytic, and high-order derivatives may not exist. Such issues can affect the validity of high-order Taylor-type arguments, and have led to misunderstandings in numerical analysis for non-analytic time-dependent problems [CC02]. We therefore begin by formalizing the solution to the operator differential equations that arise in time-dependent simulation and introducing the **Dyson series expansion**, which underlies the truncated Dyson series method.

THEOREM 14.6 (Time-ordered operator exponentials and Dyson series). *Let $A : [0,t] \to \mathbb{C}^{d\times d}$ for some positive integer d be a time-dependent linear operator that is continuous on $[0,t] \subset \mathbb{R}$. The operator differential equation $\partial_t U(t) = A(t)U(t)$ with initial condition $U(0) = I$ has a unique solution, called an ordered operator exponential, and for any $t > 0$ can be expressed as the series expansion*

$$U(t) = \mathcal{T}e^{\int_0^t A(s)\,\mathrm{d}s} = I + \sum_{n=1}^{\infty} \int_0^t \int_0^{s_n} \int_0^{s_{n-1}} \cdots \int_0^{s_2} A(s_n)\cdots A(s_1)\,\mathrm{d}s_1 \cdots \mathrm{d}s_n, \tag{14.32}$$

which is known as the Dyson series expansion.

PROOF. From the fundamental theorem of calculus,

$$\int_0^t \partial_s U(s)\,\mathrm{d}s = U(t) - U(0) = U(t) - I. \tag{14.33}$$

Substituting $\partial_s U(s) = A(s)U(s)$ yields the integral equation

$$U(t) = I + \int_0^t A(s)U(s)\,\mathrm{d}s. \tag{14.34}$$

Iterating Eq. (14.34) p times gives

$$U(t) = I + \sum_{n=1}^{p} \int_0^t \int_0^{s_n} \int_0^{s_{n-1}} \cdots \int_0^{s_2} A(s_n)\cdots A(s_1)\,\mathrm{d}s_1 \cdots \mathrm{d}s_n + R_{p+1}(t), \tag{14.35}$$

where

$$R_{p+1}(t) = \int_0^t \int_0^{s_{p+1}} \int_0^{s_p} \cdots \int_0^{s_2} A(s_{p+1})\cdots A(s_1)\,U(s_1)\,\mathrm{d}s_1 \cdots \mathrm{d}s_{p+1}. \tag{14.36}$$

It remains to show that $\lim_{p\to\infty} \|R_{p+1}(t)\| = 0$.

Let $M := \sup_{s\in[0,t]} \|A(s)\| < \infty$, which exists because A is continuous on a compact interval. Moreover, one has the bound

$$\|U(s)\| \leq \exp\Big(\int_0^s \|A(\tau)\|\;\mathrm{d}\tau\Big) \leq e^{Ms} \leq e^{Mt} \qquad (0 \leq s \leq t). \tag{14.37}$$

Using submultiplicativity and the volume of the simplex $\{0 \le s_1 \le \cdots \le s_{p+1} \le t\}$, we obtain

$$\|R_{p+1}(t)\| \le e^{Mt}\, M^{p+1} \int_0^t \int_0^{s_{p+1}} \cdots \int_0^{s_2} \mathrm{d}s_1 \cdots \mathrm{d}s_{p+1} = e^{Mt}\, \frac{(Mt)^{p+1}}{(p+1)!}. \tag{14.38}$$

Since $(p+1)!$ dominates $(Mt)^{p+1}$ as $p \to \infty$, this implies $\lim_{p\to\infty} \|R_{p+1}(t)\| = 0$, and hence the Dyson series equals $U(t)$. □

The Dyson series can be viewed as the natural analogue of the Taylor series when $A(t)$ is constant. Specifically, if $A(t) = A$ for all t, then

$$U(t) = I + \int_0^t A \, \mathrm{d}s_1 + \int_0^t \int_0^{s_2} A^2 \, \mathrm{d}s_1 \, \mathrm{d}s_2 + \cdots = I + At + \frac{A^2 t^2}{2!} + \cdots . \tag{14.39}$$

An alternative way to characterize the evolution operator is through **time-ordering**. The idea is to use a time-ordering symbol that reorders products of operators according to their time arguments. As an example, the time-ordered product of two operators $\mathcal{T}[A(s_1)A(s_2)]$ is given by

$$\mathcal{T}[A(s_1)A(s_2)] = \begin{cases} A(s_1)A(s_2), & s_1 \ge s_2; \\ A(s_2)A(s_1), & s_1 < s_2. \end{cases} \tag{14.40}$$

Note that the two possible outcomes are in general different, since the matrices A at different times might not commute. Using the identity

$$\int_0^t \cdots \int_0^t \mathcal{T}[A(s_1)\cdots A(s_n)]\, \mathrm{d}s_1 \cdots \mathrm{d}s_n = n! \int_0^t \int_0^{s_n} \int_0^{s_{n-1}} \cdots \int_0^{s_2} A(s_n)\cdots A(s_1)\, \mathrm{d}s_1 \cdots \mathrm{d}s_n, \tag{14.41}$$

we may define the time-ordered matrix exponential as

$$\mathcal{T}\Big[e^{\int_0^t A(s)\,\mathrm{d}s}\Big] = I + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^t \cdots \int_0^t \mathcal{T}[A(s_1)\cdots A(s_n)]\, \mathrm{d}s_1 \cdots \mathrm{d}s_n. \tag{14.42}$$

Therefore the solution of $\partial_t U(t) = A(t)U(t)$ with $U(0) = I$ can be written as

$$U(t) = \mathcal{T}\Big[e^{\int_0^t A(s)\,\mathrm{d}s}\Big]. \tag{14.43}$$

The time-ordering symbol is best viewed as a prescription rather than as an operator acting on the underlying Hilbert space: for each tuple $(s_1, \ldots, s_n)$, it replaces the product $A(s_1)\cdots A(s_n)$ by the product with the factors sorted in nonincreasing time order. For this reason, it is often preferable to work directly with the Dyson series definition of the ordered operator exponential. However, the time-ordered exponential notation will be useful in the truncated Dyson series algorithm.

14.4. Block encoding of time-dependent operators

A time-dependent Hamiltonian maps a tuple of the time and a vector in the Hilbert space of the simulation to another vector in the Hilbert space which is of the form $H : \mathbb{R} \times \mathbb{C}^{2^n} \to \mathbb{C}^{2^n}$. This means that a block-encoding of a time-dependent Hamiltonian must do more than just block encoding the space that the Hamiltonian acts on: it must also block encode the time.

Let us divide the interval $[0, T]$ into 2^{n_t} equal steps of size $\Delta t = \frac{T}{2^{n_t}}$. Then for any $t \in [0, T)$, we can approximate the time-dependent Hamiltonian by the piecewise-constant function

$$\widetilde{H}(t) = H(t_\ell), \quad \ell = \left\lfloor \frac{t}{\Delta t} \right\rfloor, \qquad t_\ell = \ell\, \Delta t. \tag{14.44}$$

By Taylor's theorem, the local error in the Hamiltonian is

$$\left\| H(t) - \widetilde{H}(t) \right\| \leq \max_{s\in[0,T]} \|H'(s)\| \ \Delta t, \tag{14.45}$$

and the error in the time-ordered evolution satisfies

$$\left\| \mathcal{T} e^{-i\int_0^T H(s)\ \mathrm{d}s} - \mathcal{T} e^{-i\int_0^T \widetilde{H}(s)\ \mathrm{d}s} \right\| \leq \max_{s\in[0,T]} \|H'(s)\| \ T\,\Delta t. \tag{14.46}$$

Thus the number of temporal points that we use in the discretization needs to increase as the derivative of the Hamiltonian increases. Specifically if we want to ensure that the error in the evaluation of the time evolution operator due to discretization is at most ϵ_T, then it suffices to choose

$$n_t = \mathcal{O}\left(\log\left(\frac{\max_s \|H'(s)\|\, T^2}{\epsilon_T} \right) \right). \tag{14.47}$$

Therefore, even for rapidly varying Hamiltonians, the number of qubits required for the time register scales only logarithmically in $\max_s \|H'(s)\|$ and $1/\epsilon_T$.

We can now block-encode the discretized Hamiltonian by using a clock register for the time and a standard block encoding on the system register.

Definition 14.7 (HAM-T oracle)**.** *Let $H(t) \in \mathbb{C}^{2^n\times 2^n}$ be a time-dependent Hamiltonian. Define a unitary oracle* `HAM-T` *acting on $n_t + m + n$ qubits, where m ancillas are used for the system block encoding. For a normalization constant $\alpha_T > 0$, define* `HAM-T` *by*

$$(I^{\otimes n_t} \otimes \langle 0^m| \otimes I^{\otimes n})\texttt{HAM-T}(I^{\otimes n_t} \otimes |0^m\rangle \otimes I^{\otimes n}) = \sum_{\ell=0}^{2^{n_t}-1} |\ell\rangle\langle\ell| \otimes \frac{H(\ell T/2^{n_t})}{\alpha_T}. \tag{14.48}$$

This oracle provides a block-encoding of the block-diagonal operator $\sum_\ell |\ell\rangle\langle\ell| \otimes H(\ell T/2^{n_t})$.

To construct such an oracle, we still need to implement each $H(t_\ell)$ via a unitary block encoding. We do so using a linear-combination-of-unitaries (LCU) decomposition together with a clock register. The computational basis on the clock is a convenient choice, though other bases (for example, Fourier modes) can also be used.

Definition 14.8 (Standard form for time-dependent LCU)**.** *Let $H(t) \in \mathbb{C}^{2^n\times 2^n}$ be expressed as*

$$H(t) = \sum_{j=0}^{M-1} c_j(t) U_j(t), \tag{14.49}$$

where $c_j(t) \geq 0$ and each $U_j(t)$ is unitary on $\mathbb{C}^{2^n}$. Define SELECT *so that its action on a time index ℓ and Hamiltonian index j satisfies*

$$(\langle \ell| \langle j| \otimes I^{\otimes n})\,\mathrm{SELECT}(|\ell\rangle\,|j\rangle \otimes I^{\otimes n}) = U_j(\ell T/2^{n_t}). \tag{14.50}$$

Similarly, the time-dependent coefficients are specified by a state-preparation oracle PREP-T*, which is defined for some $\alpha \geq \max_\ell \sum_{j=0}^{M-1} c_j(\ell T/2^{n_t})$ by*

$$(\text{PREP-T})\,|\ell\rangle\,|0^{\lceil \log M\rceil}\rangle = |\ell\rangle \sum_{j=0}^{M-1} \frac{\sqrt{c_j(\ell T/2^{n_t})}}{\sqrt{\alpha}}\,|j\rangle\,. \tag{14.51}$$

By Lemma 9.5, the resulting block encoding is

$$\texttt{HAM-T} = ((\text{PREP-T})^\dagger \otimes I)\ \text{SELECT}\ ((\text{PREP-T}) \otimes I). \tag{14.52}$$

Note above that we again make the seemingly restrictive assumption that $c_j(t) \geq 0$. This assumption is made only to simplify the discussion of the block-encoding as the sign of each coefficient can always be absorbed into the definition of the unitary.

Example 14.9. Let us clarify this construction by considering an elementary time-dependent Hamiltonian,

$$H(t) = X + \sin(\omega t)Z. \tag{14.53}$$

This violates the assumption $c_j(t) \geq 0$ since $\sin(\omega t)$ changes sign. We can instead write

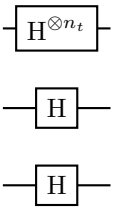
$$H(t) = X + \frac{1}{2}(-ie^{i\omega t})Z + \frac{1}{2}(ie^{-i\omega t})Z. \tag{14.54}$$

The Hamiltonian is now in standard form, with coefficients $c_j(t) = [1, 1/2, 1/2]$ and unitaries $U_j(t) = [X, -ie^{i\omega t}Z, ie^{-i\omega t}Z]$. In this case, we can further rewrite it as

$$H(t) = \frac{X}{2} + \frac{X}{2} + \frac{1}{2}(-ie^{i\omega t})Z + \frac{1}{2}(ie^{-i\omega t})Z. \tag{14.55}$$

At first sight, splitting a single X term into two identical terms seems wasteful. However, in LCU constructions the cost often depends more strongly on the number of distinct coefficient values than on the raw number of terms. Here we can implement PREP-T by preparing a uniform superposition over the index registers.

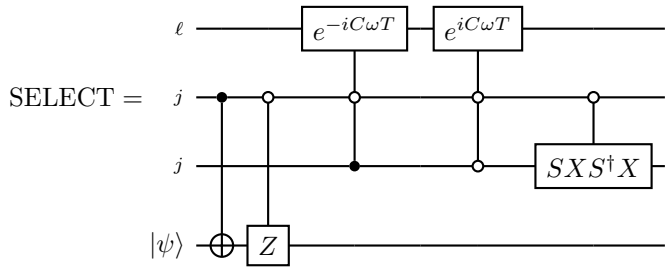
PREP-T =



Next for notational simplicity we introduce the following operator which serves to convert bit strings corresponding to the time to a fraction of the total evolution time. That is to say, we wish to construct an operator such that $|\ell\rangle \mapsto \frac{\ell}{2^{n_t}}$ for any $\ell \in \{0,1\}^{n_t}$.

$$C := \sum_{\ell=0}^{2^{n_t}-1} \frac{\ell}{2^{n_t}} |\ell\rangle\langle\ell|. \tag{14.56}$$

C is a Hermitian clock operator (not a unitary). Identifying a basis string $\ell \in \{0,1\}^{n_t}$ with the integer $\ell \in \{0, \ldots, 2^{n_t} - 1\}$, the unitary $e^{\pm i\omega TC}$ applies the phase $e^{\pm i\omega T\ell/2^{n_t}}$ to $|\ell\rangle$, which realizes the factors $e^{\pm i\omega t_\ell}$ by phase kickback. We now implement SELECT by encoding the control logic for the unitaries as follows: the first qubit selects whether we apply an X or Z term, and the second selects the sign of the frequency. The resulting SELECT circuit is



The first two gates in the circuit decide whether an X or Z Hamiltonian term is selected, whereas the last terms apply the required phases to the unitaries in the event that one of the two Z terms in the standard form decomposition of $H(t)$ is selected via the phase kickback effect. We leave it as an exercise to the reader to validate that the operation $e^{-iC\omega T}$ can be efficiently implemented using a sequence of n_t R_z rotations on the time register (and, when needed inside the select oracle, their controlled versions). The final term applies the respective $+i, -i$ phase to the Hamiltonian terms as seen from the fact that

$$SXS^\dagger X = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}, \tag{14.57}$$

which provides precisely the phases required by the standard form LCU expression.

◇

14.5. Truncated Dyson series for time-dependent Hamiltonian simulation

With the block encoding of a time-dependent Hamiltonian in hand, we turn to simulating the time-ordered evolution $\mathcal{T}e^{-i\int_0^t H(s)\,\mathrm{d}s}$. The approach was pioneered by [LW19, KSB19] and is based on implementing the **truncated Dyson series** of Theorem 14.6 as a linear combination of unitaries. This method generalizes the intuition behind the truncated Taylor series method in Section 14.2, but it is more involved because the terms must be ordered according to the times at which the Hamiltonian is queried. Here we present a simplified discussion that is not optimized for gate counts or ancilla qubits, but has essentially the same query complexity. In settings where Hamiltonian-oracle queries dominate the cost, this query complexity is a useful proxy for the overall complexity.

As in the truncated Taylor series algorithm, the truncated Dyson series algorithm simulates the evolution by dividing time into short segments and then concatenating the resulting circuits. This is needed because the block-encoding normalization factor scales exponentially with the segment duration, as in the truncated Taylor series method. The performance guarantee for a single short segment is stated next.

Lemma 14.10 (Truncated Dyson Hamiltonian simulation for short segments)**.** *Let $H : [0, T] \to \mathbb{C}^{2^n \times 2^n}$ be a differentiable time-dependent Hamiltonian that has a standard-form LCU decomposition given by the oracles* PREP-T *and* SELECT*. There exists a quantum algorithm that for any $\epsilon > 0$ and $T \in [0, \ln(2)/\alpha_T]$ implements a unitary V such that for a constant $\beta \leq 2 + \mathcal{O}(\epsilon)$,*

$$\left\| \beta(\langle 0| \otimes I)V(|0\rangle \otimes I) - \mathcal{T}e^{-i\int_0^T H(s)\,\mathrm{d}s} \right\| \leq \epsilon, \tag{14.58}$$

using a number of qubits encoding the time, n_t, that satisfies (14.47) *and a number of queries to* `HAM-T` *that is in $\mathcal{O}\big(\log(1/\epsilon)/\log\log(1/\epsilon)\big)$.*

PROOF. The first step of the algorithm involves building a truncated Dyson series expansion of the time-ordered operator exponential up to order K. We focus on queries to HAM-T, because a single query to this oracle can be simulated using $\mathcal{O}(1)$ queries to PREP-T and SELECT as in Definition 14.8.

We next show that the simulation error can be made at most ϵ. There are two sources of error: truncating the Dyson series at order K, and discretizing time using n_t bits (as discussed in (14.44)). Using the piecewise-constant approximation $\widetilde{H}$, we write

$$\begin{aligned}\left\|\beta(\langle 0|\otimes I)V(|0\rangle\otimes I)-\mathcal{T}e^{-i\int_0^T H(s)\,\mathrm{d}s}\right\| &\le \left\|\mathcal{T}e^{-i\int_0^T H(s)\,\mathrm{d}s}-\mathcal{T}e^{-i\int_0^T \widetilde{H}(s)\,\mathrm{d}s}\right\| \\ &\quad+\left\|\beta(\langle 0|\otimes I)V(|0\rangle\otimes I)-\mathcal{T}e^{-i\int_0^T \widetilde{H}(s)\,\mathrm{d}s}\right\|.\end{aligned} \tag{14.59}$$

We know from (14.46) that by choosing n_t to satisfy (14.47), we can ensure the discretization error is at most $\epsilon_T = \epsilon/2$:

$$\left\|\mathcal{T}e^{-i\int_0^T H(s)\,\mathrm{d}s}-\mathcal{T}e^{-i\int_0^T \widetilde{H}(s)\,\mathrm{d}s}\right\| \le \epsilon/2. \tag{14.60}$$

Thus it suffices to ensure that the error in the truncated Dyson series for the rounded Hamiltonian can be made at most $\epsilon/2$.

The error in the Dyson series approximation at order K has already been computed in (**??**). Since V is a block-encoding of the truncated Dyson series of the discretized-time Hamiltonian, and the truncation bound depends only on an a priori bound on $\left\|\widetilde{H}(s)\right\|$, we obtain

$$\left\|\beta(\langle 0|\otimes I)V(|0\rangle\otimes I)-\mathcal{T}e^{-i\int_0^T \widetilde{H}(s)\,\mathrm{d}s}\right\| \le \frac{(\sup_s\left\|\widetilde{H}(s)\right\| T)^{K+1}}{(K+1)!} \le \frac{(\alpha_T T)^{K+1}}{(K+1)!}. \tag{14.61}$$

Then, using the same argument as in the analysis of the truncated Taylor series simulation algorithm and the refined estimate Eq. (14.6), we obtain

$$K = \mathcal{O}\left(\frac{\log(\alpha_T T/\epsilon)}{\log\log(\alpha_T T/\epsilon)}\right) = \mathcal{O}\left(\frac{\log(1/\epsilon)}{\log\log(1/\epsilon)}\right), \tag{14.62}$$

where the last result follows from the assumption in the lemma statement that $T \le \ln(2)/\alpha_T$. This shows that for K chosen in this fashion the truncation error is at most $\epsilon/2$, and hence the overall error is at most ϵ after accounting for the discretization error.

We now show that we can construct the Dyson series expansion to order K using at most K queries to HAM-T. Using the definition of the Dyson series as given by (14.42),

$$\mathcal{T}e^{-i\int_0^T \widetilde{H}(s)\,\mathrm{d}s} \approx I + \sum_{k=1}^{K}\frac{(-i)^k}{k!}\int_0^T\int_0^T\int_0^T\cdots\int_0^T \mathcal{T}\big[\widetilde{H}(s_k)\cdots\widetilde{H}(s_1)\big]\,\mathrm{d}s_1\cdots\mathrm{d}s_k. \tag{14.63}$$

Then, because the Hamiltonian is piecewise constant, we can express this integral as

$$\int_0^T\int_0^T\int_0^T\cdots\int_0^T \mathcal{T}\big[\widetilde{H}(s_k)\cdots\widetilde{H}(s_1)\big]\,\mathrm{d}s_1\cdots\mathrm{d}s_k = \sum_{s_1,\ldots,s_k\in\mathcal{S}} \mathcal{T}\big[\widetilde{H}(s_k)\cdots\widetilde{H}(s_1)\big](\Delta t)^k, \tag{14.64}$$

where $\mathcal{S} = \{\ell\Delta t \mid \ell\in[2^{n_t}]\}$. This can be written as a linear combination of unitaries; however, the domain of integration grows exponentially with k. Fortunately, the cost of LCU depends on the one-norm of the coefficients rather than the number of terms, as in Lemma 9.5. Thus the cost of implementing this sum need not be exponential in k. The main object that we need to implement

is an operator of the form $\mathcal{T}\widetilde{H}(s_k)\cdots\widetilde{H}(s_1)$ which sorts the different Hamiltonian terms based on the time that each is evaluated at.

To implement time ordering, we need each summand in the expansion to have its own clock. Specifically, we wish to apply a transformation of the form

$$|\ell_1\rangle|\ell_2\rangle\cdots|\ell_k\rangle\otimes|\psi\rangle \to |\ell_1\rangle|\ell_2\rangle\cdots|\ell_k\rangle\otimes\mathcal{T}\widetilde{H}(s_k)\cdots\widetilde{H}(s_2)\widetilde{H}(s_1)|\psi\rangle \tag{14.65}$$

where $s_p = \ell_p\Delta t$. This transformation would allow us to build each of the terms in the truncated Dyson series (for the rounded Hamiltonian $\widetilde{H}$). However, the details of a reversible sorting process that can achieve this are complicated. An optimized version of the sorting process is described in [LW19] that includes all ancillae and gate operations needed in addition to the query operations. □

With the ability to simulate a short time segment for which $\alpha_T T = \ln(2)+\mathcal{O}(\epsilon)$, we can simulate for arbitrary durations by concatenating segments and boosting success probabilities via amplitude amplification.

THEOREM 14.11 (Truncated Dyson Simulations for Long Segments). *Let $H:\mathbb{R}\to\mathbb{C}^{2^n\times 2^n}$ be a differentiable time-dependent Hamiltonian that has a standard-form LCU decomposition given by the oracles* PREP-T *and* SELECT. *There exists a quantum algorithm that for any $\epsilon>0$ and $T>0$ implements a unitary U such that*

$$\left\|(\langle 0|\otimes I)U(|0\rangle\otimes I) - \mathcal{T}e^{-i\int_0^T H(s)\,\mathrm{d}s}\right\| \le \epsilon, \tag{14.66}$$

using $n_t = \mathcal{O}\left(\log\left(\frac{\max_{s\in[0,T]}\|H'(s)\|T^2}{\epsilon}\right)\right)$ qubits to encode the time, and $\widetilde{\mathcal{O}}\left(\alpha_T T\log(1/\epsilon)\right)$ queries to HAM-T.

PROOF SKETCH. The core idea of the strategy is to divide the total simulation time T into $r-1$ equal segments of duration $\ln(2)/\alpha_T$ and a final segment of length $T-(r-1)\ln(2)/\alpha_T$. Each of the first $r-1$ segments is chosen so that the success probability of the corresponding simulation is close to $1/4$, allowing it to be boosted to nearly 1 using a single round of oblivious amplitude amplification (see Section 11.4). The final, possibly shorter segment does not have this optimal success probability, but its amplitude can still be amplified using fixed-point amplitude amplification (see Section 13.4). The overall simulation circuit is obtained by concatenating the circuits for each segment. □

There is one subtlety in this argument. In practice, the value of α_T may depend on the chosen time interval. That is, if the Hamiltonian has a small coefficient norm over a particular segment, then this simulation method suggests using a longer timestep. However, increasing the timestep in turn changes the value of α_T for that interval. This introduces an opportunity for optimization: by choosing segment durations optimally, the overall query complexity can scale as $\widetilde{\mathcal{O}}\left(\int_0^T \alpha_T(t)\,\mathrm{d}t\cdot\log(1/\epsilon)\right)$ queries to HAM-T. This can be advantageous when $\alpha_T(t)$ is large only locally in time but the integral remains small.

Comparing the result here to Section 14.1, we find that the complexity does not reach the optimal scaling achievable via qubitization. This is expected, since truncated Dyson (like truncated Taylor) methods operate fundamentally differently from quantum signal processing and qubitization. Qubitization relies on constructing a walk operator whose spectrum directly corresponds to that of the Hamiltonian. While time-dependent Hamiltonians possess well-defined instantaneous spectra, they generally do not admit global eigenvalues or eigenvectors. As a result, it is not

possible to define a single fixed walk operator that encodes the entire time evolution and can be efficiently transformed via quantum singular value transformation. To date, no known method fully bridges the gap in query complexity between time-independent and time-dependent Hamiltonian simulation.

14.6. Interaction picture simulation method

As the truncated Dyson series method has slightly worse asymptotic scaling in t and ϵ compared to qubitization, it may seem surprising that it can still be advantageous for simulating time-independent Hamiltonians in certain regimes. The key idea is the interaction picture, which rewrites the dynamics so that the remaining time-dependent Hamiltonian term has a significantly smaller operator norm. In such cases, this reduction can offset the asymptotic overhead of truncated-Dyson methods relative to the optimal scaling achieved by qubitization.

The idea behind **interaction picture simulation** is simple. Assume that we have a time-independent Hamiltonian of the form $H = \alpha A + \beta B$, where A and B are Hermitian matrices with $\|A\| \leq 1$ and $\|B\| \leq 1$, and where $\beta \gg \alpha \geq 0$. In this regime, the dynamics is dominated by B. We can factor out this dominant part by switching to a time-dependent frame (the interaction picture with respect to B). For a state $|\psi(t)\rangle$ that obeys the Schrödinger equation under H, define

$$|\psi(t)\rangle_I := e^{i\beta Bt} |\psi(t)\rangle . \tag{14.67}$$

We now compute the corresponding evolution equation for $|\psi(t)\rangle_I$.

Proposition 14.12. *Let $H = \alpha A + \beta B$ be a Hermitian operator acting on a finite-dimensional Hilbert space with Hermitian A, B. If $|\psi(t)\rangle$ satisfies $\partial_t |\psi(t)\rangle = -iH |\psi(t)\rangle$ and $|\psi(t)\rangle_I := e^{i\beta Bt} |\psi(t)\rangle$, then $|\psi(t)\rangle_I$ satisfies*

$$\partial_t |\psi(t)\rangle_I = -iH_I(t) |\psi(t)\rangle_I , \tag{14.68}$$

*where $H_I(t)$ is called the **interaction Hamiltonian** with respect to B and is defined by*

$$H_I(t) := \alpha e^{i\beta Bt} A e^{-i\beta Bt}. \tag{14.69}$$

Proof. This follows from the product rule and the Schrödinger equation for $|\psi(t)\rangle$.

$$\begin{aligned} \partial_t |\psi(t)\rangle_I &= i\beta B e^{i\beta Bt} |\psi(t)\rangle + e^{i\beta Bt} \partial_t |\psi(t)\rangle \\ &= i\beta B e^{i\beta Bt} |\psi(t)\rangle - i e^{i\beta Bt} (\alpha A + \beta B) |\psi(t)\rangle \\ &= -i e^{i\beta Bt} (\alpha A) |\psi(t)\rangle = -i e^{i\beta Bt} (\alpha A) e^{-i\beta Bt} |\psi(t)\rangle_I \\ &= -iH_I(t) |\psi(t)\rangle_I . \end{aligned} \tag{14.70}$$

□

Since unitary conjugation preserves the operator norm, we have

$$\|H_I(t)\| = \alpha \|A\| \leq \alpha. \tag{14.71}$$

Thus the interaction picture isolates a time-dependent Hamiltonian whose operator norm is governed by α rather than β. The tradeoff is that $H_I(t)$ can vary rapidly in time when β is large. Indeed, differentiating gives

$$H_I'(t) = i\alpha\beta\, e^{i\beta Bt} [B, A] e^{-i\beta Bt}, \tag{14.72}$$

so the relevant variation scale depends on β (and on the commutator $[B, A]$). In truncated-Dyson approaches, this rapid time variation affects the time-discretization overhead (for example, the number of time-register qubits), which scales only logarithmically in such variation bounds.

This advantage, however, comes with an important caveat: one must be able to efficiently implement the evolution $e^{i\beta Bt}$ on a quantum computer. For example, if B is one-sparse (such as a Pauli string), then this evolution can be implemented efficiently. More generally, the benefit applies whenever B can be fast forwarded, meaning that its time evolution can be simulated in sublinear time in βt. While fast forwardability can arise for specific terms in a Hamiltonian decomposition, it does not hold generically. In fact, as discussed in the next section, there are Hamiltonians that provably cannot be simulated in fewer than $\mathcal{O}(\beta t)$ queries.

Example 14.13. As an example of a Hamiltonian that benefits from the interaction picture transformation let us consider the following Hamiltonian which describes a particle with mass m moving with momentum p in the presence of a periodic potential in the position x. Let us assume that the system has a physical length of L on a grid consisting of $2N + 1$ points (and grid spacing $L/2N$) then the Hamiltonian can be approximated by

$$H = \frac{p^2}{2m} + \omega \cos^2(x) \approx 4N^2 \sum_{\nu=0}^{2N} \frac{2|\nu\rangle\langle\nu| - |\nu\rangle\langle\nu+1| - |\nu+1\rangle\langle\nu|}{2mL^2} + \omega \sum_{\nu=0}^{2N} \cos^2(\nu/L)|\nu\rangle\langle\nu|. \tag{14.73}$$

Defining the incrementer operation $U_+ = \sum_\nu |\nu+1\rangle\langle\nu|$ we have that

$$\begin{aligned} H &\approx \frac{2N^2}{mL^2}(2I - U_+ - U_+^\dagger) + \omega \sum_{\nu=0}^{2N} \cos^2(\nu/L)|\nu\rangle\langle\nu| \\ &= \frac{2N^2}{mL^2}\mathrm{QFT}^\dagger \left(\sum_{\nu=0}^{2N} \big(2 - 2\cos(2\pi\nu/(2N+1))\big)|\nu\rangle\langle\nu| \right) \mathrm{QFT} + \omega \sum_{\nu=0}^{2N} \cos^2(\nu/L)|\nu\rangle\langle\nu| \end{aligned} \tag{14.74}$$

This Hamiltonian is a sum of a circulant term and a diagonal term, each of which can be block encoded efficiently, and in turn can be block encoded with a normalization constant $\alpha \in \mathcal{O}(N^2/mL^2 + |\omega|)$. Thus a simulation of the system for time T and error tolerance ϵ using the techniques of Section 14.2 can be performed using a number of queries to the block encoding oracles that scales as

$$\widetilde{\mathcal{O}}\left((N^2/mL^2 + |\omega|)T \log(1/\epsilon)\right) \tag{14.75}$$

The block encoding constant of such a Hamiltonian is potentially problematic because as the number of grid points, N, used to describe the system increases the normalization constant does as well. This means that if we wish to reduce the discretization error for the problem, the block encoding constant diverges rapidly.

Let us now examine the Hamiltonian in the interaction frame of the first term in H. In this case we have

$$\begin{aligned} H_I(t) &= \mathrm{QFT}^\dagger e^{i\left(\frac{2N^2}{mL^2}\sum_{\nu=0}^{2N}\left(2-2\cos(2\pi\nu/(2N+1))\right)|\nu\rangle\langle\nu|\right)t} \mathrm{QFT} \left(\omega \sum_{\nu=0}^{2N} \cos^2(\nu/L)|\nu\rangle\langle\nu| \right) \\ &\quad \times \mathrm{QFT}^\dagger e^{-i\left(\frac{2N^2}{mL^2}\sum_{\nu=0}^{2N}\left(2-2\cos(2\pi\nu/(2N+1))\right)|\nu\rangle\langle\nu|\right)t} \mathrm{QFT} \end{aligned} \tag{14.76}$$

From this we can see that the Truncated Dyson Simulation Algorithm of Theorem 14.11 can be used to simulate the interaction picture version of the dynamics within error ϵ using a number of

queries to the $\texttt{HAM}-\texttt{T}$ oracle that scales as

$$\widetilde{\mathcal{O}}(|\omega|T\log(1/\epsilon)) \tag{14.77}$$

which is now independent of N. This is significant because transforming to the interaction frame allows us to efficiently perform such simulations even in cases where N is exponentially large. In contrast, we saw that if we performed the simulation in the static frame then the query complexity becomes exponential. This shows that even for simple physically motivated problems, the interaction picture method can be indispensible for quantum simulation problems. In particular, this approach has yielded leading quantum query complexities for simulation of both chemistry and quantum field theories [SBW+21, RRW22]. ◇

14.7. No fast forwarding theorem

Certain Hamiltonians can be "fast-forwarded" meaning that it can be simulated using a number of gates/queries that is less than linear in αt. For instance, the complexity of implementing a single qubit rotation operation e^{iZt} is independent of t. This raises a question of whether this can be achieved more generally. The potentially surprising answer to this is that there are some Hamiltonians that cannot be simulated in less than linear time.

Before we begin with a formal argument, let us begin with an argument why it would be implausible for such an algorithm to exist. Let us imagine that all Hamiltonians could be simulated using a number of operations that scaled as, $\mathcal{O}(\sqrt{\int_0^T \alpha_T(t)dt})$. If this were true then let's take a step back and look at the quantum computer itself that solves the problem. The quantum computer is described by a time-dependent Hamiltonian $H_{QC}(t)$ that has coefficient one-norm in its decomposition that scales as $\alpha_{QC}(t)$. The total time needed to perform such a simulation would be by assumption $\mathcal{O}\left(\sqrt{\int_0^{\mathcal{O}(\sqrt{\int_0^T \alpha_T(t)dt})} \alpha_{QC}(t')dt'}\right)$. This clearly scales as $\mathcal{O}(T^{1/4})$. We don't need to stop there. We could consider a quantum computer simulation of the quantum computer performing the simulation of the simulation and achieve $\mathcal{O}(T^{1/8})$ scaling. Then by recursion, we could in effect simulate all quantum dynamics in time that is in $T^{o(1)}$. This would imply that every quantum algorithm could be implemented in near-constant time on a quantum computer, which is patently absurd. For this reason, we expect no such fast-forwarding exists for generic Hamiltonians.

How do we see, however, formally that no such fast-forwarding algorithm exists? The answer comes to us from query complexity. Specifically, we will prove the impossibility through the use of a more restrained argument by contradiction that shows if a fast forwarding algorithm existed for all Hamiltonians then such an algorithm would allow us to violate lower bounds proven for query complexity of computing the parity function. As discussed in Chapter 6, no quantum algorithm exists that can compute parity using $o(n)$ queries to the elements of a bit string of length n. Thus impossibility can be proven by reducing parity calculation to the problem of Hamiltonian simulation.

THEOREM 14.14. *Let $H : \mathbb{R} \to \mathbb{C}^{2^n \times 2^n}$ be a time-dependent Hamiltonian such that $H(t) = \sum_j \alpha_j(t)U_j(t)$ for $\alpha_j(t) \geq 0$ and $U_j(t) \in \mathbb{C}^{2^n \times 2^n}$ is a unitary operator and take $\alpha_T(t) = \sum_j \alpha_j(t)$. There does not exist a quantum algorithm that can implement an operation W such that the induced trace distance between the true evolution and the channel W satisfies*

$$D_{\mathrm{Tr}}(W, \mathcal{T}e^{-i\int_0^t H(s)\,\mathrm{d}s}) \leq 1/4$$

using a number of queries to HAM-T *that scales as $o(\int_0^t \alpha_T(t)dt)$.*

PROOF. It suffices to prove this theorem that there exists even one example of a Hamiltonian that cannot be fast forwarded without violating the assumptions of quantum theory. We will do this by showing an explicit quantum algorithm that could perform such a sub-linear time simulation on a Hamiltonian that computes the parity of a bit string. The parity problem requires that we decide between whether for a given bit string $s = [s_0, \ldots, s_{n-1}]$ obeys $\sum_j s_j \mod 2 = 0$ with probability greater than $1/2$. This can be addressed by building a "dual-rail" system that encodes the parity of the bits stored as read in sequentially in the n-bit long bit string. We will assume that a quantum oracle is provided such that $U_s |j\rangle |x\rangle = |j\rangle |x \oplus s_j\rangle$ where $\oplus$ is the exclusive or operation.

As an example imagine that we have a bit string [1101] whose parity we wish to compute. Let us begin tracking these values by starting in a state $|0\rangle_{\text{time}} |0\rangle_{\text{parity}}$. Now if we consider position 0 in the bitstring the first element is 1 and so the cumulative parity is 1 and we could encode the next configuration to be $|1\rangle_{\text{time}} |1\rangle_{\text{parity}}$. If we go to the next bit location, that bit value is 1 so the parity of all bits up to position 2 is 0. Thus the value of this partial parity state would be $|2\rangle_{\text{time}} |0\rangle_{\text{parity}}$. If we continue to compute the partial parities based on the previous one, we can see that we can compute the total parity by repeating this yielding

$$|0\rangle_{\text{time}} |0\rangle_{\text{parity}} \rightarrow |1\rangle_{\text{time}} |1\rangle_{\text{parity}} \rightarrow |2\rangle_{\text{time}} |0\rangle_{\text{parity}} \rightarrow |3\rangle_{\text{time}} |0\rangle_{\text{parity}} \rightarrow |4\rangle_{\text{time}} |1\rangle_{\text{parity}} . \tag{14.78}$$

The last qubit is 1 and so the parity of the bitstring is 1 at the end of the computation. This means that $n + 1$ values are needed to represent this.

Our next aim is to propose a dynamical system that mimics this evolution. A natural choice is to borrow intuition from angular momentum in quantum systems. Specifically, let us define the following operator J_x, which coincides (up to a constant shift in j which we will discuss later) with the x-component of the angular momentum for a spin $n/2$ system to have the following non-zero matrix elements:

$$\langle j + 1| J_x |j\rangle = \sqrt{(n - j)(j + 1)}/2 \tag{14.79}$$

This operator can be shown to have the property that

$$e^{-iJ_x\pi} |0\rangle = |n\rangle \tag{14.80}$$

Thus by simulating the dynamics for time π we can move an initial state $|0\rangle$ to $|n\rangle$, but this does not compute the parity.

To understand why an evolution for a duration of π leads to state $|n\rangle$, we will need to take a digression into the mathematics of quantum angular momentum. Quantum angular momentum operators are very similar to the Pauli matrices that we have regularly used to describe rotations on a single qubit. There are three such operators, which we denote $\hat{J}_x, \hat{J}_y, \hat{J}_z$. These operators are defined over a fixed angular momentum sector with maximum angular momentum $m = n/2$. The Z-component of the angular momentum is defined as

$$\hat{J}_z = \sum_{l=-m}^{m} l|l\rangle\langle l|, \tag{14.81}$$

which for $m = 1$ corresponds to Pauli-Z and here the variables l correspond to $l = j - n/2$. The angular momentum operators satisfy the following algebra

$$[\hat{J}_x, \hat{J}_y] = i\hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = i\hat{J}_x, \quad [\hat{J}_z, \hat{J}_x] = i\hat{J}_y. \tag{14.82}$$

The specific matrix representations of $\hat{J}_x$ and $\hat{J}_y$ are easy to find by applying $l = j - n/2$ to their original statements and we refrain from stating these forms explicitly because they will not be needed in the following argument.

The easiest way to see that $e^{-iJ_x\pi}|0\rangle = |n\rangle$ is to note that this is equivalent to $e^{-i\hat{J}_x\pi}|-n/2\rangle = |n/2\rangle$. As $\hat{J}_z$ is a diagonal operator, it is clear that this is also equivalent to

$$\langle -n/2| e^{i\hat{J}_x\pi}\hat{J}_z e^{-i\hat{J}_x\pi}|-n/2\rangle = n/2. \tag{14.83}$$

The use of the conjugation property of exponentials given in Lemma **??**

$$e^{-i\hat{J}_x\pi}\hat{J}_z e^{i\hat{J}_x\pi} = \hat{J}_z - i[\hat{J}_x,\hat{J}_z]\pi - \frac{[\hat{J}_x,[\hat{J}_x,\hat{J}_z]]\pi^2}{2!} + i\frac{[\hat{J}_x,[\hat{J}_x,[\hat{J}_x,\hat{J}_z]]]\pi^2}{3!} + \cdots \tag{14.84}$$

Using the commutation relations in (14.82),

$$e^{-i\hat{J}_x\pi}\hat{J}_z e^{i\hat{J}_x\pi} = \hat{J}_z - \hat{J}_y\pi - \frac{\hat{J}_z\pi^2}{2!} + \frac{\hat{J}_y\pi^3}{3!} + \cdots \tag{14.85}$$

Note that the above sums are simply series expansions of sin and cos, which leads to the following expression

$$e^{-i\hat{J}_x\pi}\hat{J}_z e^{i\hat{J}_x\pi} = \cos(\pi)\hat{J}_z - \hat{J}_y\sin(\pi) = -\hat{J}_z. \tag{14.86}$$

Thus we have that $\langle -n/2| e^{-i\hat{J}_x\pi}\hat{J}_z e^{i\hat{J}_x\pi}|-n/2\rangle = -\langle -n/2|\hat{J}_z|-n/2\rangle = n/2$. Which shows that $e^{-i\hat{J}_x\pi}|-n/2\rangle = |n/2\rangle$ and in turn returning to the original expression $e^{-iJ_x\pi}|0\rangle = |n\rangle$.

This intuition generalizes this to a nearly identical operator that computes the parity. To do this we will connect to the dual rail encoding of the parity discussed above. Let us define the operator G_x to be a permuted form of J_x that switches the state between the two rails depending on the value of the bit string at a given position. That is the lower-diagonal elements of the banded matrix are given by

$$\langle j+1|\langle m'|G_x|j\rangle|m\rangle = \delta_{m',m\oplus s_j}\sqrt{(n-j)(j+1)}/2 \tag{14.87}$$

As this takes the same form as J_x on a permuted basis, it is then clear that

$$e^{-iG_x\pi}|0\rangle|0\rangle = |n\rangle|\sum_j s_j \mod 2\rangle. \tag{14.88}$$

Specifically, we can see that if we permute our basis such that

$$|0\rangle|0\rangle \mapsto |0\rangle|0\rangle, \quad |1\rangle|s_0\rangle \mapsto |1\rangle|0\rangle, \ldots, \quad |n\rangle|s_0\oplus\cdots\oplus s_{n-1}\rangle \mapsto |n\rangle|0\rangle \tag{14.89}$$

and represent G_x in this basis as $\widetilde{G}_x$ we see that

$$\widetilde{G}_x = J_x \otimes I \tag{14.90}$$

Thus the evolution in this basis can be written as

$$e^{-i\widetilde{G}_x\pi}|0\rangle|0\rangle = e^{-iJ_x\otimes I\pi}|0\rangle|0\rangle = |n\rangle|0\rangle \tag{14.91}$$

As the final state is $|n\rangle|0\rangle$ in the basis of $\widetilde{G}_x$, we see that the output state in the basis of G_x is $|n\rangle|s_0\oplus\cdots\oplus s_{n-1}\rangle$. Thus the dynamics of the operator G_x can compute the parity of s.

Next let us consider block-encoding G_x. The matrix G_x is a two-sparse banded operator that has a largest matrix element that is in $\mathcal{O}(n)$. We provide a schematic argument using the block encoding discussion in Chapter 9 that provides an argument for no-fast-forwarding but uses a non-explicit construction. We will provide a more constructive block encoding in the following remark.

The Hamiltonian considered above is a 2-sparse banded matrix. It can then be block encoded using the approach given in Example 9.21. Recall that this approach construct a unitary that block encodes G_x through an amplitude oracle

(14.92)
$$O_A |0\rangle |\ell\rangle |j\rangle = \left(\frac{[G_x]_{j,c(j,\ell)}}{\max_j \sqrt{(n-j)(j+1)}/2} |0\rangle + \sqrt{1 - \frac{\left|[G_x]_{j,c(j,\ell)}\right|^2}{\left(\max_j \sqrt{(n-j)(j+1)}/2\right)^2}} |1\rangle \right) |\ell\rangle |j\rangle .$$

Followed by an entry oracle

$$O_c |\ell\rangle |j\rangle |m\rangle = |\ell\rangle |c(j,\ell)\rangle |m \oplus s_{j-\ell}\rangle = |\ell\rangle |j + (-1)^{\ell+1}\rangle |m \oplus s_{j-\ell}\rangle . \tag{14.93}$$

which follows because the only two non-zero elements for the time register, which contains j, in a given row. These occur at $j-1$ and $j+1$ and because $c(j,\ell)$ refers to the ℓ^{th} non-zero element in row j, we have that $c(j,0) = j-1$ and $c(j,1) = j+1$.

The oracle O_A does not depend on the string s. Thus it can be computed without any queries. The oracle O_c can be implemented using a controlled adder circuit followed by a query to the parity oracle. This has the action

$$U_s(U_+ \otimes |0\rangle\langle 0| + U_+^\dagger \otimes |1\rangle\langle 1|) |j\rangle |\ell\rangle |m\rangle = O_c |j\rangle |\ell\rangle |m\rangle \tag{14.94}$$

where U_+ is a modular adder such that $U_+ |x\rangle = |x+1 \mod n+1\rangle$. This requires a single query operation. Thus a block encoding of G_x can be performed that only needs $\mathcal{O}(1)$ queries to U_s.

The block encoding constant from this block encoding is given by the maximum value of the constants as shown in Example 9.21. This yields

$$\alpha = \frac{\max_j \sqrt{(n-j)(j+1)}}{2} \in \Theta(n), \tag{14.95}$$

which follows from the fact that the maximum occurs at approximately $j = n/2$. This implies that for the simulation of $e^{-iG_x\pi}$, the quantity αt satisfies $\alpha t = \alpha\pi = \Theta(n)$.

Now let us assume that a simulation algorithm existed that could simulate a any sparse Hamiltonian using a number of queries to the block-encoding operators `PREP` and `SELECT` that scales as $o(\alpha t)$. This directly implies that the number of queries to U_s needed to solve the search problem is in $o(\alpha t) = o(n)$ within trace distance at least $1/4$. As seen in Chapter 6, no quantum algorithm can exist that can solve the parity problem using $o(n)$ queries within trace distance at least $1/4$. Thus the G_x Hamiltonian cannot be fast forwarded and so no such quantum simulation algorithm can exist that can simulate all such Hamiltonians. □

There are a couple of loose ends that arise in the above discussion. First, the implementation of U_A using reversible logic requires computing $\arcsin(\sqrt{(n-j)(j+1)}/(\max_j(n-j)(j+1)))$. These reversible circuits are highly non-trivial to compute in practice and conventional methods can require thousands of qubits for even 16 bit numbers [SRWDM18]. Further, given the fact that $\arcsin(\sqrt{x})$ is not analytic on $[0,1]$, polynomial approximations will not clearly converge to the target on the entire domain. While this latter issue can be addressed by rescaling the domain so that all inputs are in $[0,1/2]$ rather than $[0,1]$, there are a number of subtle points involved in how exactly accurate approximations can be constructed to these functions. This means that it may be less than obvious to the reader how to practically construct an efficient approximation to the function on the entire interval in terms of elementary operations. Below, we give a more explicit construction that requires only reversible addition and multiplication circuits to illustrate this point and also provide a further example of LCU in action.

Remark 14.15 (Explicit block encoding of G_x)**.** Here we will seek a standard form LCU decomposition of the form $(\texttt{PREP}^\dagger \otimes I)\texttt{SELECT}(\texttt{PREP} \otimes I)$. To that end we will consider block encoding our matrix in the following form

$$G_x = \frac{(2G_{LD} + 2G_{UD})}{2} \tag{14.96}$$

where G_{LD} and G_{UD} are the lower diagonal and upper diagonal pieces of the G matrix, which we noted in the above proof is a banded matrix. We divide and multiply the result by 2 because we will use LCU to add the lower- and upper-diagonal pieces of G_x together with equal weight, which naturally leads to a factor of 2 in the averaging.

The Hilbert space that we will consider to build the LCU block encoding of G_x is of the form $|j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m$. Here the j register encodes the bit location in our simulation of G_x. The register $\ell \in [0, Q-1]$ for integer Q will be used to construct the amplitudes of the terms. The qubit r encodes whether the term is upper- or lower-diagonal with $r = 0$ corresponding to lower-diagonal and $r = 1$ meaning upper diagonal. The extra qubit b will be used to convert a phase oracle into the indicator weight that appears above. Finally, as before, the m register stores the cumulative parity bit.

The first step in constructing a decomposition for this is to first come up with a method for dealing with the varying amplitudes. We use the standard trick below to allow the amplitudes to be set uniformly, so that an equal-weight average over many terms reproduces the coefficient that we want.

$$2 \langle j+1| \langle m \oplus s_j| G_{LD} |j\rangle |m\rangle = \lim_{Q\to\infty} \frac{\max_j \sqrt{(n-j)(j+1)}}{Q} \sum_{\ell=0}^{Q-1} \mathbf{1}_{\ell^2 \leq (n-j)(j+1)}, \tag{14.97}$$

where $\mathbf{1}_{\ell^2 \leq (n-j)(j+1)}$ is the indicator function which is 1 if and only if $\ell^2 \leq (n-j)(j+1)$. This is equivalent to deciding whether $\ell \leq \sqrt{(n-j)(j+1)}$. One may ask why we choose to write the decision function like this? The answer is that by squaring both sides of the expression we can focus on an integer valued function that can be easily implemented using adder and multiplier circuits. Specifically, the comparison between two integers can be computed using the boolean function CMP, such that

$$\text{CMP}(x, y) = \begin{cases} 1 & x > y \\ 0 & \text{otherwise.} \end{cases} \tag{14.98}$$

This allows us to easily provide an explicit block encoding for the coefficients without needing to perform complex reversible arithmetic.

The error in these averages can be bounded above by ϵ by noting that the maximum deviation that each partial count can attain from its target value is 1. Thus we have that

$$\left| \langle j+1| \langle m'| G_{LD} |j\rangle |m\rangle - \frac{\delta_{m',m\oplus s_j} \max_j \sqrt{(n-j)(j+1)}}{2Q} \sum_{\ell=0}^{Q-1} \left(1 + (-1)^{\text{CMP}(\ell^2,(n-j)(j+1))}\right) \right| \leq \frac{\max_j \sqrt{(n-j)(j+1)}}{Q},$$

which is less than or equal to ϵ if we truncate the series at $Q = \max_j \sqrt{(n-j)(j+1)}/\epsilon$. Thus a modestly large number of terms is needed in the decomposition. The values in G_{UD} are the conjugates of those in G_{LD} so the process is similar, except with $j \mapsto j-1$.

The individual values of the phases for the block encoding can be set by the following operator which we denote U_ϕ whose action on a computational basis state $|j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m$

$$U_\phi |j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m = (-1)^{b\cdot \mathrm{CMP}(\ell^2,(n-j-r)(j+1-r))} |j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m . \tag{14.99}$$

This can be implemented using the following steps

$$\begin{aligned} |j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m |0\rangle &\to |j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m |\mathrm{CMP}(\ell^2,(n-j-r)(j+1-r))\rangle \\ &\to (-1)^{b\cdot \mathrm{CMP}(\ell^2,(n-j-r)(j+1-r))} |j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m |\mathrm{CMP}(\ell^2,(n-j-r)(j+1-r))\rangle \\ &\to (-1)^{b\cdot \mathrm{CMP}(\ell^2,(n-j-r)(j+1-r))} |j\rangle_j |\ell\rangle_\ell |r\rangle_r |b\rangle_b |m\rangle_m |0\rangle \end{aligned} \tag{14.100}$$

This decomposition can be implemented by first performing the comparison, then applying a controlled-Z gate from the qubit b to the comparison bit, and finally uncomputing the comparison. This process requires no query operations. Averaging over the qubit b therefore implements the factor $(I + U_\phi)/2$, which is exactly the indicator weight appearing above. We will denote this transformation U_ϕ in the following. Thus we can see that the operation

$$\texttt{SELECT} = (U_s \otimes I_{\ell rb})(I \otimes (|0\rangle\langle 0|_r \otimes U_+ + |1\rangle\langle 1|_r \otimes U_+^\dagger))U_\phi \tag{14.101}$$

here As mentioned, U_ϕ contains no query operations to U_s neither does the incremented $U_+ |j\rangle = |j+1\rangle$. Thus SELECT can be implemented using a single query.

The circuit PREP involves nothing more than applying the Hadamard transforms to the ancillary registers ℓ, r, and b:

$$\texttt{PREP} = I_j \otimes \mathrm{H}^{\otimes \log(Q)} \otimes \mathrm{H} \otimes \mathrm{H} \otimes I \tag{14.102}$$

This requires no query operations and further we see from Lemma 9.5 that

$$\max_j \sqrt{(n-j)(j+1)}(\langle 0| \otimes I)(\texttt{PREP}^\dagger \otimes I)\texttt{SELECT}(\texttt{PREP} \otimes I)(|0\rangle \otimes I) = G_x + \mathcal{O}(\epsilon) \tag{14.103}$$

provided that $Q \in \Omega(\max_j \sqrt{(n-j)(j+1)}/\epsilon)$. This is not an onerous request as increasing Q does not impact the number of queries made in the algorithm and so the error can be made arbitrarily small without changing the queries to U_s. It then follows that the normalization constant $\alpha = \mathcal{O}(n)$, and thus we see explicitly that the no-fast-forwarding Hamiltonian can be simulated without using complicated reversible operations. ◇

Notes and further reading

The use of linear combination of unitaries (LCU) for Hamiltonian simulation was developed in [CW12], and the truncated Taylor series method with nearly optimal dependence was developed in [BCK15]. The truncated Dyson series method for time-dependent simulation was developed in [LW19, KSB19]. The truncated Dyson series method is closely related to the truncated Magnus expansion method, which can be particularly suitable for highly oscillatory time-dependent problems; see, for example, [AFL22, CZA24**?**] and the references therein.

Ref. [BACS07] proved the first no-fast-forwarding theorem for time-independent Hamiltonian simulation. For more general differential equations related to Chapter 20, see [ALWZ25].

CHAPTER 15

Operator splitting based Hamiltonian simulation

In this chapter, we consider a specific class of Hamiltonian simulation algorithms where the Hamiltonian is given as a sum of simpler components: $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$, with each term H_γ generating an evolution $U_\gamma(t) = e^{-itH_\gamma}$ that is assumed to be easy to implement. The central question is: how can we combine these individually implementable unitaries to approximate the full evolution $U(t) = e^{-iHt}$? This leads to the idea of approximating the exponential of a sum by a product of exponentials, a strategy known as **operator splitting**. This approximation then seeks to find an approximation of the form

$$U(t) \approx \prod_{j=1}^{N_{\exp}} e^{-it_j H_{\gamma_j}}, \tag{15.1}$$

for some sequence of times t_j and Hamiltonian terms γ_j. Here the above holds approximately, but not precisely, because matrix multiplication is not commutative.

The above product formula approximation yields a divide and conquer scheme wherein the Hamiltonian is subdivided into smaller simulations wherein the evolution can be either brute forced or simulated using the methods in Chapter 14. This family of techniques is also commonly referred to as **product formula**, **Trotter decomposition**, Trotter splitting, or simply, splitting methods. Terms such as the Trotter-Suzuki expansion are sometimes used interchangeably with operator splitting, although they more precisely refer to specific recursive constructions derived via composition techniques. In contrast, operator splitting encompasses a broader class of methods that approximate time evolution using simpler component dynamics. Operator splitting also played a foundational role in the early development of quantum computation theory. In particular, it was used to argue that a universal quantum simulator could be realized (for local Hamiltonians) by applying a Trotter decomposition to the time evolution operator [Llo96].

It is also important to note that approximating $U(t)$ is not merely a numerical task in scientific computing. In quantum algorithms, the ability to implement $U(t)$ from easily accessible building blocks $U_\gamma(t)$ also enables indirect access to the Hamiltonian H itself. While the formal inverse operation $H = (\log U(t))/(-it)$ is generally not computed explicitly, eigenvalue transformations and other matrix processing tasks can often proceed using $U(t)$ directly, without recovering H in closed form. An approximate implementation of $U(t)$ also serves as a powerful input model for representing matrices. This is known as the **Hamiltonian simulation based input model**, also claled the **Hamiltonian evolution based input model**. Among the various approaches available, Trotter-style product formulas remain the most widely used and practically implementable method for realizing this model on quantum hardware.

We begin with the simplest case where the Hamiltonians commute exactly, and then develop first- and second-order product formulas. We proceed to higher-order generalizations, error bounds

involving commutators, and more refined norm-based estimates. We also discuss recent extensions, including randomized time-sampling strategies and adaptations to time-dependent Hamiltonians.

15.1. Warmup: the commuting case

First let us begin with the case where all terms in the Hamiltonian that we wish to simulate commute. Commuting matrices act very much like ordinary numbers. When all terms H_γ commute with each other, we simply have

$$U(t) = \prod_{\gamma=1}^{\Gamma} e^{-iH_\gamma t} = \prod_{\gamma} U_\gamma(t). \tag{15.2}$$

This arises from an elementary calculation involving the definition of the operator exponential, which we include below for completeness.

Lemma 15.1. *Let $\{A_\gamma : \gamma = 1, \ldots, \Gamma\}$ be normal matrices acting on a finite Hilbert space $\mathcal{H}$ such that $[A_\gamma, A_{\gamma'}] = 0$ for all $\gamma, \gamma' \in \{1, \ldots, \Gamma\}$. Then*

$$e^{\sum_\gamma A_\gamma} = \prod_{\gamma} e^{A_\gamma}. \tag{15.3}$$

Proof. If $\Gamma = 1$ then there is only one term in the product formula. Let us then continue to the case where $\Gamma = 2$. Assume that $[A, B] = 0$ for operators $A, B \in L(\mathcal{H})$ then we wish to show that $e^{A+B} = e^A e^B$. We can demonstrate this through Taylor's theorem (which holds because $\mathcal{H}$ is finite dimensional)

$$e^{A+B} = \sum_{j=0}^{\infty} (A+B)^j / j!. \tag{15.4}$$

Note that $(A+B)^j$ is simply the sum of all unordered sequences of A, B of length j. If $[A, B] = 0$ then $AB = BA$. Thus for example $(A+B)^2 = A^2 + AB + BA + B^2 = A^2 + 2AB + B^2$. Repeating this same pattern for larger j yields

$$(A+B)^j = \sum_{p=0}^{j} \binom{j}{p} A^{j-p} B^p. \tag{15.5}$$

Thus in the commuting case

$$e^{A+B} = \sum_{j=0}^{\infty} \sum_{p=0}^{j} \binom{j}{p} A^{j-p} B^p / j! = \sum_{j=0}^{\infty} \sum_{p=0}^{j} \frac{A^{j-p} B^p}{(j-p)! p!} = e^A e^B. \tag{15.6}$$

Thus we have demonstrated that the result holds for $\gamma = 2$.

Now let $p \geq 2$ and assume that $\prod_{\gamma=1}^{p} e^{A_\gamma} = e^{\sum_{\gamma=1}^{p} A_\gamma}$. We then have that

$$\prod_{\gamma=1}^{p} e^{A_\gamma} e^{A_{p+1}} = e^{\sum_\gamma A_\gamma} e^{A_{p+1}}. \tag{15.7}$$

Then from the above case we can combine these two exponentials because this reduces to the case $\Gamma = 2$. Thus

$$e^{\sum_\gamma A_\gamma} e^{A_{p+1}} = e^{\sum_{\gamma=1}^{p+1} A_\gamma} \tag{15.8}$$

Therefore by induction the claim holds for all $p \geq 2$ and thus the result follows. □

Example 15.2 (Sum of Pauli-Z gates)**.** Consider a sum of n Pauli-Z gates $H = \sum_{i=1}^{n} Z_i$. For instance, when $n = 2$,

$$H = Z \otimes I + I \otimes Z = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix}. \tag{15.9}$$

This is not a unitary matrix (even after normalization by a factor of 2). However, since all Z_i's commute, the Hamiltonian simulation problem

$$U(t) = e^{-itH} = \prod_{i=1}^{n} e^{-itZ_i} \tag{15.10}$$

can be solved exactly with n single qubit gates for any t. ◇

Now that we have shown that a sum of elementary Pauli-Z Hamiltonian can be simulated on a quantum computer a natural next step is to generalize this to a sum of commuting k-local Hamiltonians, which are Hamiltonians that are a sum of Pauli operations that each act non-trivially on at most k qubits. We will further also provide the explicit number of gates needed to perform this product.

THEOREM 15.3. *Let $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$ be a Hamiltonian in $L(\mathbb{C}^{2^n})$ where each $H_\gamma = \alpha_\gamma P_{\gamma_1} \cdots P_{\gamma_n}$ and each $\gamma_j \in \{0, 1, 2, 3\}$ corresponds to a Pauli operator from the set $\{I, X, Y, Z\}$. Further assume that H is k-local, i.e., for each γ at least $n - k$ of the indices satisfy $\gamma_j = 0$, and that $[H_\gamma, H_{\gamma'}] = 0$ for all γ, γ'. We then have that*

1. $e^{-iHt} = \prod_\gamma e^{-iH_\gamma t}$
2. $\prod_\gamma e^{-iH_\gamma t}$ *can be exactly implemented on a quantum computer using at most* Γ R_z *gates and at most* $2(k-1)\Gamma$ CNOT *gates and* $2k\Gamma$ *single qubit Clifford gates.*

PROOF. The first claim in the Theorem is a direct consequence of Lemma 15.1. We will now examine the second claim. Our strategy for implementing these terms is simple. We will first diagonalize each Pauli operator to turn it into a product of Pauli-Z gates. Then we will construct a simulation circuit for each of the diagonal operations by computing the eigenvalues of the diagonal operations.

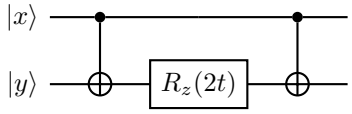
To see how this is achieved let us begin with a simple case: $e^{-iZ\otimes Zt}$. From the eigenvalue decomposition we see that the eigenvalues of the exponential are simply the exponential of the eigenvalues of the exponent. These are particularly easy to find here because Z is diagonal:

$$Z \otimes Z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \Rightarrow e^{-iZ\otimes Zt} = \begin{bmatrix} e^{-it} & 0 & 0 & 0 \\ 0 & e^{it} & 0 & 0 \\ 0 & 0 & e^{it} & 0 \\ 0 & 0 & 0 & e^{-it} \end{bmatrix} \tag{15.11}$$

From this we observe that any input $|x\rangle |y\rangle$ obtains a phase of e^{-it} if $x = y = 0$ or $x = y = 1$, and a phase of e^{it} otherwise. Note that this pattern can be more succinctly represented by seeing that, irrespective of x, y, $e^{-i(-1)^{x+y}t}$ is achieved. That is to say

$$|x\rangle |y\rangle \mapsto e^{-i(-1)^{x+y}t} |x\rangle |y\rangle . \tag{15.12}$$

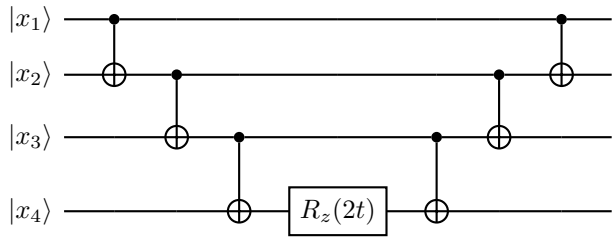
Now recall that $Xe^{-iZt}X = e^{-i(XZX)t} = e^{iZt}$. This implies that we can flip the direction of a Z-rotation by conjugating with an X gate. In effect, when $x = 1$ the sign of the phase rotation for $e^{-iZ\otimes Zt}$ is flipped. Thus we can use the following circuit for $e^{-iZ\otimes Zt}$.

(15.13)
$$e^{-iZ\otimes Zt} =$$


Next let us consider a Hamiltonian that has k Pauli-Z operations in it. We can go through the exact same reasoning to see that

(15.14)
$$e^{-i(\prod_{j=1}^{k} Z_j)t} |x_1\rangle \cdots |x_k\rangle = e^{-i(-1)^{\sum_j x_j} t} |x_1\rangle \cdots |x_k\rangle .$$

Again we see that the phase is flipped based on the parity of $\sum_j x_j$, which can be obtained by applying a chain of CNOT operations and then applying a single R_z rotation on one qubit, as in Eq. (15.13). The circuit for this for $k = 4$ is given below

(15.15)
$$e^{-iZ^{\otimes 4}t} =$$


This circuit is often simplified to have all of the targets for the CNOT operations either on the bottom-most qubit [WBAG11].

We see then that in general any Pauli operator consisting of k Pauli-Z operations can be implemented exactly using $2(k-1)$ CNOT operations and a single R_z gate.

Now let us consider the case of $e^{-iX\otimes Yt}$ for example. We can again use the property that for any unitary U and normal matrix A, $Ue^{A}U^\dagger = e^{UAU^\dagger}$. We then wish to choose U to diagonalize $X \otimes Y$. We can use the fact that $X = \mathrm{H}\,Z\,\mathrm{H}$ and $Y = S\,\mathrm{H}\,Z\,\mathrm{H}\,S^\dagger$ to see that

(15.16)
$$e^{-iX\otimes Yt} = (\mathrm{H}\otimes S\,\mathrm{H}) e^{-iZ\otimes Zt} (\mathrm{H}\otimes \mathrm{H}\,S^\dagger)$$

This logic can be extended to the case where there are at most k non-Pauli-Z operators in the exponent. We see that in each case we will have to apply one single-qubit Clifford operation per qubit to diagonalize and then another single-qubit Clifford gate to return to the original basis. Thus the cost for simulating a generic $e^{-i\alpha_\gamma P_\gamma t}$ term in the decomposition is $2k$ single-qubit Clifford gates plus the cost of simulating $Z^{\otimes k}$ (which is $2(k-1)$ CNOT operations and a single R_z gate).

By the first claim, the overall simulation of the unitary consists of Γ exponentials each of which is the exponential of a Pauli operator with at most k terms. Thus the cost is at most Γ times the aforementioned costs, which yield the result stated in the theorem. □

Example 15.4 (2D toric code)**.** Let $N = 2L^2$ spins lie on the edges of the toroidal lattice, with Hilbert space $\mathcal{H} \cong \mathbb{C}^{2^N}$. The Hamiltonian for Kitaev's 2D toric code [Kit03] is

(15.17)
$$H^{\text{toric}} = -\sum_s \mathsf{X}_s - \sum_p \mathsf{Z}_p ,$$

where s and p range over stars and plaquettes, respectively. A star consists of the four edges incident to a vertex, and a plaquette consists of the four edges surrounding a face, as shown in Fig. 15.1. The corresponding operators are

$$\mathsf{X}_s = \prod_{i \in s} \sigma_i^x, \quad \mathsf{Z}_p = \prod_{i \in p} \sigma_i^z, \tag{15.18}$$

which are all 4-local Pauli operators. Moreover,

$$[\mathsf{X}_s, \mathsf{Z}_p] = [\mathsf{X}_s, \mathsf{X}_{s'}] = [\mathsf{Z}_p, \mathsf{Z}_{p'}] = 0, \tag{15.19}$$

for all stars s, s' and plaquettes p, p'. Hence H^{toric} is a sum of commuting local Hamiltonian terms. Because of the periodic boundary condition, we also have

$$\prod_s \mathsf{X}_s = 1, \quad \prod_p \mathsf{Z}_p = 1, \tag{15.20}$$

so these commuting terms are not all independent. Even so, by Theorem 15.3, for every t we have

$$e^{-itH^{\text{toric}}} = \prod_s e^{it\mathsf{X}_s} \prod_p e^{it\mathsf{Z}_p}, \tag{15.21}$$

and this product formula is exact. Since there are L^2 star terms and L^2 plaquette terms, each supported on 4 qubits, the simulation can be implemented using at most $2L^2$ R_z gates, $12L^2$ CNOT gates, and $16L^2$ single-qubit Clifford gates.

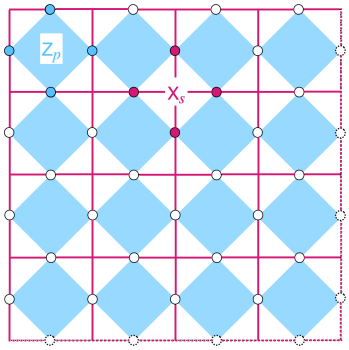


FIGURE 15.1. Illustration of 2D toric code. Each blue plaquette supports the 4-local operator $\mathsf{Z}_p = \prod_{i \in p} \sigma_i^z$, and each red star supports the 4-local operator $\mathsf{X}_s = \prod_{i \in s} \sigma_i^x$. The dashed line on the right and bottom is identified with the solid line on the left and top, respectively, due to the periodic boundary condition.

◇

15.2. First order and second order operator splitting

In quantum physics, a common task is to analyze time evolution under a Hamiltonian that is a sum of non-commuting components. The basic idea of operator splitting methods is that by rapidly alternating the application of the individual terms, the resulting dynamics can approximate the evolution generated by the full sum. This "term flickering" effect is analogous to how a rapidly flickering screen seems to be static but actually is changing incredibly quickly compared to the timescale of a video. Here this reduces the non-commuting case to controlling the errors introduced

by switching, which are governed by commutators between the terms. Quantitative bounds on these errors determine how small the switching time step must be in order to reach a target accuracy.

To analyze the complexity of operator splitting methods, we need to understand how these non-commutativity errors accumulate. The Duhamel principle (Proposition 3.22) provides a convenient way to express the effect of an inhomogeneous perturbation.

Proposition 15.5 (First-order Trotter formula, $\Gamma = 2$)**.** *Let $H = H_1 + H_2$ where $H_1, H_2 \in \mathbb{C}^{N\times N}$ are Hermitian matrices. Let $|||H||| := \|H_1\| + \|H_2\|$. The first-order Trotter approximation is defined as $\widetilde{U}(t) := e^{-itH_1}e^{-itH_2}$. For any $t \geq 0$, the local simulation error is bounded by*

$$\left\| e^{-itH} - \widetilde{U}(t) \right\| \leq t^2 |||H|||^2. \tag{15.22}$$

Consequently, to simulate e^{-itH} for a total time t with precision ϵ, the interval $[0, t]$ can be divided into L steps of size $\Delta t = t/L$, where

$$L = \left\lceil \frac{t^2 |||H|||^2}{\epsilon} \right\rceil. \tag{15.23}$$

Proof. We analyze the error using the Taylor expansion with integral remainder. For a twice differentiable matrix-valued function $f(t)$, we have

$$f(t) = f(0) + f'(0)t + \int_0^t f''(s)(t-s)\,\mathrm{d}s. \tag{15.24}$$

Let us apply this expansion to each matrix entry of the exact and approximate propagators. First, consider the exact propagator $U(t) = e^{-itH}$. Its expansion is

$$U(t) = I - itH + \int_0^t (-iH)^2 e^{-isH}(t-s)\,\mathrm{d}s. \tag{15.25}$$

Next, we examine the approximate propagator $\widetilde{U}(t) = e^{-itH_1}e^{-itH_2}$. Differentiating and using that each H_j commutes with e^{-itH_j}, we find

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\widetilde{U}(t) &= \left(\frac{\mathrm{d}}{\mathrm{d}t}e^{-itH_1}\right)e^{-itH_2} + e^{-itH_1}\left(\frac{\mathrm{d}}{\mathrm{d}t}e^{-itH_2}\right) \\ &= (-iH_1)e^{-itH_1}e^{-itH_2} + e^{-itH_1}(-iH_2)e^{-itH_2} \\ &= e^{-itH_1}(-iH_1 - iH_2)e^{-itH_2} \\ &= e^{-itH_1}(-iH)e^{-itH_2}. \end{aligned} \tag{15.26}$$

Evaluating this at $t = 0$ yields $\widetilde{U}'(0) = -iH = U'(0)$, so the zeroth and first-order terms match the exact evolution. Differentiating a second time, we obtain

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}t^2}\widetilde{U}(t) &= e^{-itH_1}(-iH_1)(-iH)e^{-itH_2} + e^{-itH_1}(-iH)(-iH_2)e^{-itH_2} \\ &= -e^{-itH_1}(H_1^2 + H_1H_2 + H_1H_2 + H_2^2)e^{-itH_2} \\ &= -e^{-itH_1}(H_1^2 + 2H_1H_2 + H_2^2)e^{-itH_2}. \end{aligned} \tag{15.27}$$

The Taylor expansion for the approximation is thus

$$\widetilde{U}(t) = I - itH - \int_0^t e^{-isH_1}(H_1^2 + 2H_1H_2 + H_2^2)e^{-isH_2}(t-s)\,\mathrm{d}s. \tag{15.28}$$

Subtracting the two expansions, the difference is given by the remainder terms:

$$U(t) - \widetilde{U}(t) = \int_0^t \left[(-iH)^2 e^{-isH} + e^{-isH_1}(H_1^2 + 2H_1H_2 + H_2^2)e^{-isH_2}\right](t-s)\,\mathrm{d}s. \tag{15.29}$$

We bound the spectral norm of the integrands. Since e^{-isH}, e^{-isH_1}, and e^{-isH_2} are unitary, each has operator norm 1. For the exact term, $\left\|(-iH)^2 e^{-isH}\right\| \leq \|H\|^2 \leq |||H|||^2$. For the approximate term,

$$\left\|e^{-isH_1}(H_1^2 + 2H_1H_2 + H_2^2)e^{-isH_2}\right\| \leq \|H_1\|^2 + 2\|H_1\|\|H_2\| + \|H_2\|^2 = |||H|||^2. \tag{15.30}$$

Applying the triangle inequality to the integral yields

$$\left\|U(t) - \widetilde{U}(t)\right\| \leq \int_0^t \left(|||H|||^2 + |||H|||^2\right)(t-s)\,\mathrm{d}s = 2|||H|||^2\frac{t^2}{2} = t^2|||H|||^2, \tag{15.31}$$

which proves Eq. (15.22).

Finally, for the global simulation over time t, we apply the product formula L times with time step $\Delta t = t/L$. Using the triangle inequality over L steps, the total error is bounded by

$$\left\|U(t) - \widetilde{U}(\Delta t)^L\right\| \leq L\left\|U(\Delta t) - \widetilde{U}(\Delta t)\right\| \leq L(\Delta t)^2|||H|||^2 = \frac{t^2}{L}|||H|||^2. \tag{15.32}$$

Setting this bound equal to ϵ and solving for L gives the stated complexity. □

Example 15.6. The Hamiltonian for the TFIM with n sites is $H = H_1 + H_2$, where

$$H_1 = -\sum_{i=1}^{n-1} JZ_iZ_{i+1}, \quad H_2 = -\sum_{i=1}^{n} gX_i. \tag{15.33}$$

Since the operators within H_1 commute, and similarly the operators within H_2 commute, the corresponding exponential propagators can be exactly decomposed into a product of local unitaries:

$$e^{-itH_1} = e^{itJ\sum_{i=1}^{n-1} Z_iZ_{i+1}} = \prod_{i=1}^{n-1} e^{itJZ_iZ_{i+1}}, \tag{15.34}$$

$$e^{-itH_2} = e^{itg\sum_{i=1}^{n} X_i} = \prod_{i=1}^{n} e^{itgX_i}. \tag{15.35}$$

Each term $e^{itJZ_iZ_{i+1}}$ (a two-qubit rotation) and e^{itgX_i} (a single-qubit rotation) can be implemented independently, with no additional approximation error arising from the decomposition within H_1 or within H_2.

To estimate the complexity of the first-order Trotter simulation $S_1(t) = e^{-itH_1}e^{-itH_2}$, we bound $|||H|||$ by the sum of the norms of the individual terms:

$$|||H||| = \|H_1\| + \|H_2\| \leq \sum_{i=1}^{n-1}\|-JZ_iZ_{i+1}\| + \sum_{i=1}^{n}\|-gX_i\|. \tag{15.36}$$

Since $\|Z_iZ_{i+1}\| = 1$ and $\|X_i\| = 1$, assuming $J, g > 0$, we have

$$|||H||| \leq J(n-1) + gn = \mathcal{O}(n). \tag{15.37}$$

Therefore, according to the error estimate $\mathcal{O}(t^2|||H|||^2/L)$ derived in Proposition 15.5, the required number of Trotter steps L to achieve precision ϵ is $L = \mathcal{O}(|||H|||^2t^2/\epsilon)$. The total query complexity is $\mathcal{O}(L)$, which scales as $\mathcal{O}\left(\frac{n^2t^2}{\epsilon}\right)$. ◇

Example 15.7. The 1D Heisenberg model Hamiltonian is given by $H = J\sum_{i=1}^{n-1}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})$, where $\mathbf{S}_i = (X_i, Y_i, Z_i)/2$, so that

$$H = \frac{J}{4}\sum_{i=1}^{n-1}\left(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1}\right). \tag{15.38}$$

We consider the common splitting $H = H_x + H_y + H_z$, where

$$H_x = \frac{J}{4}\sum_{i=1}^{n-1} X_iX_{i+1}, \quad H_y = \frac{J}{4}\sum_{i=1}^{n-1} Y_iY_{i+1}, \quad H_z = \frac{J}{4}\sum_{i=1}^{n-1} Z_iZ_{i+1}. \tag{15.39}$$

Here, the total number of terms is $\Gamma = 3$. The first-order Trotter product is $S_1(t) = e^{-itH_x}e^{-itH_y}e^{-itH_z}$. The local terms within H_x, H_y, and H_z commute, allowing for exact decomposition of the exponential propagators:

$$e^{-itH_x} = \prod_{i=1}^{n-1} e^{-it\frac{J}{4}X_iX_{i+1}}, \tag{15.40}$$

with similar expressions for e^{-itH_y} and e^{-itH_z}.

To estimate the query complexity, we compute the sum of the operator norms $|||H||| = \|H_x\| + \|H_y\| + \|H_z\|$. Since $\|X_iX_{i+1}\| = \|Y_iY_{i+1}\| = \|Z_iZ_{i+1}\| = 1$, and assuming $J > 0$:

$$|||H||| \leq \sum_{k\in\{x,y,z\}}\sum_{i=1}^{n-1}\left\|\frac{J}{4}\sigma_i^k\sigma_{i+1}^k\right\| = \frac{3J}{4}(n-1) = \mathcal{O}(n). \tag{15.41}$$

Consequently, the total query complexity for the 1D Heisenberg model scales as $\mathcal{O}\left(\frac{|||H|||^2t^2}{\epsilon}\right) = \mathcal{O}\left(\frac{n^2t^2}{\epsilon}\right)$.

Similarly, for the 2D Heisenberg model on an $n \times n$ square lattice ($N = n^2$ total qubits), the number of nearest-neighbor bonds (edges) is approximately $2N = 2n^2$. The operator norm is bounded by the total number of terms times the maximal norm of a single term. The norm sum scales linearly with the number of sites N:

$$|||H||| = \|H_x\| + \|H_y\| + \|H_z\| \leq \frac{3J}{4}(\text{Number of bonds}) \approx \frac{3J}{4}(2n^2) = \mathcal{O}(n^2). \tag{15.42}$$

The increased number of interactions leads to a larger norm sum. The query complexity then scales as $\mathcal{O}\left(\frac{|||H|||^2t^2}{\epsilon}\right) = \mathcal{O}\left(\frac{(n^2)^2t^2}{\epsilon}\right) = \mathcal{O}\left(\frac{n^4t^2}{\epsilon}\right)$. ◇

The cost of the first-order Trotter expansion is often undesirable as a function of the simulation parameters t, n, and ϵ. This scaling can be improved using the **second-order Trotter method**, also known as **symmetric Trotter splitting** or **Strang splitting**.

Proposition 15.8 (Second-order Trotter formula, $\Gamma = 2$)**.** *Let $H = H_1 + H_2$ where $H_1, H_2 \in \mathbb{C}^{N\times N}$ are Hermitian matrices. The second-order (symmetric) Trotter expansion is defined as*

$$\widetilde{U}_2(t) := e^{-i\frac{t}{2}H_2}e^{-itH_1}e^{-i\frac{t}{2}H_2}. \tag{15.43}$$

For any $t \geq 0$, the local simulation error satisfies the bound

$$\left\|e^{-itH} - \widetilde{U}_2(t)\right\| \leq \frac{t^3}{3}|||H|||^3. \tag{15.44}$$

Furthermore, for a simulation over a total time t divided into L segments of size $\Delta t = t/L$, the global error scales quadratically with the time step:

$$\left\| e^{-itH} - \left(\widetilde{U}_2(\Delta t)\right)^L \right\| = \mathcal{O}(t\Delta t^2 |||H|||^3). \tag{15.45}$$

Consequently, to achieve a precision ϵ, the required number of segments is $L = \mathcal{O}((|||H|||t)^{3/2}\epsilon^{-1/2})$, yielding a query complexity of $\mathcal{O}(L)$.

Proof. We first address the query complexity. While a single step Eq. (15.43) uses three exponentials, concatenating L steps allows adjacent half-steps to merge:

$$\left(e^{-i\frac{\Delta t}{2}H_2} e^{-i\Delta t H_1} e^{-i\frac{\Delta t}{2}H_2}\right)^L = e^{-i\frac{\Delta t}{2}H_2} \left(e^{-i\Delta t H_1} e^{-i\Delta t H_2}\right)^{L-1} e^{-i\Delta t H_1} e^{-i\frac{\Delta t}{2}H_2}. \tag{15.46}$$

The total number of exponentials is $2(L-1)+3 = 2L+1$, which is asymptotically equivalent to the first-order method.

To analyze the error, we employ the Taylor expansion with an integral remainder. The exact propagator expands as

$$U(t) = I - itH + \frac{(-itH)^2}{2} + \int_0^t (-iH)^3 e^{-isH} \frac{(t-s)^2}{2!}\, \mathrm{d}s. \tag{15.47}$$

We now compute the derivatives of $\widetilde{U}_2(t)$ at $t = 0$. For compactness, we use the multinomial coefficient notation:

$$\binom{m}{q_1, \ldots, q_k} := \frac{m!}{q_1! \cdots q_k!}. \tag{15.48}$$

The first derivative is

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{U}_2(t)\bigg|_{t=0} = -\frac{i}{2}H_2 - iH_1 - \frac{i}{2}H_2 = -iH, \tag{15.49}$$

which matches the first-order term of the exact propagator. For the second derivative, using the product rule on the three factors leads to a sum over indices $q_1 + q_2 + q_3 = 2$:

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\widetilde{U}_2(t)\bigg|_{t=0} = \sum_{q_1+q_2+q_3=2} \binom{2}{q_1, q_2, q_3} \left(-i\frac{H_2}{2}\right)^{q_1} (-iH_1)^{q_2} \left(-i\frac{H_2}{2}\right)^{q_3}. \tag{15.50}$$

Expanding the sum yields

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}t^2}\widetilde{U}_2(0) &= (-i)^2 \left[\left(\frac{H_2}{2}\right)^2 + H_1^2 + \left(\frac{H_2}{2}\right)^2 + 2\left(\frac{H_2}{2}\right) H_1 + 2H_1 \left(\frac{H_2}{2}\right) + 2\left(\frac{H_2}{2}\right)\left(\frac{H_2}{2}\right) \right] \\ &= (-i)^2 \left[H_1^2 + H_1H_2 + H_2H_1 + H_2^2\right] = (-iH)^2. \end{aligned} \tag{15.51}$$

Thus, the second-order terms also match. The error is therefore controlled by the third derivative. The norm of the third derivative of the approximation is bounded by

$$\begin{aligned} \left\| \frac{\mathrm{d}^3}{\mathrm{d}t^3}\widetilde{U}_2(t) \right\| &\le \sum_{q_1+q_2+q_3=3} \binom{3}{q_1, q_2, q_3} \left(\frac{1}{2}\|H_2\|\right)^{q_1} \|H_1\|^{q_2} \left(\frac{1}{2}\|H_2\|\right)^{q_3} \\ &= \left(\|H_1\| + \frac{1}{2}\|H_2\| + \frac{1}{2}\|H_2\|\right)^3 = |||H|||^3. \end{aligned} \tag{15.52}$$

The remainder term for the difference $U(t) - \widetilde{U}_2(t)$ is bounded by the sum of the exact and approximate remainders:

$$\left\| U(t) - \widetilde{U}_2(t) \right\| \leq \int_0^t \left(\|H\|^3 + |||H|||^3 \right) \frac{(t-s)^2}{2!} \, \mathrm{d}s \leq 2|||H|||^3 \frac{t^3}{6} = \frac{t^3}{3} |||H|||^3. \tag{15.53}$$

Finally, using the triangle inequality over L steps, the global error is bounded by

$$L \times \mathcal{O}(\Delta t^3 |||H|||^3) = \mathcal{O}(t \Delta t^2 |||H|||^3). \tag{15.54}$$

Solving for L given a target error ϵ completes the proof. □

Example 15.9. Consider the Transverse Field Ising Model (TFIM) discussed in Example 15.6, where $|||H||| = \mathcal{O}(n)$. We can now quantitatively compare the cost of the first-order and second-order Trotter schemes.

For the first-order scheme, the query complexity was found to be

$$\mathcal{O}\left(\frac{n^2 t^2}{\epsilon} \right). \tag{15.55}$$

For the second-order scheme, substituting $|||H||| \sim n$ into the complexity bound derived in Proposition 15.8, we obtain

$$\mathcal{O}\left(\frac{n^{3/2} t^{3/2}}{\epsilon^{1/2}} \right). \tag{15.56}$$

The second-order method offers a substantial asymptotic improvement, and symmetric splitting is often a standard baseline for product-formula simulation. ◇

15.3. Higher order operator splitting formula

How do we generate high-order Trotter methods? One systematic approach is via **composition methods**. For $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$, one choice of a first-order Trotter method is

$$\widetilde{U}_1(t) := e^{-itH_\Gamma} \cdots e^{-itH_1}. \tag{15.57}$$

The corresponding **adjoint method** is

$$\widetilde{U}_1^\star(t) := (\widetilde{U}_1(-t))^\dagger = e^{-itH_1} \cdots e^{-itH_\Gamma}. \tag{15.58}$$

The second-order Trotter formula can be written as the composition of the first-order method and its adjoint:

$$\widetilde{U}_2(t) := \widetilde{U}_1^\star(t/2) \widetilde{U}_1(t/2). \tag{15.59}$$

If a method is equal to its adjoint, it is called symmetric. A symmetric method must have even order of accuracy [HLW06, Theorem 3.2]. Thus $\widetilde{U}_2(t)$ must be (at least) a second-order method, agreeing with the previous analysis.

The same viewpoint applies to general product formulas. Let $U(t) := e^{-itH}$. We say that a product formula $\widetilde{U}_p(t)$ has order p if the short-time error admits an expansion

$$\widetilde{U}_p(t) = U(t) + Ct^{p+1} + \mathcal{O}(t^{p+2}), \quad t \to 0, \tag{15.60}$$

for some bounded operator C. Given real coefficients $s_1, \ldots, s_m$, we define the corresponding composition product formula by

$$\widetilde{U}_p^{\mathrm{comp}}(t) := \widetilde{U}_p(s_m t) \cdots \widetilde{U}_p(s_1 t). \tag{15.61}$$

The order of accuracy for composition methods can be analyzed by Taylor expansion (see, e.g., [HLW06, Theorem 4.1]).

THEOREM 15.10. *Assume $\widetilde{U}_p(t)$ has order p in the sense of Eq.* (15.60). *If*

$$\sum_{j=1}^{m} s_j = 1, \qquad \sum_{j=1}^{m} s_j^{p+1} = 0, \tag{15.62}$$

then the composition method $\widetilde{U}_p^{\mathrm{comp}}(t)$ in Eq. (15.61) *has order at least $p+1$.*

PROOF. Write $U_j := U(s_j t)$ and $\widetilde{U}_j := \widetilde{U}_p(s_j t)$ for brevity. By Eq. (15.60),

$$\widetilde{U}_j = U_j + C(s_j t)^{p+1} + \mathcal{O}(t^{p+2}). \tag{15.63}$$

Using the group property $U(s_m t)\cdots U(s_1 t) = U\big((\sum_{j=1}^m s_j)t\big)$ together with $U_j = I + \mathcal{O}(t)$, we obtain

$$\widetilde{U}_p^{\mathrm{comp}}(t) = U(t) + Ct^{p+1}\sum_{j=1}^{m} s_j^{p+1} + \mathcal{O}(t^{p+2}). \tag{15.64}$$

Under Eq. (15.62), the t^{p+1} term vanishes, and therefore $\widetilde{U}_p^{\mathrm{comp}}(t) = U(t) + \mathcal{O}(t^{p+2})$, i.e., the composition has order at least $p+1$. □

Example 15.11 (Yoshida–Suzuki triple jump method)**.** In Eq. (15.62), the smallest m for which the system admits a solution is $m = 3$. We then have some freedom in solving the two equations. If we impose symmetry $s_1 = s_3$, then we obtain

$$s_1 = s_3 = \frac{1}{2 - 2^{1/(p+1)}}, \quad s_2 = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}. \tag{15.65}$$

This procedure can be repeated. Starting from a symmetric method of order 2, applying Eq. (15.65) with $p = 2$ yields a method of order at least 3; by symmetry of the coefficients, the resulting method is in fact of order 4. Repeating Eq. (15.65) with $p = 4$ yields a symmetric 9-stage composition method of order 6, then with $p = 6$ a 27-stage symmetric composition method of order 8, and so on. For an order-p method, the total number of steps is $3^{p/2-1}$. ◇

Example 15.12 (Trotter–Suzuki method)**.** Consider the case $m = 5$ with $s_1 = s_2 = s_4 = s_5$. The conditions in Eq. (15.62) become

$$4s_1 + s_3 = 1, \qquad 4s_1^{p+1} + s_3^{p+1} = 0. \tag{15.66}$$

The second equation implies $s_3 = -4^{1/(p+1)} s_1$. This gives the formula [Suz91]

$$s_1 = s_2 = s_4 = s_5 = \frac{1}{4 - 4^{1/(p+1)}}, \qquad s_3 = -\frac{4^{1/(p+1)}}{4 - 4^{1/(p+1)}}. \tag{15.67}$$

If the basic method $\widetilde{U}_p(t)$ is symmetric and the coefficients are chosen as above, then $\widetilde{U}_p^{\mathrm{comp}}(t)$ is also symmetric, and therefore its order must be even. In particular, if p is even, then "order at least $p+1$" implies order at least $p+2$.

Applying this construction to the second-order Trotter method $\widetilde{U}_2(t)$ yields the **Trotter–Suzuki formula**. It recursively defines

$$\widetilde{U}_{2k}(t) := \widetilde{U}_{2k-2}^2(s_k t)\,\widetilde{U}_{2k-2}((1-4s_k)t)\,\widetilde{U}_{2k-2}^2(s_k t), \qquad s_k := \frac{1}{4 - 4^{1/(2k-1)}}, \quad k \geq 2. \tag{15.68}$$

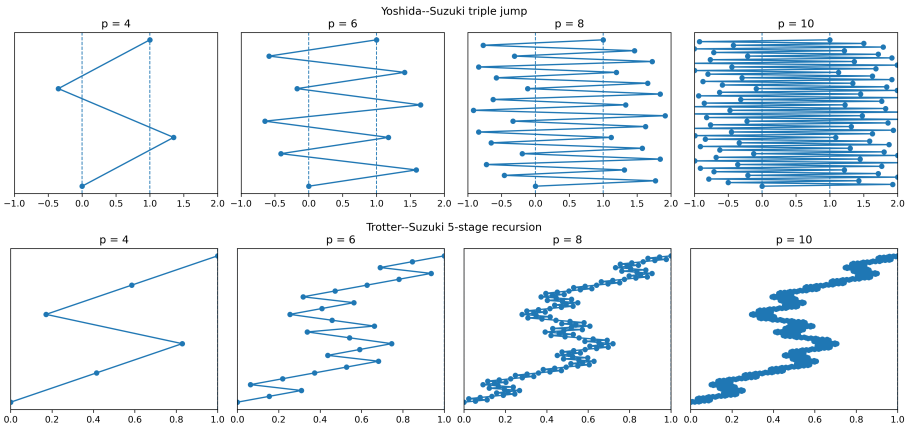


FIGURE 15.2. Comparison of steps of composition methods: the upper panel shows the Yoshida–Suzuki triple jump method, and the lower panel shows the Trotter–Suzuki 5-stage method.

Note that $\widetilde{U}_{2k}$ uses five applications of $\widetilde{U}_{2k-2}$, and hence can be written using at most 5^{k-1} applications of $\widetilde{U}_2(\cdot)$. The approximation order is $2k$, i.e.,

$$\left\| \widetilde{U}_{2k}(t) - e^{-iHt} \right\| = \mathcal{O}(t^{2k+1}), \quad t \to 0. \tag{15.69}$$

Expanding the recursion for $\widetilde{U}_{2k}(t)$ yields a composition method written directly in terms of $\widetilde{U}_2(\cdot)$. A comparison of the resulting step-size patterns for the Yoshida–Suzuki triple jump method and the Trotter–Suzuki method is shown in Fig. 15.2. The Yoshida–Suzuki coefficients oscillate between relatively large positive and negative values, which is often undesirable. By contrast, the 5-stage Trotter–Suzuki construction exhibits a pattern called "Suzuki fractals", with much smaller coefficient magnitudes. ◇

After expanding all compositions, an operator-splitting based simulation can be written as

$$\widetilde{U}(t) := \prod_{k=1}^{K} \prod_{\gamma=1}^{\Gamma} e^{-ita_{k,\gamma} H_{\pi_k(\gamma)}}, \tag{15.70}$$

where $a_{k,\gamma} \in \mathbb{R}$ and, for each k, π_k is a permutation of $\{1, \ldots, \Gamma\}$. In the Trotter–Suzuki formula above, $\widetilde{U}_{2k}(t)$ can be written in the form of Eq. (15.70) with $\Gamma = 2$ and $K = 2 \times 5^{k-1}$. We define the sum of operator norms:

$$|||H||| := \sum_{\gamma=1}^{\Gamma} \|H_\gamma\| . \tag{15.71}$$

The following result is similar to [CST+21, Lemma 1]. It provides an explicit constant without resorting to asymptotic notation.

THEOREM 15.13 (Sum of operator norm error scaling). *Let $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$ be a Hermitian operator acting on a finite-dimensional Hilbert space, and let $t \in \mathbb{R}$. Let $\widetilde{U}(t) = \prod_{k=1}^{K} \prod_{\gamma=1}^{\Gamma} e^{-ita_{k,\gamma} H_{\pi_k(\gamma)}}$ be a p-th order Trotter expansion with $|a_{k,\gamma}| \leq 1$. Then for any $t \geq 0$,*

(1) *The short-time error in the p-th order Trotter formula is*

$$\|\widetilde{U}(t) - e^{-itH}\| \leq \frac{t^{p+1}(K^{p+1}+1)}{(p+1)!}|||H|||^{p+1}. \tag{15.72}$$

(2) *We have that* $\|\widetilde{U}(t/L)^L - e^{-itH}\| \leq \epsilon$ *for the following choice of* L*:*

$$L = \left\lceil (tK|||H|||)^{1+\frac{1}{p}} \epsilon^{-\frac{1}{p}} \right\rceil. \tag{15.73}$$

The total number of operator exponentials of the form $e^{-ita_{k,\gamma}H_{\pi_k(\gamma)}}$ *required by the simulation is*

$$\Gamma KL = \Gamma \left\lceil K^{2+\frac{1}{p}} (t|||H|||)^{1+\frac{1}{p}} \epsilon^{-\frac{1}{p}} \right\rceil. \tag{15.74}$$

(3) *If we focus on the scaling with respect to* $t, |||H|||, \epsilon$*, then as* $p \to \infty$ *the gate complexity can be expressed as*

$$\mathcal{O}((t|||H|||)^{1+o(1)} \epsilon^{-o(1)}). \tag{15.75}$$

Proof. Define $F(t) := \widetilde{U}(t) - e^{-itH}$. Since $\widetilde{U}(t)$ is a p-th order formula, we have $F^{(j)}(0) = 0$ for all $0 \leq j \leq p$. Then by Taylor's theorem,

$$\widetilde{U}(t) - e^{-itH} = \frac{t^{p+1}}{p!} \int_0^1 \mathrm{d}u\, (1-u)^p \left(\widetilde{U}^{(p+1)}(ut) - (-iH)^{p+1} e^{-iutH} \right), \tag{15.76}$$

where

$$\widetilde{U}^{(p+1)}(ut) = \sum_{q_{1,1}+\cdots+q_{K,\Gamma}=p+1} \binom{p+1}{q_{1,1},\ldots,q_{K,\Gamma}} \prod_{k=1}^{K} \prod_{\gamma=1}^{\Gamma} (-ia_{k,\gamma} H_{\pi_k(\gamma)})^{q_{k,\gamma}} e^{-iuta_{k,\gamma}H_{\pi_k(\gamma)}}. \tag{15.77}$$

Using $|a_{k,\gamma}| \leq 1$ for any k, γ, we bound

$$\begin{aligned} \|\widetilde{U}^{(p+1)}(ut)\| &\leq \sum_{q_{1,1}+\cdots+q_{K,\Gamma}=p+1} \binom{p+1}{q_{1,1},\ldots,q_{K,\Gamma}} \prod_{k=1}^{K} \prod_{\gamma=1}^{\Gamma} \|H_{\pi_k(\gamma)}\|^{q_{k,\gamma}} \\ &= \left(\sum_{k=1}^{K} \sum_{\gamma=1}^{\Gamma} \|H_{\pi_k(\gamma)}\| \right)^{p+1} = (K|||H|||)^{p+1}. \end{aligned} \tag{15.78}$$

Therefore

$$\|\widetilde{U}(t) - e^{-itH}\| \leq \frac{t^{p+1}}{(p+1)!} \left[(K|||H|||)^{p+1} + |||H|||^{p+1} \right]. \tag{15.79}$$

This proves Eq. (15.72).

We now use Stirling's approximation,

$$\sqrt{2\pi} n^n \sqrt{n} \leq e^n n! \leq e n^n \sqrt{n}. \tag{15.80}$$

which in particular implies

$$n^n \leq e^n n! \leq e^n n^n. \tag{15.81}$$

For long-time simulation, we choose

$$L \frac{(t/L)^{p+1}(K^{p+1}+1)}{(p+1)!} |||H|||^{p+1} = \epsilon, \tag{15.82}$$

which gives

$$\begin{aligned} L =& \frac{(K^{p+1}+1)^{\frac{1}{p}}\,(t|||H|||)^{1+\frac{1}{p}}}{\epsilon^{\frac{1}{p}}\,((p+1)!)^{\frac{1}{p}}} \leq \left(\frac{K^{p+1}+1}{\sqrt{2\pi(p+1)}}\right)^{\frac{1}{p}} \left(\frac{e}{p+1}\right)^{1+\frac{1}{p}} (t|||H|||)^{1+\frac{1}{p}}\,\epsilon^{-\frac{1}{p}} \\ \leq& (tK|||H|||)^{1+\frac{1}{p}}\,\epsilon^{-\frac{1}{p}}. \end{aligned} \tag{15.83}$$

In the first inequality we used Stirling's approximation, and in the second inequality we used the fact that

$$\left(\frac{2}{\sqrt{2\pi(p+1)}}\right)^{\frac{1}{p}} \left(\frac{e}{p+1}\right)^{1+\frac{1}{p}} \leq 1, \quad p \geq 1, \tag{15.84}$$

which can be verified through direct computation. Finally, since $\widetilde{U}(t/L)$ and $e^{-itH/L}$ are unitary, we have

$$\|\widetilde{U}(t/L)^L - e^{-itH}\| \leq L\|\widetilde{U}(t/L) - e^{-itH/L}\|, \tag{15.85}$$

which justifies the choice of L above. This proves Eq. (15.73) and Eq. (15.74). □

When $p \to \infty$, the scaling $\mathcal{O}((t|||H|||)^{1+o(1)}\,\epsilon^{-o(1)})$ is near optimal with respect to $t, |||H|||, \epsilon$. Plugging in $p = 1, 2$, we also recover the previous results on first and second order Trotter methods.

Example 15.14 (Optimizing the cost of high-order Trotter formula)**.** Should p be chosen to be as large as possible? To answer this question, we need to take into account the preconstant $K^{2+\frac{1}{p}}$ in the gate complexity. For the Trotter–Suzuki formula of even order p, we have $K = 2 \times 5^{p/2-1}$. Therefore $K^{2+\frac{1}{p}} \leq 5^p$. An upper bound on the total number of gates is then

$$\Gamma K^{2+\frac{1}{p}}\,(t|||H|||)^{1+\frac{1}{p}}\,\epsilon^{-\frac{1}{p}} \leq \Gamma t|||H|||5^p(t|||H|||\epsilon^{-1})^{\frac{1}{p}} \tag{15.86}$$

For a fixed problem, we can assume that $t, |||H|||$ are fixed. Then the optimal value of p should be determined by the solution of the minimization problem

$$\min_{p\geq 1} \quad 5^p(t|||H|||\epsilon^{-1})^{\frac{1}{p}}. \tag{15.87}$$

Treating p as a continuous variable, the minimizer is

$$p = \max\left\{1, \sqrt{\frac{\log(t|||H|||\epsilon^{-1})}{\log 5}}\right\}. \tag{15.88}$$

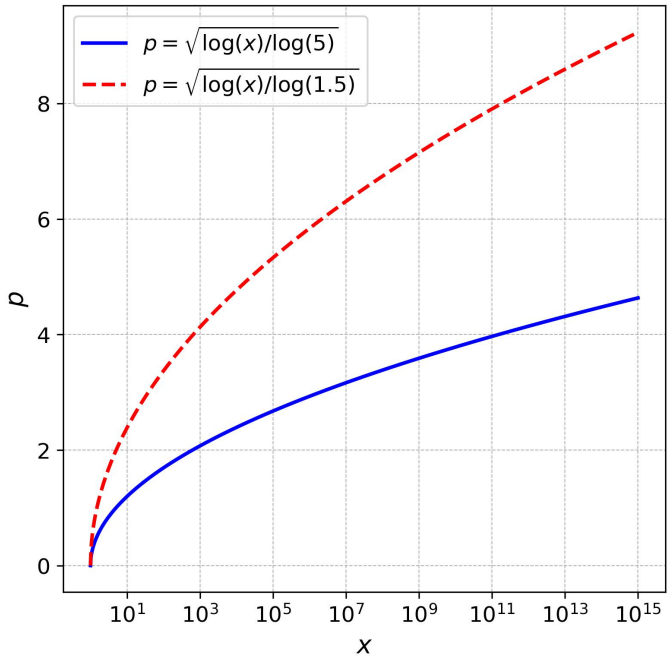


FIGURE 15.3. Optimal order p versus $x = t|||H|||\epsilon^{-1}$, assuming $K^{2+\frac{1}{p}}$ is upper bounded by 5^p and 1.5^p, respectively.

One should note that the function $\sqrt{\log(x)}$ grows very slowly as a function of x. Given $x = t|||H|||\epsilon^{-1}$, the optimal Trotter order p can be determined as shown in Fig. 15.3. The graph illustrates that the second-order Trotter method is optimal when $x \leq 10^3$, while the fourth-order method remains optimal up to $x \leq 10^{11}$. In practical applications, high-order methods can be more competitive than suggested by the above analysis, especially when more efficient methods than the Trotter–Suzuki decomposition are applied. Fig. 15.3 shows that if the factor $K^{2+\frac{1}{p}}$ can be replaced by a more modest growth 1.5^p, then the 6-th order and 8-th order methods become competitive when $t|||H|||\epsilon^{-1}$ reaches 10^7 and 10^{11}, respectively. Therefore very high-order Trotter methods provide theoretical insights, but they are often less practical in real-world situations.

◇

15.4. Commutator error bound and vector norm error bound

The error analysis in Proposition 15.5 relied on the sum of operator norms $|||H|||$. This yields a worst-case bound $\mathcal{O}(t^2|||H|||^2)$, but it does not reflect an important structural feature: if H_1 and H_2 commute (i.e., $[H_1, H_2] = 0$), then the first-order Trotter splitting is exact for all t.

To see the origin of this phenomenon, compare the Taylor expansions of the approximate and exact propagators. A direct calculation shows that the first nonzero term in the difference occurs at order t^2:

$$e^{-itH_1}e^{-itH_2} - e^{-it(H_1+H_2)} = -\frac{t^2}{2}[H_1, H_2] + \mathcal{O}(t^3). \tag{15.89}$$

This indicates that the local error is controlled by the commutator, a feature known as **commutator error scaling**. To prove a rigorous bound proportional to $\|[H_1, H_2]\|$, we first state a lemma regarding the time evolution of conjugated operators.

Lemma 15.15. *Let $A, B \in \mathbb{C}^{N\times N}$ be Hermitian matrices. Then*

$$e^{-itA} B e^{itA} = B - i\int_0^t e^{-isA}[A, B]e^{isA}\,\mathrm{d}s. \tag{15.90}$$

Consequently, the difference between a conjugated operator and the operator itself is bounded by

$$\left\|e^{-itA} B e^{itA} - B\right\| \le t\,\|[A, B]\|. \tag{15.91}$$

Proof. Define the matrix-valued function $f(t) := e^{-itA} B e^{itA}$. Differentiating with respect to t, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} f(t) = -iAe^{-itA} B e^{itA} + ie^{-itA} B A e^{itA} = -ie^{-itA}[A, B]e^{itA}. \tag{15.92}$$

Applying the fundamental theorem of calculus, $f(t) = f(0) + \int_0^t f'(s)\,\mathrm{d}s$, yields Eq. (15.90). Taking the spectral norm of both sides and using the unitarity of e^{-isA} gives the stated bound. □

We can now improve the error analysis for the first-order Trotter formula.

Proposition 15.16 (Commutator scaling of first-order Trotter error)**.** *Let $H = H_1 + H_2$ with H_1, H_2 Hermitian. For the first-order Trotter approximation $\widetilde{U}(t) = e^{-itH_1}e^{-itH_2}$, the error is bounded by*

$$\left\|\widetilde{U}(t) - e^{-itH}\right\| \le \frac{t^2}{2}\,\|[H_1, H_2]\|. \tag{15.93}$$

Proof. We begin by determining the differential equation satisfied by the approximate propagator $\widetilde{U}(t)$. Differentiating with respect to time gives

$$\begin{aligned} i\partial_t \widetilde{U}(t) &= \left(i\partial_t e^{-itH_1}\right) e^{-itH_2} + e^{-itH_1}\left(i\partial_t e^{-itH_2}\right) \\ &= H_1 e^{-itH_1} e^{-itH_2} + e^{-itH_1} H_2 e^{-itH_2}. \end{aligned} \tag{15.94}$$

We compare this to the ideal evolution $i\partial_t U(t) = (H_1 + H_2)U(t)$. Rearranging to isolate $H = H_1 + H_2$ yields

$$\begin{aligned} i\partial_t \widetilde{U}(t) &= (H_1 + H_2)\widetilde{U}(t) + e^{-itH_1} H_2 e^{-itH_2} - H_2 e^{-itH_1} e^{-itH_2} \\ &= H\widetilde{U}(t) + [e^{-itH_1}, H_2]e^{-itH_2}. \end{aligned} \tag{15.95}$$

Thus $\widetilde{U}(t)$ satisfies an inhomogeneous Schrödinger equation with inhomogeneity $B(t) := [e^{-itH_1}, H_2]e^{-itH_2}$. Applying Duhamel's principle (Proposition 3.22), we obtain

$$\left\|\widetilde{U}(t) - U(t)\right\| \le \int_0^t \|B(s)\|\,\mathrm{d}s = \int_0^t \left\|[e^{-isH_1}, H_2]\right\|\,\mathrm{d}s. \tag{15.96}$$

To bound the integrand, we observe that the norm is invariant under unitary multiplication. Multiplying the term inside the norm by e^{isH_1} on the left gives

$$\left\|[e^{-isH_1}, H_2]\right\| = \left\|e^{isH_1} H_2 e^{-isH_1} - H_2\right\|. \tag{15.97}$$

Using Lemma 15.15 with $A = -H_1$ and $B = H_2$, we have

$$\left\|e^{isH_1} H_2 e^{-isH_1} - H_2\right\| \le s\,\|[H_1, H_2]\|. \tag{15.98}$$

Substituting this back into the integral yields the final result:

$$\left\|\widetilde{U}(t) - U(t)\right\| \leq \int_0^t s \left\|[H_1, H_2]\right\| \mathrm{d}s = \frac{t^2}{2} \left\|[H_1, H_2]\right\|. \tag{15.99}$$

□

The commutator error bound implies the operator norm bound. Indeed,

$$\left\|[H_1, H_2]\right\| \leq 2 \left\|H_1\right\| \left\|H_2\right\| \leq (\left\|H_1\right\| + \left\|H_2\right\|)^2 = \left\|\!\left|H\right|\!\right\|^2, \tag{15.100}$$

which is sharper than the bound in proved in Proposition 15.5 by a factor of 2. Furthermore, commutator type error bounds can be substantially sharper than the operator norm bounds when the terms are close to commuting.

Example 15.17 (Backward error analysis and modified Hamiltonian)**.** Standard forward error analysis bounds the distance between the exact and approximate propagators. Alternatively, **backward error analysis** asks (recall Section 7.1): For what Hamiltonian $H_{\mathrm{mod}}(t)$ is the approximate propagator $\widetilde{U}(t)$ the **exact** solution?

Consider the first-order Trotter splitting $\widetilde{U}(t) = e^{-itH_1}e^{-itH_2}$. We determine the differential equation satisfied by $\widetilde{U}(t)$ by differentiating with respect to time:

$$\begin{aligned} i\partial_t \widetilde{U}(t) &= \left(i\partial_t e^{-itH_1}\right) e^{-itH_2} + e^{-itH_1}\left(i\partial_t e^{-itH_2}\right) \\ &= H_1 e^{-itH_1}e^{-itH_2} + e^{-itH_1}H_2 e^{-itH_2} \\ &= \left(H_1 + e^{-itH_1}H_2 e^{itH_1}\right)\widetilde{U}(t). \end{aligned} \tag{15.101}$$

Thus, $\widetilde{U}(t)$ exactly solves the Schrödinger equation $i\partial_t\psi(t) = H_{\mathrm{mod}}(t)\psi(t)$ governed by the time-dependent **modified Hamiltonian**:

$$H_{\mathrm{mod}}(t) = H_1 + e^{-itH_1}H_2 e^{itH_1} = H + \delta H(t), \tag{15.102}$$

where the deviation from the target Hamiltonian is $\delta H(t) = e^{-itH_1}H_2 e^{itH_1} - H_2$.

Using the conjugation expansion derived in Lemma 15.15, we can expand the backward error term $\delta H(t)$ for small t:

$$\delta H(t) = -it[H_1, H_2] + \mathcal{O}(t^2). \tag{15.103}$$

This result offers a physical intuition for the Trotter error: the simulation implements a Hamiltonian that drifts linearly away from H with time. The direction of the drift is determined by the commutator $[H_1, H_2]$.

We can relate this back to the forward error using the Magnus expansion. The propagator generated by $H_{\mathrm{mod}}(t)$ can be approximated by the exponential of the average Hamiltonian:

$$\widetilde{U}(t) \approx \exp\left(-i\int_0^t H_{\mathrm{mod}}(s)\,\mathrm{d}s\right) = \exp\left(-itH - i\int_0^t \delta H(s)\,\mathrm{d}s\right). \tag{15.104}$$

Integrating the leading order term of the backward error yields

$$\int_0^t \delta H(s)\,\mathrm{d}s \approx \int_0^t -is[H_1, H_2]\,\mathrm{d}s = -\frac{it^2}{2}[H_1, H_2]. \tag{15.105}$$

This recovers the quadratic commutator scaling $\mathcal{O}(t^2 \left\|[H_1, H_2]\right\|)$ found in the forward error analysis (Proposition 15.16). ◇

Exercise 15.1. Consider the Hamiltonian simulation problem for $H = H_1 + H_2 + H_3$. Show that the first order Trotter formula

$$\widetilde{U}(t) = e^{-itH_1}e^{-itH_2}e^{-itH_3}$$

has a commutator type error bound

$$\left\|\widetilde{U}(t) - U(t)\right\| \leq \frac{t^2}{2}(\|[H_1, H_2]\| + \|[H_1, H_3]\| + \|[H_2, H_3]\|) = \frac{t^2}{4}\sum_{\gamma_1,\gamma_2=1}^{3}\|[H_{\gamma_1}, H_{\gamma_2}]\|\,. \tag{15.106}$$

Example 15.18. For the 1D TFIM model with nearest neighbor interactions, the commutator $[Z_iZ_j, X_k]$ is non-zero only when $k = i$ or $k = j$. So the norm of the commutator $\|[H_1, H_2]\|$ scales linearly with the system size, i.e., $\|[H_1, H_2]\| = \mathcal{O}(n)$. Therefore, to achieve a precision of ϵ for constant simulation time t, using the first order Trotter method, the scaling of the total number of time steps L relative to the system size is $\mathcal{O}(n^2/\epsilon)$ if we use the estimate based on the operator norm. However, the scaling is only $\mathcal{O}(n/\epsilon)$ if we use the estimate based on the commutator norm. ⋄

Example 15.19. Consider the 1D Hubbard model, the Hamiltonian can be written in the form $H = H_1 + H_2$, where H_1 represents the kinetic energy of the electrons and H_2 describes the on-site interaction. The norms of H_1 and H_2 are proportional to the system size, thus $\|H_1\|, \|H_2\| = \mathcal{O}(n)$. However, since the commutator $[H_1, H_2]$ is non-zero only for terms where the kinetic and interaction energies correspond to the same site, we have $\|[H_1, H_2]\| = \mathcal{O}(n)$. Therefore, to achieve a precision of ϵ for constant simulation time t, using the first order Trotter method, the scaling of the total number of time steps L with respect to the system size is $\mathcal{O}(n^2/\epsilon)$ if we use the estimate based on the operator norm, but it is only $\mathcal{O}(n/\epsilon)$ if we use the estimate based on the commutator norm. ⋄

The commutator viewpoint extends to higher-order product formulas. We record the following result, parallel to Theorem 15.13, without proof; see [CST+21, Theorem 6].

THEOREM 15.20 (Commutator error scaling of Trotter expansion). *Let $H = \sum_{\gamma=1}^{\Gamma} H_\gamma$ with H_γ Hermitian and $t \in \mathbb{R}$. Let $\widetilde{U}(t) = \prod_{k=1}^{K}\prod_{\gamma=1}^{\Gamma} e^{-ita_{k,\gamma}H_{\pi_k(\gamma)}}$ be a p-th order Trotter expansion, and assume $|a_{k,\gamma}| \leq 1$ for all k, γ. Define*

$$|||H|||_{p+1,\mathrm{comm}} = \sum_{\gamma_1,\gamma_2,\ldots,\gamma_{p+1}=1}^{\Gamma} \left\|\left[H_{\gamma_{p+1}}, \left[H_{\gamma_p}, \cdots [H_{\gamma_2}, H_{\gamma_1}]\cdots\right]\right]\right\|. \tag{15.107}$$

In particular, $|||H|||_{p+1,\mathrm{comm}} = \mathcal{O}\big(2^p\Gamma^{p+1}(\max_j \|H_j\|)^{p+1}\big)$. Then for short $t \geq 0$,

$$\|\widetilde{U}(t) - e^{-itH}\| = \mathcal{O}\left(t^{p+1}K^{p+1}|||H|||_{p+1,\mathrm{comm}}\right). \tag{15.108}$$

For long time simulation, to reach precision ϵ, we can choose the number of segments

$$L = \mathcal{O}\left((tK)^{1+\frac{1}{p}}\,|||H|||_{p+1,\mathrm{comm}}^{\frac{1}{p}}\epsilon^{-\frac{1}{p}}\right), \tag{15.109}$$

and the number of gates is

$$\Gamma KL = \mathcal{O}\left(\Gamma K^{2+\frac{1}{p}}t^{1+\frac{1}{p}}|||H|||_{p+1,\mathrm{comm}}^{\frac{1}{p}}\epsilon^{-\frac{1}{p}}\right). \tag{15.110}$$

The commutator bounds above are operator-norm statements. Since the operator norm is defined by $\|A\| = \sup_{\|\psi\|=1}\|A\psi\|$, it captures a worst-case error over all states. In many applications one is instead interested in a fixed initial state $\psi(0)$; then the state-dependent error

$\left\|(U(t)-\widetilde{U}(t))\psi(0)\right\|$ can be much smaller than $\left\|U(t)-\widetilde{U}(t)\right\|$. This phenomenon is known as **vector norm scaling**.

Proposition 15.21 (Vector norm scaling for first-order Trotter)**.** *Let $H = H_1 + H_2$ with H_1, H_2 Hermitian, and let $U(t) = e^{-itH}$ and $\widetilde{U}(t) = e^{-itH_1}e^{-itH_2}$. Then for any $\psi(0) \in \mathbb{C}^N$ and any $t \geq 0$,*

$$\begin{aligned}\left\|\widetilde{U}(t)\psi(0) - U(t)\psi(0)\right\| &\leq \int_0^t \int_0^s \left\|[H_1, H_2]e^{-iuH_1}e^{-isH_2}\psi(0)\right\| \, \mathrm{d}u \, \mathrm{d}s \\ &\leq \frac{t^2}{2} \sup_{0\leq u\leq s\leq t} \left\|[H_1, H_2]e^{-iuH_1}e^{-isH_2}\psi(0)\right\|.\end{aligned} \tag{15.111}$$

In particular, since $\left\|[H_1, H_2]e^{-iuH_1}e^{-isH_2}\psi(0)\right\| \leq \|[H_1, H_2]\| \, \|\psi(0)\|$, this implies the operator-norm commutator bound $\left\|\widetilde{U}(t) - U(t)\right\| \leq \frac{t^2}{2} \|[H_1, H_2]\|$.

Proof. As in Proposition 15.16, applying Duhamel's principle to the inhomogeneous equation satisfied by $\widetilde{U}(t)\psi(0)$ yields

$$\left\|\widetilde{U}(t)\psi(0) - U(t)\psi(0)\right\| \leq \int_0^t \left\|[e^{-isH_1}, H_2]e^{-isH_2}\psi(0)\right\| \, \mathrm{d}s. \tag{15.112}$$

Using unitary invariance of the norm, we multiply by e^{isH_1} on the left and obtain

$$\left\|[e^{-isH_1}, H_2]e^{-isH_2}\psi(0)\right\| = \left\|e^{isH_1}[e^{-isH_1}, H_2]e^{-isH_2}\psi(0)\right\|. \tag{15.113}$$

Since $e^{isH_1}[e^{-isH_1}, H_2] = H_2 - e^{isH_1}H_2e^{-isH_1} = -(e^{isH_1}H_2e^{-isH_1} - H_2)$, this implies

$$\left\|[e^{-isH_1}, H_2]e^{-isH_2}\psi(0)\right\| = \left\|(e^{isH_1}H_2e^{-isH_1} - H_2)e^{-isH_2}\psi(0)\right\|. \tag{15.114}$$

Finally, applying Eq. (15.90) with $A = -H_1$ and $B = H_2$ gives

$$e^{isH_1}H_2e^{-isH_1} - H_2 = i\int_0^s e^{iuH_1}[H_1, H_2]e^{-iuH_1} \, \mathrm{d}u. \tag{15.115}$$

Therefore,

$$\left\|[e^{-isH_1}, H_2]e^{-isH_2}\psi(0)\right\| \leq \int_0^s \left\|[H_1, H_2]e^{-iuH_1}e^{-isH_2}\psi(0)\right\| \, \mathrm{d}u, \tag{15.116}$$

and substituting into the previous bound yields the stated double-integral estimate. The supremum bound follows from $\int_0^t \int_0^s \mathrm{d}u \, \mathrm{d}s = t^2/2$. □

Vector norm scaling is particularly useful when the Hamiltonian involves unbounded operators, such as differential operators in the Schrödinger equation. In such cases, the operator norm may diverge or scale poorly with discretization parameters, while the vector norm error can remain well behaved for sufficiently smooth states.

Example 15.22 (Application to the first-quantized Schrödinger equation)**.** Consider a particle in a one-dimensional potential $V(x)$ on the domain $\Omega = [0, 1]$ with periodic boundary conditions. The Hamiltonian is $H = H_1 + H_2$, where $H_1 = -\partial_x^2$ (kinetic energy) and $H_2 = V(x)$ (potential energy). We discretize the domain using a uniform grid of N points.

Using the operator norm estimates from previous sections, we have $\|H_1\| = \mathcal{O}(N^2)$ and $\|H_2\| = \mathcal{O}(1)$. The standard Trotter error bound would imply a complexity scaling of:

$$L_{\mathrm{op}} = \mathcal{O}\left(\frac{t^2 \|\|H\|\|^2}{\epsilon}\right) = \mathcal{O}\left(\frac{t^2 N^4}{\epsilon}\right), \tag{15.117}$$

which is prohibitively expensive for fine discretizations.

However, utilizing Proposition 15.21, we examine the commutator term acting on wavefunctions of the form $e^{-iuH_1}e^{-isH_2}\psi(0)$. For any smooth function $\psi(x)$,

$$[H_1, H_2]\psi = [-\partial_x^2, V]\psi = -\partial_x^2(V\psi) + V\partial_x^2\psi = -(V''\psi + 2V'\psi'). \tag{15.118}$$

In the non-asymptotic bound in Proposition 15.21, the commutator acts on split-evolved states

$$\phi_{u,s} := e^{-iuH_1}e^{-isH_2}\psi(0), \qquad 0 \le u \le s \le t. \tag{15.119}$$

Using the explicit commutator expression, we obtain

$$\|[H_1, H_2]\phi_{u,s}\| \le \|V''\|_\infty \|\phi_{u,s}\| + 2\|V'\|_\infty \left\|\phi'_{u,s}\right\|. \tag{15.120}$$

Moreover, under periodic boundary conditions, e^{-iuH_1} is a Fourier multiplier and commutes with ∂_x, so $\|\phi_{u,s}\| = \left\|e^{-isV}\psi(0)\right\| = \|\psi(0)\|$ and $\left\|\phi'_{u,s}\right\| = \left\|(e^{-isV}\psi(0))'\right\|$. Since

$$(e^{-isV}\psi(0))' = e^{-isV}(\psi'(0) - isV'\psi(0)), \tag{15.121}$$

we have the bound

$$\left\|\phi'_{u,s}\right\| \le \|\psi'(0)\| + s\|V'\|_\infty \|\psi(0)\|. \tag{15.122}$$

The bound above is written in terms of $\psi'(0)$. To obtain a statement that depends on the regularity of the **true** solution at all times, let $\psi(s) := e^{-isH}\psi(0)$ denote the exact Schrödinger evolution. Assume that $\sup_{0\le s\le t}\|\psi'(s)\|$ is finite and does not scale with the discretization size N (for instance, this holds if the initial state has bounded H^1-regularity and the potential is sufficiently regular).

To extract the global complexity scaling, apply first-order splitting with L steps of size $\Delta t = t/L$. Let $U_{\Delta t} := e^{-i\Delta t H}$ and $\widetilde{U}_{\Delta t} := e^{-i\Delta t H_1}e^{-i\Delta t H_2}$. For any initial state $\psi(0)$, a telescoping expansion gives

$$\widetilde{U}_{\Delta t}^L\psi(0) - U_{\Delta t}^L\psi(0) = \sum_{j=0}^{L-1} \widetilde{U}_{\Delta t}^{L-1-j}\big(\widetilde{U}_{\Delta t} - U_{\Delta t}\big)U_{\Delta t}^j\psi(0). \tag{15.123}$$

Since both $\widetilde{U}_{\Delta t}$ and $U_{\Delta t}$ are unitary, taking norms yields

$$\left\|\widetilde{U}_{\Delta t}^L\psi(0) - U_{\Delta t}^L\psi(0)\right\| \le \sum_{j=0}^{L-1}\left\|\big(\widetilde{U}_{\Delta t} - U_{\Delta t}\big)\psi(t_j)\right\|, \qquad \psi(t_j) := U_{\Delta t}^j\psi(0). \tag{15.124}$$

Thus it suffices to bound the one-step (local) error applied to the exact state at the beginning of each step.

We now apply Proposition 15.21 to a single step with time horizon Δt and initial state $\psi(t_j)$. In the commutator term we encounter

$$e^{-iuH_1}e^{-isH_2}\psi(t_j), \qquad 0 \le u \le s \le \Delta t. \tag{15.125}$$

Using periodic boundary conditions as above, e^{-iuH_1} commutes with ∂_x, and we obtain

$$\left\|\partial_x\big(e^{-iuH_1}e^{-isH_2}\psi(t_j)\big)\right\| = \left\|\partial_x\big(e^{-isV}\psi(t_j)\big)\right\| \le \|\psi'(t_j)\| + s\|V'\|_\infty\|\psi(t_j)\|. \tag{15.126}$$

Since $\|\psi(t_j)\| = \|\psi(0)\|$ and $s \le \Delta t$, for $\Delta t \le 1$ we can bound the right-hand side by

$$\|\psi'(t_j)\| + \|V'\|_\infty\|\psi(0)\| \le \sup_{0\le s\le t}\|\psi'(s)\| + \|V'\|_\infty\|\psi(0)\|. \tag{15.127}$$

Therefore the supremum term in Proposition 15.21 (with t replaced by Δt) is bounded by a constant depending on $\sup_{0\le s\le t}\|\psi'(s)\|$, $\|V'\|_\infty$, and $\|V''\|_\infty$, but not on N. This yields a local error per

step of order $\mathcal{O}(\Delta t^2)$ and hence a global error of order $\mathcal{O}(L\Delta t^2) = \mathcal{O}(t\Delta t) = \mathcal{O}(t^2/L)$. Choosing $L = \mathcal{O}(t^2/\epsilon)$ yields

$$L_{\text{vec}} = \mathcal{O}\left(\frac{t^2}{\epsilon}\right). \tag{15.128}$$

This result demonstrates that the number of time steps required is independent of the discretization parameter N. This explains the practical efficiency of splitting methods for quantum dynamics. ⋄

15.5. Operator splitting with randomized Hamiltonian evolution time

The Hamiltonian simulation problem can be equivalently formulated within the density matrix formalism using the Liouville–von Neumann equation

$$\partial_t \rho(t) = -i[H, \rho(t)] \coloneqq \mathcal{L}(\rho(t)), \tag{15.129}$$

where the linear map $\mathcal{L} : \mathbb{C}^{N\times N} \to \mathbb{C}^{N\times N}$ is known as the **Liouvillian**. The solution to the von Neumann equation admits a closed-form expression given by the exponential of the Liouvillian:

$$\rho(t) = e^{t\mathcal{L}}(\rho(0)) = \sum_{k=0}^{\infty} \frac{t^k \mathcal{L}^k}{k!}(\rho(0)). \tag{15.130}$$

Proposition 15.23. *Let $H \in \mathbb{C}^{N\times N}$ be a Hermitian matrix and let $\mathcal{L}(\cdot) = -i[H, \cdot]$ be the associated Liouvillian. Then the diamond norm satisfy*

$$\|\mathcal{L}\|_\diamond \leq 2\|H\|. \tag{15.131}$$

Proof. Recall that the diamond norm is defined as $\|\mathcal{L}\|_\diamond := \sup_{k\geq 1} \|\mathcal{L} \otimes \mathcal{I}_k\|_{1\to 1}$, where $\mathcal{I}_k$ is the identity map on an ancillary system of dimension k. For any dimension k and any $X \in \mathbb{C}^{Nk\times Nk}$, the action of the extended map is

$$(\mathcal{L} \otimes \mathcal{I}_k)(X) = -i(H \otimes I_k)X + iX(H \otimes I_k) = -i[H \otimes I_k, X]. \tag{15.132}$$

Thus

$$\|(\mathcal{L} \otimes \mathcal{I}_k)(X)\|_1 \leq 2\|H \otimes I_k\| \|X\|_1 = 2\|H\| \|X\|_1, \tag{15.133}$$

where we used the fact that the spectral norm is multiplicative under tensor products with the identity, $\|H \otimes I_k\| = \|H\| \|I_k\| = \|H\|$. Therefore, for any k,

$$\|\mathcal{L} \otimes \mathcal{I}_k\|_{1\to 1} \leq 2\|H\|. \tag{15.134}$$

Taking the supremum over k confirms that $\|\mathcal{L}\|_\diamond \leq 2\|H\|$. □

The **quantum stochastic drift protocol** (qDRIFT) [Cam19] provides a distinct approach to Hamiltonian simulation, particularly effective when the Hamiltonian is composed of a large number of terms. We consider a Hamiltonian H expressed as a linear combination $H = \sum_{\gamma=1}^{\Gamma} c_\gamma H_\gamma$. We assume the standard setting where H is Hermitian, the coefficients c_γ are positive real numbers, and each component H_γ is Hermitian. Without loss of generality, we assume that each component is normalized, $\|H_\gamma\| = 1$, absorbing the normalization factors into the coefficients c_γ.

The core idea of qDRIFT is to apply the individual evolution operators $U_\gamma(t) = e^{-itH_\gamma}$ stochastically. The probability of selecting the γ-th term is determined by the relative magnitude of its coefficient. We define the L_1 norm of the coefficients as

$$\|c\|_1 = \sum_{\gamma=1}^{\Gamma} c_\gamma, \tag{15.135}$$

Algorithm 15.1 qDRIFT Protocol

Require: Hamiltonian $H = \sum_{\gamma=1}^{\Gamma} c_\gamma H_\gamma$ (with $\|H_\gamma\| = 1, c_\gamma > 0$).
Access to unitaries $e^{-iH_\gamma t}$.
Initial state $|\psi\rangle$. Total evolution time $T > 0$. Number of steps N_t.
Ensure: Output state $|\Psi_{N_t}\rangle$, which is a sample from the distribution defined by the channel $\mathcal{Q}_t^{N_t}(|\psi\rangle\langle\psi|)$, approximating $e^{-iHT}|\psi\rangle$.
1: Calculate $\|c\|_1 \leftarrow \sum_{\gamma=1}^{\Gamma} c_\gamma$.
2: Define the probability distribution $p_\gamma \leftarrow c_\gamma / \|c\|_1$ for $\gamma = 1, \ldots, \Gamma$.
3: Set the time step parameter $t \leftarrow \frac{T\|c\|_1}{N_t}$.
4: Initialize $|\Psi_0\rangle \leftarrow |\psi\rangle$.
5: **for** $k = 1$ to N_t **do**
6: Randomly sample an index $\gamma_k \in \{1, \ldots, \Gamma\}$ according to the distribution $\{p_\gamma\}$.
7: Apply the unitary evolution: $|\Psi_k\rangle \leftarrow e^{-iH_{\gamma_k} t}|\Psi_{k-1}\rangle$.
8: **end for**
9: **return** $|\Psi_{N_t}\rangle$.

and the corresponding probability distribution as

$$p_\gamma = c_\gamma / \|c\|_1 . \tag{15.136}$$

This stochastic application of unitaries defines a quantum channel $\mathcal{Q}_t$:

$$\mathcal{Q}_t(\rho) = \sum_{\gamma=1}^{\Gamma} p_\gamma e^{-iH_\gamma t} \rho e^{iH_\gamma t}. \tag{15.137}$$

The key insight is that the channel $\mathcal{Q}_t$ closely approximates the ideal evolution $e^{\mathcal{L}t'}$, where $\mathcal{L}(\rho) = -i[H, \rho]$ and the effective time step is $t' = t/\|c\|_1$. To simulate the evolution for a total time T, the channel is applied repeatedly N_t times, such that $T = N_t t'$. The procedure is formalized in Algorithm 15.1.

The efficiency of the qDRIFT protocol depends on the number of steps N_t required to achieve a desired precision ϵ, measured using the diamond norm.

Proposition 15.24 (Convergence of qDRIFT)**.** *Let $H = \sum_{\gamma=1}^{\Gamma} c_\gamma H_\gamma$ be a Hamiltonian such that $\|H_\gamma\| = 1$ and $c_\gamma > 0$ for all γ. Let $\|c\|_1 = \sum_\gamma c_\gamma$. To simulate the evolution $e^{\mathcal{L}T}$ up to error ϵ in the diamond norm, it suffices to apply the qDRIFT channel $\mathcal{Q}_t$ defined in Eq.* (15.137) *for N_t steps, where*

$$N_t = \mathcal{O}\left(\frac{T^2 \|c\|_1^2}{\epsilon}\right). \tag{15.138}$$

Proof. We analyze the error introduced in a single step. Let t be the time parameter for the channel $\mathcal{Q}_t$. We aim to bound the diamond norm distance between $\mathcal{Q}_t$ and the ideal evolution $e^{\mathcal{L}t'}$, where $t' = t/\|c\|_1$.

We begin by defining a linearized approximation of the evolution. Let $W_\gamma = I - iH_\gamma t$. Since $\|H_\gamma\| = 1$, we have $\|W_\gamma\| \leq 1 + t \leq e^t$. The approximation error between the unitary $U_\gamma = e^{-iH_\gamma t}$

and W_γ is bounded by the Taylor series remainder:

$$\|U_\gamma - W_\gamma\| \leq \sum_{k=2}^{\infty} \frac{t^k}{k!} = e^t - (1+t) \leq \frac{t^2}{2} e^t. \tag{15.139}$$

Let $\mathcal{U}_\gamma(\rho) = U_\gamma \rho U_\gamma^\dagger$ and $\mathcal{W}_\gamma(\rho) = W_\gamma \rho W_\gamma^\dagger$. We bound the diamond norm distance between these two maps using Lemma 3.59.

$$\|\mathcal{U}_\gamma - \mathcal{W}_\gamma\|_\diamond \leq \|U_\gamma\| \left\|U_\gamma^\dagger - W_\gamma^\dagger\right\| + \|U_\gamma - W_\gamma\| \left\|W_\gamma^\dagger\right\|. \tag{15.140}$$

Since U_γ is unitary, $\|U_\gamma\| = 1$. We also have $\left\|U_\gamma^\dagger - W_\gamma^\dagger\right\| = \|U_\gamma - W_\gamma\|$ and $\left\|W_\gamma^\dagger\right\| = \|W_\gamma\|$ (as H_γ is Hermitian). Using the bounds derived above:

$$\begin{aligned} \|\mathcal{U}_\gamma - \mathcal{W}_\gamma\|_\diamond &\leq \|U_\gamma - W_\gamma\| \left(1 + \|W_\gamma\|\right) \\ &\leq \left(\frac{t^2}{2} e^t\right)(1 + e^t) = \frac{t^2}{2}(e^t + e^{2t}). \end{aligned} \tag{15.141}$$

For $t \geq 0$, $e^t \leq e^{2t}$, so $\|\mathcal{U}_\gamma - \mathcal{W}_\gamma\|_\diamond \leq t^2 e^{2t}$.

Let $\mathcal{W}_t = \sum_\gamma p_\gamma \mathcal{W}_\gamma$ be the averaged linearized map. The qDRIFT channel is $\mathcal{Q}_t = \sum_\gamma p_\gamma \mathcal{U}_\gamma$. By the convexity of the diamond norm:

$$\|\mathcal{Q}_t - \mathcal{W}_t\|_\diamond \leq \sum_\gamma p_\gamma \|\mathcal{U}_\gamma - \mathcal{W}_\gamma\|_\diamond \leq t^2 e^{2t}. \tag{15.142}$$

Next, we examine the structure of $\mathcal{W}_t$:

$$\begin{aligned} \mathcal{W}_t(\rho) &= \sum_\gamma p_\gamma (I - iH_\gamma t)\rho(I + iH_\gamma t) \\ &= \rho - it \sum_\gamma \frac{c_\gamma}{\|c\|_1}[H_\gamma, \rho] + t^2 \sum_\gamma p_\gamma H_\gamma \rho H_\gamma \\ &= \left(\mathcal{I} + t'\mathcal{L}\right)(\rho) + t^2 \mathcal{D}(\rho), \end{aligned} \tag{15.143}$$

where $\mathcal{D}(\rho) = \sum_\gamma p_\gamma H_\gamma \rho H_\gamma$. Let $\mathcal{I}_1 = \mathcal{I} + t'\mathcal{L}$ be the first-order approximation of the ideal evolution. The difference between $\mathcal{W}_t$ and $\mathcal{I}_1$ is $t^2\mathcal{D}$. We bound its diamond norm. Since H_γ are Hermitian and $p_\gamma \geq 0$, the map $\mathcal{D}$ is completely positive. By **??**, its diamond norm is equal to the operator norm of its adjoint acting on the identity, $\|\Phi\|_\diamond = \left\|\Phi^\dagger(I)\right\|$. Since H_γ are Hermitian, $\mathcal{D}$ is self-adjoint. Thus,

$$\|\mathcal{D}\|_\diamond = \|\mathcal{D}(I)\| = \left\|\sum_\gamma p_\gamma H_\gamma^2\right\|. \tag{15.144}$$

We bound this operator norm using the triangle inequality:

$$\|\mathcal{D}\|_\diamond \leq \sum_\gamma p_\gamma \left\|H_\gamma^2\right\| = \sum_\gamma p_\gamma \|H_\gamma\|^2 = 1. \tag{15.145}$$

Thus, $\|\mathcal{W}_t - \mathcal{I}_1\|_\diamond \leq t^2$. Combining the bounds via the triangle inequality yields

$$\|\mathcal{Q}_t - \mathcal{I}_1\|_\diamond \leq \|\mathcal{Q}_t - \mathcal{W}_t\|_\diamond + \|\mathcal{W}_t - \mathcal{I}_1\|_\diamond \leq t^2 e^{2t} + t^2 \leq 2t^2 e^{2t}. \tag{15.146}$$

Finally, we bound the error in the Taylor expansion of the ideal evolution $e^{\mathcal{L}t'}$.

$$\left\|e^{\mathcal{L}t'} - \mathcal{I}_1\right\|_\diamond \leq \sum_{k=2}^{\infty} \frac{(t')^k \|\mathcal{L}\|_\diamond^k}{k!}. \tag{15.147}$$

We use the bound $\|\mathcal{L}\|_\diamond \leq 2\|H\|$. Furthermore, $\|H\| \leq \sum_\gamma c_\gamma \|H_\gamma\| = \|c\|_1$. Thus, the expansion parameter is bounded by $t' \|\mathcal{L}\|_\diamond \leq (t/\|c\|_1)(2\|c\|_1) = 2t$. Therefore,

$$\left\| e^{\mathcal{L}t'} - \mathcal{I}_1 \right\|_\diamond \leq \sum_{k=2}^{\infty} \frac{(2t)^k}{k!} = e^{2t} - (1+2t) \leq 2t^2 e^{2t}. \tag{15.148}$$

The total error per step is the sum of these contributions:

$$\left\| e^{\mathcal{L}t'} - \mathcal{Q}_t \right\|_\diamond \leq \left\| e^{\mathcal{L}t'} - \mathcal{I}_1 \right\|_\diamond + \|\mathcal{I}_1 - \mathcal{Q}_t\|_\diamond \leq 4t^2 e^{2t}. \tag{15.149}$$

Since both $e^{\mathcal{L}t'}$ and $\mathcal{Q}_t$ are quantum channels (CPTP maps), their diamond norms are 1. By the stability of the diamond norm under composition, errors accumulate at most linearly over N_t steps. The total error for the evolution up to time $T = N_t t'$ is

$$\left\| e^{\mathcal{L}T} - \mathcal{Q}_t^{N_t} \right\|_\diamond \leq N_t \left\| e^{\mathcal{L}t'} - \mathcal{Q}_t \right\|_\diamond \leq 4N_t t^2 e^{2t}. \tag{15.150}$$

Substituting $N_t = T\|c\|_1 / t$, the total error is $4T\|c\|_1 te^{2t}$. To ensure this is bounded by ϵ, we require $4T\|c\|_1 te^{2t} \leq \epsilon$. By choosing $t = \Theta(\epsilon/(T\|c\|_1))$, the factor e^{2t} approaches 1 as $\epsilon \to 0$. Consequently, the required number of steps is $N_t = \mathcal{O}\left(\frac{T^2\|c\|_1^2}{\epsilon}\right)$. □

We can generalize this protocol to Hamiltonians $H = \sum_\gamma H_\gamma$ where the individual terms are not necessarily normalized. We define the 1-norm of the Hamiltonian as

$$|||H||| := \sum_\gamma \|H_\gamma\|. \tag{15.151}$$

We can rewrite $H = \sum_\gamma \|H_\gamma\| (H_\gamma / \|H_\gamma\|)$. Applying qDRIFT to this decomposition, we identify $c_\gamma = \|H_\gamma\|$ and $\|c\|_1 = |||H|||$. The probability distribution becomes $p_\gamma = \|H_\gamma\| / |||H|||$, and the evolution applied in each step corresponds to the normalized Hamiltonian terms. The resulting complexity scaling is

$$N_t = \mathcal{O}\left(\frac{T^2 |||H|||^2}{\epsilon}\right), \tag{15.152}$$

which matches the error scaling of the first-order Trotter method with respect to T and ϵ.

The primary advantage of the qDRIFT method is that its cost depends on the aggregate norm $|||H|||$ and is independent of the number of terms Γ. This is particularly beneficial when the Hamiltonian comprises a large number of terms, provided their cumulative norm remains manageable.

However, qDRIFT presents some disadvantages compared to deterministic methods like Trotterization. Its inherent randomized nature can complicate its use as a subroutine in algorithms requiring a coherent implementation of the unitary evolution e^{-iHT}. Furthermore, the error bound in qDRIFT depends directly on $|||H|||^2$, rather than on the norms of the commutators between the terms. This often results in a larger prefactor in the error compared to higher-order Trotter formulas, especially when the Hamiltonian terms nearly commute.

Moreover, the nature of the output state differs significantly. If the target precision ϵ is defined in terms of the diamond norm (or trace distance), both the first-order Trotter method and qDRIFT exhibit a cost scaling of $\mathcal{O}(\epsilon^{-1})$. However, the Trotter method implements a unitary evolution, resulting in a pure state if the input is pure. In contrast, qDRIFT implements a quantum channel, generally producing a mixed state (represented as an ensemble of the pure states generated by the algorithm). If we measure accuracy in terms of infidelity (recall **??**), the infidelity of the

deterministic first-order Trotter method scales as $\mathcal{O}(\epsilon^2)$. This is often quadratically better than the infidelity achievable by a randomized method such as qDRIFT, where the infidelity typically scales linearly with the trace distance error, $\mathcal{O}(\epsilon)$.

Readers may wonder whether the random choices made within qDRIFT introduce an additional source of variance. For measurements performed at the end of the computation, the answer is no: once the protocol has produced a final density matrix ρ, the expectation value and variance of any observable A are determined by ρ through $\mathrm{Tr}[A\rho]$ and $\mathrm{Tr}[A^2\rho] - \mathrm{Tr}[A\rho]^2$. Thus the internal randomness used to sample the sequence of Hamiltonian terms is already incorporated into the output channel $\mathcal{Q}_t^{N_t}(\rho(0))$. Consequently, if $\mathcal{Q}_t^{N_t}(\rho(0))$ is equal or close to the target final state, then the resulting measurement statistics are equal or close as well. Measurements on the final state alone cannot reveal whether that density matrix arose from a deterministic unitary evolution or from a randomized channel.

15.6. Sparse Hamiltonian simulation with product formulas

15.7. Operator splitting for time-dependent problems

In Section 14.3 we introduced the time-ordered operator exponential formalism for time-dependent Hamiltonian simulation. The time-ordered operator exponential is also directly related to the Trotter formulæ. This definition of the ordered operator exponential, for an arbitrary matrix, is given below.

Proposition 15.25. *Let $A : [0,t] \to \mathbb{C}^{2^n \times 2^n}$ be a differentiable matrix valued function. We then have that if we define $\mathcal{T}[e^{\int_0^t A(s)\,\mathrm{d}s}]$ to be the solution to the operator valued differential equation*

$$\partial_t \mathcal{T}[e^{\int_0^t A(s)\,\mathrm{d}s}] = A(t)\mathcal{T}[e^{\int_0^t A(s)\,\mathrm{d}s}] \quad \textit{subject to} \quad \mathcal{T}[e^{\int_0^t A(s)\,\mathrm{d}s}]\Big|_{t=0} = I \tag{15.153}$$

$$\mathcal{T}[e^{\int_0^t A(s)\,\mathrm{d}s}] = \lim_{r\to\infty} \prod_{k=0}^{r-1} e^{A(kt/r)t/r}. \tag{15.154}$$

Proof. Let $U(t+\delta,t) = \mathcal{T}[e^{\int_t^{t+\delta} A(s)\,\mathrm{d}s}]$. We then have by the fact that the ordered operator is the solution to a first order homogeneous differential equation with differential operator $A(s)$ we can write

$$\frac{\partial}{\partial\delta}U(t+\delta,t) = A(t+\delta)U(t+\delta,t) = A(t)U(t+\delta,t) + \mathcal{O}(\max_s \|A'(s)\| e^{\max_s \|A\|\delta}\delta). \tag{15.155}$$

We can see from this that this Taylor expanded time-evolution operator is, up to errors that are first order in δ, identical to the solution to the time-independent differential equation. Specifically, the solution is of the form

$$U(t+\delta,t) = e^{A(t)\delta} + \mathcal{O}(\max_s \|A'(s)\| e^{\max_s \|A(s)\|\delta}\delta^2) \tag{15.156}$$

Thus we have that

$$\begin{aligned} \prod_{k=0}^{r-1} U((k+1)t/r, kt/r) &= \prod_{k=0}^{r-1} (e^{A(kt/r)t/r} + \mathcal{O}(\max_s \|A'(s)\| e^{\max_s \|A(s)\|t/r} t^2/r^2)) \\ &= \prod_{k=0}^{r-1} (e^{A(kt/r)t/r}) + \mathcal{O}(\max_s \|A'(s)\| e^{\max_s \|A(s)\|t} t^2/r) \end{aligned} \tag{15.157}$$

Given that we have assumed that $A(s)$ is differentiable, it is also bounded on the interval. Thus as $r \to \infty$ the error in the Taylor series goes to zero. □

This naturally leads to a first-order Trotter-based simulation method for time-dependent Hamiltonians. Further, higher-order variants are also known to exist that require a smaller value of r to achieve a given error tolerance given that $A(s)$ is differentiable many times and is anti-Hermitian (i.e. $A(s) = -iH(s)$ for Hermitian $H(s)$).

Higher-order formulas are more formidable to construct for ordered operator exponentials because of the fact that the Hamiltonian changes with time. This in turn means that any formula that we choose needs to properly take into account not just the commutation structure of the Hamiltonian terms with each other, but also each term's commutation structure with itself. The key tool that is used again and again when analyzing Trotter-Suzuki formulas is the fundamental theorem of Calculus. Specifically, this tool is useful because it generalizes Taylor's theorem and allows us to estimate the error without losing the commutator structure of the error terms. As a specific example of how integration by parts can be useful, consider the following

$$\begin{aligned} e^{iAt} - e^{iBt} &= it \int_0^1 \frac{\partial}{\partial s} e^{i(As+B(1-s))t} ds \\ &= \int_0^1 \int_0^1 e^{i(As+B(1-s))tu}(A-B)e^{-i(As+B(1-s))tu} du \; e^{i(As+B(1-s))t} ds, \end{aligned} \tag{15.158}$$

using Duhamel's formula for the derivative of the exponential because, recall, that the chain rule of differentiation does not hold for matrix calculus unless the derivative of the exponent commutes with the exponential. This reveals not only the difference between two operators, but also the commutator structure of the solution because of the fact that

$$\begin{aligned} e^{i(As+B(1-s))tu}(A-B)e^{-i(As+B(1-s))tu} &= (A-B) \\ +it[As+B(1-s), A-B] - \frac{t^2}{2!}[As+B(1-s), [As+B(1-s), A-B]] + \cdots \end{aligned} \tag{15.159}$$

Higher order generalizations of this formula can be found if we assume that the Hamiltonian is at least twice differentiable. This may be anticipated because if the Hamiltonian is sufficiently smooth then it is easy to see from the midpoint rule that we have that $\int_0^t H(s)ds = H(t/2)t + O(t^3)$. Thus we expect that if we just perform a Trotter decomposition with the Hamiltonian evaluated at the midpoint of the step then the error should be third order rather than the second order errors seen above. We show this below for the case where $A(t) = -iH(t)$ where $H(t)$ is a Hermitian operator valued function in a form that can be used directly in a Trotter decomposition [WHW+15].

Proposition 15.26. *Let $H : [0,t] \to \mathbb{C}^{2^n \times 2^n}$ be a twice-differentiable Hermitian matrix valued function then*

$$\|\mathcal{T} e^{-i\int_0^t H(u)\,\mathrm{d}u} - e^{-iH(t/2)t}\| \leq \frac{\|[H(t/2), \dot{H}(t/2)]\|t^3}{12} + \frac{\max_s \|\ddot{H}(s)\|t^3}{24}. \tag{15.160}$$

Proof. Our proof follows by using a common strategy that underlies Trotter formula analysis: the fundamental theorem of calculus. Specifically, we have that $H(u) = \int_{t/2}^u \frac{\partial}{\partial v} H(v)dv + H(t/2)$. Then by applying this trick again to remove the existing integral, we find that under the assumption that the Hamiltonian is at least twice differentiable

$$H(u) = H(t/2) + (u - t/2)\dot{H}(t/2) + \int_{t/2}^u (u-s)\ddot{H}(s)ds. \tag{15.161}$$

As a result we have that the time-evolution operator can be expressed as

$$\mathcal{T}e^{-i\int_0^t H(u)du} = \mathcal{T}e^{-i\int_0^t \left(H(t/2)+(u-t/2)\dot{H}(t/2)+\int_{t/2}^u (u-s)\ddot{H}(s)ds\right)du} \tag{15.162}$$

We then have that the error that is incurred by dropping the remaining integral term in $H(u)$ can be again understood by a clever application of the fundamental theorem of calculus. Specifically, let

$$H(u,v) = H(t/2) + (u-t/2)\dot{H}(t/2) + v\Delta(u). \tag{15.163}$$

for $\Delta(u) = \int_{t/2}^u (u-s)\ddot{H}(s)ds$. We then have that

$$\int_0^1 \frac{\partial}{\partial v}\mathcal{T}e^{-i\int_0^t H(u,v)du}dv = \mathcal{T}e^{-i\int_0^t H(u)du} - \mathcal{T}e^{-i\int_0^t \left(H(t/2)+(u-t/2)\dot{H}(t/2)\right)}. \tag{15.164}$$

Then using the definition of the ordered operator exponential, we see that for a differentiable $H(u,v)$

$$\frac{\partial}{\partial v}\mathcal{T}e^{-i\int_0^t H(u,v)du} = \frac{\partial}{\partial v}\lim_{r\to\infty}\prod_{j=0}^{r-1} e^{-iH(jt/r,v)t/r}. \tag{15.165}$$

Using the product rule, which applies for matrix calculus (although the product rule is another matter), we find that

$$\begin{aligned}
\frac{\partial}{\partial v}\lim_{r\to\infty}\prod_{j=0}^{r-1} e^{-iH(jt/r,v)t/r} &= \lim_{r\to\infty}\sum_{p=0}^{r-1}\left(\prod_{j=p+1}^{r-1} e^{-iH(jt/r,v)t/r}\right)(-i\Delta(pt/r)t/r)\left(\prod_{j=0}^{p} e^{-iH(jt/r,v)t/r}\right) \\
&= \int_0^t \left(\mathcal{T}e^{-i\int_u^t H(w,v)dw}\right)(-i\Delta(u))\left(\mathcal{T}e^{-i\int_0^u H(w,v)dw}\right)du. \qquad (15.166)
\end{aligned}$$

Thus from the triangle inequality

$$\begin{aligned}
\left\|\mathcal{T}e^{-i\int_0^t H(u)du} - \mathcal{T}e^{-i\int_0^t \left(H(t/2)+(u-t/2)\dot{H}(t/2)\right)du}\right\| &\leq \int_0^t \|\Delta(u)\|\,du \leq \frac{\max_s \|\ddot{H}(s)\|}{2}\int_0^t (u-t/2)^2 du \\
&\leq \frac{\max_s \|\ddot{H}(s)\| t^3}{24}. \qquad (15.167)
\end{aligned}$$

Next let us define

$$\dot{H}_u(t/2) := e^{-i(t/2-u)H(t/2)}\dot{H}(t/2)e^{i(t/2-u)H(t/2)} \tag{15.168}$$

and analyze the operator exponential by transforming into an interaction frame:

$$\mathcal{T}e^{-i\int_0^t (H(t/2)+(u-t/2)\dot{H}(t/2))du} = e^{-iH(t/2)t/2}\left(\mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}_u(t/2)du}\right)e^{-iH(t/2)t/2} \tag{15.169}$$

We then have by the unitary invariance of the operator norm

$$\|\mathcal{T}e^{-i\int_0^t (H(t/2)+(u-t/2)\dot{H}(t/2))du} - e^{-iH(t/2)t}\| = \|\mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}_u(t/2)du} - \mathcal{I}\| \tag{15.170}$$

Next using the fact that $\int_0^t (u-t/2)du = 0$ and the fact that $[(u-t/2)\dot{H}(t/2), (u'-t/2)\dot{H}(t/2)] = 0$ for all u, u' we can write

$$\mathcal{I} = e^{-i\int_0^t (u-t/2)\dot{H}(t/2)du} = \mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}(t/2)du}. \tag{15.171}$$

It then follows that

$$\|\mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}_u(t/2)du} - \mathcal{I}\| = \|\mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}_u(t/2)du} - \mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}(t/2)du}\| \tag{15.172}$$

We then have that

$$\|\mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}_u(t/2)du} - \mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}(t/2)du}\| \leq \int_0^t |u-t/2|\|\dot{H}_u(t/2) - \dot{H}(t/2)\|du \tag{15.173}$$

We can then again use the fundamental theorem of calculus to rewrite the difference between the two operators via

$$\begin{aligned}\|\dot{H}_u(t/2) - \dot{H}(t/2)\| &= \left\| \int_0^1 \frac{\partial}{\partial x}\left(e^{-i(t/2-u)(1-x)H(t/2)}\dot{H}(t/2)e^{i(t/2-u)(1-x)H(t/2)}\right)dx\right\| \\ &= \left\| \int_0^1 i(t/2-u)\left(e^{-i(t/2-u)(1-x)H(t/2)}(H(t/2)\dot{H}(t/2) - \dot{H}(t/2)H(t/2))e^{i(t/2-u)(1-x)H(t/2)}\right)dx\right\|\end{aligned} \tag{15.174}$$

An application of the triangle inequality yields

$$\|\dot{H}_u(t/2) - \dot{H}(t/2)\| \leq \|[H(t/2), \dot{H}(t/2)]\||u-t/2|. \tag{15.175}$$

Thus substituting this into our expression for the error we then see that

$$\begin{aligned}\|\mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}_u(t/2)du} - \mathcal{T}e^{-i\int_0^t (u-t/2)\dot{H}(t/2)du}\| &\leq \int_0^t (u-t/2)^2\|[H(t/2), \dot{H}(t/2)]\|du \\ &\leq \frac{t^3\|[H(t/2), \dot{H}(t/2)]\|}{12}\end{aligned} \tag{15.176}$$

Therefore it follows that

$$\|\mathcal{T}e^{-i\int_0^t H(u)du} - e^{-iH(t/2)t}\| \leq \frac{\|[H(t/2), \dot{H}(t/2)]\|t^3}{12} + \frac{\max_s \|\ddot{H}(s)\|t^3}{24}. \tag{15.177}$$

□

This result shows that by simply taking the midpoint rule for the evolution, we can build a second-order product formula (because the error is $\mathcal{O}(t^3)$). This naturally leads to an elementary quantum algorithm for simulating time-dependent Hamiltonians as claimed by the following Theorem. Note that in the following theorem, for simplicity, we focus on the case where we simply have a single Hamiltonian term and introduce a subroutine for simplicity that exponentiates the Hamiltonian at any fixed time. Any of the previously discussed time-independent Hamiltonian simulation methods could be used to implement such a subroutine if a concrete cost for a specific time-dependent Hamiltonian is desired.

THEOREM 15.27. *Let $H : \mathbb{R} \to L(\mathbb{C}^{2^n})$ be a time-dependent Hamiltonian. Assume that we have a subroutine, S, that can simulate $e^{-iH(t)\Delta}$ for any t and Δ. There exists a quantum algorithm that can, for any $t > 0$ and $\epsilon > 0$, construct a unitary $V \in L(\mathbb{C}^{2^n})$ such that $\|V - \mathcal{T}e^{-i\int_0^t H(s)ds}\| \leq \epsilon$ using a number of queries to S, or equivalently number of matrix exponentials, that are bounded above*

$$N_{\text{query}} \leq \frac{t^{3/2}\sqrt{2\max_s \|[H(s), \dot{H}(s)]\| + \max_s \|\ddot{H}(s)\|}}{\sqrt{24\epsilon}}$$

PROOF. If we split our evolution into N_{query} segments then we can approximate the time-evolution operator by

$$\mathcal{T}e^{-i\int_0^t H(u)du} \approx \prod_{j=0}^{N_{\text{query}}-1} e^{-iH((j+1/2)t/N_{\text{query}})t/N_{\text{query}}}. \tag{15.178}$$

Then each exponential in the approximation can be simulated using a single query to S. Thus the entire algorithm simply requires N_{query} applications of S. Next note that by definition we can also write

$$\mathcal{T}e^{-i\int_0^t H(u)du} = \prod_{j=0}^{N_{\text{query}}-1} \mathcal{T}e^{-i\int_{jt/N_{\text{query}}}^{(j+1)t/N_{\text{query}}} H(u)du} \tag{15.179}$$

and thus by Proposition 3.21 and Proposition 15.26 the error in the approximation can be expressed as

$$\begin{aligned} &\left\| \prod_{j=0}^{N_{\text{query}}-1} \mathcal{T}e^{-i\int_{jt/N_{\text{query}}}^{(j+1)t/N_{\text{query}}} H(u)du} - \prod_{j=0}^{N_{\text{query}}-1} e^{-iH((j+1/2)t/N_{\text{query}})t/N_{\text{query}}} \right\| \\ &\leq \left(\frac{\max_s \|[H(s), \dot{H}(s)]\|}{12} + \frac{\max_s \|\ddot{H}(s)\|}{24} \right) \left(\frac{t^3}{N_{\text{query}}^2} \right) = \epsilon \end{aligned} \tag{15.180}$$

due to the sub-additivity of unitary errors. The result then follows by solving for N_{query}. □

This shows very similar scaling to what we saw for the second order (symmetric) Trotter formula. In a sense, the use of the midpoint as the approximation is the temporal analogue of the symmetric Trotter formula and removes the contribution of the $\mathcal{O}(t^2)$ terms that depend on $\dot{H}(s)$ from the error. It is also perhaps unsurprising that such a formula can be used as the base to construct high-order versions of the time-dependent Trotter formula as is explicitly studied in [WBHS10]; however, for brevity we omit the discussion of that construction.

Perhaps the most interesting, and seldom remarked upon, aspect of this complexity is that the error in the simulation scales with the commutator of the Hamiltonian and its derivative. This means that the cost of simulation for rapidly varying Hamiltonians may be modest using product formulas in cases where the commutator of the Hamiltonian and its derivative is small. In contrast, the Truncated Dyson series approach (the reigning champion for simulation of time-dependent Hamiltonians at the time of publication) does not have this property and the cost depends explicitly on the coefficient norm of the LCU decomposition (which upper bounds the norm of the Hamiltonian). This shows that product formula approximations can outperform other known simulation methods in cases where the Hamiltonian approximately commutes with itself (given the second derivative term is negligible). This in turn illustrates again that, while Trotter formulas may fall short of optimal asymptotic query complexity, it can often provide the best known simulation costs for spatially local Hamitlonians.

15.8. Lieb-Robinson Bounds for Local Hamiltonians

15.9. Phase Estimation and Operator Splitting

Notes and further reading

The high-order operator splitting methods discussed in this chapter are constructed by composing lower-order methods. Such composition techniques were extensively developed in the 1990s [Suz90, Yos90, McL95], and we refer readers to the classical textbook [HLW06] for a comprehensive treatment of composition methods in the context of geometric numerical integration. The time-independent Schrödinger equation offers a concrete setting for analyzing the error behavior of operator splitting methods, both in low- and high-order regimes [JL00, Tha08, DT10]. For instance, [JL00] first observed that in some quantum settings, the actual error scales only with the size of commutators (with the vector norm scaling), leading to error bounds that are significantly smaller than one might expect from standard order analysis.

In the context of quantum algorithms, these ideas have been extended and refined to address bounded operators such as spin systems, as well as unbounded operators like Schrödinger operators in first quantization. A detailed and increasingly nuanced understanding of error behavior in Hamiltonian simulation has since emerged as a highly active area of research. Theoretical developments have led to continued improvements in both asymptotic and practical error bounds [WBHS10, BCG14, BCK15, CMN$^+$18, COS19, Low19, CS19, CST$^+$21, CHKT21, ŞS20, AFL21, SBW$^+$21, AFL22, RWW24, HHB$^+$25].

Beyond the Trotter-Suzuki family of composition methods, a wide variety of other approaches have been developed for constructing high-order operator splitting schemes for Hamiltonian simulation. These include Magnus expansion techniques [BCOR09, CZA24, FLS25], multiproduct formulas [LKW19, AAT24], and other generalizations, each with their own trade-offs in terms of cost, accuracy, and suitability for quantum implementation.

CHAPTER 16

Quantum phase estimation and Fourier transforms

Quantum phase estimation is one of the most versatile and powerful tools in the arsenal of the quantum algorithm designer. It is the workhorse behind Shor's famous factorization algorithm, the Harrow Hassidim and Lloyd algorithm for solving linear systems and is the basis behind the majority of chemistry applications for quantum simulation. The reason for this is that phase estimation provides a way to learn the eigenvalues of a unitary, and project onto the eigenvectors, using a number of operations that scales poly-logarithmically with the dimension of the Hilbert space that the unitary acts on. In contrast, standard classical algorithms for achieving this such as the Lancosz algorithm or Gaussian ellimination scale polynomially with the Hilbert space dimension. An informal statement of the phase estimation problem is given below.

Problem 16.1. *Let $U \in U(N)$ be a unitary matrix and let ϵ be an error tolerance, and let $U|\psi_i\rangle = e^{2\pi\phi_i}|\psi_i\rangle$ where $0 \leq \phi_i < 1$ further assume that a state is without loss of generality of the form $|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle$. The goal of phase estimation is to provide an encoding of a randomly sampled ϕ_i in a quantum or classical register within error ϵ such that each ϕ_i is provided with probability. Optionally, some phase estimation problems require that we project onto $|\psi_j\rangle$ with probability approximately equal to $|\alpha_j|^2$.*

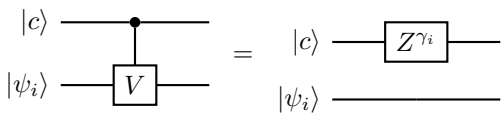
We see above that quantum phase estimation involves two closely related goals. One is eigenvalue estimation, where the output is a classical approximation to the phase. The other is eigenstate preparation, where the algorithm also filters the input toward a spectral component. We begin with the quantum Fourier transform because it gives the cleanest mechanism for turning phase information into computational-basis data. Standard quantum phase estimation can then be expressed as a coherent spectral readout procedure that serves both goals at once. This in turn leads to the analysis of finite precision and imperfect input states, to coherent eigenvalue transformation, and to iterative single-ancilla methods when only a classical estimate is needed. The same viewpoint also clarifies why phase estimation can achieve Heisenberg-limited scaling and how amplitude estimation fits into this framework.

Quantum phase estimation accomplishes this goal by using quantum gates to transform the eigenvalues of a unitary matrix into bit flips. The operation that achieves this is known as the quantum Fourier transform, which is a generalization of the Hadamard transform. The eigenvalues are then fed into the quantum Fourier transform through a cunning application of the phase kickback effect.

The simplest version of phase estimation can be illustrated as follows. Let us assume that V is a unitary and Hermitian matrix. This means that for any eigenvector $|\psi_i\rangle$ we have that $V|\psi_i\rangle = (-1)^{\gamma_i}|\psi_i\rangle$ for simplicity. The phase kickback effect then shows us that by controlling the unitary, the eigenvalue γ_i can be kicked back onto the phase onto a control qubit as shown in the

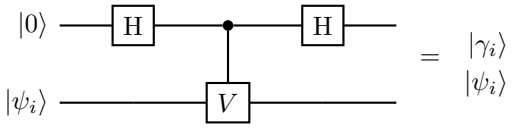
following diagram.

(16.1)



We can then find this eigenvalue γ_i by applying Hadamard transforms through the identity $HZH = X$, which implies that

(16.2)



Thus by measuring the top-most qubit, we can learn the eigenvalue. This observation has been widely used throughout the algorithms seen so far including the Deutsch Josza algorithm, and also appears in measuring errors in quantum error correcting codes as well as in applying a projector using LCU.

While the quantum application of this idea is relatively new, the roots of the phase estimation algorithm run deep. The idea was essentially pioneered by Jules Jamin in 1856, where the ideas were subsequently developed into a field that we now know as interferometry which allows precise estimation of phase differences to be estimated via one (of many possible) wave interference experiment. These ideas have profoundly changed radio astronomy (where interference between radio waves are used to perform high-sensitivity experiments).

The quantum phase estimation method works in precisely the same way as interferometry, as we see in Figure 16.1. The state of a control qubit defines a path for the quantum system to evolve through, such that only states of the form $|1\rangle|\psi\rangle$ receive a phase. The final Hadamard gate then recombines the two signals and then we will see that the eigenphase can then be inferred from the probability of measuring zero or one after the recombination. Note however, that the eigenstate projection property is unique to quantum phase estimation and does not have a direct analogue in interferometry.

This chapter is laid out as follows. First we discuss the quantum Fourier transform and show how it generalizes the Hadamard gate in generalized Pauli matrices. We then apply these techniques to build Fourier-based quantum phase estimation methods. We discuss the Heisenberg limit next, which places lower bounds on the cost of performing phase estimation and then discuss Iterative methods which allow statistical inference to be used in place of Fourier transforms to estimate eigenvalues.

16.1. Quantum Fourier transform

The Fourier transform is ubiquitous in scientific computing, and the fast Fourier transform (FFT) is a backbone for many fast classical algorithms. The quantum Fourier transform (QFT) plays a similar role in quantum algorithms, appearing in phase estimation, Shor's algorithm, and related constructions such as the fast Fermionic Fourier transform (FFFT) [BWM+18]. Beyond serving as a subroutine, it provides a concrete mechanism for converting information stored in phase into information stored in the computational basis, and it leads naturally to generalized Pauli matrices on multi-qubit systems. For these reasons, a clear understanding of the quantum Fourier transform is useful throughout quantum algorithms.

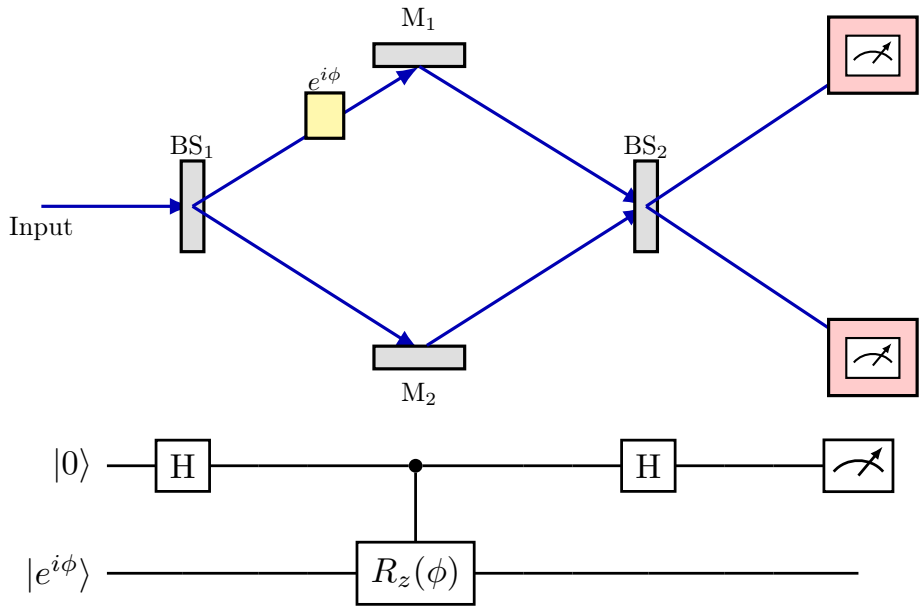


FIGURE 16.1. (Above) Diagram showing an optical interferometer that describes light bouncing through a 50/50 beamsplitters such that light going through the top path experiences a phase of $e^{i\phi}$ relative to the path on the bottom and then bounces off a mirror (M_1, M_2) before the light interferes with itself at the second 50/50 beam splitter before the reflected and transmitted beams are measured where the intensity of light in the top-most branch measured is proportional to the probability of measuring 0 in an experiment whereas the bottom-most intensity corresponds to the probability of measuring 1 in a Bernoulli experiment. (Below) Quantum circuit for a quantum phase estimation experiment that is mathematically equivalent to the above interferometer wherein the first qubit sets the analogue of the top and bottom paths in the interferometer and the controlled R_z gate plays the analogue of the phase delay in the interferometer.

For any j in the computational basis of an n-qubit system with $N = 2^n$, the (discrete) forward Fourier transform is defined as follows:

$$U_{\mathrm{FT}} |j\rangle = \frac{1}{\sqrt{N}} \sum_{k \in [N]} e^{i2\pi \frac{kj}{N}} |k\rangle . \tag{16.3}$$

The transformation is also often abbreviated in terms of the root of unity $\omega = e^{i2\pi/N}$ as

$$U_{\mathrm{FT}} |j\rangle = \frac{1}{\sqrt{N}} \sum_{k \in [N]} \omega^{kj} |k\rangle . \tag{16.4}$$

In particular

$$U_{\mathrm{FT}} |0^n\rangle = \frac{1}{\sqrt{N}} \sum_{k \in [N]} |k\rangle = \mathrm{H}^{\otimes n} |0^n\rangle . \tag{16.5}$$

The (discrete) inverse Fourier transform is

$$U_{\mathrm{FT}}^{\dagger}\left|j\right\rangle = \frac{1}{\sqrt{N}} \sum_{k\in[N]} e^{-i2\pi \frac{kj}{N}} \left|k\right\rangle . \tag{16.6}$$

Using the binary representation of integers

$$k = (k_{n-1}\cdots k_0.), \quad j = (j_{n-1}\cdots j_0.) \tag{16.7}$$

we have

$$\begin{aligned}\frac{kj}{N} =& k_0\frac{j}{2^n} + k_1\frac{j}{2^{n-1}} + \cdots + k_{n-1}\frac{j}{2} \\ =& k_0(.j_{n-1}\cdots j_0) + k_1(j_{n-1}.j_{n-2}\cdots j_0) + \cdots + k_{n-1}(j_{n-1}\cdots j_1.j_0).\end{aligned}$$

Since $e^{i2\pi x}$ depends only on the fractional part of x, we may discard the integer parts in the binary expansions above. Therefore the exponential can be written as

$$e^{i2\pi\frac{kj}{N}} = e^{i2\pi k_0(.j_{n-1}\cdots j_0)} e^{i2\pi k_1(.j_{n-2}\cdots j_0)} \cdots e^{i2\pi k_{n-1}(.j_0)}. \tag{16.8}$$

A standard calculation gives the following factorized form:

(16.9)

$$\begin{aligned}U_{\mathrm{FT}}\left|j_{n-1}\cdots j_0\right\rangle =& \frac{1}{\sqrt{2^n}} \sum_{k_{n-1},\ldots,k_0} e^{i2\pi k_0(.j_{n-1}\cdots j_0)} e^{i2\pi k_1(.j_{n-2}\cdots j_0)} \cdots e^{i2\pi k_{n-1}(.j_0)} \left|k_{n-1}\cdots k_0\right\rangle \\ =& \frac{1}{\sqrt{2^n}} \left(\sum_{k_{n-1}} e^{i2\pi k_{n-1}(.j_0)} \left|k_{n-1}\right\rangle\right) \otimes \left(\sum_{k_{n-2}} e^{i2\pi k_{n-2}(.j_1 j_0)} \left|k_{n-2}\right\rangle\right) \\ & \otimes \cdots \otimes \left(\sum_{k_0} e^{i2\pi k_0(.j_{n-1}\cdots j_0)} \left|k_0\right\rangle\right) \\ =& \frac{1}{\sqrt{2^n}} \left(\left|0\right\rangle + e^{i2\pi(.j_0)}\left|1\right\rangle\right) \otimes \left(\left|0\right\rangle + e^{i2\pi(.j_1 j_0)}\left|1\right\rangle\right) \otimes \cdots \otimes \left(\left|0\right\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)}\left|1\right\rangle\right).\end{aligned}$$

Eq. (16.9) involves a series of controlled rotations of the form

$$\left|0\right\rangle \to \frac{1}{\sqrt{2}} \left(\left|0\right\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)}\left|1\right\rangle\right). \tag{16.10}$$

Before describing the full QFT circuit, let us first work out a circuit for implementing this controlled rotation. We use the relation

$$e^{i2\pi(.j_{n-1}\cdots j_0)} = e^{i2\pi(.j_{n-1})} e^{i2\pi(.0 j_{n-2})} \cdots e^{i2\pi(.0\cdots 0 j_0)}. \tag{16.11}$$

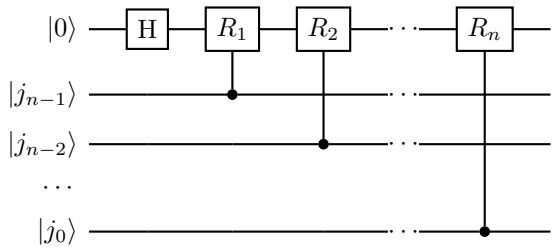
Example 16.2 (Implementation of controlled rotation)**.** Consider the implementation of

$$\left|0\right\rangle\left|j\right\rangle \to \frac{1}{\sqrt{2}} \left(\left|0\right\rangle + e^{i2\pi(.j_{n-1}\cdots j_0)}\left|1\right\rangle\right)\left|j\right\rangle, \tag{16.12}$$

Let us define

$$R_j = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2^{j-1}} \end{pmatrix}. \tag{16.13}$$

In particular, $R_1 = Z$. The quantum circuit is



◇

The implementation of QFT follows the same principle, but **does not** require a separate signal qubit to store the phase information. Let us see a few examples.

When $n = 1$, we need to implement

$$|j_0\rangle \to \frac{1}{\sqrt{2}}\left(|0\rangle + e^{i2\pi(.j_0)}|1\rangle\right). \tag{16.14}$$

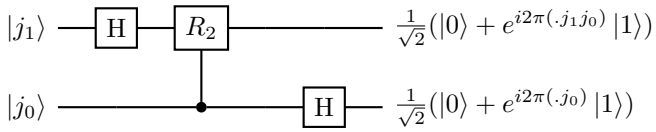
This is the Hadamard gate:

$$|j_0\rangle \to \mathrm{H}|j_0\rangle. \tag{16.15}$$

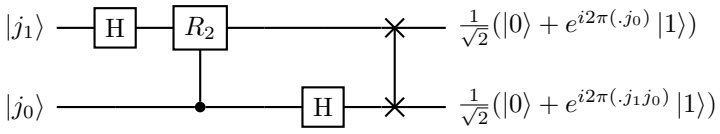
When $n = 2$, we need to implement

$$|j\rangle \to \frac{1}{\sqrt{2^2}}\left(|0\rangle + e^{i2\pi(.j_0)}|1\rangle\right) \otimes \left(|0\rangle + e^{i2\pi(.j_1 j_0)}|1\rangle\right). \tag{16.16}$$

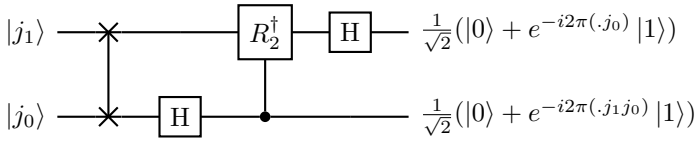
This can be implemented using the following circuit:



Comparing the result with that in Eq. (16.16), we find that the ordering of the qubits is reversed. To recover the desired result in QFT, we can apply a SWAP gate to the outcome, i.e.,



In order to implement the inverse Fourier transform, we only need to apply the Hermitian conjugate as



Similarly one can construct the circuit for U_{FT} and its inverse for $n = 3$.

In general, the QFT circuit is given by Fig. 16.2. Compare the circuit in Fig. 16.2 with Eq. (16.9), we find again that the ordering is reversed in the output. To restore the correct order as defined in QFT, we can use $\mathcal{O}(n/2)$ swap operations. The total gate complexity of QFT is $\mathcal{O}(n^2)$. We summarize this in the following theorem.

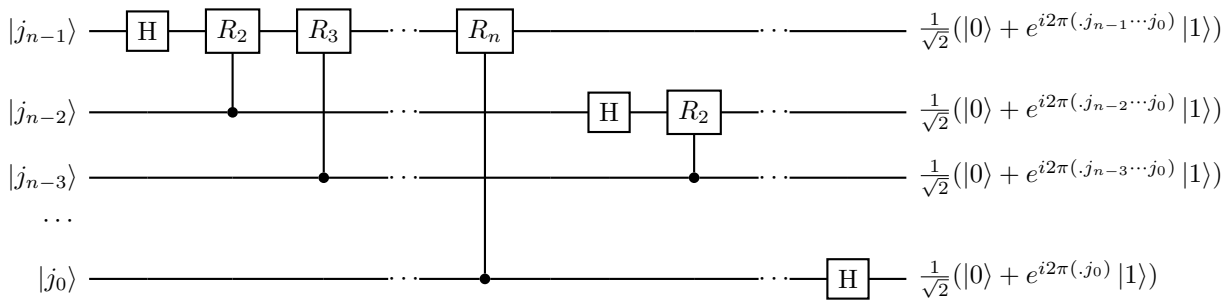


FIGURE 16.2. Circuit diagram for quantum Fourier transform (before applying swap operations).

THEOREM 16.3. *Let $U_{\mathrm{FT}} \in L(\mathbb{C}^{2^n})$ be the n-qubit quantum Fourier transform. There exists a quantum circuit of length $\mathcal{O}(n^2)$ containing gates drawn from the library $\mathrm{H}, \mathrm{CNOT}, R_z(\theta)$ that can precisely implement U_{FT}.*

Exercise 16.1. For a 3 qubit system, explicitly construct the circuit for U_{FT} and its inverse.

Exercise 16.2. For a n-qubit system, write down the quantum circuit for the swap operation used in QFT.

16.2. Example: Generalized Pauli matrices

As we saw above, the quantum Fourier transform generalizes the Hadamard transform to dimensions greater than 2. The Hadamard gate is an element of the Clifford group, and hence it maps the single-qubit Pauli matrices to themselves under conjugation. For $n \geq 2$, the quantum Fourier transform is not a Clifford unitary, so it does not stabilize the n-qubit Pauli group. Nevertheless, there is a natural family of Pauli-like matrices that is stabilized by conjugation with the quantum Fourier transform. These are Sylvester's **generalized Pauli matrices** (also known as **Weyl-Heisenberg matrices**), which will also be useful later in the discussion of phase estimation and arithmetic.

Sylvester's generalized Pauli matrices are defined as follows.

Definition 16.4 (Sylvester's generalized Pauli matrices)**.** *Let $\mathcal{Z}_n \in L(\mathbb{C}^{2^n})$ be the n-qubit generalized Z matrix, defined by*

$$\mathcal{Z}_n := \sum_{j=0}^{2^n-1} e^{i2\pi j/2^n} |j\rangle\langle j|. \tag{16.17}$$

and let $\mathcal{X}_n \in L(\mathbb{C}^{2^n})$ be the n-qubit generalized X matrix, defined by

$$\mathcal{X}_n := U_{\mathrm{FT}}^\dagger \mathcal{Z}_n U_{\mathrm{FT}}. \tag{16.18}$$

Up to global phases, the 2^{2n} elements of the n-qubit generalized Pauli group are

$$P_{k,j} = \mathcal{X}_n^k \mathcal{Z}_n^j = \sum_{\ell=0}^{2^n-1} \omega^{j\ell} |\ell + k\rangle\langle\ell|, \tag{16.19}$$

where the addition $\ell + k$ is taken modulo 2^n.

This shows that $\mathcal{X}_n$ plays the role of a bit-flip (Pauli-X) matrix in this setting: it is the Fourier transform of the diagonal generalized Pauli-Z matrix. Although the generalized Pauli group has 2^{2n} elements, the matrices have enough structure that we can often manipulate them without expanding them entrywise.

Example 16.5. As a simple example of finding an explicit expression for the generalized Pauli matrices, let us verify the property that

$$\mathcal{X}_n = \sum_{\ell=0}^{2^n-1} |\ell + 1\rangle\langle\ell|, \tag{16.20}$$

where $\ell + 1$ is understood modulo 2^n. Using the definition of U_{FT} and $\mathcal{Z}_n$ we compute

$$\begin{aligned} U_{\mathrm{FT}}^\dagger \mathcal{Z}_n U_{\mathrm{FT}} &= \frac{1}{2^n} \sum_{j,m=0}^{2^n-1} \left(\sum_{\ell=0}^{2^n-1} e^{i2\pi\ell(m-j+1)/2^n} \right) |j\rangle\langle m| \\ &= \sum_{m=0}^{2^n-1} |m+1\rangle\langle m|, \end{aligned} \tag{16.21}$$

where we used $\sum_{\ell=0}^{2^n-1} e^{i2\pi\ell t/2^n} = 2^n$ if $t \equiv 0 \pmod{2^n}$ and 0 otherwise. ◇

This example illustrates a basic property of the Fourier transform: it turns phase rotations into shifts in the computational basis. This observation leads to an in-place adder construction known as the Draper adder.

Corollary 16.6 (Draper adder)**.** *There exists a quantum algorithm that implements a unitary n-qubit modular adder that maps, for any n-bit integers p, q, $|p\rangle |q\rangle \mapsto |p\rangle |q + p \mod 2^n\rangle$. This algorithm uses no ancillary qubits and requires $\mathcal{O}(n^2)$ two-qubit operations.*

Proof. Write $a = \sum_{r=0}^{n-1} a_r 2^r$ with $a_r \in \{0, 1\}$. Then

$$\begin{aligned} |a\rangle |b\rangle &\to |a\rangle \ \mathcal{X}_n^a |b\rangle \\ &= |a\rangle \ \mathcal{X}_n^{a_0 2^0} \cdots \mathcal{X}_n^{a_{n-1} 2^{n-1}} |b\rangle \\ &= |a\rangle \ U_{\mathrm{FT}}^\dagger \mathcal{Z}_n^{a_0 2^0} \cdots \mathcal{Z}_n^{a_{n-1} 2^{n-1}} U_{\mathrm{FT}} |b\rangle . \end{aligned} \tag{16.22}$$

Each $\mathcal{Z}_n$ can be implemented using a sequence of n single-qubit phase rotations. Specifically, using the same binary expansion used above in the Fourier transform,

$$\mathcal{Z}_n = \bigotimes_{m=0}^{n-1} e^{i2\pi 2^{m-n} |1\rangle\langle 1|}. \tag{16.23}$$

In turn for any integer power $p \geq 0$ we then have that

$$\mathcal{Z}_n^p = \bigotimes_{m=0}^{n-1} e^{i2\pi p 2^{m-n} |1\rangle\langle 1|}, \tag{16.24}$$

which requires only n single-qubit rotations. In the adder construction, these rotations are controlled by the bits of a, and hence are implemented as controlled phase rotations between the registers. There are $\mathcal{O}(n^2)$ such controlled rotations, each realizable using $\mathcal{O}(1)$ CNOT gates and single-qubit R_z gates, so the overall two-qubit gate complexity is $\mathcal{O}(n^2)$.

As noted in Theorem 16.3, the n-qubit quantum Fourier transform can be implemented using $\mathcal{O}(n^2)$ two-qubit gates. Thus the overall two-qubit gate complexity is $\mathcal{O}(n^2) + \mathcal{O}(n^2) = \mathcal{O}(n^2)$. Finally, since neither the quantum Fourier transform nor the controlled rotations require ancillary qubits, the entire adder algorithm can be implemented in place. □

We see from the above corollary that, in this setting, the identity $Z = \mathrm{H}\,X\,\mathrm{H}$ generalizes to a construction of adders that do not require additional qubits, unlike traditional reversible circuits such as the carry ripple adder. This example will set the stage in the following section, where we use similar reasoning to show that the quantum Fourier transform can be used to learn the eigenvalues of a unitary, even when those eigenvalues are not of the form $e^{i2\pi j/2^n}$ for $j \in \mathbb{Z}_{2^n}$.

The generalized Pauli matrices further satisfy similar commutation relations to ordinary Pauli matrices that reduce to the familiar anti-commutation relation when $n = 1$:

$$\mathcal{X}_n \mathcal{Z}_n = e^{-i2\pi/2^n} \mathcal{Z}_n \mathcal{X}_n. \tag{16.25}$$

Further, these generalized Pauli matrices form a complete orthonormal basis with respect to the Hilbert-Schmidt inner product: $\langle P_{j,k}, P_{\ell,m} \rangle = 2^{-n} \operatorname{Tr}[P_{j,k}^\dagger P_{\ell,m}] = \delta_{(j,k),(\ell,m)}$. Consequently, any matrix M can be decomposed as $M = \sum_{j,k} P_{j,k} \langle P_{j,k}, M \rangle$.

16.3. Quantum phase estimation

Let U be a unitary, and let $|\psi\rangle$ be an eigenvector, i.e.,

$$U|\psi\rangle = e^{i2\pi\varphi} |\psi\rangle, \quad \varphi \in [0, 1). \tag{16.26}$$

We would like to estimate the phase φ to a prescribed precision. Using a classical computer, one could in principle recover φ from the element-wise quotient $U|\psi\rangle \oslash |\psi\rangle$, where $\oslash$ denotes element-wise division. Specifically, if $\langle j|\psi\rangle \neq 0$ for some computational-basis index j, then

$$\langle j|U|\psi\rangle \,/\, \langle j|\psi\rangle = e^{i2\pi\varphi}. \tag{16.27}$$

Such an element-wise division operation is not available as an efficient quantum subroutine. Even in this idealized setting, we need a different mechanism for converting phase information into data in the computational basis.

More generally, there are two closely related tasks. One is eigenvalue estimation, where the output is a classical approximation to φ. The other is eigenstate preparation, where the algorithm also filters the input, which is usually a linear combination of eigenstates, toward a spectral component.

In this section, we introduce the standard quantum phase estimation algorithm, which is based on the quantum Fourier transform (QFT) and uses d ancilla qubits to store the phase information.

From now on, we assume that $\varphi = 0.j_{d-1} \cdots j_0$ has an exact d-bit representation. From the availability of U^j we can define a controlled unitary operation

$$\mathcal{U} = \sum_{j \in [2^d]} |j\rangle\langle j| \otimes U^j. \tag{16.28}$$

When $d = 1$, $\mathcal{U}$ is simply the controlled U operation. For a general d, it seems that we need to implement all 2^d different U^j. However, this is not necessary. Writing $j = \sum_{i=0}^{d-1} j_i 2^i$ with

$j_i \in \{0,1\}$, we have $U^j = U^{\sum_{i=0}^{d-1} j_i 2^i} = \prod_{i=0}^{d-1} U^{j_i 2^i}$. Therefore, similarly to the operations in QFT,

$$\begin{aligned}
\mathcal{U} &= \sum_{j\in[2^d]} |j\rangle\langle j| \otimes U^j \\
&= \sum_{j_{d-1},\dots,j_0} (|j_{d-1}\rangle\langle j_{d-1}|) \otimes \cdots \otimes (|j_0\rangle\langle j_0|) \otimes \prod_{i=0}^{d-1} U^{j_i 2^i} \\
&= \prod_{i=0}^{d-1}{}' \left(\sum_{j_i} |j_i\rangle\langle j_i| \otimes U^{j_i 2^i} \right) \\
&= \prod_{i=0}^{d-1}{}' \left(|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U^{2^i} \right).
\end{aligned} \tag{16.29}$$

Here the primed product $\prod'$ is a slightly awkward notation: the factors act on different control qubits in the first register, while they are multiplied (i.e., applied sequentially) on the second register. It is in fact much clearer to observe the structure in the quantum circuit in Fig. 16.3.

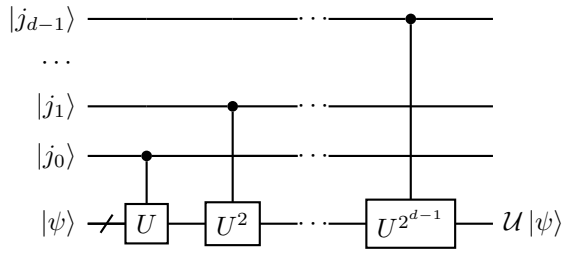


FIGURE 16.3. Circuit for controlled matrix power of U.

Now let the initial state in the ancilla qubits be $|0^d\rangle$. Using $\mathrm{H}^{\otimes d}$ (equivalently, the QFT acting on $|0^d\rangle$) and $\mathcal{U}$, we transform the initial state according to

$$\begin{aligned}
|0^d\rangle|\psi\rangle &\xrightarrow{\mathrm{H}^{\otimes d}\otimes I} \frac{1}{\sqrt{2^d}} \sum_{j\in[2^d]} |j\rangle|\psi\rangle \\
&\xrightarrow{\mathcal{U}} \frac{1}{\sqrt{2^d}} \sum_{j\in[2^d]} |j\rangle U^j|\psi\rangle = \frac{1}{\sqrt{2^d}} \sum_{j\in[2^d]} |j\rangle e^{i2\pi\varphi j}|\psi\rangle \\
&\xrightarrow{U_{\mathrm{FT}}^\dagger\otimes I} \sum_{k'\in[2^d]} \left(\frac{1}{2^d} \sum_{j\in[2^d]} e^{i2\pi j\left(\varphi - \frac{k'}{2^d}\right)} \right) |k'\rangle|\psi\rangle .
\end{aligned} \tag{16.30}$$

Since $\varphi = \frac{k}{2^d}$ for some $k \in [2^d]$, measuring the first register yields the outcome k with certainty, and hence recovers the phase information. Therefore the quantum circuit for QFT-based QPE is given by Fig. 16.4. Here we have used Eq. (16.5). We should note that $U_{\mathrm{FT}}^\dagger$ includes the swapping operations.

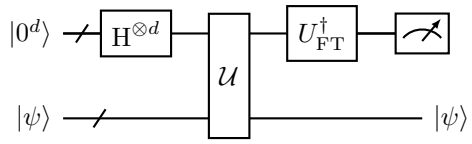


FIGURE 16.4. Quantum circuit for quantum phase estimation using quantum Fourier transform.

Example 16.7 (Hadamard test viewed as QPE)**.** When $d = 1$, note that $U_{\mathrm{FT}}^\dagger = \mathrm{H}$, so the QFT based QPE in Fig. 16.4 is exactly the Hadamard test in Fig. 2.1. Note that φ does not need to be exactly represented by a one bit number! ◇

16.4. Analysis of Fourier-based quantum phase estimation

Assume that U has the eigendecomposition

$$U|\psi_j\rangle = e^{i2\pi\varphi_j}|\psi_j\rangle. \tag{16.31}$$

Without loss of generality we label the eigenphases so that $0 \le \varphi_0 \le \varphi_1 \le \cdots \le \varphi_{N-1} < 1$. To analyze QPE, it is useful to separate the idealizations used above. So far we have assumed that

(1) The initial state $|\psi\rangle$ is an exact eigenstate satisfying $U|\psi\rangle = e^{i2\pi\varphi}|\psi\rangle$.
(2) The unitary U can be implemented exactly.
(3) The eigenphase φ has a d-bit binary representation.

In practical calculations, these conditions generally cannot all be satisfied **exactly**, so we must analyze how each deviation affects the accuracy of QPE.

We first consider condition (2), namely that U can only be implemented approximately. Since $e^{i2\pi x}$ is 1-periodic, phase estimation can only determine a phase modulo 1. It is therefore natural to measure the estimation error using the 1-periodic distance

$$|\theta|_1 \equiv |\theta|_{\bmod 1} := \min\{(\theta \bmod 1), 1 - (\theta \bmod 1)\} \in [0, 1/2]. \tag{16.32}$$

For later use, note that

$$|\sin(\pi\theta)| \ge 2|\theta|, \quad \theta \in [-1/2, 1/2]. \tag{16.33}$$

Then for $\varphi, \varphi' \in [0, 1)$, we have

$$\left|e^{2\pi i\varphi} - e^{2\pi i\varphi'}\right| = 2|\sin(\pi(\varphi - \varphi'))| = 2\sin(\pi|\varphi - \varphi'|_1) \ge 4|\varphi - \varphi'|_1, \tag{16.34}$$

If we only have an approximate implementation of U denoted by $\widetilde{U}$ satisfying

$$\left\|U - \widetilde{U}\right\| \le \epsilon, \tag{16.35}$$

then according to the perturbation theory of unitary matrices in Theorem 7.8, the perturbation of the eigenvalue on the unit circle satisfies $\left|e^{2\pi i\varphi} - e^{2\pi i\varphi'}\right| \le \epsilon$, and the perturbation of the corresponding phase angle is bounded by $\epsilon/4$. Thus we may account for implementation error separately as an additive contribution to the phase-estimation error, and then continue the analysis under the assumption that U is implemented exactly.

We next consider condition (3), namely that φ cannot be represented exactly by a d-bit number. To estimate φ to d bits of precision with high probability, we apply the QPE circuit using $t > d$

ancilla qubits and interpret the measurement outcome k' as the estimator $\widetilde{\varphi}_{k'} = k'/T$. The exact relation between the t and the desired accuracy d will be determined later. Let $T = 2^t$. Similar to Eq. (16.30), we obtain the state

$$\begin{aligned} |0^t\rangle |\psi\rangle &\to \sum_{k' \in [T]} \left(\frac{1}{T} \sum_{j \in [T]} e^{i2\pi j \left(\varphi - \frac{k'}{T}\right)} \right) |k'\rangle |\psi\rangle \\ &= \sum_{k'} \gamma_{k'} |k'\rangle |\psi\rangle . \end{aligned} \tag{16.36}$$

Here

$$\gamma_{k'} = \frac{1}{T} \sum_{j \in [T]} e^{i2\pi j \left(\varphi - \frac{k'}{T}\right)} = \frac{1}{T} \frac{1 - e^{i2\pi T(\varphi - \widetilde{\varphi}_{k'})}}{1 - e^{i2\pi(\varphi - \widetilde{\varphi}_{k'})}}, \quad \widetilde{\varphi}_{k'} = \frac{k'}{T}. \tag{16.37}$$

Therefore if φ has an exact t-bit representation, i.e., $\varphi = \widetilde{\varphi}_{k'_0}$ for some k'_0, then $\gamma_{k'} = \delta_{k',k'_0}$. We recover the previous result that one run of the QPE circuit gives the value φ deterministically.

Now assume that $\varphi \neq \widetilde{\varphi}_{k'}$ for any k'. The probability of measuring the first register and obtaining k' is

$$\mathbb{P}(k') = |\gamma_{k'}|^2 = \frac{1}{T^2} \frac{\sin^2(\pi T(\varphi - \widetilde{\varphi}_{k'}))}{\sin^2(\pi(\varphi - \widetilde{\varphi}_{k'}))} =: F_T(\varphi - \widetilde{\varphi}_{k'}). \tag{16.38}$$

The function

$$F_T(x) = \frac{1}{T^2} \frac{\sin^2(\pi T x)}{\sin^2(\pi x)} . \tag{16.39}$$

is called the **Fejér kernel**.

In terms of the phase, we would like to find k'_0 such that

$$\left|\varphi - \widetilde{\varphi}_{k'_0}\right|_1 < \epsilon. \tag{16.40}$$

Here $\epsilon = 2^{-d} = 2^{t-d}/T$ is the precision parameter. In particular, for any k' we have

$$|\varphi - \widetilde{\varphi}_{k'}|_1 \leq \frac{1}{2}. \tag{16.41}$$

Applying Eq. (16.33) with $\theta = |\varphi - \widetilde{\varphi}_{k'}|_1$, we obtain

$$F_T(\varphi - \widetilde{\varphi}_{k'}) = |\gamma_{k'}|^2 \leq \frac{1}{4T^2 |\varphi - \widetilde{\varphi}_{k'}|_1^2}. \tag{16.42}$$

Let k'_0 be the measurement outcome, which can be viewed as a random variable. The probability of obtaining some $\widetilde{\varphi}_{k'_0}$ that is at least ϵ distance away from φ is

$$\begin{aligned} \mathbb{P}(\left|\varphi - \widetilde{\varphi}_{k'_0}\right|_1 \geq \epsilon) &= \sum_{|\varphi - \widetilde{\varphi}_{k'}|_1 \geq \epsilon} F_T(\varphi - \widetilde{\varphi}_{k'}) \\ &\leq \sum_{|\varphi - \widetilde{\varphi}_{k'}|_1 \geq \epsilon} \frac{1}{4T^2 |\varphi - \widetilde{\varphi}_{k'}|_1^2} \\ &\leq \frac{2}{4T} \int_{\epsilon}^{\infty} \frac{1}{x^2} \, \mathrm{d}x + \frac{2}{4T^2\epsilon^2} = \frac{1}{2T\epsilon} + \frac{1}{2(T\epsilon)^2}. \end{aligned} \tag{16.43}$$

Set $t - d = \lceil \log_2 \delta^{-1} \rceil$, then $T\epsilon = 2^{t-d} \geq \delta^{-1}$. Hence for any $0 < \delta < 1$, the failure probability satisfies

$$\mathbb{P}(\big|\varphi - \widetilde{\varphi}_{k'_0}\big|_1 \geq \epsilon) \leq \frac{\delta + \delta^2}{2} \leq \delta. \tag{16.44}$$

In other words, in order to obtain the phase φ to accuracy $\epsilon = 2^{-d}$ with a success probability at least $1 - \delta$, we need $d + \lceil \log_2 \delta^{-1} \rceil$ ancilla qubits to store the value of the phase. On top of that, it suffices to take the simulation time so that $T \geq (\epsilon\delta)^{-1}$.

Remark 16.8 (Quantum median method)**.** One problem with QPE is that in order to obtain a success probability $1-\delta$, we must use $\log_2 \delta^{-1}$ ancilla qubits, and the maximal simulation time also needs to be increased by a factor δ^{-1}. The increase of the maximal simulation time is particularly undesirable since it increases the circuit depth and hence the required coherence time of the quantum device. When $|\psi\rangle$ is an exact eigenstate, this can be improved by the median method, which uses $\log \delta^{-1}$ copies of the result from QPE without using ancilla qubits or increasing the circuit depth. When $|\psi\rangle$ is a linear combination of eigenstates, the problem of the aliasing effect becomes more difficult to handle. One possibility is to generalize the median method into the quantum median method [NWZ09], which uses classical arithmetics to evaluate the median using a quantum circuit. To reach success probability $1 - \delta$, we still need $\log_2 \delta^{-1}$ ancilla qubits, but the maximal simulation time does not need to be increased. ◇

We summarize the preceding discussion as a theorem.

THEOREM 16.9. *Assume that an exact eigenstate $|\psi\rangle$ is available and $U|\psi\rangle = e^{i2\pi\varphi}|\psi\rangle$ for some $\varphi \in [0, 1)$. Let $\epsilon \in (0, 1/2)$ and $\delta \in (0, 1)$, and apply the standard t-qubit QPE circuit with $T = 2^t$ to the input $|0^t\rangle|\psi\rangle$. If $T \geq (\epsilon\delta)^{-1}$ and we output the estimator $\widetilde{\varphi} = k'/T$ from the measurement outcome $k' \in [T]$, then*

$$\mathbb{P}\big(|\widetilde{\varphi} - \varphi|_1 \geq \epsilon\big) \leq \delta.$$

Moreover, in the standard implementation via controlled powers $U^{2^0}, \ldots, U^{2^{t-1}}$, the number of queries to U is $\mathcal{O}(T) = \mathcal{O}\big(1/(\delta\epsilon)\big)$.

PROOF. From the derivation above (using Eq. (16.42) and summing the tail), we have

$$\mathbb{P}\big(\big|\varphi - \widetilde{\varphi}_{k'_0}\big|_1 \geq \epsilon\big) \leq \frac{1}{2T\epsilon} + \frac{1}{2(T\epsilon)^2}.$$

If $T\epsilon \geq \delta^{-1}$, then the right-hand side is at most $(\delta + \delta^2)/2 \leq \delta$. Finally, implementing the controlled powers U^{2^i} (without fast-forwarding) uses $\sum_{i=0}^{t-1} 2^i = T - 1$ calls to U, hence $\mathcal{O}(T)$ queries. □

We finish this section by stating a general proposition for the outcome of QPE, which relaxes conditions (1) and (3) simultaneously and subsumes the previous calculations.

Proposition 16.10. *Let U be a unitary with an eigendecomposition $U|\psi_k\rangle = e^{2\pi i\varphi_k}|\psi_k\rangle$, and let $|\psi\rangle = \sum_k c_k|\psi_k\rangle$ be a normalized initial state. Apply the standard t-qubit QPE circuit with $T = 2^t$ to the input $|0^t\rangle|\psi\rangle$. Then, upon measuring the first register in the computational basis and obtaining outcome $k' \in \{0, \ldots, T-1\}$, the probability of that outcome is*

$$\mathbb{P}(k') = \sum_k \big|c_k\big|^2 \, F_T\big(\varphi_k - k'/T\big).$$

where F_T is the Fejér kernel.

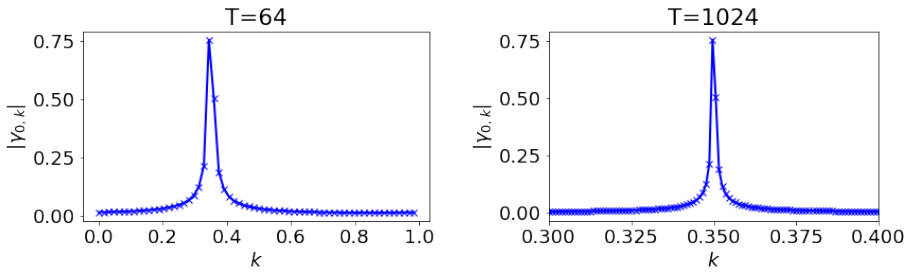


FIGURE 16.5. For $\varphi = 0.35$, the shape of $|\gamma_{0,k}|$ with $T = 64$ and $T = 1024$.

PROOF. We start with

$$|0^t\rangle\,|\psi\rangle \xrightarrow{U_{\mathrm{FT}}\otimes I} \sum_k c_k \frac{1}{\sqrt{T}} \sum_{j=0}^{T-1} |j\rangle\,|\psi_k\rangle \xrightarrow{\mathcal{U}} \sum_k c_k \frac{1}{\sqrt{T}} \sum_{j=0}^{T-1} |j\rangle\, e^{2\pi i \varphi_k j}\,|\psi_k\rangle\ .$$

After applying the inverse Fourier transform on the first register,

$$\sum_k c_k \frac{1}{\sqrt{T}} \sum_{j=0}^{T-1} |j\rangle\, e^{2\pi i \varphi_k j}\,|\psi_k\rangle \xrightarrow{U_{\mathrm{FT}}^\dagger\otimes I} \sum_{k'}\sum_k c_k \Big(\tfrac{1}{T} \sum_{j=0}^{T-1} e^{2\pi i j(\varphi_k - k'/T)}\Big)\,|k'\rangle\,|\psi_k\rangle\ ,$$

where

$$\gamma_{k,k'} = \frac{1}{T}\sum_{j=0}^{T-1} e^{2\pi i j(\varphi_k - k'/T)} = \frac{1}{T}\,\frac{1-e^{2\pi i T(\varphi_k - k'/T)}}{1-e^{2\pi i(\varphi_k - k'/T)}}.$$

Hence the probability of observing $|k'\rangle$ in the first register is

$$\mathbb{P}(k') = \Big\|\sum_k c_k\,\gamma_{k,k'}\,|\psi_k\rangle\Big\|^2 = \sum_k |c_k|^2\,|\gamma_{k,k'}|^2 = \sum_k |c_k|^2\,F_T\big(\varphi_k - k'/T\big),$$

which completes the proof. □

16.5. Eigenvalue transformation with quantum phase estimation

As an application of the preceding analysis, we show how QPE can be used as a coherent eigenvalue readout primitive for implementing matrix functions. Let H be a Hermitian matrix, and let $f(H)$ be a matrix function that we would like to apply to a quantum state. We assume access to a unitary U whose eigenphases encode the eigenvalues of H. For concreteness, and consistent with the QPE setup in Chapter 16, we take

$$U = e^{i2\pi H}, \tag{16.45}$$

which can be implemented, for instance, by Hamiltonian simulation. In this discussion we ignore the simulation error. The function $f : \mathbb{R} \to \mathbb{R}$ is assumed to satisfy $|f(x)| \le 1$ for $x \in [-1, 1]$. Let H have the eigendecomposition

$$H\,|v_j\rangle = \lambda_j\,|v_j\rangle\,. \tag{16.46}$$

To simplify the discussion, we assume $0 < \lambda_0 \le \lambda_1 \le \ldots \le \lambda_{N-1} < 1$ and that all eigenvalues have an exact d-bit representation. More general spectra can be handled by shifting and rescaling H so

that its spectrum lies in $[0, 1)$, but then the QPE output must be interpreted modulo 1. Our goal is to prepare a state $|\psi\rangle \propto f(H)\,|b\rangle$.

If the input state is an eigenvector, say $|b\rangle = |v_j\rangle$, then QPE implements the mapping

$$U_{\mathrm{QPE}}\,|0^d\rangle\,|v_j\rangle = |\lambda_j\rangle\,|v_j\rangle\,. \tag{16.47}$$

In general, write the input state as

$$|b\rangle = \sum_j \beta_j\,|v_j\rangle\,. \tag{16.48}$$

Then by linearity,

$$U_{\mathrm{QPE}}\,|0^d\rangle\,|b\rangle = \sum_j \beta_j\,|\lambda_j\rangle\,|v_j\rangle\,. \tag{16.49}$$

Note that

$$f(H)\,|b\rangle = \sum_j \beta_j f(\lambda_j)\,|v_j\rangle\,, \tag{16.50}$$

so it suffices to use the eigenvalue information stored in the ancilla register to multiply each coefficient β_j by the factor $f(\lambda_j)$. For this purpose the eigenvalues must be stored coherently, exactly as QPE provides. We therefore apply the following controlled rotation (see Proposition 5.7):

$$U_{\mathrm{CR}}\,|0\rangle\,|\lambda_j\rangle = \left(\sqrt{1 - \left|f(\widetilde{\lambda}_j)\right|^2}\,|0\rangle + f(\widetilde{\lambda}_j)\,|1\rangle\right)|\lambda_j\rangle\,. \tag{16.51}$$

Here $\widetilde{\lambda}_j$ denotes the value extracted from the QPE register; under the present exact-representation assumption, $\widetilde{\lambda}_j = \lambda_j$.

Finally, we uncompute by applying $U_{\mathrm{QPE}}^\dagger$, which returns the eigenvalue register from $|\lambda_j\rangle$ to $|0^d\rangle$. The overall algorithm is in Fig. 16.6.

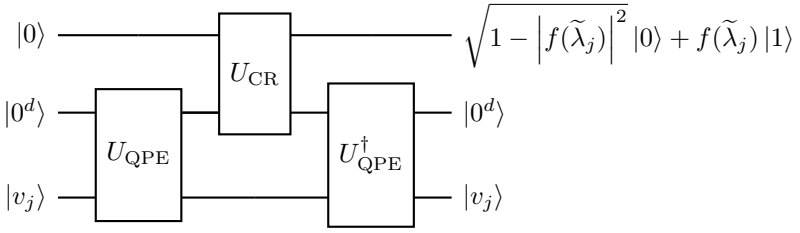


FIGURE 16.6. Circuit for the QPE based algorithm for implementing matrix functions.

After this uncomputation, the d ancilla qubits used for storing the eigenvalues become available again as workspace. Discarding all working registers, the resulting unitary, denoted by $\mathcal{U}$, satisfies

$$\mathcal{U}\,|0\rangle\,|b\rangle = \sum_j \left(\sqrt{1 - \left|f(\widetilde{\lambda}_j)\right|^2}\,|0\rangle + f(\widetilde{\lambda}_j)\,|1\rangle\right)\beta_j\,|v_j\rangle\,. \tag{16.52}$$

Measuring the signal qubit, if the outcome is 1, the normalized vector stored in the system register is

$$|\psi\rangle \propto \sum_j \beta_j f(\widetilde{\lambda}_j) |v_j\rangle \approx f(H) |b\rangle . \tag{16.53}$$

The discussion in Section 16.4 shows that this picture is simplest when two idealized assumptions hold: the relevant eigenvalues admit exact d-bit representations, and the input is decomposed in an eigenbasis that QPE can resolve cleanly. Once these assumptions are relaxed, the bookkeeping becomes more involved because one must track both phase-estimation error and the distribution over different eigencomponents. In the applications below we will therefore work mainly in this idealized regime, while keeping in mind that a complete analysis requires the more general bounds developed above. On the other hand, QSVT-based eigenvalue transformation does not require such idealized assumptions, and the analysis is much more straightforward.

16.6. Heisenberg-limited scaling

A central theme in quantum metrology is the trade-off between the precision of an estimate and the quantum resources consumed. This trade-off leads to scaling laws that characterize the efficiency of an estimation protocol.

Consider estimating a parameter φ encoded by a quantum process, given R uses of that process. The most direct strategy uses the R resources independently: prepare R identical probe states, apply the process to each, measure them individually, and analyze the results. According to the quantum Cramér-Rao bound (see Section 8.6), for any unbiased estimator the variance satisfies $\mathbb{V} = \Omega(1/R)$. Thus the precision scales as $\epsilon = \mathcal{O}(R^{-1/2})$, and achieving precision ϵ requires $R = \mathcal{O}(\epsilon^{-2})$. This is known as the shot-noise-limited scaling (SNL) or the standard quantum limit (SQL), and it is optimal when probes are used independently (see also Example 8.10). Quantum mechanics also permits strategies that surpass the SNL. By utilizing entanglement across the R probes, or using the resources sequentially on a single probe, one can increase the quantum Fisher information and achieve **Heisenberg-limited scaling** (HL) [GLM04, GLM06]. At the Heisenberg limit the precision scales as $\epsilon = \mathcal{O}(R^{-1})$, corresponding to the quadratic improvement $R = \mathcal{O}(\epsilon^{-1})$.

In quantum algorithms involving phase estimation, the parameter of interest is often an eigenphase φ of a Hamiltonian H, accessed through a unitary oracle $U(t) = e^{-iHt}$. In this setting the relevant resource is the total evolution time T. The scaling laws can be stated in terms of T: the SNL corresponds to $\epsilon = \mathcal{O}(T^{-1/2})$, whereas the HL corresponds to $\epsilon = \mathcal{O}(T^{-1})$. The term "Heisenberg-limited" reflects the time–energy heuristic $\Delta E\, \Delta t \geq 1/2$ (in units where $\hbar = 1$), which suggests that resolving an energy to uncertainty ΔE requires time on the order of $1/\Delta E$, matching the $1/T$ scaling.

To connect these scaling laws to information-theoretic bounds, we relate the mean-square error and the variance via $\mathbb{V} \approx \epsilon^2$. Under this identification, the SNL corresponds to $\mathbb{V} = \mathcal{O}(T^{-1})$ (equivalently $T = \mathcal{O}(\epsilon^{-2})$), and the HL corresponds to $\mathbb{V} = \mathcal{O}(T^{-2})$ (equivalently $T = \mathcal{O}(\epsilon^{-1})$).

When estimating a circular quantity such as a phase $\varphi \in [0, 2\pi)$, the standard variance depends on an arbitrary choice of reference angle. A rotation-invariant alternative is the **Holevo variance** $\mathbb{V}_H$. Given an estimator $\hat{\varphi}$, it is defined by

$$\mathbb{V}_H(\hat{\varphi}) = \frac{1}{|\mathbb{E}(e^{i\hat{\varphi}})|^2} - 1. \tag{16.54}$$

Asymptotically, if the distribution of the estimator is sufficiently peaked around the true value, the Holevo variance coincides with the standard variance $\mathbb{V}(\hat{\varphi})$. Specifically, if we choose coordinates

such that the mean error is zero, Taylor expansion shows [BHB+09]:

$$\begin{aligned}\mathbb{V}_H(\hat{\varphi}) &= \frac{1}{1-\mathbb{E}(\hat{\varphi}^2)+\mathcal{O}(\mathbb{E}(\hat{\varphi}^4))}-1 \\ &= \mathbb{V}(\hat{\varphi})+\mathcal{O}\left(\mathbb{V}(\hat{\varphi})^2\right).\end{aligned} \tag{16.55}$$

Thus, for asymptotic scaling statements, the Holevo variance serves as a proxy for the phase uncertainty. We now formalize scaling in terms of how $\mathbb{V}_H$ behaves as a function of the total evolution time T.

Definition 16.11. *Let a quantum phase estimation protocol use a sequence of evolution times $\{t_1,\dots,t_N\}$ to produce an estimator $\hat{\varphi}$ for an unknown phase φ^*. Let $T=\sum_{p=1}^{N}|t_p|$ be the total evolution time. Assume the estimator has bias at most $\widetilde{\mathcal{O}}(T^{-\beta/2})$. We characterize the scaling by the behavior of the Holevo variance as T increases:*

$$\mathbb{V}_H(\hat{\varphi})=\widetilde{\mathcal{O}}\left(T^{-\beta}\right). \tag{16.56}$$

*For quantum phase estimation, $\beta=1$ is referred to as **shot-noise-limited scaling**, and $\beta=2$ is called **Heisenberg-limited scaling**.*

The Heisenberg limit ($\beta=2$) is the best possible scaling in this model. It follows from the quantum Cramér–Rao bound (QCRB) [BC94], which lower bounds the variance of any locally unbiased estimator [BHB+09, WK97, WK98].

THEOREM 16.12 (Optimality of Heisenberg-limited scaling). *Consider a quantum protocol with the following properties:*

1. *It applies controlled phase queries with evolution times $t_1,\dots,t_N$ to an eigenstate $|\psi\rangle$ satisfying $U(t)|\psi\rangle=e^{it\varphi^*}|\psi\rangle$ for all queried times t.*
2. *It interleaves these queries with an arbitrary sequence of unitaries $\{G_i\}$ acting only on the ancillary register, so the target register remains fixed in the state $|\psi\rangle$.*

Then for any estimator $\hat{\varphi}$ that is locally unbiased at φ^*, the variance satisfies

$$\mathbb{V}(\hat{\varphi})\geq\frac{1}{4T^2}. \tag{16.57}$$

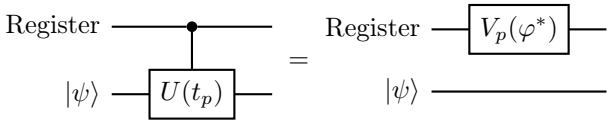
Moreover, if the estimator is sufficiently concentrated so that Eq. (16.55) applies (in particular, $\mathbb{V}(\hat{\varphi})=o(1)$), then

$$\mathbb{V}_H(\hat{\varphi})\geq\frac{1-o(1)}{4T^2}, \tag{16.58}$$

and hence no protocol in this model can achieve $\beta>2$ in Definition 16.11.

PROOF. We apply the QCRB directly to the phase parameter. The assumptions ensure that the target state remains fixed in the eigenstate $|\psi\rangle$ throughout the protocol, so we may focus on the evolution of the auxiliary register. The application of the controlled query $C(U(t_p))$ induces an effective phase rotation on that register:

(16.59)



For each query there is an orthogonal projector Π_p on the register such that

$$V_p(\varphi^*) = (I - \Pi_p) + e^{it_p\varphi^*}\Pi_p = e^{it_p\varphi^*\Pi_p}. \tag{16.60}$$

Indeed, Π_p projects onto the subspace of register states for which the controlled query is activated. Since Π_p is a projector, $\|\Pi_p\| = 1$.

Let $|\Psi_0\rangle$ be the initial state of the register. The final state $|\Psi(\varphi^*)\rangle$, parameterized by φ^*, is

$$|\Psi(\varphi^*)\rangle = G_N V_N(\varphi^*) G_{N-1} \cdots V_1(\varphi^*) G_0 \,|\Psi_0\rangle\,. \tag{16.61}$$

By Proposition 8.16, the QFI of this pure-state family is

$$\mathcal{F}_Q(\varphi^*) = 4\left(\langle\dot\Psi|\dot\Psi\rangle - |\,\langle\Psi|\dot\Psi\rangle\,|^2\right) \le 4\left\||\dot\Psi(\varphi^*)\rangle\right\|^2, \tag{16.62}$$

where $|\dot\Psi(\varphi^*)\rangle = \frac{\partial}{\partial\varphi^*}|\Psi(\varphi^*)\rangle$.

We compute the derivative using the product rule. Let $U_{\text{total}}(\varphi^*)$ be the total evolution operator. Then $|\dot\Psi(\varphi^*)\rangle = \frac{\partial U_{\text{total}}(\varphi^*)}{\partial\varphi^*}|\Psi_0\rangle$. We bound the norm using the triangle inequality:

$$\left\||\dot\Psi(\varphi^*)\rangle\right\| \le \sum_{p=1}^{N}\left\|G_N V_N \cdots G_p\left(\frac{\partial V_p(\varphi^*)}{\partial\varphi^*}\right)G_{p-1}\cdots G_0\,|\Psi_0\rangle\right\|. \tag{16.63}$$

Since G_i and $V_j(\varphi^*)$ are unitary, they preserve the norm. Using the submultiplicativity of the operator norm and $\||\Psi_0\rangle\| = 1$, we have:

$$\left\||\dot\Psi(\varphi^*)\rangle\right\| \le \sum_{p=1}^{N}\left\|\frac{\partial V_p(\varphi^*)}{\partial\varphi^*}\right\|. \tag{16.64}$$

Since $V_p(\varphi^*) = e^{it_p\varphi^*\Pi_p}$, its derivative is $\frac{\partial V_p(\varphi^*)}{\partial\varphi^*} = it_p\Pi_p V_p(\varphi^*)$. The norm is bounded by

$$\left\|\frac{\partial V_p(\varphi^*)}{\partial\varphi^*}\right\| = |t_p|\,\|\Pi_p V_p(\varphi^*)\| \le |t_p|\,\|\Pi_p\| = |t_p|. \tag{16.65}$$

Substituting this back, we obtain

$$\left\||\dot\Psi(\varphi^*)\rangle\right\| \le \sum_{p=1}^{N}|t_p| = T. \tag{16.66}$$

Consequently, the QFI is bounded by $\mathcal{F}_Q(\varphi^*) \le 4T^2$. The QCRB then implies

$$\mathbb{V}(\hat\varphi) \ge \frac{1}{\mathcal{F}_Q(\varphi^*)} \ge \frac{1}{4T^2}. \tag{16.67}$$

If additionally $\mathbb{V}(\hat\varphi) = o(1)$ so that Eq. (16.55) applies, then $\mathbb{V}_H(\hat\varphi) = \mathbb{V}(\hat\varphi)\,(1 + o(1))$, and the same T^{-2} lower bound holds for the Holevo variance. □

A minor subtlety in interpreting Theorem 16.12 is that the usual (linear) variance $\mathbb{V}(\hat\varphi)$ depends on a choice of branch cut for the representative of $\hat\varphi \in [0, 2\pi)$, and can therefore be large even when $\hat\varphi$ is accurate modulo 2π. This issue is most relevant when proving **upper** bounds, where one wishes to compare an estimator to the true phase in a rotation-invariant manner (hence the use of the Holevo variance in Definition 16.11).

For the lower bound in Theorem 16.12, however, the argument is local: the QCRB constrains any estimator that is locally unbiased at φ^* through derivatives of the likelihood in a neighborhood of φ^*. Consequently, the branch-cut ambiguity does not affect the scaling conclusion. In particular,

when the estimator is sufficiently concentrated so that Eq. (16.55) applies, the lower bound transfers directly to $\mathbb{V}_H(\hat{\varphi})$ up to $1 + o(1)$ factors, as stated in Theorem 16.12.

This result shows that $\beta = 2$ is the optimal scaling that can be achieved by any phase estimation protocol under these conditions, regardless of whether the protocol uses entanglement or intersperses the queries with additional unitaries (provided these operations act trivially on the eigenstate whose phase is being estimated). Subsequent work shows that, under additional regularity assumptions and for appropriate covariant measurements, one can optimize the constant factor in front of T^{-2}, with an optimal constant of order π^2 in this setting [GDDWB20].

We next show that Heisenberg-limited scaling is achievable. We illustrate this using the quantum Fourier transform based phase estimation scheme described above.

Proposition 16.13. *Quantum Fourier transform based phase estimation using the Fejér kernel, as described in Fig. 16.4, achieves Heisenberg-limited scaling according to Definition 16.11 as the number of bits of precision d increases, provided the register size is $t = d + 2$ and $\hat{\varphi}$ is taken to be the median of $\Theta(d)$ repetitions of the estimates.*

Proof. We analyze the performance in terms of the desired precision $\epsilon = 2^{-d}$. With register size $t = d + 2$, a single execution uses controlled powers up to $U^{2^{t-1}}$, so the evolution time is $\Theta(2^t) = \Theta(2^d)$. Repeating this procedure $\Theta(d)$ times gives total evolution time

$$T = \sum_i |t_i| = \Theta(d2^d). \tag{16.68}$$

With register size $t = d + 2$, a single run yields an estimate within error 2^{-d} of φ^* with probability at least $1/4$. By taking the median of $\Theta(d)$ repetitions, the failure probability, i.e., the probability that the resulting estimate $\hat{\varphi}$ is more than $\mathcal{O}(2^{-d})$ away from φ^* is suppressed exponentially. The Chernoff bound applied to the median gives $\mathbb{P}(\text{fail}) = e^{-\Theta(d)} = \mathcal{O}(2^{-d})$.

First, we analyze the bias. The maximum possible error is bounded by 2π.

$$|\mathbb{E}(\hat{\varphi} - \varphi^*)| \leq \mathbb{E}(|\hat{\varphi} - \varphi^*|) \leq \epsilon + 2\pi\,\mathbb{P}(\text{fail}) = \mathcal{O}(2^{-d}). \tag{16.69}$$

We relate this to the total time T. Since $T = \Theta(d2^d)$, we have $2^{-d} = \Theta(d/T)$. The bias is $\mathcal{O}(d/T)$. The requirement for $\beta = 2$ in Definition 16.11 is $\widetilde{\mathcal{O}}(T^{-1})$. Since d is logarithmic in T, this holds in the $\widetilde{\mathcal{O}}(\cdot)$ sense.

Next, we analyze the variance. We account for the contribution from both successful and failed estimations.

$$\mathbb{V}(\hat{\varphi}) \leq \mathbb{E}((\hat{\varphi} - \varphi^*)^2) \leq \epsilon^2 + (2\pi)^2\,\mathbb{P}(\text{fail}). \tag{16.70}$$

Using statistical amplification in Section 8.2, if we choose the constant implicit in $\Theta(d)$ repetitions large enough, we may ensure $\mathbb{P}(\text{fail}) = \mathcal{O}(2^{-2d})$, and hence $\mathbb{V}(\hat{\varphi}) = \mathcal{O}(2^{-2d})$. Using Eq. (16.55), we obtain

$$\mathbb{V}_H(\hat{\varphi}) = \mathcal{O}(2^{-2d}) = \mathcal{O}(d^2T^{-2}) = \widetilde{\mathcal{O}}(T^{-2}). \tag{16.71}$$

This establishes Heisenberg-limited scaling. □

Theorem 16.12 gives an information-theoretic lower bound on the variance. While the QFT-based approach achieves the optimal scaling exponent, it does not saturate the constant factor in Theorem 16.12 because of the logarithmic overhead and the shape of the Fejér kernel. One can

improve the constant by optimizing the input state. For example, using input states derived from the Kaiser window [GDDWB20, BSG+24a] leads to a Holevo variance bound of the form

$$\mathbb{V}_H(\hat{\varphi}) \leq \tan^2\left(\frac{\pi}{T+2}\right) \approx \frac{\pi^2}{T^2}. \tag{16.72}$$

This demonstrates that the exact Heisenberg limit (including the preconstant) is achievable. Furthermore, practical optimizations can improve constant factors. For instance, using directionally controlled rotations $V(t) := |0\rangle\langle 0| \otimes U^\dagger(t) + |1\rangle\langle 1| \otimes U(t)$ instead of the standard controlled unitary $\mathrm{CU}(t)$ effectively doubles the phase kickback per query ($e^{\pm i\varphi t}$ versus $e^{i\varphi t}$), which can halve the required evolution time [BGB+18].

16.7. Amplitude estimation

Let $|\psi_0\rangle$ be prepared by an oracle U_{ψ_0}, i.e., $U_{\psi_0}|0^n\rangle = |\psi_0\rangle$. Assume that

$$|\psi_0\rangle = \sqrt{\mathbb{P}(0)}\,|\psi_{\mathrm{good}}\rangle + \sqrt{1-\mathbb{P}(0)}\,|\psi_{\mathrm{bad}}\rangle\,, \tag{16.73}$$

where $|\psi_{\mathrm{bad}}\rangle$ is orthogonal to $|\psi_{\mathrm{good}}\rangle$, and $\sqrt{\mathbb{P}(0)} = \sin\frac{\theta}{2}$. The goal of amplitude estimation is to estimate $\mathbb{P}(0)$ to additive precision ϵ. If $\mathbb{P}(0)$ is bounded away from 0 and 1, then estimating it by Monte Carlo sampling requires $\mathcal{N} = \mathcal{O}(\epsilon^{-2})$ samples.

Let $G = R_{\psi_0} R_{\mathrm{good}}$ be the Grover operator as in Section 11.2. Then in the basis $\mathcal{B} = \{|\psi_{\mathrm{good}}\rangle, |\psi_{\mathrm{bad}}\rangle\}$, the subspace $\mathcal{H} = \operatorname{span}\mathcal{B}$ is an invariant subspace of G. Recall the computation of **??**, the matrix representation is

$$[G]_{\mathcal{B}} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}. \tag{16.74}$$

Its two eigenstates are

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\psi_{\mathrm{good}}\rangle \pm i\,|\psi_{\mathrm{bad}}\rangle\right), \tag{16.75}$$

with eigenvalues $e^{\pm i\theta}$, respectively.

Therefore the problem of estimating θ can be solved with phase estimation with an imperfect initial state. Note that

$$|\langle\psi_0|\psi_+\rangle|^2 = \frac{1}{2}\left|\sin\frac{\theta}{2} + i\cos\frac{\theta}{2}\right|^2 = \frac{1}{2} = |\langle\psi_0|\psi_-\rangle|^2. \tag{16.76}$$

Consider a QPE circuit with t ancilla qubits and (in the Fourier-based implementation) controlled powers up to $G^{2^{t-1}}$, so that the total "Grover time" is $T = \Theta(2^t)$. Then each execution with the system register will be in $|\psi_+\rangle$ or $|\psi_-\rangle$ states each with probability 1/2. This corresponds to the estimation of $\pm\theta$, respectively, and no postselection is needed.

Let

$$t = d + \lceil \log \delta^{-1} \rceil \tag{16.77}$$

be the number of ancilla qubits with $\epsilon' = 2^{-d}$. Then QPE obtains an estimate denoted by $\widetilde{\theta}$, which approximates θ to precision ϵ' with success probability $1-\delta$. Define the corresponding estimate

$\widetilde{\mathbb{P}}(0) := \sin^2 \frac{\widetilde{\theta}}{2}$. Since $\mathbb{P}(0) = \sin^2 \frac{\theta}{2}$, we have

$$\begin{aligned} &\sin^2 \frac{\widetilde{\theta}}{2} - \sin^2 \frac{\theta}{2} \\ =&\sin^2 \frac{\widetilde{\theta}-\theta}{2} \cos^2 \frac{\theta}{2} + \cos^2 \frac{\widetilde{\theta}-\theta}{2} \sin^2 \frac{\theta}{2} + 2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \sin \frac{\widetilde{\theta}-\theta}{2} \cos \frac{\widetilde{\theta}-\theta}{2} - \sin^2 \frac{\theta}{2} \\ =&\sin \frac{\theta}{2} \cos \frac{\theta}{2} \sin(\widetilde{\theta}-\theta) + \left(1 - 2\sin^2 \frac{\theta}{2}\right) \sin^2 \frac{\widetilde{\theta}-\theta}{2}. \end{aligned} \tag{16.78}$$

Using the fact that $\left|\sin(\widetilde{\theta}-\theta)\right| \leq \left|\widetilde{\theta}-\theta\right| \leq \epsilon'$, we have

$$\left|\widetilde{\mathbb{P}}(0) - \mathbb{P}(0)\right| \leq \sqrt{\mathbb{P}(0)(1-\mathbb{P}(0))}\,\epsilon' + |1-2\mathbb{P}(0)|\,\frac{\epsilon'^2}{4}. \tag{16.79}$$

Let ϵ' be sufficiently small. If $\mathbb{P}(0)(1-\mathbb{P}(0)) = \Omega(1)$, we can choose $\epsilon' = \mathcal{O}(\epsilon)$, and the total complexity of QPE is $\mathcal{O}(\epsilon^{-1})$.

If $\mathbb{P}(0)$ is small, it is natural to estimate $\mathbb{P}(0)$ to multiplicative accuracy ϵ instead. Using

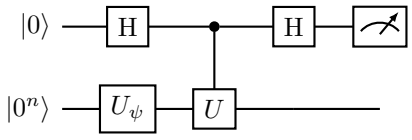
$$\left|\widetilde{\mathbb{P}}(0) - \mathbb{P}(0)\right| \approx \sqrt{\mathbb{P}(0)}\epsilon' < \mathbb{P}(0)\epsilon, \tag{16.80}$$

we take $\epsilon' = \sqrt{\mathbb{P}(0)}\,\epsilon$. Therefore the runtime of QPE is $\mathcal{O}(\mathbb{P}(0)^{-\frac{1}{2}}\epsilon^{-1})$. If $\mathbb{P}(0)$ is estimated to multiplicative accuracy ϵ using Monte Carlo sampling, the number of samples is $\mathcal{N} = \mathcal{O}(\mathbb{P}(0)^{-1}\epsilon^{-2})$.

In terms of the resource T used in Definition 16.11, phase estimation yields an estimate of θ with error $\mathcal{O}(1/T)$, which is Heisenberg-limited scaling for the eigenphase of G. Translating this into an estimate of $\mathbb{P}(0) = \sin^2(\theta/2)$ introduces a factor of $\sqrt{\mathbb{P}(0)(1-\mathbb{P}(0))}$ in the error, as shown above.

As for success probability, one may increase t so that a single run succeeds with probability $1-\delta$, which yields total Grover time polynomial in $1/\delta$ (for the standard Fourier-based QPE analysis, this is $\mathcal{O}(\epsilon'^{-1}\delta^{-1})$). A better method is to choose $t = d + \Theta(1)$ and repeat independently $\Theta(\log(1/\delta))$ times (taking the median), giving total Grover time $\widetilde{\mathcal{O}}(\epsilon'^{-1})$.

Example 16.14 (Amplitude estimation to accelerate Hadamard test)**.** Consider the circuit for the Hadamard test in Fig. 2.1 to estimate $\mathrm{Re}\,\langle\psi|U|\psi\rangle$. Let the initial state $|\psi\rangle$ be prepared by a unitary U_ψ, then the following combined circuit



maps $|0\rangle\,|0^n\rangle$ to

$$|\psi_0\rangle = \frac{1}{2}\,|0\rangle\,(|\psi\rangle + U\,|\psi\rangle) + \frac{1}{2}\,|1\rangle\,(|\psi\rangle - U\,|\psi\rangle) := \sqrt{\mathbb{P}(0)}\;|\psi_{\mathrm{good}}\rangle + \sqrt{1-\mathbb{P}(0)}\;|\psi_{\mathrm{bad}}\rangle\,, \tag{16.81}$$

and the goal is to estimate $\mathbb{P}(0)$. This also gives the implementation of the reflector R_{ψ_0}.

Note that R_{good} can be implemented by simply reflecting against the signal qubit, i.e.,

$$R_{\mathrm{good}} = (I - 2\,|0\rangle\,\langle 0|) \otimes I^{\otimes n} = -Z \otimes I^{\otimes n}. \tag{16.82}$$

Then we can run QPE to the Grover unitary $G = R_{\psi_0} R_{\mathrm{good}}$ to estimate $\mathbb{P}(0)$, and the circuit depth is $\mathcal{O}(\epsilon^{-1})$. ◇

Amplitude estimation is sometimes called Heisenberg-limited (despite the fact that it only measures a phase as an intermediate step) because it reduces to phase estimation of the Grover eigenphase and achieves $\mathcal{O}(1/T)$ scaling for estimating that phase as a function of Grover time T. This should be interpreted with care: the metrological Heisenberg limit in Section 16.6 concerns phase parameters generated by time evolution, whereas amplitude estimation reduces the problem to a phase-estimation task for a constructed unitary G.

16.8. Iterative phase estimation and Cramér-Rao bound

Quantum Fourier transform is not the only way to approach the problem of phase estimation. If we seek only a classical estimate of an eigenvalue of a unitary, then we can replace the Fourier analysis discussed previously by statistical inference on the measurement outcomes returned by the experiment. This approach has a major advantage: instead of a logarithmic number of ancilla qubits, iterative approaches require at most one additional qubit and involve **iteratively** measuring the control qubit for a controlled unitary evolution and then inferring the phase from the resulting data. The best methods can perform comparably to the Fourier-based methods described above. The main disadvantage is that these methods project the input irreversibly onto the eigenbasis of the unitary. Therefore iterative phase estimation, unlike the Fourier-based approach discussed above, cannot be used as a subroutine inside a larger coherent quantum algorithm.

The general form of iterative phase estimation can be described by the circuit in Fig. 16.7. Here the circuit $W(t;\theta)$ is the basic building block. The parameter t determines the power of the unitary applied to the input state $|\psi\rangle$, and the angle θ determines a rotation applied to the control qubit before measurement. One then applies $W(t;\theta)$ repeatedly with different choices of t and θ, and uses the resulting measurement outcomes to infer an estimate of the eigenvalue of the input state $|\psi\rangle$. The choices of t and θ can be made adaptively from previous measurement results or fixed in advance. The difference between Fig. 16.7(b) and Fig. 16.7(c) is whether the input state $|\psi\rangle$ is reset for each iteration, or whether the output state from one iteration is used as the input to the next.

Direct computation shows

$$(\langle 0| \otimes I) W(t;\theta) (|0\rangle \otimes I) = \frac{e^{i\theta/2} I + e^{-i\theta/2} U^t}{2}. \tag{16.83}$$

For simplicity, consider an eigenstate $|\psi\rangle$ of U with eigenvalue $e^{i\phi}$. In this case there is no difference between the circuits in Fig. 16.7(b) and Fig. 16.7(c), because conditioning on any measurement outcome multiplies the target state only by a scalar. For each block $W(t,\theta)$, the probability of measuring the control qubit to be zero is then

$$\mathbb{P}(0) = \left| \frac{e^{i\theta/2} + e^{-i\theta/2} e^{i\phi t}}{2} \right|^2 = \frac{1}{2} + \frac{e^{i(\phi t - \theta)} + e^{-i(\phi t - \theta)}}{4} = \cos^2\left(\frac{\phi t - \theta}{2} \right). \tag{16.84}$$

To understand the fundamental limitations of iterative phase estimation and determine whether Heisenberg-limited scaling is possible, we can apply the Cramér-Rao bound (Theorem 8.12). This gives a simple upper bound on the amount of information that can be extracted from a prescribed sequence of experiments, analogous to the general result in Theorem 16.12.

THEOREM 16.15 (Cramér-Rao bound for iterative phase estimation). *Let $|\psi\rangle$ be an eigenstate of U with eigenvalue $e^{i\phi}$. Consider the iterative phase-estimation experiment in Fig. 16.7 with evolution times $t_1, \ldots, t_N$ (chosen independently of the previous measurement outcomes), where at*

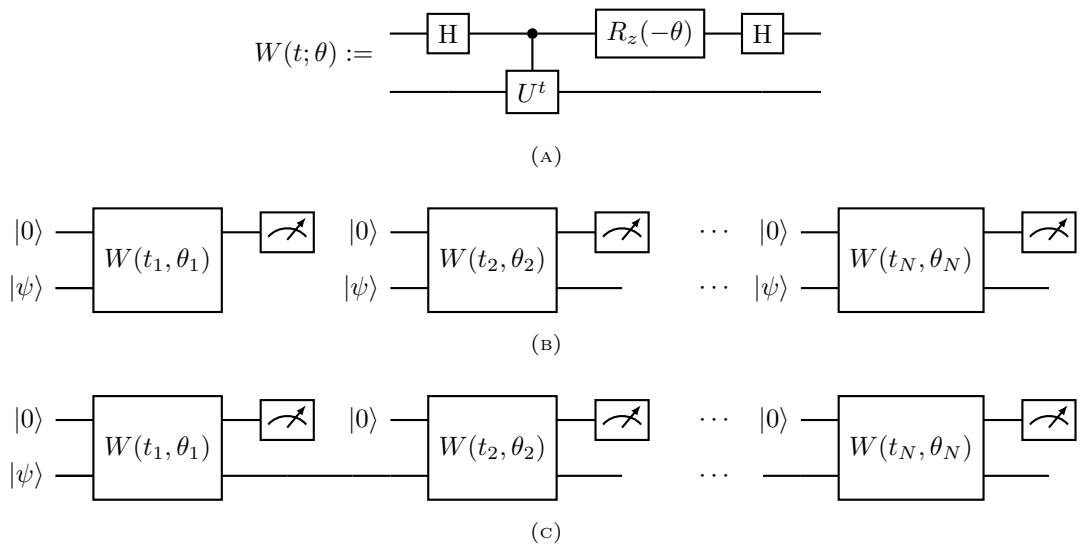


FIGURE 16.7. Generic form of circuits for iterative phase estimation. (a) The building block $W(t;\theta)$, a modified version of the Hadamard test. (b) A sequence of experiments in which the initial state $|\psi\rangle$ is reset for each run. (c) A sequence of experiments in which the output state from the previous experiment is used as the input to the next one.

step j the feedback angle θ_j may be any function of the previous measurement outcomes. Let $\hat{\phi}$ be an estimator that is locally unbiased at the true phase ϕ. Then

$$\mathbb{V}(\hat{\phi}) \geq \frac{1}{\sum_{j=1}^{N} t_j^2}. \tag{16.85}$$

PROOF. The Cramér-Rao bound states that $\mathbb{V}(\hat{\phi}) \geq 1/I_F^{(N)}(\phi)$, where $I_F^{(N)}(\phi)$ is the Fisher information of the full measurement record. Write the measurement outcomes as $\nu_1, \ldots, \nu_N \in \{0,1\}$. Because the feedback angle θ_j may depend on previous outcomes, the joint distribution factorizes only conditionally:

$$\mathbb{P}(\nu_1, \ldots, \nu_N|\phi) = \prod_{j=1}^{N} \mathbb{P}(\nu_j|\nu_1, \ldots, \nu_{j-1}; \phi). \tag{16.86}$$

For an eigenstate input, each conditional probability is again given by the same one-step likelihood with the chosen value of θ_j. Therefore it suffices to compute the Fisher information contributed by one step and then use additivity of the score function for the product likelihood.

Let us calculate the Fisher information $I_F^{(j)}(\phi)$ for a single experiment j. Let $\nu_j \in \{0,1\}$ be the measurement outcome. The probability distribution is given by Eq. (16.84).

$$\mathbb{P}(0|\phi) = \cos^2(\alpha_j), \quad \mathbb{P}(1|\phi) = 1 - \cos^2(\alpha_j) = \sin^2(\alpha_j), \tag{16.87}$$

where $\alpha_j = (\phi t_j - \theta_j)/2$. Note that $\frac{\partial \alpha_j}{\partial \phi} = t_j/2$. The Fisher information for the jth experiment is

$$I_F^{(j)}(\phi) = \sum_{\nu_j \in \{0,1\}} \frac{1}{\mathbb{P}(\nu_j|\phi)} \left(\frac{\partial \mathbb{P}(\nu_j|\phi)}{\partial \phi} \right)^2. \tag{16.88}$$

The derivatives of the probabilities are

$$\frac{\partial \mathbb{P}(0|\phi)}{\partial \phi} = 2\cos(\alpha_j)(-\sin(\alpha_j))\frac{t_j}{2} = -t_j \sin(\alpha_j)\cos(\alpha_j) \tag{16.89}$$

and similarly,

$$\frac{\partial \mathbb{P}(1|\phi)}{\partial \phi} = t_j \sin(\alpha_j)\cos(\alpha_j). \tag{16.90}$$

Substituting these into the expression for the Fisher information gives

$$\begin{aligned} I_F^{(j)}(\phi) &= \frac{(-t_j \sin(\alpha_j)\cos(\alpha_j))^2}{\cos^2(\alpha_j)} + \frac{(t_j \sin(\alpha_j)\cos(\alpha_j))^2}{\sin^2(\alpha_j)} \\ &= t_j^2 \sin^2(\alpha_j) + t_j^2 \cos^2(\alpha_j) = t_j^2, \end{aligned} \tag{16.91}$$

which is independent of ϕ and of the chosen feedback angle θ_j.

Now let

$$S_j(\phi) := \partial_\phi \log \mathbb{P}(\nu_j|\nu_1, \ldots, \nu_{j-1}; \phi) \tag{16.92}$$

be the conditional score for step j. The score of the full record is

$$S^{(N)}(\phi) = \sum_{j=1}^{N} S_j(\phi). \tag{16.93}$$

For any fixed previous record $(\nu_1, \ldots, \nu_{j-1})$, the conditional expectation of $S_j(\phi)$ is zero:

$$\mathbb{E}[S_j(\phi)|\nu_1, \ldots, \nu_{j-1}] = \sum_{\nu_j \in \{0,1\}} \mathbb{P}(\nu_j|\nu_1, \ldots, \nu_{j-1}; \phi) \partial_\phi \log \mathbb{P}(\nu_j|\nu_1, \ldots, \nu_{j-1}; \phi) \tag{16.94}$$

$$= \sum_{\nu_j \in \{0,1\}} \partial_\phi \mathbb{P}(\nu_j|\nu_1, \ldots, \nu_{j-1}; \phi) = \partial_\phi \sum_{\nu_j \in \{0,1\}} \mathbb{P}(\nu_j|\nu_1, \ldots, \nu_{j-1}; \phi) = \partial_\phi 1 = 0. \tag{16.95}$$

Now if $k < j$, then $S_k(\phi)$ depends only on $\nu_1, \ldots, \nu_k$ and is therefore measurable with respect to $\nu_1, \ldots, \nu_{j-1}$. Using the tower property,

$$\mathbb{E}[S_k(\phi) S_j(\phi)] = \mathbb{E}\left[S_k(\phi)\, \mathbb{E}[S_j(\phi)|\nu_1, \ldots, \nu_{j-1}] \right] = 0. \tag{16.96}$$

Thus all cross terms vanish, and hence

$$I_F^{(N)}(\phi) = \mathbb{E}\left[(S^{(N)}(\phi))^2 \right] = \sum_{j=1}^{N} \mathbb{E}\left[S_j(\phi)^2 \right] = \sum_{j=1}^{N} I_F^{(j)}(\phi) = \sum_{j=1}^{N} t_j^2. \tag{16.97}$$

Applying the Cramér-Rao bound yields

$$\mathbb{V}(\hat{\phi}) \geq \frac{1}{\sum_{j=1}^{N} t_j^2}. \tag{16.98}$$

□

Theorem 16.15 shows that the Fisher information grows quadratically with each evolution time t_j, but only linearly with the number of experiments when the t_j are comparable. Thus, at the level of Fisher information, long evolutions are substantially more informative than short ones.

Example 16.16 (Linearly spaced evolution times cannot achieve the Heisenberg limit)**.** Let us consider a sequence of measurements with linearly spaced simulation times $t_j = j\tau$ for $j = 1, \dots, N$, where τ is a constant step size. To achieve a precision ϵ, from Theorem 16.15, this implies we need $\sum_{j=1}^{N} t_j^2 \gtrsim 1/\epsilon^2$. We calculate the sum of squares of the evolution times:

$$\sum_{j=1}^{N} t_j^2 = \tau^2 \sum_{j=1}^{N} j^2 = \tau^2 \frac{N(N+1)(2N+1)}{6} = \Theta(\tau^2 N^3). \tag{16.99}$$

Setting this to be $\Theta(1/\epsilon^2)$ to satisfy the CRB, we can solve for the required number of experiments N:

$$\tau^2 N^3 = \Theta(1/\epsilon^2) \implies N = \Theta(\epsilon^{-2/3}). \tag{16.100}$$

The total evolution time, which represents the total resource cost, is

$$T = \sum_{j=1}^{N} t_j = \tau \sum_{j=1}^{N} j = \tau \frac{N(N+1)}{2} = \Theta(\tau N^2). \tag{16.101}$$

Substituting the scaling for N, we find the total time required:

$$T = \Theta(\tau(\epsilon^{-2/3})^2) = \Theta(\epsilon^{-4/3}). \tag{16.102}$$

This scaling is better than the shot-noise limit $\mathcal{O}(\epsilon^{-2})$, but worse than the Heisenberg limit $\mathcal{O}(\epsilon^{-1})$. Therefore a uniform grid of simulation times cannot yield Heisenberg-limited scaling. When the CRB is saturated, the error ϵ scales with the maximum evolution time $t_{\max} = N\tau$ as $\epsilon = \Theta(N^{-3/2}) = \Theta(t_{\max}^{-3/2})$. This scaling can in fact be achieved by classical signal-processing algorithms such as ESPRIT [RK89]; see the analysis in [DELZ24]. ◇

Example 16.17 (Exponentially spaced evolution times can achieve the Heisenberg limit)**.** Let us now consider a sequence of measurements with exponentially spaced simulation times, $t_j = \tau 2^{j-1}$ for $j = 1, \dots, N$. The maximum evolution time is $t_{\max} = \tau 2^{N-1}$. We calculate the sum of squares of the evolution times:

$$\sum_{j=1}^{N} t_j^2 = \tau^2 \sum_{j=1}^{N} (2^{j-1})^2 = \tau^2 \sum_{j=1}^{N} 4^{j-1} = \tau^2 \frac{4^N - 1}{3} = \Theta(\tau^2 4^N). \tag{16.103}$$

To satisfy the CRB for a precision ϵ, we set this to be $\Theta(1/\epsilon^2)$:

$$\tau^2 4^N = \Theta(1/\epsilon^2) \implies 2^N = \Theta(1/(\tau\epsilon)). \tag{16.104}$$

This implies that the number of experiments required, N, scales logarithmically with the desired precision: $N = \Theta(\log(1/\epsilon))$.

The total evolution time, which represents the total resource cost, is

$$T = \sum_{j=1}^{N} t_j = \tau \sum_{j=1}^{N} 2^{j-1} = \tau(2^N - 1) = \Theta(\tau 2^N). \tag{16.105}$$

Substituting the scaling for 2^N, we find the total time required:

$$T = \Theta(\tau \cdot (1/(\tau\epsilon))) = \Theta(\epsilon^{-1}). \tag{16.106}$$

Thus the total evolution time satisfies $T = \mathcal{O}(\epsilon^{-1})$, which is the Heisenberg scaling. This is precisely the resource scaling used by algorithms such as Kitaev's phase estimation, which we will discuss next in Section 16.9. ◇

An important remaining question is whether special deterministic structure in the times t_j is necessary for Heisenberg scaling. The next example shows that random long-time samples are not ruled out by the Cramér-Rao bound.

Example 16.18 (Randomly chosen evolution times)**.** Let us revisit Example 16.16. The key limitation of using linearly spaced times is that the sum of squares of the evolution times grows too slowly with the maximum evolution time. This suggests that we should sample longer times more frequently.

Consider a sequence of N measurements where each evolution time t_j is chosen independently and randomly from a Gaussian distribution with mean 0 and variance σ^2, i.e., $t_j \sim \mathcal{N}(0, \sigma^2)$. The sum of squares of the evolution times is a random variable, which can be approximated by its expected value:

$$\sum_{j=1}^{N} t_j^2 \approx N\mathbb{E}[t_j^2] = N\sigma^2. \tag{16.107}$$

To satisfy the CRB for a precision ϵ, we set

$$N\sigma^2 = \Theta(1/\epsilon^2). \tag{16.108}$$

If we set $\sigma = \Theta(1/\epsilon)$, then it is sufficient to choose $N = \Theta(1)$, which is a constant independent of ϵ. The total evolution time is

$$T = \sum_{j=1}^{N} |t_j| \approx N\mathbb{E}[|t_j|] = N\sigma\sqrt{\frac{2}{\pi}} = \Theta(1/\epsilon). \tag{16.109}$$

At the level of Fisher information, this is compatible with Heisenberg scaling. Note that the Cramér-Rao bound gives only a lower bound on the variance of locally unbiased estimators and does not show that the bound is attained. Therefore one cannot conclude from this calculation alone that a constant number of random samples suffices for a fixed success probability. A practical randomized strategy will be discussed in Section 18.5. ◇

16.9. Kitaev's phase estimation algorithm

Kitaev's method (see, for example, [KSV02, Section 13.5]) provides an easy-to-understand example of an iterative phase estimation algorithm that, unlike the previous example, is capable of reaching Heisenberg-limited scaling. Other approaches have also been proposed, with different tradeoffs in computational resources, queries to the underlying unitaries, and qubits [SHF13, WG16, KLY15]. Kitaev's main advantage lies in the simplicity of its analysis. It estimates the bits in a binary expansion of the phase recursively, using Hadamard-test data to localize the phase modulo 1 at each scale. The result is stated below.

Pseudo-code for Kitaev's phase estimation algorithm is given in Algorithm 16.1, where M is a parameter that controls the number of repetitions of the Hadamard test at each scale. The main claim that we wish to prove about the algorithm is given below. We state it for the simpler case where the phase is an exact binary fraction. This restriction can be removed, but doing so complicates the argument. We also focus on the case where the input is a single eigenstate of the

Algorithm 16.1 Kitaev's phase estimation algorithm

Prepare state $|\psi\rangle$.
for $j = d, \dots, 1$ **do**
  for $k = 1, \dots, M$ **do**
    Apply $W(2^{j-1}; \theta = 0)$ to $|0\rangle |\psi\rangle$ and measure the ancillary qubit.
    Store the outcome as $\nu_C[j,k] \in \{0,1\}$.
    Apply $W(2^{j-1}; \theta = \pi/2)$ to $|0\rangle |\psi\rangle$ and measure the ancillary qubit.
    Store the outcome as $\nu_S[j,k] \in \{0,1\}$.
  end for
  $P_C[j] \leftarrow \frac{1}{M} \sum_{k=1}^{M} (-1)^{\nu_C[j,k]}$
  $P_S[j] \leftarrow \frac{1}{M} \sum_{k=1}^{M} (-1)^{\nu_S[j,k]}$
  $\hat{\beta}[j] \leftarrow \frac{1}{2\pi} \operatorname{atan2}(P_S[j], P_C[j]) \bmod 1$
  $\beta[j] \leftarrow$ the element of $\{0.000, \dots, 0.111\}$ closest to $\hat{\beta}[j]$
end for
Set $0.b_d b_{d+1} b_{d+2} \leftarrow \beta[d]$.
for $j = d-1, \dots, 1$ **do**
  $b_j \leftarrow \begin{cases} 0 & \text{if } |0.0 b_{j+1} b_{j+2} - \beta[j]| \bmod 1 < 1/4 \\ 1 & \text{if } |0.1 b_{j+1} b_{j+2} - \beta[j]| \bmod 1 < 1/4 \end{cases}$
end for
return $\phi = 2\pi(0.b_1 \cdots b_{d+2})$ as estimate of phase

unitary. As discussed previously, for a general input the method projects the state onto one of the eigenvectors in its support.

Proposition 16.19 (Complexity of Kitaev's phase estimation algorithm)**.** *Let U be a unitary operator and let $|\psi\rangle$ be an eigenstate such that, for an integer $d > 0$,*

$$U |\psi\rangle = e^{i\phi} |\psi\rangle, \qquad \phi = 2\pi(0.b_1 \dots b_{d+2}), \qquad b_j \in \{0,1\}. \tag{16.110}$$

There exists a choice $M = \mathcal{O}(\log(d/\delta))$ such that Algorithm 16.1 returns the correct value of ϕ with probability at least $1 - \delta$ using

$$\mathcal{O}(2^d \log(d/\delta)) \tag{16.111}$$

queries to U. In particular, for precision $\epsilon = 2^{-d}$, the query complexity is $\widetilde{\mathcal{O}}(\epsilon^{-1})$, so Kitaev's phase estimation algorithm achieves Heisenberg-limited scaling up to logarithmic factors.

Proof. For each $j \in \{1, \dots, d\}$, define

$$\alpha_j := \frac{2^{j-1}\phi}{2\pi} \bmod 1 = 0.b_j b_{j+1} \cdots b_{d+2}. \tag{16.112}$$

We first identify the quantities estimated by the Hadamard-test data. Let $t_j = 2^{j-1}$. By Eq. (16.84), for an eigenstate input with eigenvalue $e^{i\phi}$,

$$\mathbb{P}(0 \mid t_j, \theta) = \cos^2\left(\frac{t_j \phi - \theta}{2}\right). \tag{16.113}$$

Therefore, if $\nu_C[j,k]$ is the measurement outcome obtained from $W(t_j;\theta=0)$ and $\nu_S[j,k]$ is the outcome obtained from $W(t_j;\theta=\pi/2)$, then

$$\mathbb{E}[(-1)^{\nu_C[j,k]}] = \cos(t_j\phi) = \cos(2\pi\alpha_j), \tag{16.114}$$

and

$$\mathbb{E}[(-1)^{\nu_S[j,k]}] = \sin(t_j\phi) = \sin(2\pi\alpha_j). \tag{16.115}$$

Hence $P_C[j]$ and $P_S[j]$ are unbiased estimators for the cosine and sine of the phase $2\pi\alpha_j$.

We next control the estimation error. Since each random variable $(-1)^{\nu_C[j,k]}$ and $(-1)^{\nu_S[j,k]}$ takes values in $\{\pm1\}$, Hoeffding's inequality gives, for any $\eta>0$,

$$\mathbb{P}\Big(|P_C[j]-\cos(2\pi\alpha_j)|\ge\eta\Big)\le 2e^{-M\eta^2/2}, \tag{16.116}$$

and the same bound holds for $P_S[j]$. Choosing $\eta=1/16$ and then choosing $M\ge c\log(d/\delta)$ for a sufficiently large absolute constant c, a union bound over all $2d$ such events shows that, with probability at least $1-\delta$,

$$|P_C[j]-\cos(2\pi\alpha_j)|\le\frac{1}{16},\qquad |P_S[j]-\sin(2\pi\alpha_j)|\le\frac{1}{16},\qquad j=1,\dots,d. \tag{16.117}$$

Let $z_j:=e^{i2\pi\alpha_j}, w_j:=P_C[j]+iP_S[j]$. Then $|w_j-z_j|\le\frac{\sqrt{2}}{16}<\frac{1}{8}$. Since $|z_j|=1$, it follows that $|w_j|\ge 7/8$. On the annulus $\{w\in\mathbb{C}:|w|\ge 7/8\}$, the argument map is Lipschitz with a universal constant, so the phase extracted from w_j by atan2 differs from the phase of z_j by less than $\pi/8$. Equivalently,

$$\Big|\hat\beta[j]-\alpha_j\Big|_{\bmod 1}<\frac{1}{16},\qquad j=1,\dots,d. \tag{16.118}$$

By definition, $\beta[j]$ is the 3-bit fraction closest to $\hat\beta[j]$, so

$$\Big|\beta[j]-\hat\beta[j]\Big|_{\bmod 1}\le\frac{1}{16}. \tag{16.119}$$

Hence

$$|\beta[j]-\alpha_j|_{\bmod 1}<\frac{1}{8},\qquad j=1,\dots,d. \tag{16.120}$$

We now prove that the classical post-processing recovers all bits correctly. For the base case $j=d$, the number $\alpha_d=0.b_db_{d+1}b_{d+2}$ is itself a 3-bit fraction. Since the distinct elements of $\{0.000,\dots,0.111\}$ are separated by distance $1/8$ modulo 1, Eq. (16.120) implies that $\beta[d]=\alpha_d$. Thus the initialization step recovers b_d,b_{d+1},b_{d+2} exactly.

For the induction step, assume that b_{j+1} and b_{j+2} have already been determined correctly. Set

$$\gamma_0:=0.0b_{j+1}b_{j+2},\qquad \gamma_1:=0.1b_{j+1}b_{j+2}. \tag{16.121}$$

Then γ_{b_j} agrees with the first three bits of α_j, so

$$\Big|\alpha_j-\gamma_{b_j}\Big|_{\bmod 1}<\frac{1}{8}. \tag{16.122}$$

Combining this with Eq. (16.120) gives

$$\Big|\beta[j]-\gamma_{b_j}\Big|_{\bmod 1}\le|\beta[j]-\alpha_j|_{\bmod 1}+\Big|\alpha_j-\gamma_{b_j}\Big|_{\bmod 1}<\frac{1}{16}+\frac{1}{8}<\frac{1}{4}. \tag{16.123}$$

On the other hand,

$$|\gamma_0 - \gamma_1|_{\bmod 1} = \frac{1}{2}, \tag{16.124}$$

so both inequalities in the decision rule cannot hold simultaneously. Therefore the rule

$$b_j \leftarrow \begin{cases} 0 & \text{if } |0.0b_{j+1}b_{j+2} - \beta[j]|_{\bmod 1} < 1/4, \\ 1 & \text{if } |0.1b_{j+1}b_{j+2} - \beta[j]|_{\bmod 1} < 1/4 \end{cases} \tag{16.125}$$

recovers the correct value of b_j. By descending induction, all bits $b_1, \ldots, b_{d+2}$ are recovered exactly.

It remains to count queries. For each fixed j, one execution of $W(2^{j-1}; \theta)$ uses 2^{j-1} queries to U, and the algorithm performs $2M$ such experiments, one for each of the two values of θ, so the query cost at level j is

$$\mathcal{O}(M 2^{j-1}). \tag{16.126}$$

Summing over $j = 1, \ldots, d$ gives the total query complexity

$$\sum_{j=1}^{d} \mathcal{O}(M 2^{j-1}) = \mathcal{O}(M 2^d) = \mathcal{O}(2^d \log(d/\delta)). \tag{16.127}$$

Since $\epsilon = 2^{-d}$, this is $\widetilde{\mathcal{O}}(\epsilon^{-1})$, which is Heisenberg-limited scaling up to logarithmic factors. □

If only the first d bits of the phase are retained, the natural accuracy guarantee is

$$\left|\widetilde{\phi}/(2\pi) - \phi/(2\pi)\right|_{\bmod 1} < 2^{-d}, \tag{16.128}$$

where $\widetilde{\phi}$ denotes the truncated d-bit output.

Now that we have gone over the theory, it may be instructive to consider a small instance of Kitaev's phase estimation procedure.

Example 16.20. Consider $\frac{\phi}{2\pi} = 0.b_1b_2b_3b_4b_5 = 0.11111$, and take $d = 3$. Then

$$\alpha_1 = 0.11111, \qquad \alpha_2 = 0.1111, \qquad \alpha_3 = 0.111. \tag{16.129}$$

The possible rounded values of $\beta[j]$ are

j	α_j	possible $\beta[j]$
1	0.11111	$\{0.111, 0.000\}$
2	0.1111	$\{0.111, 0.000\}$
3	0.111	$\{0.111\}$

Start with $j = 3$. Since $\beta[3] = 0.111$, the initialization step recovers $0.b_3b_4b_5 = 0.111$. For $j = 2$, if $\beta[2] = 0.111$, then Eq. (16.125) yields $b_2 = 1$. If $\beta[2] = 0.000$, then

$$|0.011 - 0.000|_{\bmod 1} = \frac{3}{8} > \frac{1}{4}, \qquad |0.111 - 0.000|_{\bmod 1} = \frac{1}{8} < \frac{1}{4}, \tag{16.130}$$

so the same rule still gives $b_2 = 1$. Repeating the argument for $j = 1$ gives $b_1 = 1$. Hence the algorithm recovers $\phi/(2\pi) = 0.11111$ exactly. ◇

Example 16.21. Let us try to relax the requirement of Kitaev's algorithm as follows: for each j, α_j is determined to precision $1/8$, and we round the result to $\beta[j] \in \{\,0.00, 0.01, 0.10, 0.11\,\}$. Start from the 2-bit estimate obtained from $\beta[3]$. Then for $j = 2, 1$, we assign

$$b_j = \begin{cases} 0, & |0.0b_{j+1} - \beta[j]|_{\bmod 1} < 1/2, \\ 1, & |0.1b_{j+1} - \beta[j]|_{\bmod 1} < 1/2. \end{cases} \tag{16.131}$$

Here the two candidates are separated by exactly $1/2$ modulo 1, so the threshold $< 1/2$ leaves open the possibility that both candidates are compatible with the observed value.

Let us run the algorithm above for

$$\frac{\phi}{2\pi} = 0.b_1b_2b_3b_4 = 0.1111. \tag{16.132}$$

Then

j	α_j	possible $\beta[j]$
1	0.1111	$\{\,0.11, 0.00\,\}$
2	0.111	$\{\,0.11, 0.00\,\}$
3	0.11	$\{\,0.11\,\}$

Start with $j = 3$. Since $\beta[3] = 0.11$, we recover $0.b_3b_4 = 0.11$. Then for $j = 2$, if $\beta[2] = 0.11$, we obtain $b_2 = 1$. But if $\beta[2] = 0.00$, then

$$|0.01 - 0.00|_{\bmod 1} = \frac{1}{4} < \frac{1}{2}, \qquad |0.11 - 0.00|_{\bmod 1} = \frac{1}{4} < \frac{1}{2}. \tag{16.133}$$

Both candidates satisfy the decision rule, so b_2 is not determined uniquely. Thus this variant fails. ◇

16.10. Eigenstate projection for iterative phase estimation

The previous discussion shows that iterative phase estimation (IPE) can be used to learn an eigenphase to high precision with Heisenberg-limited scaling. The reader may notice, however, that the analysis provided was given only for the case where the initial state is an eigenstate of the unitary U. In contrast, the Fourier-based phase estimation process discussed in Section 16.4 can simultaneously estimate a phase and project the input state onto the corresponding eigenvector. Our aim in this section is to show that IPE possesses an analogous projective property. We demonstrate that the sequential application of IPE, as depicted in Fig. 16.7(c), can statistically approximate spectral projectors.

We begin by developing intuition for this behavior. Consider an arbitrary initial state expanded in the eigenbasis of U:

$$|\psi\rangle = \sum_j \beta_j \,|\psi_j\rangle\,, \tag{16.134}$$

where $U\,|\psi_j\rangle = e^{i\phi_j}\,|\psi_j\rangle$. For simplicity in this intuitive discussion, we assume the eigenphases ϕ_j are distinct modulo 2π.

Let us examine the effect of applying a single step of the IPE procedure, involving the unitary $W(t, \theta)$ followed by a measurement of the control qubit. Based on the likelihood derived in (16.84), the state evolves stochastically. If the outcome 0 is measured, the probability of this event is

$\mathbb{P}(0) = \sum_j |\beta_j|^2 \cos^2((\phi_j t - \theta)/2)$. The normalized post-measurement state is (ignoring global phases):

$$|\psi\rangle \mapsto \frac{1}{\sqrt{\mathbb{P}(0)}} \sum_j \beta_j \cos((\phi_j t - \theta)/2) \, |\psi_j\rangle \, . \tag{16.135}$$

A similar transformation involving sine terms occurs if the outcome 1 is measured.

This process can be viewed as a random walk, a topic that we will discuss in detail in **??** (alternatively it can be seen as a quantum analogue of Bayesian inference [WG15]). Note here that the probabilities of the outcomes of the measurements depend on the distribution of the β_j. If the process is repeated many times, we see that all the components of the vector will be multiplied by a sequence of cosines or sines of angles. This means that the coefficient β_j will be dramatically reduced for eigenvalues, ϕ_j, that are unlikely to produce the measured outcome. As the product of these outcomes leads to exponentially shrinking amplitudes, we would expect all but the most consistent eigenvectors with the measurement settings to all but vanish from the quantum state.

The stationary distributions for this process are simply $\beta_j = \delta_{jk}$ for any integer k. We can see by substituting this into the above equation that regardless of the outcome, the eigenstate remains stationary. Further, these stationary states are complete under the assumption that the ϕ_j are distinct modulo 2π. Thus if the iterative phase estimation process approaches a stationary distribution it must correspond to one of the eigenvectors.

While the above argument provides a strong intuitive case for why we expect iterative phase estimation to converge to a stationary distribution, it is difficult to reason about because of the fact that the update rule for the amplitudes is a non-linear function of the β_j. This means that it is difficult to rule out aperiodic transitions such as a chain of states of the form $|\psi\rangle \to |\phi\rangle \to |\psi\rangle$.

To provide a rigorous proof that IPE can statistically approximate the spectral projectors, we circumvent the complexities of the non-linear state dynamics by employing the principle of deferred measurement (see Section 2.6), which allows us to replace the sequence of intermediate measurements and classical feedback (used for adaptive choices of parameters) with an equivalent coherent quantum circuit where all measurements occur at the end. Writing each eigenphase as $\phi_k = 2\pi\varphi_k$ with $\varphi_k \in [0, 1)$, we measure phase errors using the periodic distance introduced in Eq. (16.32).

THEOREM 16.22. *Let U be a unitary operator with an orthonormal eigenbasis $\{|\psi_k\rangle\}$ and corresponding normalized eigenphases $\{\varphi_k\} \subset [0, 1)$, so that*

$$U \, |\psi_k\rangle = e^{i2\pi\varphi_k} \, |\psi_k\rangle \, . \tag{16.136}$$

Consider an iterative phase estimation (IPE) algorithm of the form in Fig. 16.7(c) involving N measurements, and let $\mathbf{m} \in \{0, 1\}^N$ denote the measurement record. Let $F : \{0, 1\}^N \to [0, 1)$ be the classical estimator for the normalized phase.

Assume the IPE algorithm satisfies the following performance guarantee: for any input eigenstate $|\psi_k\rangle$, the probability that the estimated phase is far from the true phase φ_k is bounded by δ, i.e.,

$$\mathbb{P}(|F(\mathbf{m}) - \varphi_k|_1 > \epsilon \,|\, \textit{input } \, |\psi_k\rangle) \leq \delta. \tag{16.137}$$

Then, for an arbitrary input state $|\psi\rangle = \sum_k \beta_k \, |\psi_k\rangle$, the IPE algorithm returns an estimate within ϵ of some true eigenphase φ_k with total probability at least $1 - \delta$. Moreover, for each k, the joint probability of obtaining an estimate within ϵ of φ_k and then finding the system in state $|\psi_k\rangle$ under an additional measurement in the eigenbasis is at least $|\beta_k|^2(1 - \delta)$.

PROOF. We construct a unitary circuit, denoted C_{IPE}, that coherently represents the entire N-step IPE protocol. This circuit acts on the system register, initialized to $|\psi\rangle$, and an N-qubit ancilla register, initialized to $|0\rangle^{\otimes N}$. The adaptive choices of parameters (t_j, θ_j), which depend on previous classical outcomes in the original protocol, are implemented coherently in C_{IPE} by controls on the preceding ancilla qubits. This yields a sequence of coherent operations $\mathcal{W}_j$, illustrated schematically below.

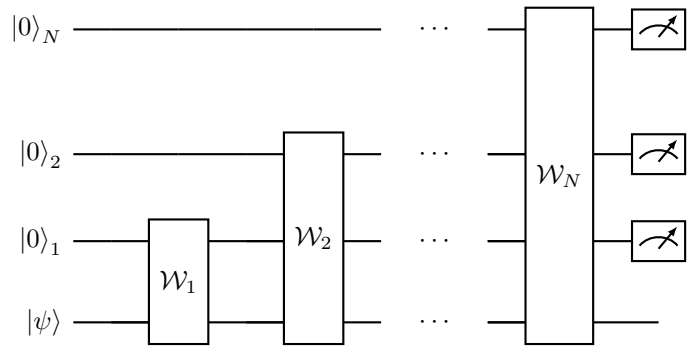


FIGURE 16.8. The structure of the deferred measurement circuit C_{IPE}. The unitaries $\mathcal{W}_j$ implement the adaptive steps coherently, entangling the j-th ancilla with the system.

We first analyze the action of C_{IPE} on an input eigenstate $|\psi_k\rangle$. In the IPE protocol, if the input is an eigenstate, then the system state remains unchanged throughout the process because the controlled-U operations only add phases. Therefore C_{IPE} preserves the system state:

$$C_{\mathrm{IPE}}(|0\rangle^{\otimes N} |\psi_k\rangle) = \sum_{\mathbf{m}\in\{0,1\}^N} \alpha_{\mathbf{m},k}(|\mathbf{m}\rangle |\psi_k\rangle). \tag{16.138}$$

The coefficients $\alpha_{\mathbf{m},k}$ determine the probability distribution of the measurement outcomes for the input $|\psi_k\rangle$, namely $|\alpha_{\mathbf{m},k}|^2 = \mathbb{P}(\mathbf{m}|\,|\psi_k\rangle)$.

Now consider the action of C_{IPE} on the superposition $|\psi\rangle = \sum_k \beta_k |\psi_k\rangle$. By the linearity of quantum mechanics, the final state before measurement is

$$|\Psi_{\mathrm{final}}\rangle = C_{\mathrm{IPE}}(|0\rangle^{\otimes N} |\psi\rangle) = \sum_{\mathbf{m},k} \beta_k \alpha_{\mathbf{m},k} |\mathbf{m}\rangle |\psi_k\rangle . \tag{16.139}$$

We now translate the performance guarantee into constraints on the coefficients $\alpha_{\mathbf{m},k}$. Define the success set S_k to be the set of measurement records that yield an estimate close to φ_k:

$$S_k = \{\mathbf{m} \in \{0,1\}^N : |F(\mathbf{m}) - \varphi_k|_1 \leq \epsilon\}. \tag{16.140}$$

The performance guarantee implies that for any k,

$$\sum_{\mathbf{m}\notin S_k} |\alpha_{\mathbf{m},k}|^2 \leq \delta, \quad \text{and consequently,} \quad \sum_{\mathbf{m}\in S_k} |\alpha_{\mathbf{m},k}|^2 \geq 1 - \delta. \tag{16.141}$$

We first bound the overall probability that the algorithm fails to return an accurate estimate for any of the eigenphases. Let $S = \bigcup_k S_k$ be the set of all outcomes that are successful for at least

one eigenphase. A failure occurs if we measure an outcome $\mathbf{m} \notin S$. Let $E = S^c$ be the set of failure outcomes.

The probability of failure is calculated from the state $|\Psi_{\text{final}}\rangle$:

$$\begin{aligned} \mathbb{P}(\text{Failure}) &= \sum_{\mathbf{m}\in E} \| (\langle \mathbf{m}| \otimes I) |\Psi_{\text{final}}\rangle \|^2 \\ &= \sum_{\mathbf{m}\in E} \left\| \sum_k \beta_k \alpha_{\mathbf{m},k} |\psi_k\rangle \right\|^2 . \end{aligned} \tag{16.142}$$

Since the eigenstates $\{|\psi_k\rangle\}$ are orthonormal, we have

$$\begin{aligned} \mathbb{P}(\text{Failure}) &= \sum_{\mathbf{m}\in E} \sum_k |\beta_k|^2 |\alpha_{\mathbf{m},k}|^2 \\ &= \sum_k |\beta_k|^2 \left(\sum_{\mathbf{m}\in E} |\alpha_{\mathbf{m},k}|^2 \right). \end{aligned} \tag{16.143}$$

By definition, if $\mathbf{m} \in E$, then $\mathbf{m} \notin S_k$ for all k. Thus $E \subseteq S_k^c$. Using the bound from Eq. (16.141), we have $\sum_{\mathbf{m}\in E} |\alpha_{\mathbf{m},k}|^2 \leq \sum_{\mathbf{m}\notin S_k} |\alpha_{\mathbf{m},k}|^2 \leq \delta$. Therefore,

$$\mathbb{P}(\text{Failure}) \leq \sum_k |\beta_k|^2 \delta = \delta \left(\sum_k |\beta_k|^2 \right) = \delta. \tag{16.144}$$

Thus, the total probability of success (obtaining an estimate within ϵ of some φ_k) is at least $1 - \delta$.

Finally, we determine the probability that the measurement record lies in S_k and that a subsequent ideal measurement of the system in the eigenbasis returns $|\psi_k\rangle$. This probability is obtained by applying the projector $\Pi_k = (\sum_{\mathbf{m}\in S_k} |\mathbf{m}\rangle\langle\mathbf{m}|) \otimes |\psi_k\rangle\langle\psi_k|$ to the final state $|\Psi_{\text{final}}\rangle$.

$$\mathbb{P}(S_k \text{ and system found in } |\psi_k\rangle) = \| \Pi_k |\Psi_{\text{final}}\rangle \|^2. \tag{16.145}$$

Applying the projector to the state in Eq. (16.139):

$$\begin{aligned} \Pi_k |\Psi_{\text{final}}\rangle &= \Pi_k \left(\sum_{\mathbf{m}',j} \beta_j \alpha_{\mathbf{m}',j} |\mathbf{m}'\rangle |\psi_j\rangle \right) \\ &= \sum_{\mathbf{m}\in S_k} \beta_k \alpha_{\mathbf{m},k} |\mathbf{m}\rangle |\psi_k\rangle . \end{aligned} \tag{16.146}$$

The probability is the squared norm of this state:

$$\begin{aligned} \mathbb{P}(S_k \text{ and system found in } |\psi_k\rangle) &= \sum_{\mathbf{m}\in S_k} |\beta_k|^2 |\alpha_{\mathbf{m},k}|^2 \\ &= |\beta_k|^2 \sum_{\mathbf{m}\in S_k} |\alpha_{\mathbf{m},k}|^2. \end{aligned} \tag{16.147}$$

Using the bound from Eq. (16.141), we conclude

$$\mathbb{P}(S_k \text{ and system found in } |\psi_k\rangle) \geq |\beta_k|^2 (1 - \delta). \tag{16.148}$$

This confirms that the IPE procedure assigns to each spectral projector essentially the same weight as the ideal Born rule, provided the algorithm is reliable for individual eigenstates. □

If we want the algorithm to identify the eigenphase unambiguously, the phases must be well separated. If $|\varphi_j - \varphi_k|_1 > 2\epsilon$ for all $j \neq k$, then the success sets S_j and S_k are disjoint. Otherwise there would exist an outcome $\mathbf{m} \in S_j \cap S_k$, and the triangle inequality would imply

$$|\varphi_j - \varphi_k|_1 \leq |\varphi_j - F(\mathbf{m})|_1 + |\varphi_k - F(\mathbf{m})|_1 \leq 2\epsilon, \tag{16.149}$$

which is a contradiction. This separation guarantees that a successful outcome $\mathbf{m}$ corresponds to a unique eigenphase. We generally cannot control deterministically which eigenstate the system collapses onto.

Theorem 16.22 shows that the measurement record assigns total weight close to $|\beta_j|^2$ to outcomes associated with φ_j. Equivalently, if one follows the protocol by an ideal measurement in the eigenbasis, then the joint probability of reporting a phase near φ_j and finding $|\psi_j\rangle$ is at least $|\beta_j|^2(1-\delta)$. This conclusion is determined solely by the initial amplitudes and is independent of the strategy used to select the control phases θ_k and evolution times t_k, provided the strategy is reliable on each eigenstate.

The IPE process can therefore be interpreted as a measurement channel that approximately resolves the spectral projectors of U. If we ignore the classical measurement record D, the induced channel suppresses coherences between eigencomponents that produce distinguishable outcome distributions. When the eigenphases are well resolved by the protocol, this behaves like an approximate dephasing channel in the eigenbasis of U.

If we possess prior knowledge about the spectrum and wish to target a specific eigenstate, we may choose the control phases θ_k appropriately to infer the final state by conditioning on the measurement outcomes D. Specifically, if we align the control phase with the target eigenphase, we maximize the probability of obtaining the 0 outcome for that state. Observing a sequence of 0 outcomes then strongly correlates with successful filtering toward the target state. Proposition 16.23 shows that if we observe a sequence of all zeros when the control phases θ_k are aligned with a known eigenvalue ϕ_{k^*}, then the posterior state has high fidelity with the corresponding eigenstate.

Proposition 16.23. *Let $|\psi\rangle = \sum_j \beta_j |\psi_j\rangle$ be the initial state. Suppose we aim to prepare the eigenstate $|\psi_{k^*}\rangle$ corresponding to a known eigenphase ϕ_{k^*}. Assume $|\beta_{k^*}|^2 > 0$. We perform N IPE steps using a fixed evolution time $t_k = t$ and a fixed control phase $\theta_k = t\phi_{k^*}$. Assume t is chosen such that for all $j \neq k^*$ (where $\beta_j \neq 0$), $(\phi_{k^*} - \phi_j)t \neq 0 \pmod{2\pi}$. Let $D = \{0\}^N$ be the event that all measurement outcomes are 0. Then, conditioned on observing $D = \{0\}^N$, the squared fidelity with the target pure state satisfies*

$$F(|\psi_N\rangle\langle\psi_N|, |\psi_{k^*}\rangle\langle\psi_{k^*}|)^2 \geq 1 - \frac{1 - |\beta_{k^*}|^2}{|\beta_{k^*}|^2} R^N, \tag{16.150}$$

where

$$R = \max_{j \neq k^*, \beta_j \neq 0} \cos^2((\phi_{k^*} - \phi_j)t/2) < 1. \tag{16.151}$$

The probability of observing $D = \{0\}^N$ is at least $|\beta_{k^*}|^2$.

Proof. In each step k, the likelihood of observing outcome 0 given the state $|\psi_j\rangle$ is

$$\mathbb{P}(0 \,|\, \text{input } |\psi_j\rangle) = \cos^2((\phi_{k^*} - \phi_j)t/2). \tag{16.152}$$

For the target state $|\psi_{k^*}\rangle$, the likelihood is $\mathbb{P}(0 \,|\, \text{input } |\psi_{k^*}\rangle) = \cos^2(0) = 1$. For $j \neq k^*$, let $R_j = \cos^2((\phi_{k^*} - \phi_j)t/2)$. By the assumption on t, $R_j < 1$. Let R be the maximum as defined in the proposition statement. The probability for observing $D = \{0\}^N$ given $|\psi_j\rangle$ is $\mathbb{P}(D \,|\, \text{input } |\psi_j\rangle) = R_j^N$.

The probability of observing this specific outcome sequence D is:

$$\mathbb{P}(D) = \sum_j |\beta_j|^2 \mathbb{P}(D \,|\, \text{input } |\psi_j\rangle) = |\beta_{k^*}|^2 + \sum_{j \neq k^*} |\beta_j|^2 R_j^N. \tag{16.153}$$

Thus, we have $\mathbb{P}(D) \geq |\beta_{k^*}|^2$.

For pure states, fidelity satisfies

$$F(|\psi_N\rangle\langle\psi_N|, |\psi_{k^*}\rangle\langle\psi_{k^*}|) = |\langle\psi_{k^*}|\psi_N\rangle|. \tag{16.154}$$

Hence the squared fidelity is determined by the posterior probability $\mathbb{P}(\phi_{k^*}|D) = |\langle\psi_{k^*}|\psi_N\rangle|^2$. We have

$$\begin{aligned} F(|\psi_N\rangle\langle\psi_N|, |\psi_{k^*}\rangle\langle\psi_{k^*}|)^2 = \mathbb{P}(\phi_{k^*}|D) &= \frac{|\beta_{k^*}|^2 \mathbb{P}(D \,|\, \text{input } |\psi_{k^*}\rangle)}{\mathbb{P}(D)} \\ &= \frac{|\beta_{k^*}|^2}{|\beta_{k^*}|^2 + \sum_{j \neq k^*} |\beta_j|^2 R_j^N} \\ &= 1 - \frac{\sum_{j \neq k^*} |\beta_j|^2 R_j^N}{|\beta_{k^*}|^2 + \sum_{j \neq k^*} |\beta_j|^2 R_j^N} \\ &\geq 1 - \frac{\sum_{j \neq k^*} |\beta_j|^2 R^N}{|\beta_{k^*}|^2} = 1 - \frac{1 - |\beta_{k^*}|^2}{|\beta_{k^*}|^2} R^N, \end{aligned} \tag{16.155}$$

where we used $R_j \leq R$ for all $j \neq k^*$. The fidelity thus approaches 1 exponentially with the number of measurements N. □

Notes and further reading

In this chapter we have provided the foundation of quantum phase estimation including specific implementations for the most popular forms of phase estimation: Fourier-based QPE and Kitaev's Iterative QPE algorithm. However, the subfield of phase estimation (and more broadly quantum metrology) is much broader than the discussion that we can fit in here. We will now provide a guide to help the reader further explore other approaches to either coherent or iterative phase estimation methods.

In many works, Kitaev's phase estimation algorithm is often used synonymously with iterative phase estimation but this is certainly not true. As we discussed above, there are many ways that we can choose experiments to improve upon these results. Examples of this strategy include the work of [SHF13] which provides two iterative phase estimation algorithms that yield advantages over Kitaev. The first involves directly using Bayesian inference to learn the phase through a sequence of chosen with t taken uniformly on $[0, 2^n - 1]$. This result is shown to yield optimal scaling with the number of measurements. It requires, however, an inefficient inference algorithm that requires a uniform grid of 2^n potential phases. The second result in this work that is relevant for iterative phase estimation uses an efficient inference scheme for learning the phase at price of requiring a small constant factor more applications of the unitary than the measurement optimal Bayesian strategy [GFWC12, WG16].

Other approaches seeking to achieve the optimal constant factor for the variance for Heisenberg-limited scaling use adaptive experiment design to learn eigenphases in iterative frameworks [BWB01, HBB$^+$07, HS10, WG16]. The method explicitly tracks the prior distribution for the phase and then actively designs the experiment that minimizes the posterior variance. Heuristic optimization to

this problem lead to scaling that approaches the optimal variance, often being within less than 10% deviation from the ultimate Heisenberg limit [RWS+17].

A further technique that has been widely used for phase estimation is robust phase estimation [KLY15]. Robust Phase Estimation comes from a very different genealogy than other phase estimation protocols: it arises from the quantum characterization community rather than the algorithms or quantum optics communities. The approach has several advantages including the fact that it does not require any ancillary qubits (as opposed to the one needed for iterative phase estimation). It further can be used to characterize the unknown angles in the single qubit unitary $e^{-i(\alpha X+\beta Y+\gamma Z)}$ while achieving Heisenberg limited scaling. However, despite these strengths it is not known to achieve the ideal constant factor in the Heisenberg limit.

Further parallelized versions of phase estimation have been developed [KOS07, RWS+17, ACC+22]. The idea behind these approaches is inspired by NOON state methods developed in the quantum optics community [BHB+09] to prepare a state of the form $(|0\rangle |\psi\rangle^{\otimes N} + |1\rangle U^{\otimes N} |\psi\rangle^{\otimes N})/\sqrt{2}$ which will multiply the eigenphase observed by a factor of N. This not only allows phase estimation to be parallelized in cases where copies of the same eigenstate can be efficiently prepared, it also allows the simulation time to be shortened for cases where we are interested in estimating the eigenvalues of a Hamiltonian and in turn allow methods such as QDrift to allow phase estimation to be performed in constant depth [ACC+22]. Additionally, in cases where Bayesian methods are used to combine at least two independent phase estimation experiments it can be seen that even without an entangled state that N independent quantum computers can combine their data from phase estimation to achieve a variance of $\pi/2N$, which is the optimal scaling possible for non-entangled inputs [RWS+17].

There is the remaining issue about optimality of phase estimation. While iterative phase estimation can achieve the Heisenberg limit, the arguments given above do not actually show that this is the ultimate limit in precision estimation. This ultimate limit has been shown to coincide with the Heisenberg limit using more sophisticated arguments based on the quantum Cramèr-Rao bound, which provides a limit on the achievable variance for an unbiased estimator after optimizing over all possible quantum POVMs that could be used to learn the parameter [ZPDK10]. This shows that the central intuition first gleaned from the energy-time uncertainty principle in fact does represent the ultimate limits of learning a fixed phase. The quantum Cramèr-Rao bound can also be used to understand ultimate limits yielded also are understood for the case where we have a phase that stochastically varies over time. For example, in the case of Brownian motion scaling of $\mathcal{O}(\epsilon^{-2/3})$ is optimal and can be saturated by modifying the phase estimation algorithm to track the drift of phase [BHW13].

Subsequent work has also led to improvements in amplitude estimation. The use of priors has also been shown to provide a substantial advantage for estimation of expectation values of projectors. Using the fact that a projector can be easily square-rooted, it is possible to use LCU circuitry to subtract an apriori estimate of the variable to be estimated and then use amplitude estimation to estimate the smaller value. Since amplitude estimation is polynomially more efficient for small angle estimation, this can lead to a substantial improvement in such estimates and even surpass the Heisenberg-limit if such prior knowledge is provided [SDM+24]. Additionally, other works have used gradient estimation to obtain expectation of vector valued quantities to obtain quadratically better scaling than amplitude estimation allows in the number of variables [HWM+22]. These results illustrate that more work can be done to optimize quantum expectation value estimation beyond amplitude amplification.

Part IV

Application

CHAPTER 17

Quantum walks

Classical random walks and Markov chain Monte Carlo methods are powerful tools for designing randomized algorithms, with applications including sampling, optimization, and approximate counting. A motivating example comes from the early internet: to rank the importance of a website, one could start at a well-known site and walk randomly by following links with equal probability. The probability that this random walk visits a particular site reflects its importance within the network. This intuition underlies Google's PageRank algorithm.

Quantum walks provide a natural quantum generalization of classical random walks and have been employed to design quantum algorithms that outperform their classical counterparts in several scenarios. We focus on reversible Markov chains because they admit a Hermitian representation via the discriminant matrix. This allows tools from block encoding, qubitization, and phase estimation to act directly on the quantized version of the walk dynamics.

We then discuss continuous-time quantum walks, where the graph adjacency matrix defines a Hamiltonian and the quantum state evolves via Schrödinger dynamics. We introduce the glued trees problem which demonstrates an exponential query separation. In this example, classical random walks become trapped near the graph center with exponentially small probability of reaching the exit, while continuous-time quantum walks exhibit coherent transport through the column space and reach the exit in polynomial time.

17.1. Markov chains and classical random walks

We first review basic notions for Markov chains, using the column-stochastic convention to align with a quantum formulation.

Definition 17.1 (Markov chain)**.** *Let Σ be a state space. A Markov chain on Σ is a sequence of random variables $X_1, X_2, \ldots$ taking values in Σ, and the probability of moving to the next state depends only on the current state. More precisely,*

(17.1)
$$\mathbb{P}(X_{t+1} = i \mid X_t = j, X_{t-1} = i_{t-1}, \ldots, X_1 = i_1) = \mathbb{P}(X_{t+1} = i \mid X_t = j), \qquad \forall t \geq 1,\ i, j, i_1, \ldots, i_{t-1} \in \Sigma.$$

When the state space Σ is finite, we say the Markov chain is finite. In this case, we may identify Σ with $\{0, 1, \ldots, N-1\}$ where $N := |\Sigma|$, and denote

$$\mathbb{P}(X_{t+1} = i \mid X_t = j) = P_{ij}, \qquad \forall t \geq 1,\ i, j \in \Sigma. \tag{17.2}$$

Here P is a column-stochastic (left-stochastic) matrix: $\sum_i P_{ij} = 1$ for all j and $P_{ij} \geq 0$.

The **stationary distribution** of the Markov chain is an eigenvector π of the transition matrix P with eigenvalue 1:

$$P\pi = \pi, \qquad \pi_i \geq 0, \qquad \sum_i \pi_i = 1. \tag{17.3}$$

Given a stationary distribution π, the goal of quantum algorithms is to prepare the coherent version of π:

$$|\pi\rangle = \sum_i \sqrt{\pi_i}\,|i\rangle\,, \tag{17.4}$$

which is a normalized quantum state. For a classical observable O (i.e., O is diagonal in the computational basis), the expectation of O with respect to π can be computed as $\langle\pi|O|\pi\rangle$, which is the same as the classical expectation $\mathbb{E}_\pi(O) = \sum_i \pi_i O_{ii}$.

The stationary distribution need not be unique. Even if P has a unique stationary distribution, the direct sum $P' := P \oplus P$ has at least two linearly independent stationary distributions, corresponding to probability mass supported on the first or the second copy. This corresponds to a Markov chain on the disjoint union of two copies of the same state space.

A Markov chain is called **irreducible** if for any two states $i, j \in \Sigma$ there exists a $t \in \mathbb{N}$ such that $[P^t]_{ij} > 0$. Let $\mathcal{T}(i) := \{t \geq 1 : [P^t]_{ii} > 0\}$ be the set of return times to i. The **period** of i is defined as the greatest common divisor of $\mathcal{T}(i)$. A Markov chain is called **aperiodic** if the period of every state is one. For a finite, irreducible, and aperiodic Markov chain, there exists $t \in \mathbb{N}$ such that $[P^t]_{ij} > 0$ for all $i, j \in \Sigma$ [LP17, Proposition 1.7].

To proceed further, we first introduce the Perron theorem for matrices with positive entries [HJ91, Theorem 8.2.8]. This is a special case of the Perron–Frobenius theorem for nonnegative matrices.

THEOREM 17.2 (Perron). *Let $A \in \mathbb{R}^{N\times N}$ with all positive entries. Then it has a simple eigenvalue equal to its spectral radius $\rho(A)$. The corresponding eigenvector v can be chosen to have positive entries, i.e., $v_i > 0$ for all i, and is unique up to scaling. All other eigenvalues λ of A satisfy $|\lambda| < \rho(A)$.*

For stochastic matrices, the spectral radius is 1. Let us use Perron's theorem to show the existence of a **spectral gap**.

Proposition 17.3. *Let P be the transition matrix of a finite, irreducible and aperiodic Markov chain. Then it has a unique stationary distribution π with eigenvalue 1. Moreover, there exists $\gamma \in (0, 1]$ such that every eigenvalue $\lambda \neq 1$ of P satisfies $|\lambda| \leq 1 - \gamma$.*

PROOF. From the assumptions, there exists $t \in \mathbb{N}$ such that P^t is a positive matrix. Let π be the eigenvector of P^t corresponding to the unique maximal eigenvalue with positive entries. Since P^t is column-stochastic,

$$\sum_{i,j} (P^t)_{ij}\pi_j = \sum_j \pi_j. \tag{17.5}$$

Therefore the corresponding eigenvalue is 1. We may normalize π so that $\sum_i \pi_i = 1$. From

$$P^t(P\pi) = P(P^t\pi), \tag{17.6}$$

we find that $P\pi$ is also an eigenvector of P^t with eigenvalue 1. By the uniqueness of the eigenvector, we have $P\pi = \pi$, i.e., π is the unique stationary distribution of P. By the Perron theorem, all other eigenvalues of P^t have absolute value strictly less than 1, so there exists $\gamma' > 0$ such that they are all bounded in absolute value by $1 - \gamma'$. Therefore if there is an eigenvector v of P with eigenvalue $\lambda \neq 1$, then v is an eigenvector of P^t and $|\lambda|^t \leq 1 - \gamma'$. The result then follows once we define $1 - \gamma = (1 - \gamma')^{1/t}$. □

Throughout most of this chapter, we will study a narrower family of Markov chains known as **reversible Markov chains**, for which every allowed transition has a corresponding reverse transition.

Definition 17.4 (Reversibility, or detailed balance)**.** *A Markov chain is **reversible** if there is a stationary distribution π such that the transition matrix P satisfies the **detailed balance condition**:*

$$P_{ji}\pi_i = P_{ij}\pi_j, \qquad \forall i, j \in \Sigma. \tag{17.7}$$

One immediate consequence of reversibility is that π must be a stationary distribution, since summing over i yields $\sum_i P_{ji}\pi_i = \sum_i P_{ij}\pi_j = \pi_j$.

Example 17.5. Let Σ be the set of all n-bit strings $\{0,1\}^n$, and $E(i)$ be a real-valued function on Σ, which is called the energy of the state i. The stationary distribution of interest is the Gibbs distribution

$$\pi_i := \frac{e^{-\beta E(i)}}{Z}, \qquad Z := \sum_{i\in\Sigma} e^{-\beta E(i)}, \tag{17.8}$$

with inverse temperature $\beta > 0$.

The **Metropolis–Hastings Markov chain** is constructed as follows. Given a current state $i \in \Sigma$, pick a uniformly random bit position $\ell \in \{1, \dots, n\}$, and let j be the configuration obtained from i by flipping the ℓ-th bit. This defines a proposal kernel Q by

$$Q_{ji} := \frac{1}{n} \quad \text{if } i \text{ and } j \text{ differ in exactly one bit}, \qquad Q_{ji} := 0 \text{ otherwise}, \tag{17.9}$$

so that $Q_{ji} = Q_{ij}$. Accept the proposal with probability

$$\alpha_{ji} := \min\{1, e^{-\beta(E(j)-E(i))}\}. \tag{17.10}$$

The resulting transition matrix P is given by

$$P_{ji} := Q_{ji}\alpha_{ji} \quad (j \neq i), \qquad P_{ii} := 1 - \sum_{j\neq i} P_{ji}. \tag{17.11}$$

Then P is column-stochastic by construction, and π is stationary because P satisfies detailed balance: for $i \neq j$ with $Q_{ji} > 0$,

$$\begin{aligned} \pi_i P_{ji} &= \frac{e^{-\beta E(i)}}{Z} Q_{ji} \min\{1, e^{-\beta(E(j)-E(i))}\} \\ &= \frac{e^{-\beta E(j)}}{Z} Q_{ij} \min\{1, e^{-\beta(E(i)-E(j))}\} = \pi_j P_{ij}, \end{aligned} \tag{17.12}$$

and summing over i yields $\sum_i P_{ji}\pi_i = \pi_j$. ◇

We define the **discriminant matrix** associated with a Markov chain as

$$D := \sum_{i,j} \sqrt{P_{ij}P_{ji}}\, |i\rangle\langle j|, \tag{17.13}$$

which is real symmetric and hence Hermitian. For a reversible Markov chain, the stationary state can be encoded as an eigenvector of D. This is shown in the following proposition.

Proposition 17.6 (Discriminant matrix of a reversible Markov chain)**.** *For a finite, irreducible, aperiodic and reversible Markov chain, the coherent version of the stationary state in Eq.* (17.4) *is an eigenvector of the discriminant matrix D satisfying*

$$D\,|\pi\rangle = |\pi\rangle\,. \tag{17.14}$$

Furthermore, we have

$$D = \mathrm{diag}(\sqrt{\pi})P^\top \,\mathrm{diag}(\sqrt{\pi})^{-1} = \mathrm{diag}(\sqrt{\pi})^{-1}P\,\mathrm{diag}(\sqrt{\pi}). \tag{17.15}$$

Therefore the set of eigenvalues of P and the set of the eigenvalues of D are the same.

Proof. Direct computation shows

$$\langle i|\,D\,|\pi\rangle = \sum_j \sqrt{P_{ij}P_{ji}\pi_j} = \sum_j P_{ji}\sqrt{\pi_i} = \sqrt{\pi_i}. \tag{17.16}$$

In the second equality we use the detailed balance condition, and the third equality uses the column-stochasticity of P. Therefore $|\pi\rangle$ is an eigenvector of D with eigenvalue 1.

Next we will proceed to prove (17.15):

(17.17)

$$\mathrm{diag}(\sqrt{\pi})P^\top \,\mathrm{diag}(\sqrt{\pi})^{-1} = \sum_{i,j}\frac{\sqrt{\pi_i}}{\sqrt{\pi_j}}P_{ji}|i\rangle\langle j| = \sum_{i,j}\frac{\sqrt{P_{ji}\pi_i}}{\sqrt{P_{ij}\pi_j}}\sqrt{P_{ij}P_{ji}}|i\rangle\langle j| = \sum_{i,j}\sqrt{P_{ij}P_{ji}}|i\rangle\langle j| = D.$$

Here we again use the detailed balance condition. Similarly

(17.18)

$$\mathrm{diag}(\sqrt{\pi})^{-1}P\,\mathrm{diag}(\sqrt{\pi}) = \sum_{i,j}\frac{\sqrt{\pi_j}}{\sqrt{\pi_i}}P_{ij}|i\rangle\langle j| = \sum_{i,j}\frac{\sqrt{P_{ij}\pi_j}}{\sqrt{P_{ji}\pi_i}}\sqrt{P_{ij}P_{ji}}|i\rangle\langle j| = \sum_{i,j}\sqrt{P_{ij}P_{ji}}|i\rangle\langle j| = D.$$

□

Since the discriminant matrix is real and symmetric, D is diagonalizable with real eigenvalues and orthogonal eigenvectors.

$$D\,|v_j\rangle = \lambda_j\,|v_j\rangle\,, \quad \langle v_j|v_k\rangle = \delta_{jk}. \tag{17.19}$$

Proposition 17.6 immediately implies that the transition matrix P corresponding to a reversible Markov chain is also diagonalizable as $P|\lambda_j\rangle\!\rangle = \lambda_j|\lambda_j\rangle\!\rangle$. Here the (unnormalized) eigenvectors $|\lambda_j\rangle\!\rangle$ can be chosen as

$$|\lambda_j\rangle\!\rangle = \mathrm{diag}(\sqrt{\pi})\,|v_j\rangle\,. \tag{17.20}$$

We order the eigenvalues $\{\lambda_j\}$ in non-increasing order with $\lambda_0 = 1$ and $|v_0\rangle = |\pi\rangle$. Then $|\lambda_0\rangle\!\rangle = \pi$, viewed as a column vector.

The following is often referred to as the **convergence theorem** for Markov chains.

Theorem 17.7. *Let P be the transition matrix of a finite, irreducible and aperiodic Markov chain with stationary distribution π. Then there exists a constant $\gamma \in (0,1]$ and $C > 0$ such that for any initial probability distribution ρ,*

$$\left\|P^t\rho - \pi\right\|_1 \le C(1-\gamma)^t, \qquad t \in \mathbb{N}. \tag{17.21}$$

While we do not prove Theorem 17.7 directly (see e.g. [LP17, Theorem 4.9]), we will show a more refined result for reversible Markov chains.

Proposition 17.8. *Let P be the transition matrix of a finite, irreducible, aperiodic and reversible Markov chain on a state space Σ of size $N := |\Sigma|$, and let γ be its spectral gap. Let π be the unique stationary distribution. Then from any initial distribution ρ, for any $\delta > 0$, there exists a positive integer t^* such that*

$$\left\|P^t\rho - \pi\right\|_1 \leq \delta, \qquad t \geq t^*. \tag{17.22}$$

where

$$t^* = \left\lceil \log\left(\frac{\sqrt{N/\min_i \pi_i}}{\delta}\right) / \log\left(\frac{1}{1-\gamma}\right) \right\rceil. \tag{17.23}$$

Proof. Because P is diagonalizable with real eigenvalues $\{\lambda_j\}_{j=0}^{N-1}$, using Eq. (17.19), we can express the probability vector ρ in the eigenbasis of P as

$$\rho = \sum_{j=0}^{N-1} \alpha_j |\lambda_j\rangle\!\rangle = \sum_{j=0}^{N-1} \alpha_j \operatorname{diag}(\sqrt{\pi})\,|v_j\rangle\,. \tag{17.24}$$

Here we set $\lambda_0 = 1$ and $|\lambda_0\rangle\!\rangle = \pi$, and we define the spectral gap γ by $1 - \gamma := \max_{j\geq 1} |\lambda_j|$. We then have

$$\alpha_j = \langle v_j| \operatorname{diag}(\sqrt{\pi})^{-1}\rho\rangle\,. \tag{17.25}$$

In particular,

$$\alpha_0 = \sum_i \rho_i = 1, \tag{17.26}$$

For any positive integer t,

$$P^t\rho = \pi + \sum_{j=1}^{N-1} \alpha_j \lambda_j^t \operatorname{diag}(\sqrt{\pi})\,|v_j\rangle\,. \tag{17.27}$$

Then using the Cauchy-Schwarz inequality,

$$\left\|\operatorname{diag}(\sqrt{\pi})\,|v_j\rangle\right\|_1 \leq \sqrt{\sum_i \pi_i}\ \||v_j\rangle\| = 1, \tag{17.28}$$

and

$$\left\|P^t\rho - \pi\right\|_1 \leq \sum_{j=1}^{N-1} |\alpha_j|\,|\lambda_j|^t \leq (1-\gamma)^t \sum_{j=1}^{N-1} |\alpha_j| \leq (1-\gamma)^t\sqrt{N}\sqrt{\sum_{j=1}^{N-1} |\alpha_j|^2}. \tag{17.29}$$

Furthermore by the resolution of the identity and the fact that $\{|v_j\rangle\}$ is an orthonormal basis,

$$\sum_{j=1}^{N-1} |\alpha_j|^2 \leq \sum_{j=1}^{N-1} \langle \operatorname{diag}(\sqrt{\pi})^{-1}\rho|v_j\rangle\,\langle v_j|\operatorname{diag}(\sqrt{\pi})^{-1}\rho\rangle \leq \sum_i \rho_i^2\pi_i^{-1} \leq \frac{\sum_i \rho_i}{\min_i \pi_i} = \frac{1}{\min_i \pi_i}, \tag{17.30}$$

we obtain

$$\left\|P^t\rho - \pi\right\|_1 \leq (1-\gamma)^t\sqrt{\frac{N}{\min_i \pi_i}}. \tag{17.31}$$

For the ℓ_1 distance (or total variation distance) to be at most δ, it suffices to take

$$t \geq \frac{\log(\frac{\sqrt{N/\min_i \pi_i}}{\delta})}{\log\left(\frac{1}{1-\gamma}\right)}. \tag{17.32}$$

□

Using the fact that $\frac{1}{\log \frac{1}{1-\gamma}} \approx \frac{1}{\gamma}$ when γ is small, we find that the time t^* is inversely proportional to the spectral gap γ.

Example 17.9. Consider the simple random walk on the d-dimensional hypertorus $(\mathbb{Z}_L)^d$, viewed as a graph $G = (V, E)$ with vertex set $V = (\mathbb{Z}_L)^d$ and edges between vertices at graph distance one. Assume that $L \geq 3$ is odd, so that the walk is aperiodic, and note that $|V| = L^d$. The walker can move in each of the $2d$ cardinal directions.

For $x, y \in V$, let $\mathrm{dist}(x, y)$ denote the graph distance. In the column-stochastic convention,

$$P_{yx} := \mathbb{P}(X_{t+1} = y \mid X_t = x) = \begin{cases} \frac{1}{2d}, & \text{if } \mathrm{dist}(x,y) = 1, \\ 0, & \text{otherwise.} \end{cases} \tag{17.33}$$

By symmetry the stationary distribution is uniform, i.e.,

$$\pi_x = \frac{1}{|V|}, \qquad x \in V. \tag{17.34}$$

It is stationary since $P\pi = \pi$. Moreover, for any $x, y \in V$ with $\mathrm{dist}(x, y) = 1$,

$$P_{yx}\pi_x = \frac{1}{2d\,|V|} = P_{xy}\pi_y. \tag{17.35}$$

Thus the detailed balance condition is satisfied and the walk is reversible.

Since P is symmetric, the discriminant matrix satisfies $D = P$. Let

$$T := \sum_{i \in \mathbb{Z}_L} |i+1\rangle\langle i|, \tag{17.36}$$

where addition is modulo L. Then

$$D = P = \frac{1}{2d} \sum_{\nu=1}^{d} I^{\otimes(\nu-1)} \otimes (T + T^\top) \otimes I^{\otimes(d-\nu)}. \tag{17.37}$$

As shown earlier during our discussion of the Fourier transform, such operators are diagonalized by the discrete Fourier transform on $\mathbb{Z}_L$. In particular,

$$\mathrm{DFT}^{\otimes d}\, D \left((\mathrm{DFT})^\dagger\right)^{\otimes d} = \sum_{k_1,\ldots,k_d \in \mathbb{Z}_L} |k_1 \ldots k_d\rangle\langle k_1 \ldots k_d| \frac{1}{d}\Big(\cos(2\pi k_1/L) + \cdots + \cos(2\pi k_d/L)\Big). \tag{17.38}$$

The largest eigenvalue occurs when $k_1 = k_2 = \cdots = k_d = 0$, and the second largest eigenvalue occurs when exactly one of the k_ν equals 1 or $L-1$. Thus

$$\gamma = \frac{1 - \cos(2\pi/L)}{d} = \frac{2\sin^2(\pi/L)}{d}. \tag{17.39}$$

The number of steps needed for the walk to approach the stationary distribution within ℓ_1 distance δ is therefore approximately

$$\frac{1}{\gamma}\log\left(\frac{\sqrt{|V|\,/\min_x \pi_x}}{\delta}\right) = \frac{1}{\gamma}\log\left(\frac{|V|}{\delta}\right) = \mathcal{O}\left(dL^2\log(|V|\,/\delta)\right). \tag{17.40}$$

◇

17.2. Block encoding of the discriminant matrix

Now that we have discussed the fundamentals of Markov Chains, we can examine how we would implement such a walk on a quantum computer. The simplest approach to do this is to build a block encoding of the discriminant matrix. This block-encoding can then be used to sample from the stationary distribution for the Markov chain. This allows us to represent the non-unitary process as a block of a larger unitary matrix.

Our first goal in the encoding of the elements of the Markov chain is to build a circuit that gives access to the entries of the transition matrix P. Assume that we have access to an oracle O_P that will construct a weighted superposition over all the neighbors of a vertex j in the graph as follows:

$$O_P\,|0^n\rangle\,|j\rangle = \sum_k \sqrt{P_{kj}}\,|k\rangle\,|j\rangle\,. \tag{17.41}$$

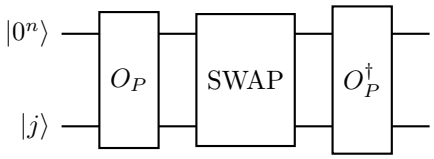
Since P is a left stochastic matrix, the right hand side is already a normalized vector. Hence the map defined by Eq. (17.41) is an isometry and can be extended to a unitary O_P without introducing an additional signal qubit. We also need the n-qubit SWAP operation:

$$\mathrm{SWAP}\,|i\rangle\,|j\rangle = |j\rangle\,|i\rangle\,, \tag{17.42}$$

which swaps the value of the two registers in the computational basis, and can be directly implemented using n SWAP operations between two qubits, and in turn $3n$ CNOT operations. The role of the SWAP operation is to easily prepare $D = \sum_{ij}\sqrt{P_{ij}P_{ji}}|i\rangle\langle j|$ from (17.13), since we need to ensure that the P_{ij} elements get paired with their transposes. This pairing is guaranteed by the use of a SWAP operation as seen in the following proposition.

Proposition 17.10. *Let D be a discriminant matrix associated with a transition matrix $P \in \mathbb{R}^{N\times N}$ with $N = 2^n$, then the following circuit provides a Hermitian block encoding of the matrix D via $(\langle 0^n|\otimes I)U_D(|0^n\rangle\otimes I) = D$ where*

$U_D :=$



Proof. Clearly U_D is unitary and Hermitian. Now we compute as before

$$|0^n\rangle\,|j\rangle \xrightarrow{O_P} \sum_k \sqrt{P_{kj}}\,|k\rangle\,|j\rangle \xrightarrow{\mathrm{SWAP}} \sum_k \sqrt{P_{kj}}\,|j\rangle\,|k\rangle\,. \tag{17.43}$$

Meanwhile

$$|0^n\rangle\,|i\rangle \xrightarrow{O_P} \sum_{k'} \sqrt{P_{k'i}}\,|k'\rangle\,|i\rangle\,. \tag{17.44}$$

So the inner product gives

$$\langle 0^n| \langle i| U_D |0^n\rangle |j\rangle = \sum_{k,k'} \sqrt{P_{k'i}P_{kj}}\delta_{j,k'}\delta_{i,k} = \sqrt{P_{ji}P_{ij}} = D_{ij}. \tag{17.45}$$

This proves the claim. □

How can we use this to solve a computational problem? Since D is a Hermitian matrix, it can be viewed as a Hamiltonian. This implies that we can use an algorithm such as quantum phase estimation to project onto the principal eigenvector corresponding to the equilibrium distribution π.

Proposition 17.11. *Let $P \in \mathbb{R}^{N\times N}$ be the transition matrix that corresponds to a finite, irreducible, aperiodic and reversible Markov chain, and let π be the stationary distribution and $|\pi\rangle$ be the coherent version of the distribution. Assume that we are provided a quantum state $|\psi\rangle \in \mathbb{C}^N$ such that $|\langle\psi|\pi\rangle| \geq \sqrt{1-\delta^2}$. Let $\gamma > 0$ be the spectral gap of P. Then for any $\epsilon > 0$ and $0 < \delta < 1$, there exists a quantum algorithm that can prepare a state $|\tilde{\pi}\rangle$ such that $|\langle\pi|\tilde{\pi}\rangle| \geq 1-\epsilon$ with success probability at least $1 - 3\delta^2/2$ using*

$$\mathcal{O}\left(\frac{\log(1/(\epsilon\gamma))\log(1/\delta)}{\gamma}\right) \tag{17.46}$$

queries to O_P and $O_P^\dagger$.

Proof. According to Proposition 17.6, the spectral gap of P is equal to the gap between the largest eigenvalue and the next largest eigenvalue of the discriminant matrix D.

As D is a Hermitian matrix with $\|D\| \leq 1$, we can implement a unitary W such that $\|W - e^{-iD\pi/2}\| \leq \epsilon_0$ using

$$\mathcal{C}_W = \mathcal{O}\left(1 + \frac{\log(1/\epsilon_0)}{\log\log(1/\epsilon_0)}\right) \tag{17.47}$$

queries to a block encoding of D. By Proposition 17.10, implementing such a block encoding uses $\mathcal{O}(1)$ calls to O_P and $O_P^\dagger$.

Phase estimation with precision $\mathcal{O}(\gamma)$ distinguishes the principal eigenphase (corresponding to the eigenvalue 1 of D) from the rest of the spectrum using $\mathcal{O}(1/\gamma)$ controlled applications of W. Using statistical amplification, achieving failure probability at most $\delta^2/2$ for this discrimination step incurs an additional factor $\mathcal{O}(\log(1/\delta))$.

Since $|\langle\psi|\pi\rangle|^2 \geq 1-\delta^2$, the probability of not projecting onto $|\pi\rangle$ due to the initial overlap is at most δ^2. Therefore, by the union bound, the overall probability of failure is at most $\delta^2 + \delta^2/2 = 3\delta^2/2$.

As a last step, we need to discuss the quality of the eigenstate that we prepare. Here we note that the eigenvalue 1 of D is simple for the equilibrium distribution. Using eigenvector perturbation bounds for a simple eigenvalue in Theorem 7.9, we find that

$$1 - |\langle\pi|\tilde{\pi}\rangle| = \mathcal{O}(\epsilon_0/\gamma). \tag{17.48}$$

Therefore it suffices to choose $\epsilon_0 = \Theta(\epsilon\gamma)$.

Combining the above bounds yields an overall query complexity of

$$\mathcal{O}\left(\frac{\log(1/(\epsilon\gamma))\log(1/\delta)}{\gamma}\right) \tag{17.49}$$

in calls to O_P and $O_P^\dagger$. □

This shows that we can prepare the stationary distribution using quantum phase estimation (QPE), providing an alternative to the classical approach of iteratively applying the transition matrix. However, as Proposition 17.8 indicates, the overall cost of this quantum method remains comparable to that of classical algorithm (with respect to the gap γ). This motivates a deeper question: can we truly accelerate convergence using quantum analogues of Markov chains? We will see that it is possible to quadratically amplify the spectral gap, thereby demonstrating that quantum effects can fundamentally speed up the mixing of Markov processes.

17.3. Szegedy's quantum walk and qubitization

For a Markov chain defined on a graph $G = (V, E)$ with $|V| = N = 2^n$, Szegedy constructed the following quantum walk operator [Sze04], which can be used to achieve quadratic speedup for a range of problems, using a strategy similar to that in Grover type algorithms in Chapter 11. For any input vertex j, we construct a state $O_P |0^n\rangle |j\rangle$, which is the coherent version of the probability distribution over the neighboring vertices of j according to the transition matrix P. It then swaps the role of the outgoing and incoming vertices: $\mathrm{SWAP} \cdot O_P |0^n\rangle |j\rangle$. These operators are exactly the same ones used above for block encoding the discriminant matrix D. However, as we will see below, after re-arranging the terms, we can quadratically increase the effective gap of the Markov chain. This means that we can achieve a fundamental advantage by using quantum as opposed to classical walks to solve problems.

Using the O_P oracle in Eq. (17.41) and the multi-qubit SWAP gate, we can define two sets of quantum states

$$\begin{aligned} |\psi_j^1\rangle &= O_P |0^n\rangle |j\rangle = \sum_k \sqrt{P_{kj}} |k\rangle |j\rangle , \\ |\psi_j^2\rangle &= \mathrm{SWAP}(O_P |0^n\rangle |j\rangle) = \sum_k \sqrt{P_{kj}} |j\rangle |k\rangle . \end{aligned} \tag{17.50}$$

This gives rise to two $2n$-qubit projection operators and reflection operators

$$\Pi_l = \sum_{j\in[N]} |\psi_j^l\rangle \langle\psi_j^l| , \quad R_{\Pi_l} = 2\Pi_l - I_{2n}, \quad l = 1, 2. \tag{17.51}$$

Using the resolution of identity, the reflection operators can also be written as

$$R_{\Pi_1} = O_P(Z_\Pi \otimes I_n)O_P^\dagger, \qquad Z_\Pi := 2|0^n\rangle\langle 0^n| - I_n. \tag{17.52}$$

Similarly

$$R_{\Pi_2} = \mathrm{SWAP}\, O_P(Z_\Pi \otimes I_n)O_P^\dagger \,\mathrm{SWAP}\, . \tag{17.53}$$

Szegedy's quantum walk operator is defined as the product of these two reflection operators

$$\mathcal{U}_Z = R_{\Pi_2} R_{\Pi_1} , \tag{17.54}$$

which is a rotation operator that resembles that in Grover's algorithm.

We first note that

$$O_P^\dagger \mathcal{U}_Z O_P = \Big(O_P^\dagger \,\mathrm{SWAP}\, O_P(Z_\Pi \otimes I_n)\Big)^2 =: O_Z^2, \tag{17.55}$$

where the circuit for $O_Z := O_P^\dagger \,\mathrm{SWAP}\, O_P(Z_\Pi \otimes I_n)$ is shown in Fig. 17.1 and is often called the **walk operator**. Let $U_D = O_P^\dagger \,\mathrm{SWAP}\, O_P$ be the Hermitian block encoding of D in Proposition 17.10. Compare this with Fig. 10.1, we find that the walk operator O_Z is exactly the qubitization circuit associated with the block encoding of D. Therefore, Szegedy's quantum walk operator is the same

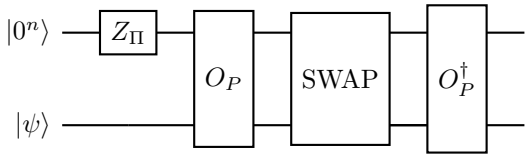


FIGURE 17.1. Circuit implementing one step of the O_Z operator which corresponds to the Szegedy walk. This circuit is precisely the same form of the circuit to that used in qubitization-based simulation algorithms.

as a block encoding of $T_2(D)$, up to a matrix similarity transformation, where $T_2(x) = 2x^2 - 1$ is the 2nd order Chebyshev polynomial. Furthermore, the matrix power O_Z^{2k} provides a block encoding of the Chebyshev matrix polynomial $T_{2k}(D)$.

From the eigendecomposition $D|v_i\rangle = \lambda_i |v_i\rangle$, for each $|v_i\rangle$, the associated basis in the 2-dimensional subspace is $\mathcal{B}_i = \{|0^n\rangle |v_i\rangle, |\perp_i\rangle\}$. Then the qubitization procedure gives

$$[O_Z]_{\mathcal{B}_i} = \begin{pmatrix} \lambda_i & -\sqrt{1-\lambda_i^2} \\ \sqrt{1-\lambda_i^2} & \lambda_i \end{pmatrix}. \tag{17.56}$$

The eigenvalues of O_Z in the 2×2 matrix block are

$$e^{\pm i \arccos(\lambda_i)}. \tag{17.57}$$

This relation is important for the following reasons. By Proposition 17.6, if a Markov chain is reversible and ergodic, the eigenvalues of D and P are the same. In particular, the largest eigenvalue of D is unique and is equal to 1, and the second largest eigenvalue of D is $1-\gamma$, where $\gamma > 0$ is called the spectral gap. Since $\arccos(1) = 0$, and $\arccos(1-\gamma) \approx \sqrt{2\gamma}$, we find that the spectral gap of O_Z on the unit circle is in fact $\mathcal{O}(\sqrt{\gamma})$ instead of $\mathcal{O}(\gamma)$. This is called the **spectral gap amplification**. Thus, applying quantum phase estimation to O_Z instead of $e^{-iD\pi/2}$ as in Proposition 17.11 yields a quadratic improvement in the dependence on the spectral gap γ for preparing the stationary distribution.

Here is an example illustrating how Szegedy's walk construction can be used to prepare a Gibbs state when the Hamiltonian is explicitly diagonalizable.

Example 17.12 (Preparing a Gibbs state for explicitly diagonalizable Hamiltonians)**.** Assume that the Hamiltonian $H \in \mathbb{C}^{2^n \times 2^n}$ can be written as

$$H = U\mathcal{E}U^\dagger, \tag{17.58}$$

where U is a unitary and $\mathcal{E} = \sum_{j=0}^{2^n-1} E(j)|j\rangle\langle j|$ is a diagonal matrix of energies. Assume furthermore that the map $|j\rangle \mapsto E(j)$ can be computed in poly(n) time on a quantum computer, and that U can be implemented in poly(n) time. For inverse temperature $\beta > 0$, the Gibbs state is

$$\rho_\beta := \frac{e^{-\beta H}}{\mathrm{Tr}\left[e^{-\beta H}\right]} = U\left(\frac{e^{-\beta \mathcal{E}}}{\mathrm{Tr}\left[e^{-\beta \mathcal{E}}\right]}\right)U^\dagger. \tag{17.59}$$

Thus preparing ρ_β reduces to preparing the classical Gibbs distribution over the eigenbasis of $\mathcal{E}$ and conjugating by U.

Let $\Sigma = \{0,1\}^n$. Consider the Metropolis–Hastings chain in Example 17.5, with symmetric proposal kernel Q given by single-bit flips and acceptance probability

$$\alpha_{ji} := \min\{1, e^{-\beta(E(j)-E(i))}\}. \tag{17.60}$$

Define the transition matrix P by

$$P_{ji} := Q_{ji}\alpha_{ji} \quad (j \neq i), \qquad P_{ii} := 1 - \sum_{j \neq i} P_{ji}. \tag{17.61}$$

Then P is column-stochastic and reversible with stationary distribution

$$\pi_i := \frac{e^{-\beta E(i)}}{Z}, \qquad Z := \sum_{i \in \Sigma} e^{-\beta E(i)}. \tag{17.62}$$

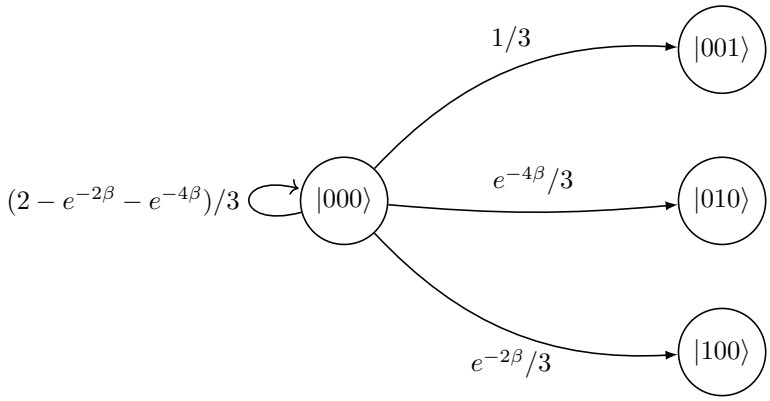
In order to visualize this process, let us assume that we have a Hamiltonian that is already diagonal in the computational basis:

$$H = (I - Z_0) + 2(I - Z_1) - 4(I - Z_2). \tag{17.63}$$

Note that $(I - Z_k)$ contributes 0 on $|0\rangle$ and 2 on $|1\rangle$. Therefore the energy of $|b_0 b_1 b_2\rangle$ is

$$E(b_0 b_1 b_2) = 2b_0 + 4b_1 - 8b_2. \tag{17.64}$$

From the state $|000\rangle$, the three single-bit-flip proposals lead to $|100\rangle$ (energy change $+2$), $|010\rangle$ (energy change $+4$), and $|001\rangle$ (energy change -8). Using the Metropolis acceptance rule, the corresponding acceptance probabilities are $e^{-2\beta}$, $e^{-4\beta}$, and 1, respectively. Since $Q_{ji} = 1/3$ for these proposals, the transition probabilities out of $|000\rangle$ are as shown in the following figure.



The figure shows the transition probabilities out of $i = 000$. Substituting the above energy changes into the Metropolis rule gives the displayed values. In the present example, single-bit flips connect all vertices of $\{0,1\}^3$, so the chain is irreducible. Moreover, $P_{ii} > 0$ for every i (because proposals can be rejected), so the chain is aperiodic. Therefore the stationary distribution is unique.

Let $\gamma > 0$ denote the spectral gap of P, meaning that the second-largest eigenvalue of P is at most $1-\gamma$ in absolute value. The associated Szegedy walk has eigenphases related to the eigenvalues of P: if $\lambda \in [-1,1]$ is an eigenvalue of P (equivalently, of the discriminant matrix), then the walk has eigenphases $\pm \arccos(\lambda)$. In particular, the smallest nonzero eigenphase is

$$\arccos(1-\gamma) = \Theta(\sqrt{\gamma}), \tag{17.65}$$

when γ is small. Consequently, given an initial state with non-negligible overlap with the coherent stationary state, one can prepare a state close to

$$|\pi\rangle = \sum_{i\in\Sigma} \sqrt{\pi_i}\,|i\rangle\,. \tag{17.66}$$

We then append $|0^n\rangle$ to this state, yielding

$$\sum_{i\in\Sigma} \sqrt{\pi_i}\,|i\rangle\,|0^n\rangle\,. \tag{17.67}$$

By applying n CNOT gates with the first register as control and the second register as target, and subsequently applying the unitary U to the first register, we prepare the state

$$\sum_{i\in\Sigma} \sqrt{\pi_i}(U\,|i\rangle)\,|i\rangle\,. \tag{17.68}$$

This is a purification of ρ_β. Indeed, tracing out the second register leads to

$$\sum_{i\in\Sigma} \pi_i\, U|i\rangle\langle i|U^\dagger = \frac{e^{-\beta H}}{\operatorname{Tr}\left[e^{-\beta H}\right]}. \tag{17.69}$$

Each step in the Szegedy walk can be implemented using a constant number of evaluations of $E(\cdot)$ (to compute the acceptance probabilities) together with elementary gates, and the total cost is $\mathrm{poly}(n)$. Suppressing logarithmic factors in the target precision and success probability, the number of walk steps required to resolve the eigenphase gap scales as $\mathcal{O}\big(1/\sqrt{\gamma}\big)$. Compared to Proposition 17.8, where the number of applications of the transition matrix scales as $\mathcal{O}(1/\gamma)$, this yields a quadratic improvement in the dependence on the spectral gap.

It is worth contrasting this with the results in Section 13.5, where a quadratic quantum speedup is obtained under the assumption that a block encoding of H is available via QSVT. The key difference lies in the input model. In the block-encoding oracle model for $H \in \mathbb{C}^{2^n\times 2^n}$, the cost typically includes a prefactor of $\sqrt{2^n/\operatorname{Tr}\left[e^{-\beta H}\right]}$, which is efficient only at sufficiently high temperatures. In contrast, the Markov chain-based cost model depends on the spectral gap γ rather than directly on the Hilbert space dimension, although γ itself may become small at low temperatures. ⋄

The discussion so far has focused on reversible Markov chains. However, Szegedy's quantum walk framework can also be applied to irreversible chains. As demonstrated in the example below, the quantum walk operator is constructed from the discriminant matrix of an irreversible chain. While the spectrum of the discriminant matrix generally differs from that of the original transition matrix, it still encodes useful information. In particular, by comparing the spectra of discriminant matrices for graphs with and without a marked vertex, one can determine the existence of a marked vertex.

Example 17.13 (Determining whether there is a marked vertex in a complete graph)**.** Let $G = (V, E)$ be a complete graph of $N = 2^n$ vertices. We would like to distinguish the following two scenarios:

(1) All vertices are the same, and the random walk is given by the transition matrix

$$P = \frac{1}{N} ee^\top, \quad e = (1, \ldots, 1)^\top. \tag{17.70}$$

(2) There is one *marked* vertex. Without loss of generality we may assume this is the 0-th vertex (of course we do not have access to this information). In this case, the transition matrix is

$$\widetilde{P}_{ij} = \begin{cases} \delta_{i0}, & j = 0, \\ P_{ij}, & j > 0. \end{cases} \tag{17.71}$$

In other words, in the case (2), the random walk will stop at the marked index. The transition matrix can also be written in the block partitioned form as

$$\widetilde{P} = \begin{pmatrix} 1 & \frac{1}{N}\widetilde{e}^\top \\ 0 & \frac{1}{N}\widetilde{e}\widetilde{e}^\top \end{pmatrix}. \tag{17.72}$$

Here $\widetilde{e}$ is an all 1 vector of length $N-1$.

For the random walk defined by P, the stationary state is $\pi = \frac{1}{N}e$, and the spectral gap is 1. For the random walk defined by $\widetilde{P}$, the stationary state is $\widetilde{\pi} = (1, 0, \ldots, 0)^\top$, and the spectral gap is $\gamma = N^{-1}$. Starting from the uniform state π (as a column vector), the probability distribution after k steps of random walk is $\widetilde{P}^k\pi$. This converges to the stationary state of $\widetilde{P}$, and hence reach the marked vertex after $\mathcal{O}(N)$ steps of walks.

Since P is symmetric, the discriminant matrix D is equal to P. Even though $\widetilde{P}$ is not reversible, the discriminant matrix $\widetilde{D}$ is still well-defined:

$$\widetilde{D} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{N}\widetilde{e}\widetilde{e}^\top \end{pmatrix}. \tag{17.73}$$

To distinguish the two cases, we are given a Szegedy quantum walk operator called O, which can be either O_Z or $\widetilde{O}_Z$, which is associated with $D, \widetilde{D}$, respectively. The initial state is

$$|\psi_0\rangle = |0^n\rangle \left(\mathrm{H}^{\otimes n} |0^n\rangle\right). \tag{17.74}$$

Our strategy is to measure the expectation

$$m_k = \langle\psi_0|O^k|\psi_0\rangle\,, \tag{17.75}$$

which can be obtained via the Hadamard test.

Before determining the value of k, first notice that if $O = O_Z$, then $O_Z|\psi_0\rangle = |\psi_0\rangle$. Hence $m_k = 1$ for all values of k.

On the other hand, if $O = \widetilde{O}_Z$, we use the fact that $\widetilde{D}$ only has two nonzero eigenvalues 1 and $(N-1)/N = 1-\gamma$, with associated eigenvectors denoted by $|\widetilde{\pi}\rangle$ and $|\widetilde{v}\rangle = \frac{1}{\sqrt{N-1}}(0, 1, 1 \ldots, 1)^\top$, respectively. Furthermore,

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} |0^n\rangle\,|\widetilde{\pi}\rangle + \sqrt{\frac{N-1}{N}}\,|0^n\rangle\,|\widetilde{v}\rangle\,. \tag{17.76}$$

Due to qubitization, we have

$$\widetilde{O}_Z^k\,|\psi_0\rangle = \frac{1}{\sqrt{N}}\,|0^n\rangle\,T_k(1)\,|\widetilde{\pi}\rangle + \sqrt{\frac{N-1}{N}}\,|0^n\rangle\,T_k(1-\gamma)\,|\widetilde{v}\rangle + |\perp\rangle\,, \tag{17.77}$$

where $|\perp\rangle$ is an unnormalized state satisfying $(|0^n\rangle\langle 0^n|) \otimes I_n\,|\perp\rangle = 0$. Then using $T_k(1) = 1$ for all k, we have

$$m_k = \frac{1}{N} + \left(1 - \frac{1}{N}\right) T_k(1-\gamma). \tag{17.78}$$

Use the fact that $T_k(1-\gamma) = \cos(k \arccos(1-\gamma))$, in order to have $T_k(1-\gamma) \approx 0$, the smallest k satisfies

$$k \approx \frac{\pi}{2\arccos(1-\gamma)} \approx \frac{\pi}{2\sqrt{2\gamma}} = \frac{\pi\sqrt{N}}{2\sqrt{2}}. \tag{17.79}$$

Therefore taking $k = \lceil \frac{\pi\sqrt{N}}{2\sqrt{2}} \rceil$, we have $m_k \approx 1/N$. Running Hadamard's test to constant accuracy allows us to distinguish the two scenarios.

Alternatively, we may evaluate the success probability of obtaining 0^n in the ancilla qubits, i.e.,

$$p(0^n) = \left\| (|0^n\rangle\langle 0^n| \otimes I_n) O^k |\psi_0\rangle \right\|^2. \tag{17.80}$$

When $O = O_Z$, we have $p(0^n) = 1$ with certainty. When $O = \widetilde{O}_Z$, according to Eq. (17.77),

$$p(0^n) = \frac{1}{N} + \left(1 - \frac{1}{N}\right) T_k^2(1-\gamma). \tag{17.81}$$

So running the problem with $k = \lceil \frac{\pi\sqrt{N}}{2\sqrt{2}} \rceil$, we can distinguish between the two cases.

It is natural to draw comparisons between Szegedy's quantum walk and Grover's search. The two algorithms make queries to different oracles, and both yield quadratic speedup compared to the classical algorithms. The quantum walk is slightly weaker, since it only tells whether there is one marked vertex or not. On the other hand, Grover's search also finds the location of the marked vertex. Both algorithms consist of repeated usage of the product of two reflectors. The number of iterations need to be carefully controlled. Indeed, choosing a polynomial degree four times as large as Eq. (17.79) would result in $m_k \approx 1$ for the case with a marked vertex.

Another possible solution of the problem of finding the marked vertex is to perform QPE on the Szegedy walk operator O (which can be O_Z or $\widetilde{O}_Z$). The effectiveness of the method rests on the spectral gap amplification discussed above. We refer to [Chi21, Chapter 17] for more details. ⋄

17.4. Glued tree problem and continuous time quantum walk

The continuous time quantum walk on the glued tree is one of the most important quantum algorithms. This is because it provides an example of an algorithmic task wherein there is a provable exponential separation in quantum and classical query complexity for solving the problem. Further, this algorithm was discovered first within the paradigm of continuous time quantum walks rather than using existing discrete paradigms. Note that this does not yet imply that $\mathsf{BQP} \neq \mathsf{BPP}$ because this exponential separation is relative to an oracle. Nonetheless, an exponential separation in query complexity strongly suggests that something is profoundly different between the quantum and classical computation.

17.4.1. Glued tree problem. The **glued tree problem** is a graph traversal problem that consists of two binary trees of depth n (our convention is that the root has depth 0) rooted at two vertices that we will label s and t drawn from an exponentially large set of labels. These two trees are then glued together by a random bipartite cycle graph that alternates between the leaf nodes of the two balanced binary trees (see Fig. 17.2).

Definition 17.14 (Glued Tree Graph)**.** *A glued tree graph $G(V, E)$ of depth $2n$ is constructed in the following manner.*

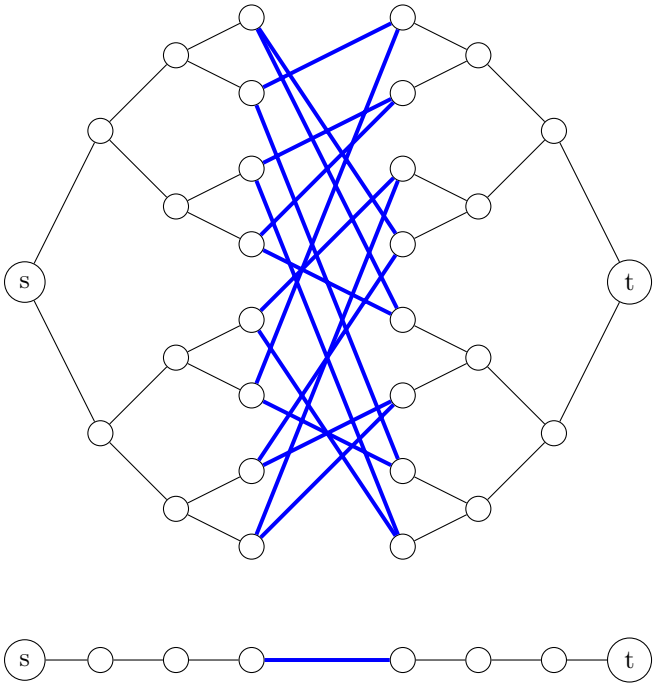


FIGURE 17.2. (Top) Glued-tree graph with parameter $n = 3$, with entrance node s on the left and exit node t on the right. The thick lines in blue color indicate the edges of the bipartite cycle graph. (Bottom): Column-space representation, where each vertex represents all nodes in the corresponding column of the original graph.

(1) *Divide the vertex set such that* $V = V_s \bigcup V_t$ *such that* V_s *and* V_t *are disjoint sets of vertices of size* $2^{n+1} - 1$*, and construct* $G_s = (V_s, E_s)$ *as a balanced binary tree of depth* n *rooted at a vertex* s*, and similarly construct* $G_t = (V_t, E_t)$ *as a balanced binary tree graph of depth* n *rooted at* t*.*
(2) *Construct a random bipartite cycle graph,* $C = ((L_s \bigcup L_t), E_C)$ *where* L_s *and* L_t *are the sets of leaf nodes in the tree* G_s *and* G_t*. Specifically, for the bipartite cycle graph we have that if* $x \in L_s$ *then the neighbors of* x *are only in* L_t *and vice-versa and every vertex in the graph has degree precisely* 2*.*
(3) *Construct the graph* $G = G_s \bigcup C \bigcup G_t$ *where the graph union is formed by constructing the union of the vertex and edge sets of the constituent graphs.*

The goal of the problem is to find the label of t using as few queries to an oracle that provides the labels of all vertices adjacent to any requested labeled vertex. This is an example of the **hitting problem**. The aim of the bipartite cycle graph is to create a maze in which a classical algorithm can easily get lost.

First, note that the exit label t here cannot be found by brute force due to the exponentially large size of the graph. Even Grover's algorithm would take an exponentially long time to find the exit vertex.

Algorithm 17.1 Classical Markov Chain for Glued Trees

Input: Oracle that yields the neighboring vertex of any vertex in the graph $G = (V, E)$ where V is the vertex set and E is the edge set and label of the starting node label(s).

1: Initialize $x \leftarrow \text{label}(s)$.
2: **while** $x \neq \text{label}(t)$ **do**
3: Query oracle to get the neighbor set of x $N(x) := \{y : (x, y) \in E\}$.
4: Draw vertex $x' \in N(x)$ uniformly over the set $N(x)$.
5: $x \leftarrow x'$.
6: **end while**

Next, intuitively we expect as n increases for any random walk algorithm to become increasingly trapped near the center of the graph. To see this, consider the following Markov chain Monte Carlo algorithm (Algorithm 17.1). At first, this algorithm can efficiently explore the graph. After starting at s, it moves to an adjacent vertex which will always be closer to the vertex t. In the second step, because the Markov Chain does not have memory, it will have a 1/3 probability of moving back to s and a 2/3 probability of moving closer to t. This situation reverses, however, after reaching the center of the graph. Now the probability of progressing towards the label t is only 1/3 and the probability of returning closer to the center is 2/3. This means that the walker tends to be trapped near the center for a long time without moving towards the label t.

We may analyze the long-time behavior of the Markov chain by examining its stationary distribution. The specific vertex occupied by the random walker is not essential. Rather, what matters is the **column** in which the walker resides. Since the walker begins in the first column and terminates in the last, the individual vertex labels in the intermediate steps carry no additional information. Consequently, it suffices to track the column-level transitions rather than individual vertex transitions. When we aggregate the graph by columns, the graph simplifies dramatically to a path graph, as shown in the lower panel of Fig. 17.2. Labeling the first $n+1$ columns as $0, \ldots, n$ and the remaining $n+1$ columns as $n+1, \ldots, 2n+1$, the transition probability from the column i to the column j is:

$$P_{ji} = \begin{cases} 1 & \text{if } i = 0 \text{ and } j = 1, \text{ or if } i = 2n+1 \text{ and } j = 2n \\ 2/3 & \text{if } 1 \leq i \leq n \text{ and } j = i+1, \text{ or if } n+1 \leq i \leq 2n \text{ and } j = i-1 \\ 1/3 & \text{if } 1 \leq i \leq n \text{ and } j = i-1, \text{ or if } n+1 \leq i \leq 2n \text{ and } j = i+1 \\ 0 & \text{otherwise} \end{cases}. \tag{17.82}$$

The stationary distribution π can be obtained from the detailed balance condition $P_{ji}\pi_i = P_{ij}\pi_j$. We have that $\pi_0 \cdot (1) = \pi_1 \cdot (1/3)$ and similarly, $\pi_1 \cdot (2/3) = \pi_2 \cdot (1/3)$ and so forth. We then see that $\pi_n(2/3) = \pi_{n+1}(2/3)$ which implies that the two columns in the middle of the graph must have the same probabilities (as anticipated from symmetry). From this, we see that the following is a stationary distribution that satisfies the detailed balance condition and further because the graph is irreducible we know that the state is unique.

$$\pi = \left[1/(3 \cdot 2^{n-1}), 1/2^{n-1}, \ldots, 1/2, 1, 1, 1/2, \ldots, 1/2^{n-1}, 1/(3 \cdot 2^{n-1})\right] / \|\pi\|_1. \tag{17.83}$$

As the stationary distribution has exponentially small probability at the vertices s and t, the walker sampled from the stationary distribution will have a vanishingly small probability of reaching the exit vertex t. Thus, even if we are able to efficiently prepare the stationary distribution, it does not

help us solve the hitting problem. This also implies that Szegedy's quantum walk, which accelerates the process of reaching the stationary distribution, cannot resolve this problem either.

In fact, it can be shown that actually **no** classical algorithm can find the label of the exit vertex t using a sub-exponential in n number of queries to the graph. The proof of this theorem involves a series of reductions and is omitted here.

THEOREM 17.15 ([CCD+03, Theorem 6]). *For the glued tree problem of depth $2n$, any classical algorithm that finds the exit vertex t with success probability at least $\Omega(2^{-n/6})$ must make at least $\Omega(2^{n/6})$ queries to the adjacency matrix, where the adjacency matrix serves as an oracle that returns the neighbors of a vertex $x \in V$.*

17.4.2. Continuous-time quantum walk. For an undirected graph $G = (V, E)$, its adjacency matrix A is a real symmetric matrix with

$$A_{x,y} = \begin{cases} 1 & \text{if } (x,y) \in E, \\ 0 & \text{otherwise.} \end{cases} \tag{17.84}$$

Therefore A can be viewed as a Hamiltonian that defines a quantum dynamics. The **continuous-time quantum walk** refers to the following time-evolved state

$$|\psi(t)\rangle = e^{-iAt} |\psi(0)\rangle . \tag{17.85}$$

We first note that, unlike in the classical random walk, a continuous-time quantum walk cannot drive an arbitrary initial state to the stationary distribution. The only stationary states are the eigenvectors of the adjacency matrix A. To solve a hitting problem, that is, to reach a target state $|\phi\rangle$, we instead evolve the system for a random amount of time chosen uniformly from the interval $[0, T]$. The success probability is then given by the time-averaged transition probability, computed as

$$p = \frac{1}{T} \int_0^T |\langle \phi | \psi(t) \rangle|^2 \ \mathrm{d}t. \tag{17.86}$$

As noted earlier, the adjacency matrix generates transitions between the columns of the glued trees graph. Specifically, let $|C_j\rangle$ denote a quantum state in column j which is supported over the set of all vertices that are graph distance j away from s (where the graph distance gives the minimum number of edges that need to be traversed to go between two vertices). Specifically, we have that if x is in the second column of the glued tree and y is in the fourth column then $A_{x,y} = 0$ because the two vertices are not adjacent. Similarly, if x, y are in the same column then $A_{x,y} = 0$ because the glued tree has no edges between the same column of vertices. Thus the adjacency matrix only leads to non-trivial dynamics in the columns of the matrix as does the graph Laplacian.

This observation allows us to define a **column space** for the graph. In particular, if we let C_j be the set of vertices in column j then

$$|C_j\rangle = \frac{1}{\sqrt{|C_j|}} \sum_{x \in C_j} |x\rangle . \tag{17.87}$$

This notation also then directly implies that $|C_0\rangle = |s\rangle$ and $|C_{2n+1}\rangle = |t\rangle$. We then have that in this sub-space of column states

$$\begin{aligned}\langle C_{j+1}| A |C_j\rangle &= \frac{1}{\sqrt{|C_{j+1}||C_j|}} \sum_{x\in C_{j+1}} \sum_{y\in C_j} \langle x| A |y\rangle \\ &= \begin{cases} \frac{2|C_j|}{\sqrt{|C_{j+1}||C_j|}} & 0 \leq j \leq n, \\ \frac{|C_j|}{\sqrt{|C_{j+1}||C_j|}} & n+1 \leq j \leq 2n. \end{cases} \\ &= \begin{cases} \sqrt{2} & j \neq n, \\ 2 & j = n. \end{cases}\end{aligned} \tag{17.88}$$

This is true because if we consider all columns less than n then the subsequent column will contain twice as many vertices in it than the previous column. Past this point there will be half as many in every subsequent column. This implies that $|C_{j+1}| = 2|C_j|$ if $j < n$, $|C_{n+1}| = |C_n|$, and $|C_{j+1}| = |C_j|/2$ if $j > n$, and the final claim in Eq. (17.88) follows by substitution.

Furthermore the matrix A will only generate transitions between vectors within this space. The simplest way to see this is by considering the following complete basis whose elements are defined for any $p \in \mathbb{Z}_{|C_j|}$

$$|C_j^{(p)}\rangle := \sum_{x\in C_j} \frac{1}{\sqrt{|C_j|}} e^{-i2\pi p r_j(x)/|C_j|} |x\rangle , \tag{17.89}$$

where $r_j(x)$ gives the location of the vertex x in a sorted list of the vertices in the set C_j (the particular sorting order does not matter for the definition). As argued in our discussion of the quantum Fourier transform, these states form an orthonormal basis in each column C_j which implies that $\langle C_j^{(q)}|C_j^{(p)}\rangle = \delta_{pq}$. Also note that $|C_j^{(0)}\rangle = |C_j\rangle$. Similarly, we see that the inner product between any two vectors from different columns is zero because they contain disjoint sets of vertices. We then have that for any $j \leq n-1$ and $p > 0$

$$\begin{aligned}\langle C_{j+1}^{(p)}| A |C_j^{(0)}\rangle &= \frac{1}{\sqrt{|C_{j+1}||C_j|}} \sum_{x\in C_{j+1}} \sum_{y\in C_j} e^{-i2\pi p r_{j+1}(x)/|C_{j+1}|} \langle x| A |y\rangle \\ &= \frac{\sqrt{2}}{\sqrt{|C_{j+1}||C_j|}} \sum_{x\in C_{j+1}} e^{-i2\pi p r_{j+1}(x)/|C_{j+1}|} = 0.\end{aligned} \tag{17.90}$$

The same argument can be repeated for the remaining cases, which shows that the matrix A does not generate transitions between the $p = 0$ vectors of this complete basis and the remainder of the space. Thus as the vector space is complete, we then have that set $\{|C_j\rangle : j = 0, \ldots, 2n+1\}$ forms a basis for $A^k |C_0\rangle = A^k |s\rangle$ without needing to include $p > 0$. Thus by Taylor's theorem, it also forms a basis for every state of the form $e^{-iAt} |s\rangle$ for $t \in \mathbb{R}$.

From this perspective, we can see that the A matrix is the adjacency matrix for a path graph when represented in the column space, as illustrated by Figure 17.2. If we were to examine the dynamics in the continuum, A could be easily diagonalized with the eigenvectors being sine/cosine functions with appropriate periods. However, this intuition breaks down, apart from the obvious fact that we are focusing on a discrete problem, due to the defect at the center of the graph where $\langle C_{n+1}^{(p)}| A |C_n^{(p)}\rangle = 2$ rather than $\sqrt{2}$.

Now let us consider the reflection operator R such that for any $j < n$

$$R\,|C_j\rangle = |C_{2n+1-j}\rangle\,. \tag{17.91}$$

Hence the set $\{|C_j\rangle\}$ also remains closed under applications of R. We then further have that

$$AR\,|C_j\rangle = RA\,|C_j\rangle\,. \tag{17.92}$$

If we define $\hat{A}$ and $\hat{R}$ to be the restriction of the operators onto the subspace formed by the span of these column space vectors, then $[\hat{A}, \hat{R}] = 0$. Then the eigenvectors of $\hat{A}$ can be re-written in terms of simultaneous eigenvectors of $\hat{A}$ and $\hat{R}$. We can find eigenvectors by noting that due to the required symmetry (or anti-symmetry) under reflection imposed on any eigenvector of $\hat{R}$, the eigenvectors must also possess the same reflection parity. Thus, a reasonable guess to make is that the solution will be a linear combination of sine functions, with appropriate periodicity, and with the parity of the solution flipping at $j = n+1$ if the eigenvalue of $\hat{R}$ is negative for the eigenvector in question and positive otherwise. This guess can be written as [CCD+03]

$$|E_k^{\pm}\rangle := \sum_{j=0}^{n} \sin(p_k^{\pm}(j+1))\,|C_j\rangle \pm \sum_{j=n+1}^{2n+1} \sin(p_k^{\pm}(2n+2-j))\,|C_j\rangle \tag{17.93}$$

with eigenvalues $E_k^{\pm} = 2\sqrt{2}\cos(p_k^{\pm})$ where $p_k^{\pm}$ is a solution of the equation

$$\frac{\sin((n+2)p_k^{\pm})}{\sin((n+1)p_k^{\pm})} = \pm\sqrt{2}. \tag{17.94}$$

We will also prove these relations below.

Algorithm 17.2 describes a quantum algorithm for solving the glued tree problem using continuous-time quantum walk. The walker is initialized in the known state $|\text{label}(s)\rangle$, and the goal is to reach the target state $|\phi\rangle = |\text{label}(t)\rangle$. Crucially, this target state is not directly accessible; it can only be identified via a projective measurement onto $|\phi\rangle$. Similar to Grover's search, the ability to verify a candidate label t does not imply knowledge of how to construct or locate the state $|\text{label}(t)\rangle$.

Algorithm 17.2 Continuous-Time Quantum Walk for Glued Trees

Input: Maximum simulation time T; oracle that implements Hamiltonian evolution e^{-iAu} for any $u \in [0, T]$, where A is the adjacency matrix of the glued tree graph; oracle that performs projective measurement onto $P = |\text{label}(t)\rangle\langle\text{label}(t)|$.

1: Prepare the initial state $|\psi(0)\rangle = |\text{label}(s)\rangle$.
2: Sample a time u uniformly at random from the interval $[0, T]$, and evolve the state as $|\psi(u)\rangle = e^{-iAu}\,|\psi(0)\rangle$.
3: Perform a projective measurement onto P. If the outcome is successful, return label(t) in the computational basis. Otherwise, repeat the procedure.

To justify the efficiency of Algorithm 17.2 for solving the glued tree problem, we analyze the quantum dynamics of the continuous-time walk in the column space of the graph. In this reduced representation, the quantum walk exhibits coherent propagation from the entrance to the exit, in stark contrast to the classical random walk which becomes trapped near the central region. As a result, we can find the exit vertex label with high probability using only poly(n) quantum queries to the Hamiltonian and measurement oracles (Theorem 17.18).

Proposition 17.16. *For the glued tree problem of depth $2n$, let $\min|E-E'|$ be the minimum difference between any two eigenvalues of $\hat{A}$ (that is, A restricted to the column subspace). Then for any $T>0$, the time averaged probability of the continuous time quantum walk transitioning from the entrance, $|s\rangle$, to the exit, $|t\rangle$ is bounded below as*

$$\frac{1}{T}\int_0^T \left|\langle t|\, e^{-iAu}\,|s\rangle\right|^2 \mathrm{d}u \geq \frac{1}{2n+2} - \frac{2}{T\min|E-E'|}. \tag{17.95}$$

Proof. We will argue by symmetry and the Cauchy–Schwarz inequality that the time averaged probability of transitioning from the entrance to the exit is only polynomially small in the depth of the glued trees. As a unitary process cannot have a unique fixed point for all inputs, we compute this probability in terms of a time averaged probability of finding the exit node for times chosen uniformly over the interval $[0,T]$. Specifically we have that if we expand the time average in an eigenbasis $|E\rangle$ of $\hat{A}$,

$$\begin{aligned}\frac{1}{T}\int_0^T \langle t|\, e^{-iAu}|s\rangle\langle s|e^{iAu}\,|t\rangle \;\mathrm{d}u &= \frac{1}{T}\sum_{E,E'}\int_0^T \langle t|E\rangle\,\langle E'|t\rangle\,\langle E|s\rangle\,\langle s|E'\rangle\, e^{i(E-E')u}\,\mathrm{d}u \\ &= \sum_E |\langle t|E\rangle|^2\,|\langle E|s\rangle|^2 + \frac{1}{T}\sum_{E\neq E'}\frac{e^{i(E-E')T}-1}{i(E-E')}\,\langle t|E\rangle\,\langle E'|t\rangle\,\langle E|s\rangle\,\langle s|E'\rangle\,.\end{aligned} \tag{17.96}$$

Next using the symmetry condition set by the fact that $|E\rangle$ is a simultaneous eigenvector of the reflection operator $\hat{R}$, we know that $|\,\langle t|E\rangle\,|^4 = |\,\langle s|E\rangle\,|^4$. Thus the Cauchy–Schwarz inequality implies that

$$(2n+2)\sum_E |\langle t|E\rangle|^4 \geq \left(\sum_E |\langle t|E\rangle|^2\right)^2 = 1. \tag{17.97}$$

Hence

$$\sum_E |\langle t|E\rangle|^2\,|\langle E|s\rangle|^2 \geq 1/(2n+2). \tag{17.98}$$

Repeating a similar argument using the Cauchy–Schwarz inequality allows us to bound the term where $E\neq E'$ by

$$\left|\frac{1}{T}\sum_{E\neq E'}\frac{e^{i(E-E')T}-1}{i(E-E')}\,\langle t|E\rangle\,\langle E'|t\rangle\,\langle E|s\rangle\,\langle s|E'\rangle\right| \leq \frac{2}{T\min|E-E'|}. \tag{17.99}$$

Thus from the triangle inequality

$$\frac{1}{T}\int_0^T \langle t|\, e^{-iAu}|s\rangle\langle s|e^{iAu}\,|t\rangle\, du \geq \frac{1}{(2n+2)} - \frac{2}{T\min|E-E'|}. \tag{17.100}$$

□

The above result shows that if the eigenvalue gap is large enough then we can simply simulate the evolution under A for randomly chosen evolution times t chosen from $[0,T]$ and then if T is large enough then the probability of finding the exit is $\Omega(1/n)$. This means that the number of trials needed to find the exit vertex t is geometrically distributed with a mean of $O(n)$. Thus we

can show that the total evolution time needed to find the label of t is polynomial if the gap is at least polynomial. The following lemma demonstrates precisely such a claim.

Lemma 17.17. *Let $\hat{A}$ be the restriction of the adjacency matrix to the column subspace described in Proposition 17.16. The minimum eigenvalue gap between any two eigenvalues of $\hat{A}$ obeys*

$$\min |E - E'| > \frac{2\sqrt{2}\pi^2}{(1+\sqrt{2})(n+1)^3} + \mathcal{O}(1/n^4). \tag{17.101}$$

Proof. The eigenvalue equation implies that

$$\langle C_j| A |E_k^{\pm}\rangle = 2\sqrt{2}\cos(p)\langle C_j|E_k^{\pm}\rangle \tag{17.102}$$

Then by explicitly evaluating the action of the adjacency matrix on the column space vectors,

$$\sqrt{2}\langle C_{n+2}|E_k^{\pm}\rangle + \langle C_n|E_k^{\pm}\rangle = 2\cos(p)\langle C_{n+1}|E_k^{\pm}\rangle . \tag{17.103}$$

Similarly, the use of (17.93) further allows us to see that

$$\pm\sqrt{2}\sin((n+2)p_k^{\pm}) + \sin((n+1)p_k^{\pm}) = 2\sin((n+1)p_k^{\pm})\cos(p_k^{\pm}). \tag{17.104}$$

This yields the following non-linear expression for the quantization condition p,

$$\frac{\sin((n+2)p_k^{\pm})}{\sin((n+1)p_k^{\pm})} = \pm\sqrt{2}. \tag{17.105}$$

as alluded to previously.

Let us consider for simplicity the negative branch of the expression. An analytic solution to this expression is difficult to obtain, however, we can find an asymptotic solution for large n. In particular, let

$$p_k^- = \pi(k+1)/(n+1) - \delta_k \tag{17.106}$$

where $\delta_k = 0$ corresponds to the root of $\sin((n+1)p_k^-)$ so we are looking, in essence, for solutions that are perturbations away from the k^{th} root of the denominator which is justified because the function will vary rapidly in this vicinity as it approaches the singularity at $\delta_k = 0$. Expressing the eigenvalue relation in this limit gives

$$\sin((n+1)\delta_k - \frac{(k+1)\pi}{(n+1)} + \delta_k) = -\sqrt{2}\sin((n+1)\delta_k). \tag{17.107}$$

Expanding δ_k^- in powers of $1/(n+1)$ yields $\delta_k^{-1} = c_0 + c_1/(n+1) + O(1/n^2)$. Substituting this into (17.107) and eliminating any terms that are first order or higher in $1/(n+1)$

$$-\sqrt{2}\sin(c_0) = \sin(c_0). \tag{17.108}$$

This expression must hold for all n thus we must have that $c_0 = m\pi$ for integer π. For simplicity, we choose the trivial root of $c_0 = 0$. The expression for all first order terms in $1/(n+1)$ (neglecting all higher order terms) is

$$\begin{aligned} &-\sqrt{2}\sin\left(\frac{c_1}{n+1}\right) = \sin\left(\frac{c_1}{n+1} - \frac{(k+1)\pi}{(n+1)}\right) \\ \Rightarrow\quad &-\sqrt{2}\left(\frac{c_1}{n+1}\right) + O(1/n^3) = \left(\frac{c_1}{n+1} - \frac{(k+1)\pi}{(n+1)}\right) + O(1/n^3) \end{aligned} \tag{17.109}$$

This expression must be true for all n sufficiently large. As a result, the only way this expression can asymptotically hold is if

$$p_k^- = \frac{(k+1)\pi}{(n+1)} - \frac{(k+1)\pi}{(1+\sqrt{2})(n+1)^2} + O(1/n^3). \tag{17.110}$$

We can apply similar reasoning to find the positive roots are asymptotically

$$p_k^+ = \frac{(k+1)\pi}{(n+1)} + \frac{(k+1)\pi}{(1+\sqrt{2})(n+1)^2} + O(1/n^3). \tag{17.111}$$

From these expressions, we note that the two closest solutions to p_k^- will both be positive solutions corresponding to the same k and the subsequent one. This gives us that the gap between the two nearest $p_k^\pm$ to p_k^- is

$$\Delta_k := \min\left(\frac{(k+1)\pi\sqrt{2}}{(1+\sqrt{2})(n+1)^2}, \frac{(k+1)\pi}{(1+\sqrt{2})(n+1)^2}\right) + O(1/n^3). \tag{17.112}$$

The smallest gap corresponds to $k = 0$ which yields

$$\Delta_{\min} := \frac{\pi}{(1+\sqrt{2})(n+1)^2} + O(1/n^3). \tag{17.113}$$

The minimum eigenvalue gap then can be found by substituting this into the eigenvalue expression to find that the eigenvalue gap is minimal for $k' = 0$ and $k = 1$ and hence is of the form

$$\begin{aligned}
\min(|E_k - E_{k'}|) &= 2\sqrt{2}\left(\cos(p_k^+(k+1)) - \cos(p_{k'}^-(k'+1))\right) \\
&\geq 2\sqrt{2}\left(\cos(p_1^+) - \cos(p_0^-)\right) \\
&= 2\sqrt{2}\left|\int_0^{p_1^+ - p_0^-} \frac{\partial}{\partial_s}\cos(p_0^- + s)ds\right| \\
&= 2\sqrt{2}\left|\int_0^{p_1^+ - p_0^-} \sin(p_0^- + s)ds\right| \\
&= 2\sqrt{2}|p_1^+ - p_0^-||\sin(p_0^-(k+1))| + O(1/n^4) \\
&\geq \frac{2\sqrt{2}\pi}{(1+\sqrt{2})(n+1)^2}\sin\left(\frac{\pi}{n+1}\right) + O(1/n^4) \\
&\geq \frac{2\sqrt{2}\pi^2}{(1+\sqrt{2})(n+1)^3} + O(1/n^4)
\end{aligned} \tag{17.114}$$

□

From this result we have a bound on the minimum eigenvalue gap for the adjacency matrix. This allows us to then use this result to prove a bound on the total time needed to find the vertex label of t with inverse polynomial probability in n.

THEOREM 17.18. *For the glued tree problem of depth $2n$, it is sufficient to choose $T = \Theta(n^3)$ so that the time averaged probability of the continuous time quantum walk transitioning from the entrance, $|s\rangle$, to the exit, $|t\rangle$ is bounded below by $1/4(n+1)$.*

PROOF. Proof follows directly from substituting the result of Lemma 17.17 into Proposition 17.16 and requiring that the higher-order terms in the probability expansion add up to at most half of the probability that would be seen in the limit of $T \to \infty$. □

Notes and further reading

Classical Markov chains, including both discrete-time and continuous-time variants (the latter not discussed here), provide the foundation for quantum walks. Their convergence properties, mixing times, and spectral characteristics are treated in [Liu01, LP17], and they underpin the definition of the discriminant matrix used in Szegedy's quantum walk [Sze04]. Historically, Szegedy's construction directly inspired the development of block encodings for Hermitian matrices, with applications in Hamiltonian simulation [BC12] and quantum algorithms for solving linear systems of equations [CKS17]. As discussed in earlier chapters, the Szegedy walk operator is now best understood as a special case of qubitization; see also [AGJ21].

We introduced both discrete-time and continuous-time quantum walks. These two models differ significantly in their operational mechanisms; for a comparative overview, see [Chi10b]. The exponential query advantage of the continuous-time quantum walk was demonstrated in the glued trees problem [CCD$^+$03], which subsequently motivated further research in quantum adiabatic algorithms [SNK12, GHV21].

CHAPTER 18

Solving eigenvalue problems

In this chapter, we study quantum algorithms for estimating low-lying eigenvalues of Hermitian matrices and for preparing the corresponding eigenstates. These two related tasks differ in an important way: estimating the ground-state energy can remain meaningful even when nearby eigenvalues are clustered, whereas preparing the ground state requires spectral separation. This distinction guides the discussion throughout the chapter.

We first analyze repeated quantum phase estimation as a baseline. In particular, the analysis exposes how imperfect initial overlap and Fourier tails affect the cost of ground-state energy estimation. This motivates the use of quantum singular value transformation, which implements sharper spectral filters and leads to near-optimal procedures for both ground-state preparation and energy estimation. We then show that these guarantees are essentially best possible by proving lower bounds. Finally, we discuss what remains possible in the Hamiltonian-simulation input model using single-ancilla, statistically post-processed measurements, which is complementary to the iterative phase estimation method discussed in Chapter 16.

18.1. Problem setup

Let $H \in \mathbb{C}^{N\times N}$ with $N = 2^n$ be a Hermitian matrix with eigendecomposition

$$H\,|\psi_j\rangle = \lambda_j\,|\psi_j\rangle\,. \tag{18.1}$$

The eigenvalues are ordered non-decreasingly $\lambda_0 \le \lambda_1 \le \cdots \le \lambda_{N-1}$. We are interested in estimating one or a few eigenvalues λ_j, and prepare the associated eigenstate $|\psi_j\rangle$. For concreteness, we will focus on the smallest eigenvalue λ_0, also called the ground-state energy, as well as $|\psi_0\rangle$ called the ground state. All other eigenvalues are called excited-state energies. Estimating ground energy and obtaining information on the ground state of a given quantum Hamiltonian have numerous applications in condensed matter physics, quantum chemistry, and quantum information. However, even for quantum computer, estimating the ground-state energy is a hard problem.

Recall from Example 2.55 that a Hamiltonian $H \in \mathbb{C}^{2^n\times 2^n}$ is called a k-local Hamiltonian if it can be written as $H = \sum_{i=1}^{m} H_i$, where each term H_i acts nontrivially on at most k qubits. In addition, we assume $\|H_i\| \le 1$ for all $i = 1, \ldots, m$. Given two real numbers a and b with $b - a > 1/\operatorname{poly}(n)$, the task is to decide whether the ground-state energy λ_0 of H is less than a or greater than b. This decision problem is known as the local Hamiltonian ground-state energy problem, or simply the local Hamiltonian (LH) problem. It is known that the LH problem is QMA-complete for any $k > 1$ [KSV02]. That is, the problem belongs to the complexity class QMA, and any other problem in QMA can be reduced to an instance of the LH problem with only polynomial overhead. Furthermore, if one can prepare the ground-state wavefunction with sufficient accuracy, then the ground-state energy can be estimated efficiently using quantum phase estimation (QPE). Therefore, the task of preparing the ground state is at least as hard as solving the LH problem and

is thus QMA-hard. However, it is important to note that ground-state preparation is not a decision problem, and does not formally belong to the complexity class QMA.

What the QMA-hardness of the local Hamiltonian (LH) problem tells us is that one should not expect to design a quantum algorithm that can efficiently solve all LH instances, unless BQP = QMA, which is widely believed to be unlikely. However, it is important to emphasize that QMA-hard instances represent the worst-case scenarios among all local Hamiltonians. To make the problem more tractable in practice, there are two possible approaches. One is to provide additional information beyond just the Hamiltonian H, such as a good initial state or structural insight. The other is to focus on specific classes of Hamiltonians, with the hope that physically motivated models may exhibit better computational behavior. This chapter focuses on the former approach, since making use of specific properties of Hamiltonians typically requires additional tools.

One of the most widely adopted sufficient conditions to circumvent QMA-hardness is to assume access to a good initial state:

$$|\phi\rangle = \sum_{k\in[N]} c_k |\psi_k\rangle , \tag{18.2}$$

where the initial overlap $p_0 = |\langle\phi|\psi_0\rangle|^2 = |c_0|^2 > 1/\operatorname{poly}(n)$. The initial overlap is sometimes denoted by $\gamma = \sqrt{p_0}$. One special case is that the ground state is already prepared and $|\phi\rangle = |\psi_0\rangle$, i.e., $p_0 = 1$. If we further have access to $U = e^{i\tau H}$ for some suitable τ, then this reduces to a phase estimation problem discussed in Chapter 16. Compared to phase estimation, this chapter mainly focuses on the scenario when the initial state is not a perfect eigenstate, i.e., $p_0 < 1$. We will also consider the problem of solving eigenvalue problems when H is provided by a block encoding U_H.

It is worth noting that there is some subtle difference between preparing the ground state and estimating the ground-state energy. The former task requires a positive spectral gap $\Delta := \lambda_1 - \lambda_0 > 0$, otherwise the problem is ill-posed according to perturbation theory (Davis-Kahan $\sin\theta$ theorem in Theorem 7.5). The latter however does not require a positive spectral gap. This is because the eigenvalue is stable with respect to perturbation (Weyl's inequality in Theorem 7.4), and any estimate λ with $|\lambda - \lambda_0| < \epsilon$ is a good approximation to the ground-state energy, even if λ is an eigenvalue corresponding to an excited state.

18.2. Quantum phase estimation

In this section, we will study the following simple algorithm to estimate the ground state energy of a Hamiltonian.

Algorithm 18.1 Ground State Energy Estimation via Repeated QPE

Input: Hamiltonian H with eigenvalues in $(0, 1/2)$; Oracle $U = e^{i2\pi H}$; Initial state $|\phi\rangle$; number of trials M; QPE precision parameters as needed.

Output: Estimation of the ground state energy.

1: **for** $\ell = 1$ to M **do**
2: Perform QPE by querying U and the initial state to obtain phase estimate $\widetilde{\varphi}_{k'}^{(\ell)}$.
3: **end for**
4: **return** $\min_{\ell} \widetilde{\varphi}_{k'}^{(\ell)}$

We first note that if **all** eigenvalues of the Hamiltonian can be exactly represented by a d-bit number, the algorithm is easy to analyze. Let $\epsilon = 2^{-d}$. Consider the general initial state in

Eq. (18.2). If we apply the QPE circuit in Fig. 16.4 to $|0^t\rangle|\phi\rangle$ with $t = d$ and measure the ancilla qubits, we obtain a fixed point number representation of λ_0 with probability p_0. Furthermore, the system register returns the eigenstate $|\psi_0\rangle$ with probability p_0. In each run, the probability of *not* obtaining the ground state is $1 - p_0$. Therefore after M runs, the failure probability is $(1-p_0)^M \leq e^{-p_0 M}$. Hence setting $M = \lceil \log(1/\delta)/p_0 \rceil$, the success probability of obtaining the exact ground state energy is at least $1 - \delta$.

When an exact eigenstate is available (in particular when $p_0 = 1$), the standard QPE accuracy and cost tradeoff is summarized in Theorem 16.9.

Unfortunately, when the eigenvalues do not have an exact d-bit binary representation, the analysis becomes more complex, and the results are less favorable than those in the previous analysis.

Let t be the number of ancilla qubits used in the QPE circuit and let $T = 2^t$. Recall from Proposition 16.10 that the probability of measuring the first register and obtain k' is

$$\mathbb{P}(k') = \left\| \sum_k c_k \gamma_{k,k'} |\psi_k\rangle \right\|^2 = \sum_k |c_k \gamma_{k,k'}|^2 = \sum_k |c_k|^2 F_T(\lambda_k - \widetilde{\varphi}_{k'}). \tag{18.3}$$

Here $F_T(\cdot)$ is the Fejér kernel arising in the standard Fourier-transform-based QPE analysis in Chapter 16, and $\widetilde{\varphi}_{k'} = k'/T$ is the phase estimator.

Note that for any λ_k that does not have an exact t-bit binary representation, the tail of the Fejér kernel implies that we may obtain $\widetilde{\varphi}_{k''} < \lambda_0$, i.e., we obtain an energy estimate that is lower than the ground state energy! The probability of ending up in the state $|k''\rangle|\psi_k\rangle$ is $|c_k|^2 F_T(\lambda_k - \widetilde{\varphi}_{k''})$.

We now demonstrate that by choosing a sufficiently large T, the probability of underestimating the ground state energy can be effectively controlled. Recall the periodic distance Eq. (16.32). For simplicity we further restrict all eigenvalues to be in $(\epsilon, 1/2)$. Since λ_0 is the ground state energy, when $\widetilde{\varphi}_{k'} \leq \lambda_0 - \epsilon$, we have

$$|\lambda_k - \widetilde{\varphi}_{k'}|_1 \geq |\lambda_0 - \widetilde{\varphi}_{k'}|_1 = \lambda_0 - \widetilde{\varphi}_{k'} \geq \epsilon, \quad \forall k \in [N]. \tag{18.4}$$

Using the pointwise bound on the Fejér kernel (Eq. (16.42), cf. the proof of Theorem 16.9), the probability of underestimating the ground state energy by ϵ is

$$\begin{aligned}
\mathbb{P}(\widetilde{\varphi}_{k'} \leq \lambda_0 - \epsilon) =& \sum_k \sum_{\lambda_0 - \widetilde{\varphi}_{k'} \geq \epsilon} |c_k|^2 F_T(\lambda_k - \widetilde{\varphi}_{k'}) \\
\leq& \sum_k \sum_{\lambda_0 - \widetilde{\varphi}_{k'} \geq \epsilon} |c_k|^2 \frac{1}{4T^2 |\lambda_k - \widetilde{\varphi}_{k'}|_1^2} \\
\leq& \sum_k \sum_{\lambda_0 - \widetilde{\varphi}_{k'} \geq \epsilon} |c_k|^2 \frac{1}{4T^2 |\lambda_0 - \widetilde{\varphi}_{k'}|^2} \\
=& \sum_{\lambda_0 - \widetilde{\varphi}_{k'} \geq \epsilon} \frac{1}{4T^2 |\lambda_0 - \widetilde{\varphi}_{k'}|^2} \\
\leq& \frac{1}{4T\epsilon} + \frac{1}{4(T\epsilon)^2}.
\end{aligned} \tag{18.5}$$

Let $T\epsilon = \delta'^{-1}$ with $\delta' < 1/2$, we have

$$\mathbb{P}(\widetilde{\varphi}_{k'} \leq \lambda_0 - \epsilon) \leq \frac{\delta'}{2}. \tag{18.6}$$

Therefore by the union bound, after M repetitions,

$$\mathbb{P}\left(\min_\ell \widetilde{\varphi}_{k'}^{(\ell)} \le \lambda_0 - \epsilon\right) \le \frac{M\delta'}{2}. \tag{18.7}$$

In order to obtain $\mathbb{P}\left(\min_\ell \widetilde{\varphi}_{k'}^{(\ell)} \le \lambda_0 - \epsilon\right) < \frac{\delta}{2}$, we need to set $\delta' = M^{-1}\delta$.

We also need to upper bound $\mathbb{P}\left(\min_\ell \widetilde{\varphi}_{k'}^{(\ell)} \ge \lambda_0 + \epsilon\right)$. To this end, first note that $\widetilde{\varphi}_{k'} \ge \lambda_0 + \epsilon$ implies $|\widetilde{\varphi}_{k'} - \lambda_0|_1 \ge \epsilon$. Moreover,

$$\begin{aligned}
\mathbb{P}(|\widetilde{\varphi}_{k'} - \lambda_0|_1 < \epsilon) =& \sum_k \sum_{|\widetilde{\varphi}_{k'} - \lambda_0|_1 < \epsilon} |c_k|^2 F_T(\lambda_k - \widetilde{\varphi}_{k'}) \\
\ge& p_0 \sum_{|\widetilde{\varphi}_{k'} - \lambda_0|_1 < \epsilon} F_T(\lambda_0 - \widetilde{\varphi}_{k'}) \\
=& p_0 \left(1 - \sum_{|\widetilde{\varphi}_{k'} - \lambda_0|_1 \ge \epsilon} F_T(\lambda_0 - \widetilde{\varphi}_{k'})\right) \\
\ge& p_0 \left(1 - \frac{1}{2T\epsilon} - \frac{1}{2(T\epsilon)^2}\right) \\
\ge& p_0(1 - \delta').
\end{aligned} \tag{18.8}$$

Here we have used the normalization condition that

$$\sum_{k'} F_T(\lambda_k - \widetilde{\varphi}_{k'}) = 1, \quad \forall k. \tag{18.9}$$

Therefore

$$\mathbb{P}(|\widetilde{\varphi}_{k'} - \lambda_0|_1 \ge \epsilon) = 1 - \mathbb{P}(|\widetilde{\varphi}_{k'} - \lambda_0|_1 < \epsilon) \le 1 - p_0(1 - \delta') \le 1 - \frac{p_0}{2}. \tag{18.10}$$

This means that

$$\mathbb{P}\left(\min_\ell \widetilde{\varphi}_{k'}^{(\ell)} \ge \lambda_0 + \epsilon\right) \le \mathbb{P}(|\widetilde{\varphi}_{k'} - \lambda_0|_1 \ge \epsilon)^M = (1 - p_0/2)^M \le e^{-\frac{p_0 M}{2}}. \tag{18.11}$$

We can then take $M = \lceil \frac{2}{p_0} \log \frac{2}{\delta} \rceil$ so that

$$\mathbb{P}\left(\min_\ell \widetilde{\varphi}_{k'}^{(\ell)} \ge \lambda_0 + \epsilon\right) \le \frac{\delta}{2}. \tag{18.12}$$

To summarize, according to the relation $\delta' = M^{-1}\delta$, in order to estimate the ground state energy to precision $\epsilon = 2^{-d}$ with success probability $1 - \delta$, we need

$$t = d + \lceil \log_2 \delta'^{-1} \rceil = d + \mathcal{O}(\log p_0^{-1} + \log \delta^{-1} + \log\log \delta^{-1}) \tag{18.13}$$

ancilla qubits in QPE. The circuit depth is

$$T = \mathcal{O}\left((\epsilon p_0 \delta)^{-1} \log \delta^{-1}\right). \tag{18.14}$$

Taking the number of repetitions M into account, the total cost of the method is

$$\mathcal{O}\left(\epsilon^{-1}\delta^{-1}p_0^{-2}(\log \delta^{-1})^2\right). \tag{18.15}$$

Remark 18.1 (Dependence on the initial overlap p_0)**.** The analysis above shows that the cost of QPE grows at least linearly in p_0^{-1}. For efficient ground state estimation, the initial state must satisfy $p_0^{-1} = \mathcal{O}(\text{poly}(n))$. The tail of the Fejér kernel decays slowly, and this introduces additional cost in p_0^{-1}. First, in order to reduce the possibility of overshooting, the number of repetitions M needs to be large enough and is $\mathcal{O}(p_0^{-1})$. However, this also increases the probability of undershooting the eigenvalue, and hence δ' needs to be chosen to be $\mathcal{O}(M^{-1}) = \mathcal{O}(p_0)$. This means that the circuit depth should be $\mathcal{O}(\delta'^{-1}) = \mathcal{O}(p_0^{-1})$. The total complexity is thus $TM = \mathcal{O}(p_0^{-2})$. Therefore, when the initial overlap p_0 is small, using QPE to find the ground state energy can be very costly. The dependence on p_0 can be improved to $\mathcal{O}(p_0^{-1})$ using the quantum median method in Remark 16.8. It can be further improved to $\mathcal{O}(p_0^{-\frac{1}{2}})$, as we will see in Section 18.3. ⋄

18.3. Near-optimal ground state preparation and ground state energy estimation

Let $H \in \mathbb{C}^{2^n \times 2^n}$ be a Hermitian matrix with eigenvalues in the interval $(0, 1)$, and assume access to a unitary U_I that prepares an initial state $|\phi\rangle = U_I |0^n\rangle$ with overlap $p_0 = |\langle\phi|\psi_0\rangle|^2$. To simplify the discussion, we assume that the ground and first excited energies λ_0, λ_1 are known and separated by a positive gap $\Delta = \lambda_1 - \lambda_0$. Our goal is to use quantum singular value transformation (QSVT) to filter the initial state toward $|\psi_0\rangle$ and to estimate the ground-state energy.

18.3.1. Ground state preparation. For simplicity, we assume that we are given $U_H \in \text{BE}_{\alpha,m}(H)$ as a block-encoding of a Hamiltonian H, and a number μ such that $\lambda_0 \leq \mu - \frac{\Delta}{2} < \mu + \frac{\Delta}{2} \leq \lambda_1$, and use this information to prepare the ground state.

We construct a polynomial approximation to the step function

$$\theta(x - \mu) = \frac{1}{2}\left(1 - \text{sign}(x - \mu)\right), \tag{18.16}$$

which equals 1 for $x < \mu$ and 0 for $x > \mu$. Without loss of generality we assume $0 \preceq H \preceq 1$. Since QSVT requires a polynomial defined on $[-1, 1]$, we extend the construction to $[-1, 1]$ by choosing a real even polynomial. Since the step function is discontinuous, the polynomial should only aim at approximating the step function outside $(\mu - \Delta/2, \mu + \Delta/2)$. The polynomial also needs to satisfy the conditions in Theorem 12.2. We need to find an even polynomial $F(x)$ satisfying

$$|F(x) - 1| \leq \epsilon', \quad \forall x \in [0, \mu - \Delta/2]; \quad |F(x)| \leq \epsilon', \quad \forall x \in [\mu + \Delta/2, 1]. \tag{18.17}$$

We can achieve this by approximating the sign function, with $\deg(F) = \mathcal{O}(\log(1/\epsilon')\Delta^{-1})$ (see e.g. [LC17a, Corollary 7] and [GSLW19, Corollary 16]). This construction is based on an approximation to the error function. Fig. 18.1 gives a concrete construction of the even polynomial obtained via numerical optimization, and the phase factors are obtained via QSPPACK. This generates a polynomial $P(x)$ such that $\text{Re}\, P(x) = F(x)$.

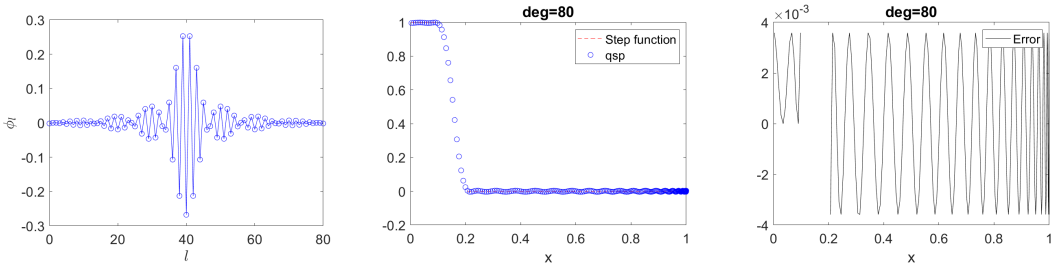


FIGURE 18.1. QSP representation for approximating a step function using an even polynomial on $[0, 0.1] \cup [0.2, 1]$. The phase factors plotted removes a factor of $\pi/4$ on both ends (see **??**).

We set $\mu = (\lambda_0 + \lambda_1)/2$ and apply the QSVT circuit U_F implementing the polynomial filter $F(H)$ to the initial state $|\phi\rangle$:

$$U_F |0^m\rangle |\phi\rangle = |0^m\rangle F(H) |\phi\rangle + |\perp\rangle = \sqrt{p_0} |0^m\rangle F(H) |\psi_0\rangle + \sqrt{1 - p_0} |0^m\rangle F(H) |\psi_\perp\rangle + |\perp\rangle . \tag{18.18}$$

Here $|\psi_\perp\rangle$ is a state in the system register orthogonal to $|\psi_0\rangle$, while $|\perp\rangle$ is orthogonal to all states $|0^m\rangle |\phi\rangle$. Note that

$$\|F(H) |\psi_\perp\rangle\| \leq \epsilon', \quad \|F(H) |\psi_0\rangle\| \geq 1 - \epsilon'. \tag{18.19}$$

Therefore, upon measuring the ancilla qubits, the probability of obtaining the outcome 0^m in the ancilla register is at least $p_0(1 - \epsilon')^2$. Conditioned on this outcome, the postselected system state is proportional to $F(H) |\phi\rangle$ and has fidelity at least $1 - \mathcal{O}(\epsilon'^2/p_0)$ with $|\psi_0\rangle$. In a single execution of the circuit, the maximal number of queries to U_H and $U_H^\dagger$ (referred to as the query depth for short) is $\mathcal{O}(\alpha\Delta^{-1} \log(1/\epsilon'))$, and the total number of queries to U_H and $U_H^\dagger$ using naive repetition is $\mathcal{O}(\alpha\Delta^{-1} p_0^{-1} \log(1/\epsilon'))$. Using amplitude amplification, the query depth becomes $\mathcal{O}(\alpha\Delta^{-1} p_0^{-\frac{1}{2}} \log(1/\epsilon'))$, and the total number of queries to U_H and $U_H^\dagger$ becomes $\mathcal{O}(\alpha\Delta^{-1} p_0^{-\frac{1}{2}} \log(1/\epsilon'))$. Here ϵ' controls the polynomial approximation error, whereas ϵ below denotes the target infidelity. To obtain fidelity at least $1 - \epsilon$, it suffices to take $\epsilon' = \Theta(\sqrt{\epsilon p_0})$, which yields a logarithmic dependence $\log(1/\epsilon') = \mathcal{O}(\log(p_0^{-1}\epsilon^{-1}))$. The result is summarized in Proposition 18.2. This also matches the query lower bound in Section 18.4.

Proposition 18.2 (Ground state preparation with *a priori* information)**.** *Let $U_H \in \mathrm{BE}_{\alpha,m}(H)$ be a block-encoding of a Hamiltonian $H \in \mathbb{C}^{2^n \times 2^n}$, and suppose H has a positive spectral gap $\Delta = \lambda_1 - \lambda_0$. Assume access to an initial state $|\phi\rangle = U_I |0^n\rangle$ such that $p_0 = |\langle\phi|\psi_0\rangle|^2 > 0$. Let μ be a real number satisfying $\lambda_0 \leq \mu - \frac{\Delta}{2} < \mu + \frac{\Delta}{2} \leq \lambda_1$. Then, the ground state $|\psi_0\rangle$ can be prepared to fidelity at least $1 - \epsilon$ using $\mathcal{O}\left(\alpha\Delta^{-1} p_0^{-1/2} \log(p_0^{-1}\epsilon^{-1})\right)$ queries to U_H and its inverse, and $\mathcal{O}\left(p_0^{-1/2}\right)$ queries to U_I and its inverse.*

18.3.2. Ground-state energy estimation. Once the ground state $|\psi_0\rangle$ has been prepared to sufficient accuracy, one natural approach to computing the ground-state energy is to estimate the expectation value $\langle\psi_0|H|\psi_0\rangle$. A straightforward sampling method requires $\mathcal{O}(1/\epsilon^2)$ repetitions to achieve additive error ϵ, but this can be improved to the Heisenberg limit $\mathcal{O}(1/\epsilon)$ using amplitude estimation.

However, in general, an accurate estimate μ of the ground-state energy is not known in advance and must be computed by an algorithm. To address this, we introduce a method based on binary search that does not require a precise initial estimate of μ, yet still allows the ground-state energy to be estimated to precision ϵ with a total cost of $\mathcal{O}(1/\epsilon)$, thereby achieving Heisenberg-limited scaling. The binary search procedure relies on solving a subproblem called the fuzzy bisection problem, which is described in detail in Section 18.3.3. The main result is stated as follows:

THEOREM 18.3 (Ground state energy estimation without **a priori** information). *Let $U_H \in \mathrm{BE}_{\alpha,m}(H)$ be a block-encoding of a Hamiltonian $H \in \mathbb{C}^{2^n \times 2^n}$ with eigenvalues in the interval $(0,1)$, and assume access to an initial state $|\phi\rangle = U_I |0^n\rangle$ such that $p_0 = |\langle\phi|\psi_0\rangle|^2 > 0$. Then the ground energy can be estimated to precision ϵ with probability $1-\delta$ with $\widetilde{\mathcal{O}}(\alpha\epsilon^{-1}p_0^{-\frac{1}{2}}\log(\delta^{-1}))$ queries to U_H and its inverse, and $\widetilde{\mathcal{O}}\left(p_0^{-1/2}\log(\alpha\epsilon^{-1})\log(\delta^{-1})\right)$ queries to U_I and its inverse.*

Note that Theorem 18.3 does not assume the presence of a positive spectral gap. In this setting, the target precision ϵ effectively plays the role of a spectral gap: estimating λ_0 to precision ϵ also allows one to prepare a state supported on eigenvectors with eigenvalues within ϵ of λ_0. However, when a positive spectral gap Δ is known, the result can be further improved. In this case, it suffices to estimate the ground-state energy to within precision $\Delta/2$, and then apply the ground-state preparation algorithm using the estimated energy as input. We then have the following corollary:

Corollary 18.4 (Ground state preparation without *a priori* information)**.** *Let $U_H \in \mathrm{BE}_{\alpha,m}(H)$ be a block-encoding of a Hamiltonian $H \in \mathbb{C}^{2^n \times 2^n}$ with eigenvalues in the interval $(0,1)$, and suppose H has a positive spectral gap $\Delta = \lambda_1 - \lambda_0$. Assume access to an initial state $|\phi\rangle = U_I|0^n\rangle$ such that $p_0 = |\langle\phi|\psi_0\rangle|^2 > 0$. Then, the ground state $|\psi_0\rangle$ can be prepared to fidelity at least $1-\epsilon$ with probability $1-\delta$ using $\widetilde{\mathcal{O}}\left(\alpha\Delta^{-1}p_0^{-1/2}\log(\delta^{-1}\epsilon^{-1})\right)$ queries to U_H and its inverse, and $\widetilde{\mathcal{O}}\left(p_0^{-1/2}\log(\alpha\Delta^{-1})\log(\delta^{-1})\right)$ queries to U_I and its inverse.*

18.3.3. Proof of Theorem 18.3. Again for simplicity of the discussion we assume the block encoding factor $\alpha = 1$. The ground state energy estimation algorithm relies on solving the following **fuzzy bisection problem**:

Definition 18.5 (Fuzzy bisection problem)**.** *Given a real number μ and a tolerance parameter $h > 0$, the goal is to design a quantum algorithm that, with probability at least $1-\delta'$, satisfies the following behavior:*

1. *Outputs 0 if $\lambda_0 \le \mu - h$,*
2. *Outputs 1 if $\lambda_0 \ge \mu + h$,*

under the promise that one of the two cases holds. In the intermediate case where $\mu - h < \lambda_0 < \mu + h$, the algorithm is allowed to output either 0 or 1.

In order to solve the fuzzy bisection problem, we first construct a real even polynomial $F(x)$ satisfying

$$|F(x)-1| \le \epsilon', \quad \forall x \in [0, \mu-h]; \quad |F(x)| \le \epsilon', \quad \forall x \in [\mu+h, 1]. \tag{18.20}$$

The degree of $F(x)$ is $\mathcal{O}(h^{-1}\log(\epsilon'^{-1}))$. If $\lambda_0 \ge \mu + h$, then $\|F(H)|\phi\rangle\|^2 \le (\epsilon')^2$; if $\lambda_0 \le \mu - h$, then

$$\|F(H)|\phi\rangle\|^2 \ge \|F(\lambda_0)|\psi_0\rangle\|^2 \ge (1-\epsilon')^2 p_0. \tag{18.21}$$

The quantity $\|F(H)\,|\phi\rangle\,\|^2$ can be estimated from the success probability of measuring the ancilla qubits in a block-encoded implementation $U_F \in \mathrm{BE}_{1,m'}(F,\epsilon')$ of the operator $F(H)$.

To improve efficiency, we define two projectors:

$$\Pi = |0^{m'}\rangle\langle 0^{m'}| \otimes I, \qquad \Pi' = |0^{m'+n}\rangle\langle 0^{m'+n}|. \tag{18.22}$$

We observe that the relevant quantity is the amplitude

$$\left\|(\langle 0^{m'}| \otimes I)U_F\,|0^{m'}\rangle\,|\phi\rangle\right\| = \left\|\Pi U_F(I\otimes U_I)\,|0^{m'+n}\rangle\right\|, \tag{18.23}$$

which we only need to estimate to precision related to $\sqrt{p_0}$ in order to distinguish between two cases in a binary decision problem. This can be viewed as a **binary amplitude estimation** problem.

We choose parameters for the amplitude gap as follows:

$$\gamma_1 = \epsilon' = \frac{\sqrt{p_0}}{4}, \quad \gamma_2 = (1-\epsilon')\sqrt{p_0}, \tag{18.24}$$

so that the gap satisfies $\gamma_2 - \gamma_1 \geq \sqrt{p_0}/2$. Note that $W = \Pi U_F(I\otimes U_I)\Pi'$ has a single nonzero singular value. The binary amplitude estimation problem then reduces to deciding whether this singular value is at most γ_1 or at least γ_2.

To solve this, we construct an even polynomial $G(x)$ satisfying

$$|G(x)-1| \leq \delta', \quad \forall x \in [0,\gamma_1]; \qquad |G(x)| \leq \delta', \quad \forall x \in [\gamma_2, 1]. \tag{18.25}$$

We then apply the singular value transformation $G^{\triangleright}(W)$ using QSVT. Applying the resulting circuit to the initial state $|0^{n+m'}\rangle$ enables us to distinguish between the two cases with failure probability at most $\mathcal{O}(\delta')$. The number of queries to W is $\mathcal{O}\left((\gamma_2-\gamma_1)^{-1}\log(1/\delta')\right) = \mathcal{O}\left(p_0^{-1/2}\log(1/\delta')\right)$. This implies that, in order to solve the fuzzy bisection problem, the number of queries to U_H and its inverse is $\mathcal{O}\left(p_0^{-1/2}h^{-1}\log(p_0^{-1})\log(1/\delta')\right)$, and the number of queries to U_I and its inverse is $\mathcal{O}\left(p_0^{-1/2}\log(1/\delta')\right)$.

With these preparations, we find λ_0 by iteratively shrinking an interval (l,r) known to contain it (in the worst case, $l=0$ and $r=1$). In each iteration, we solve the fuzzy bisection problem that outputs 0 when $\lambda_0 \leq (2l+r)/3$ and outputs 1 when $\lambda_0 \geq (l+2r)/3$. This is achieved by setting $\mu = (l+r)/2$ and $h = (r-l)/6$. If the output is 0, we update $r \leftarrow (l+2r)/3$; if the output is 1, we update $l \leftarrow (2l+r)/3$. In either case, we maintain $l \leq \lambda_0 \leq r$ and shrink the interval length by a factor $2/3$.

The values of l and r will converge to λ_0 from both sides. Therefore when $r-l \leq 2\epsilon$, λ_0 will be within ϵ distance from $(l+r)/2$. This gives us the ground-state energy estimate. This will take $\left\lceil \log_{3/2}\left((r-l)/(2\epsilon)\right)\right\rceil$ iterations because $r-l$ shrinks by a factor $2/3$ in each iteration.

To ensure a final success probability of at least $1-\delta$, we need to choose $\delta' = \Theta(\delta/\log(\epsilon^{-1}))$ when solving each fuzzy bisection step. By setting the precision parameter $h=\epsilon$, and taking into account that there are $\log(1/\epsilon)$ steps in total, the total number of queries to U_H and its inverse is thus $\widetilde{\mathcal{O}}(\epsilon^{-1}p_0^{-\frac{1}{2}}\log(\delta^{-1}))$. In particular, it achieves the Heisenberg-limited scaling with respect to the precision ϵ. The number of queries to U_I and its inverse is $\widetilde{\mathcal{O}}\left(p_0^{-1/2}\log(1/\delta)\log(1/\epsilon)\right)$. This proves Theorem 18.3.

18.4. Lower bound for ground state preparation

We have shown that the cost for preparing the ground state to precision ϵ with success probability at least $1-\delta$ is $\widetilde{\mathcal{O}}(\Delta^{-1}p_0^{-\frac{1}{2}}\log(\delta^{-1}))$, regardless of whether the ground state energy is known *a priori*. Is it possible to further reduce the query complexity with respect to Δ, p_0? In this section we prove that the cost of ground state preparation is near-optimal. We prove both lower bounds by reducing from the unstructured search problem, for which Grover's algorithm achieves the optimal query complexity. We treat two complementary regimes: constant spectral gap and vanishing overlap, and constant overlap and vanishing spectral gap. For simplicity, we denote by $\gamma = \sqrt{p_0}$. If the ground state preparation problem is formulated under additional normalization constraints (e.g., $0 \preceq H \preceq I$), one may replace H by an affine transformation of H; this does not change the ground state and only rescales the spectral gap by a constant factor.

Proposition 18.6. *When $\Delta = \Omega(1)$, and $\gamma \to 0^+$, the number of queries to U_H needed to prepare the ground state $|\psi_0\rangle$ to fidelity at least $\sqrt{3}/2$ is $\Omega(1/\gamma)$.*

Proof. Let $N = 2^n$. Consider an oracle

$$U_t = I - 2\,|t\rangle\,\langle t|\,, \tag{18.26}$$

where t is an n-bit string. The operator U_t is Hermitian and unitary, with eigenvalue -1 on $|t\rangle$ and eigenvalue 1 on $|t\rangle^{\perp}$. Hence $|t\rangle$ is the unique ground state and the spectral gap equals 2. Moreover, U_t is an $(1,0,0)$-block-encoding of itself, so we may take $U_H = U_t$.

Let $|u\rangle = \frac{1}{\sqrt{N}}\sum_s |s\rangle$ be the uniform superposition of all n-strings, then we have $\langle u|t\rangle = \frac{1}{\sqrt{N}}$, and $|u\rangle$ can be efficiently prepared by the Hadamard transform since $\mathrm{H}^{\otimes n}\,|0^n\rangle = |u\rangle$. If the ground state preparation problem can be solved with $o(1/\gamma)$ queries to U_H for fixed Δ to produce an approximate ground state with fidelity at least $\sqrt{3}/2$, then from the above setup we have $\gamma = 1/\sqrt{N}$, and measuring the output state in the computational basis yields t with probability at least $3/4$. Therefore the unstructured search problem can be solved with $o(\sqrt{N})$ queries to the oracle U_t, contradicting Grover's lower bound. □

Proposition 18.7. *When $\gamma = \Omega(1)$, and $\Delta \to 0^+$, the number of queries to U_H needed to prepare the ground state $|\psi_0\rangle$ to fidelity at least $\sqrt{3}/2$ is $\Omega(1/\Delta)$.*

Proof. We want to create a situation in which the overlap is bounded from below by a constant but the gap vanishes. Consider $U_t = I - 2\,|t\rangle\,\langle t|$ where t is an n-bit string. Let $|u\rangle = \frac{1}{\sqrt{N}}\sum_s |s\rangle$ be the uniform superposition of all n-bit strings. The reflection operator

$$D = I - 2|u\rangle\langle u| \tag{18.27}$$

can be efficiently implemented using Hadamard gates. Then we define

$$H(\tau) = (1-\tau)D + \tau U_t, \tag{18.28}$$

and consider $H(1/2)$. Since D and U_t are Hermitian, $H(\tau)$ is Hermitian for all $\tau \in [0,1]$. Because both $\mathrm{span}\{|u\rangle, |t\rangle\}$ and its orthogonal complement are invariant subspaces of D and U_t, and both operators equal the identity when restricted to $\mathrm{span}\{|u\rangle, |t\rangle\}^{\perp}$, it suffices to analyze $H(1/2)$ on the two-dimensional subspace $\mathrm{span}\{|u\rangle, |t\rangle\}$. Let $a := \langle u|t\rangle = 1/\sqrt{N}$ and write

$$|u\rangle = a\,|t\rangle + \sqrt{1-a^2}\,|t^{\perp}\rangle\,, \qquad |t^{\perp}\rangle := \frac{|u\rangle - a\,|t\rangle}{\sqrt{1-a^2}}, \tag{18.29}$$

so that $\{|t\rangle, |t^\perp\rangle\}$ is an orthonormal basis of $\mathrm{span}\{|u\rangle, |t\rangle\}$. In this basis, $U_t = \mathrm{diag}(-1, 1)$ and

$$[D]_{\{|t\rangle,|t^\perp\rangle\}} = \begin{pmatrix} 1-2a^2 & -2a\sqrt{1-a^2} \\ -2a\sqrt{1-a^2} & 2a^2-1 \end{pmatrix}. \tag{18.30}$$

Therefore

$$[H(1/2)]_{\{|t\rangle,|t^\perp\rangle\}} = \frac{1}{2}\left([D]_{\{|t\rangle,|t^\perp\rangle\}} + [U_t]_{\{|t\rangle,|t^\perp\rangle\}}\right) = \begin{pmatrix} -a^2 & -a\sqrt{1-a^2} \\ -a\sqrt{1-a^2} & a^2 \end{pmatrix}. \tag{18.31}$$

The eigenvalues of this matrix are $\pm a = \pm 1/\sqrt{N}$. Hence the ground-state energy of $H(1/2)$ is $-1/\sqrt{N}$, the first excited energy is $1/\sqrt{N}$, and the gap is $\Delta(1/2) = 2/\sqrt{N}$. A direct calculation shows that the corresponding ground state is

$$|\Psi\rangle = \frac{|u\rangle + |t\rangle}{\sqrt{2 + \frac{2}{\sqrt{N}}}}, \tag{18.32}$$

and therefore $\langle\Psi|u\rangle = \langle\Psi|t\rangle = 1/\sqrt{2} + \mathcal{O}(1/\sqrt{N})$ for large N.

Therefore $|t\rangle$ can be prepared in the following way: we first prepare the ground state of $H(1/2)$, whose block-encoding can be constructed using $\mathcal{O}(1)$ controlled applications of U_t (as well as controlled-D) per query. The resulting approximate ground state we denote by $|\widetilde{\Psi}\rangle$. Then we measure $|\widetilde{\Psi}\rangle$ in the computational basis.

If the desired lower bound does not hold, then $|\widetilde{\Psi}\rangle$ can be prepared with $o(1/\Delta(1/2)) = o(\sqrt{N})$ queries to the block-encoding of $H(1/2)$ and therefore the same number of queries to U_t. Because the angle corresponding to fidelity is the great-circle distance on the unit sphere, we have the triangle inequality

$$\arccos|\langle\widetilde{\Psi}|t\rangle| \leq \arccos|\langle\Psi|t\rangle| + \arccos|\langle\widetilde{\Psi}|\Psi\rangle| \leq \frac{5\pi}{12} + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right). \tag{18.33}$$

Here we use $|\langle\widetilde{\Psi}|\Psi\rangle| \geq \sqrt{3}/2$. Therefore for large N we have $|\langle\widetilde{\Psi}|t\rangle| \geq \cos(5\pi/12) + \mathcal{O}(1/\sqrt{N}) > 1/4$. The probability of obtaining t upon measuring in the computational basis is at least $1/16$. Since Grover's lower bound applies for any constant success probability bounded away from 0, this would yield an $o(\sqrt{N})$-query algorithm for unstructured search, a contradiction.

□

18.5. Single ancilla eigenvalue estimation

So far we have demonstrated that in the block-encoding input model, one can design efficient quantum algorithms that achieve near-optimal complexity for both ground-state energy estimation and ground-state preparation. However, block encoding requires significant quantum resources. A natural question is what can be achieved in the Hamiltonian simulation input model, where the available queries are of the form e^{-iHt}, and Hamiltonian simulation can be implemented using methods such as Trotter decomposition.

Recall the iterative phase estimation algorithm discussed in Section 16.8, which uses only a single ancilla qubit and controlled Hamiltonian simulation. Through iterative refinement, this algorithm can estimate the eigenphase and prepare the corresponding eigenstate. A different approach is to consider what can be achieved using just a single invocation of the circuit block from Fig. 16.7, queried in parallel. While the resulting procedure cannot prepare an eigenstate, it may still allow us to estimate the eigenvalue efficiently.

When the input state $|\phi\rangle$ is an exact eigenstate of H, the Hadamard test can be used to estimate the corresponding eigenvalue with cost $\mathcal{O}(\epsilon^{-2})$, and this can be improved to $\mathcal{O}(\epsilon^{-1})$ using Kitaev's algorithm described in Section 16.9. The algorithm presented in this section can be interpreted as a robust version of the Kitaev algorithm, which estimates the eigenvalue even when the input state has only partial overlap with an eigenstate, that is, when $p_0 = |\langle\phi|\psi_0\rangle|^2 < 1$. For concreteness, we focus on ground-state energy estimation, although the method can be applied more generally.

The basic idea is that instead of coherently constructing a filter in the energy eigenbasis using quantum eigenvalue transformation, as in Section 18.3, we collect data from the quantum computer and then use classical signal processing to construct such a filter incoherently.

To understand how this works, we first describe how the quantum data are collected. Using the circuit in Fig. 18.2, setting $t = t_j$, we may define a complex random variable Z_j

$$Z_j = X_j + iY_j, \quad X_j, Y_j \in \{\pm 1\}, \tag{18.34}$$

such that

$$\mathbb{E}(Z_j) = \langle\phi| \exp(-it_j H) |\phi\rangle\,, \quad |Z_j| \le 2\,. \tag{18.35}$$

Therefore Z_j gives an unbiased estimator of

$$\langle\phi| \exp(-it_j H) |\phi\rangle = \sum_{m\in[N]} p_m \exp(-i\lambda_m t_j) = \int_{-\pi}^{\pi} e^{-it_j x} p(x)\,\mathrm{d}x. \tag{18.36}$$

Here $p(x) = \sum_{m\in[N]} p_m \delta(x - \lambda_m)$ is the spectral density (also called the density of states) of H.

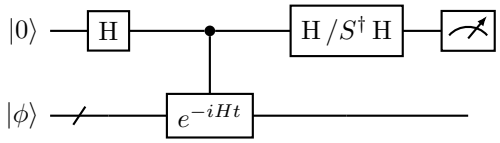


FIGURE 18.2. Circuit for estimating the real part (by applying the H gate) or the imaginary part (by applying the $S^\dagger$ H gate) of the quantity $\langle\phi|e^{-itH}|\phi\rangle$ on a quantum computer. The measurement outcome defines a random variable that takes the value 1 if the result is 0, and -1 if the result is 1. Here, H denotes the Hadamard gate and S denotes the phase gate.

Without loss of generality we assume $\|H\| < \pi/3$. Given a set of time points $\{t_j\}_{j=1}^{N_t}$, where each t_j is an **integer** drawn from a probability distribution $a(t)$ to be specified later, we run the circuits Fig. 18.2 for the real and imaginary parts only once, to prepare the following noisy data set:

$$D = \{(t_j, Z_j)\}_{j=1}^{N_t}\,, \quad Z_j \in \{\pm 1 \pm i\}. \tag{18.37}$$

Our goal is to approximate the cumulative distribution function (CDF), defined as

$$C(\mu) = \int_{-\pi}^{\mu} p(x)\,\mathrm{d}x. \tag{18.38}$$

We first rewrite $C(\mu)$ as the convolution between the spectral density and a periodized step function

$$\hat{\theta}(x) = \sum_{k\in\mathbb{Z}} \mathbf{1}_{[2k\pi,(2k+1)\pi)}(x). \tag{18.39}$$

Since p is supported on $[-\pi/3, \pi/3]$, we have

$$(\hat{\theta} * p)(\mu) = \int_{-\pi}^{\pi} \hat{\theta}(\mu - x)p(x)\,\mathrm{d}x = \int_{-\pi/3}^{\mu} p(x)\,\mathrm{d}x = C(\mu), \quad \mu \in [-\pi/3, \pi/3]. \tag{18.40}$$

Here we use the fact that $\mu - x \in [-2\pi/3, 2\pi/3] \subset [-\pi, \pi]$. Expressing $\hat{\theta}(x)$ as a Fourier series, $\hat{\theta}(x) = \sum_{t\in\mathbb{Z}} \theta(t)e^{itx}$, the Fourier series coefficients are

$$\theta(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{\theta}(x)e^{-itx}\,\mathrm{d}x = \frac{1}{2\pi}\int_{0}^{\pi} e^{-itx}\,\mathrm{d}x = \frac{1}{2\pi(-it)}(e^{-it\pi} - 1) = \begin{cases} \frac{1}{i\pi t}, & t \text{ is odd}, \\ \frac{1}{2}, & t = 0, \\ 0, & t \neq 0 \text{ and is even}. \end{cases} \tag{18.41}$$

Ideally, we draw i.i.d. random variables $t_j \in \mathbb{Z}$ according to the distribution proportional to $|\theta(t)|$, and let $\theta(t) = |\theta(t)|\, e^{i\zeta(t)}$, where the phase convention is $\zeta(0) = 0$, $\zeta(t) = -\pi/2$ if $t > 0$, and $\zeta(t) = \pi/2$ if $t < 0$. Then the sample average $\frac{1}{N_t}\sum_{j=1}^{N_t} e^{it_j\mu}e^{i\zeta(t_j)}Z_j$ is an unbiased estimator up to the normalization constant $\sum_{t\in\mathbb{Z}} |\theta(t)|$ of

$$\sum_{t\in\mathbb{Z}} \theta(t)e^{it\mu}\,\langle\phi|\exp(-itH)\,|\phi\rangle = \int_{-\pi}^{\pi}\sum_{t\in\mathbb{Z}} \theta(t)e^{it(\mu-x)}p(x)\,\mathrm{d}x = \int_{-\pi}^{\pi} \hat{\theta}(\mu-x)p(x)\,\mathrm{d}x = C(\mu). \tag{18.42}$$

However, the expected total evolution time of this strategy will be proportional to $\sum_{t\in 2\mathbb{Z}+1} |\theta(t)|\,|t| = \infty$! This is not surprising considering that $C(\mu)$ is a discontinuous function. For instance, if $\mu = \lambda_0$, then $C(\lambda_0 - \epsilon) = 0$ and $C(\lambda_0 + \epsilon) = p_0$ for any $\epsilon > 0$. So even solving the decision problem of whether $C(\mu) > p_0/2$ or $C(\mu) < p_0/4$ requires resolving the spectral density to infinite precision, which requires an infinite evolution time.

Below we will show that the problem becomes much more manageable if we are to solve a fuzzy decision problem as in Section 18.3.3 with a precision parameter $h > 0$. Then we may perform a binary search process to estimate λ_0 to precision ϵ. We will convolve the periodized step function $\hat{\theta}(x)$ with a periodized Gaussian function

$$\hat{b}(x) = \frac{T}{\sqrt{2\pi}}\sum_{k\in\mathbb{Z}} e^{-\frac{(x+2k\pi)^2T^2}{2}}, \tag{18.43}$$

where T is a tunable parameter related to the Hamiltonian simulation time that will be chosen later. The Fourier series coefficients are

$$b(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{b}(x)e^{-itx}\,\mathrm{d}x = \frac{1}{2\pi}e^{-\frac{t^2}{2T^2}}, \quad t \in \mathbb{Z}. \tag{18.44}$$

We now define the desired function

$$a(t) = 2\pi A b(t)\theta(t) = \begin{cases} \frac{A}{i\pi t}e^{-\frac{t^2}{2T^2}}, & t \text{ is odd}, \\ \frac{A}{2}, & t = 0, \\ 0 & t \neq 0 \text{ and is even}. \end{cases} \tag{18.45}$$

Here $A > 0$ is a normalization factor chosen so that

$$\sum_{t\in\mathbb{Z}} |a(t)| = 1. \tag{18.46}$$

Note that

$$\frac{1}{2} + \sum_{t\in 2\mathbb{Z}+1} \frac{1}{\pi\,|t|} e^{-\frac{t^2}{2T^2}} = \Theta(\log T), \tag{18.47}$$

so the normalization factor $A = \Theta((\log T)^{-1})$. By the convolution formula,

$$\hat{a}(x) = \sum_{t\in\mathbb{Z}} a(t)e^{itx} = A\int_{-\pi}^{\pi} \hat{\theta}(x-y)\hat{b}(y)\,\mathrm{d}y. \tag{18.48}$$

As a result, if we draw i.i.d. random variables $t_j \in \mathbb{Z}$ according to the probability distribution $|a(t)|$, and let $a(t) = |a(t)|\, e^{i\zeta(t)}$, then the sample average $\frac{1}{N_t}\sum_{j=1}^{N_t} e^{it_j\mu} e^{i\zeta(t_j)} Z_j$ is an unbiased estimator of

$$\begin{aligned} &\sum_{t\in\mathbb{Z}} a(t)e^{it\mu}\,\langle\phi|\exp(-itH)\,|\phi\rangle = \int_{-\pi}^{\pi}\sum_{t\in\mathbb{Z}} a(t)e^{it(\mu-x)}p(x)\,\mathrm{d}x \\ &= A\int_{-\pi}^{\pi} (\hat{\theta}*\hat{b})(\mu-x)p(x)\,\mathrm{d}x = A\int_{-\pi}^{\pi} \hat{b}(\mu-x)(\hat{\theta}*p)(x)\,\mathrm{d}x = A\int_{-\pi}^{\pi} \hat{b}(\mu-x)C(x)\,\mathrm{d}x, \end{aligned} \tag{18.49}$$

which is the CDF smeared by a Gaussian distribution of width T^{-1}.

In order to reach the tolerance $h = \Theta(\epsilon)$ in the last step of the binary search process, we need to choose $T = \Theta(\epsilon^{-1})$. Then the expected evolution time is

$$\sum_{t\in\mathbb{Z}} |a(t)t| = \Theta(AT) = \widetilde{\mathcal{O}}(T) = \widetilde{\mathcal{O}}(\epsilon^{-1}), \tag{18.50}$$

and the second moment satisfies

$$\sum_{t\in\mathbb{Z}} |a(t)|\, t^2 = \Theta(AT^2) = \widetilde{\mathcal{O}}(T^2) = \widetilde{\mathcal{O}}(\epsilon^{-2}). \tag{18.51}$$

At each step of the bisection process, we need to estimate the smeared CDF well enough to distinguish the two promised cases; after rescaling by A^{-1}, this amounts to additive precision $p_0/4$ with success probability at least $1-\delta'$. Using a Monte Carlo sampling strategy and majority voting, the number of samples is $N_s = \widetilde{\mathcal{O}}(p_0^{-2}\log(1/\delta'))$. Since there are $\mathcal{O}(\log(\epsilon^{-1}))$ steps in total, we can set $\delta' = \delta/\log(\epsilon^{-1})$, and the total evolution time is $\widetilde{\mathcal{O}}(p_0^{-2}\epsilon^{-1}\log(\delta^{-1}))$. This achieves the Heisenberg-limited scaling.

Notes and further reading

For the repeated-QPE approach in Section 18.2, the quadratic dependence on the initial overlap p_0 comes from the slowly decaying tails of the Fejér kernel in the standard Fourier-based implementation. In that setting, the Fejér kernel corresponds to the uniform resource state $\mathrm{H}^{\otimes n}\,|0^n\rangle$. Replacing this resource state by windowed constructions, such as Kaiser-window states [BSG+24b, BTK+25] or Gaussian states [MGB22], suppresses the tails exponentially and improves the overlap dependence from quadratic to linear.

The near-optimal algorithm in Section 18.3 proceeds differently: it reduces ground-state energy estimation to a sequence of decision problems and then combines them with a binary search [LT20a].

The same decision-problem viewpoint can also be implemented in Hamiltonian-simulation input models, as discussed in Section 13.6, with matching asymptotic complexity [DLT22].

For ground-state preparation, Section 18.4 proves separate lower bounds $\Omega(\Delta^{-1})$ and $\Omega(\gamma^{-1})$, where Δ is the spectral gap and $\gamma = \sqrt{p_0}$. Ref. [MdW23] strengthens this to the joint lower bound $\Omega((\Delta\gamma)^{-1})$, matching the upper bounds in their simultaneous dependence on gap and overlap.

The single-ancilla method in Section 18.5 keeps the Hadamard-test circuit but shifts the work to classical post-processing of the resulting samples. In this sense it is closely related to Kitaev-type phase estimation, but with a different estimator and a different robustness guarantee. The use of such post-processing for early fault-tolerant phase and energy estimation was developed in [LT22, WBC22, ZWJ22, WFZ$^+$23, DL23a, NLY23, BCI$^+$23]. Under stronger assumptions, the same data can also be used for spectral density estimation; see [Som19, RRMB21, DL23b, LNY23, DLL$^+$24b, SCS$^+$23, DELZ24]. Closely related methods based on quantum Krylov diagonalization begin with [PM19, SHE20] and were developed further in [CG22, SHT22, ELN22, DTO22, BHS$^+$23, SKS$^+$23, SKR$^+$24, YAK$^+$25, YMI$^+$25]. For some Hamiltonians, the controlled simulation in these methods can be replaced by control-free constructions [RRMB21, DLT22, YCB$^+$24, CCGP$^+$24].

The QMA-completeness of the local Hamiltonian problem was proved first for $k = 5$ in [KSV02] and then refined to $k = 2$ in [KKR06, OT05, AGIK09]. In the standard formulation, the promise gap satisfies $b-a > 1/\operatorname{poly}(n)$. Whether the problem remains QMA-complete for a constant promise gap $b - a = \Omega(1)$ is open; this is the quantum PCP conjecture, for which [AAV13, NN24] provide background. The inverse-precision dependence in this promise problem is not merely an artifact of the reduction. Even if an exact ground state were available, estimating its energy to additive error ϵ still requires cost of order ϵ^{-1} in the phase-estimation model. A related question asks whether a family of local Hamiltonians is gapped, namely whether $\lambda_1 - \lambda_0$ stays bounded below by a positive constant as the system size grows. That problem is undecidable in general.

CHAPTER 19

Solving linear systems of equations

In this chapter, we study quantum algorithms for the quantum linear systems problem (QLSP). Given a matrix $A \in \mathbb{C}^{N\times N}$ and a vector $b \in \mathbb{C}^N$, the goal is to prepare a quantum state proportional to the solution $x = A^{-1}b$. The main difficulty is not only to implement the inverse map on the spectrum of A, but to do so with controlled dependence on the condition number, the target precision, and the success probability in an oracle model for both A and b.

We first study the HHL algorithm, where matrix inversion is achieved through phase estimation and controlled rotations. This makes the basic mechanism transparent, but it also exposes the main sources of inefficiency, especially the need for accurate eigenvalue estimation and the cost of postselection. These limitations motivate the move to QSVT, which implements the inverse more directly through polynomial approximation and yields better precision dependence. We then turn to Poisson's equation and fermionic Green's functions to show how the abstract solver interfaces with concrete operators and observables. The chapter ends with adiabatic and quantum Zeno methods, where the problem is recast as eigenpath traversal and the focus shifts from polynomial approximation to gap-dependent state preparation, leading to near-optimal dependence on the condition number.

19.1. Problem setup

The quantum linear system problem (QLSP) solves the linear systems of equations $Ax = b$ on a quantum computer for some $A \in \mathbb{C}^{N\times N}$ and $b \in \mathbb{C}^N$ with $N = 2^n$. Without loss of generality we may assume A is Hermitian. This is because we can always consider a dilated linear system

$$\widetilde{A}\begin{pmatrix}0\\x\end{pmatrix} = \begin{pmatrix}b\\0\end{pmatrix}, \quad \widetilde{A} = \begin{bmatrix}0 & A\\ A^\dagger & 0\end{bmatrix}, \tag{19.1}$$

which is equivalent to the original system $Ax = b$. The matrix A can be accessed via a block encoding $U_A \in \mathrm{BE}_{\alpha,m}(A)$, or via a Hamiltonian evolution oracle $U = e^{i2\pi A}$ if A is Hermitian. The right hand side vector is a normalized vector $|b\rangle$ that can be accessed through an oracle U_b:

$$U_b\,|0^n\rangle = |b\rangle\,. \tag{19.2}$$

Solving QLSP means approximating the normalized solution state $|x\rangle = x/\,\|x\|$. A QLSP solver constructs a block encoding $\widetilde{U} \in \mathrm{BE}_{\gamma,m}(A^{-1},\epsilon)$, which produces a quantum state $|\widetilde{x}\rangle$ so that

$$\||\widetilde{x}\rangle - |x\rangle\| \le \epsilon, \quad |x\rangle = \frac{A^{-1}\,|b\rangle}{\|A^{-1}\,|b\rangle\|}. \tag{19.3}$$

What about the norm of the solution x? Let $|\widetilde{x}\rangle\!\rangle = \langle 0^m|\,\widetilde{U}\,|0^m\rangle\,|b\rangle$ be an unnormalized vector and $|\widetilde{x}\rangle = |\widetilde{x}\rangle\!\rangle\,/\,\||\widetilde{x}\rangle\!\rangle\|$, then

$$\|x - \gamma|\widetilde{x}\rangle\!\rangle\| \le \epsilon. \tag{19.4}$$

Using the triangle inequality,

$$\left| \|x\| - \gamma \||\widetilde{x}\rangle\| \right| \leq \epsilon. \tag{19.5}$$

Therefore $\gamma \||\widetilde{x}\rangle\|$ can be a good approximation to the norm of the solution vector $\|x\|$.

The QLSP solver is frequently used as a quantum subroutine for other tasks. For an end-to-end task, we can compute observables from the QLSP solution of the form $x^\dagger O x = \langle x|O|x\rangle \|x\|^2$. If we write $|y\rangle = y/\|y\|$, then the overlap between the solution vector and a given vector y satisfies $y^\dagger x = \|y\| \|x\| \langle y|x\rangle$.

19.2. Quantum phase estimation and HHL algorithm

The **Harrow–Hassidim–Lloyd (HHL) algorithm** [HHL09], which uses the quantum Fourier transform based QPE, is the first quantum algorithm for solving QLSP. The Hermitian matrix A is queried using Hamiltonian evolution oracle $U = e^{i2\pi A}$. The eigendecomposition of A is given by $A|v_j\rangle = \lambda_j |v_j\rangle, j \in [N]$. Due to the nuances associated with the analysis of QPE, it is not easy to give a precise analysis of the performance of the HHL algorithm in the most general setting. To avoid such complications, we will assume each eigenvalue of A is in $(0, 1)$ and has an exact d-bit representation. Under these assumptions, the first step of the eigenvalue-transformation in Section 16.5 is to apply QPE so that, if

$$|b\rangle = \sum_j c_j |v_j\rangle, \tag{19.6}$$

then by linearity,

$$U_{\mathrm{QPE}} |0^d\rangle |b\rangle = \sum_j c_j |\lambda_j\rangle |v_j\rangle. \tag{19.7}$$

Note that the unnormalized solution satisfies

$$x = A^{-1}|b\rangle = \sum_j \frac{c_j}{\lambda_j} |v_j\rangle, \tag{19.8}$$

so the second step is to use the eigenvalue register $|\lambda_j\rangle$ to apply a controlled rotation that multiplies each component by λ_j^{-1}. Using a coherent implementation of classical arithmetic operations, we can implement the controlled rotation

$$U_{\mathrm{CR}} |0\rangle |\lambda_j\rangle = \left(\sqrt{1 - \frac{C^2}{\widetilde{\lambda}_j^2}} |0\rangle + \frac{C}{\widetilde{\lambda}_j} |1\rangle \right) |\lambda_j\rangle. \tag{19.9}$$

Here C is a normalization constant to be chosen later. Note that $\widetilde{\lambda}_j$ is not exactly the same as λ_j even when λ_j is expressed exactly in a d-bit representation. This discrepancy arises because, for each λ_j, the rotation requires classical arithmetic operations to compute $\frac{1}{\pi} \arcsin\left(\frac{C}{\lambda_j}\right)$ and store a finite bit representation of this angle, denoted by θ_j, in a working quantum register. After this, we can implement $\sin(\pi\theta_j) = \frac{C}{\widetilde{\lambda}_j}$ via the controlled rotation circuit. Here, each $\widetilde{\lambda}_j$ approximates λ_j.

Next, we perform uncomputation by applying $U_{\mathrm{QPE}}^\dagger$, we convert the information from the ancilla register $|\lambda_j\rangle$ back to $|0^d\rangle$. Therefore the quantum circuit for the HHL algorithm is in Fig. 19.1.

Note that through the uncomputation, the d ancilla qubits for storing the eigenvalues also becomes a working register. Discarding all working registers, the resulting unitary denoted by

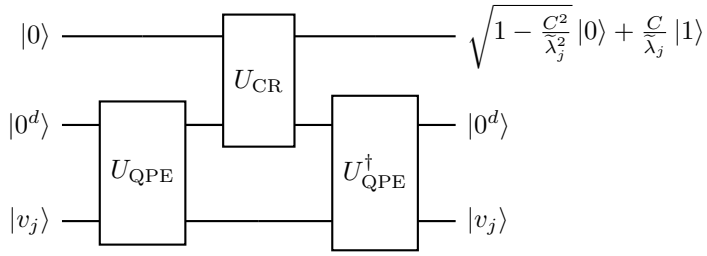


FIGURE 19.1. Circuit for the HHL algorithm.

U_{HHL} satisfies

$$U_{\mathrm{HHL}}\,|0\rangle\,|b\rangle=\sum_j\left(\sqrt{1-\frac{C^2}{\widetilde{\lambda}_j^2}}\,|0\rangle+\frac{C}{\widetilde{\lambda}_j}\,|1\rangle\right)c_j\,|v_j\rangle\,. \tag{19.10}$$

Finally, measuring the signal qubit (the only ancilla qubit left), if the outcome is 1, we obtain the (unnormalized) vector

$$|\widetilde{x}\rangle\!\rangle=\sum_j\frac{C}{\widetilde{\lambda}_j}c_j\,|v_j\rangle\,. \tag{19.11}$$

Upon success of measurement, the system register stores a normalized state

$$|\widetilde{x}\rangle=\frac{|\widetilde{x}\rangle\!\rangle}{\||\widetilde{x}\rangle\!\rangle\|}\approx|x\rangle\,, \tag{19.12}$$

which is the desired approximate solution to QLSP. From Eq. (19.10), the success probability for measuring the signal qubit with outcome 1 is the square of the norm of the unnormalized solution

$$p(1)=\||\widetilde{x}\rangle\!\rangle\|^2\approx C^2\left\|A^{-1}\,|b\rangle\right\|^2. \tag{19.13}$$

Therefore the success probability is determined by

(1) the choice of the normalization constant C,
(2) the norm of the true solution $\xi:=\left\|A^{-1}\,|b\rangle\right\|$.

To maximize the success probability, C should be chosen to be as large as possible, and satisfies the constraint $|C/\lambda_j|\le 1$ for all λ_j. For simplicity assume $\|A\|=1$, and let $\kappa=\|A\|\left\|A^{-1}\right\|$ be the condition number. This means $\lambda_0^{-1}=\left\|A^{-1}\right\|=\kappa/\|A\|=\kappa$. Under these assumptions, it is sufficient to choose $C=\kappa^{-1}$. Also use the fact $\left\|A^{-1}\,|b\rangle\right\|\ge 1$, the success probability satisfies

$$p(1)=\Omega(\kappa^{-2}). \tag{19.14}$$

In other words, in the worst case, we need to repeatedly run the HHL algorithm for $\mathcal{O}(\kappa^2)$ times to obtain the outcome 1 in the signal qubit. The choice of the constant C does not contribute to the normalized solution $|\widetilde{x}\rangle$.

Although the HHL algorithm uses additional quantum resources for e.g., quantum Fourier transform and quantum implementation of classical arithmetic operations, we assume that the gate complexity of U_{HHL} is mainly determined by the number of queries to the Hamiltonian evolution oracle $U=e^{i2\pi A}$.

Remark 19.1 (Multiplicative accuracy for estimating eigenvalues)**.** Since $\widetilde{\lambda}_j$ and λ_j cannot be the same even in the best case scenario, we need to identify the accuracy needed for approximating each λ_j. In order to solve QLSP to precision ϵ according to the criterion Eq. (19.3), we need to estimate the eigenvalues to **multiplicative accuracy** ϵ.

To see why this is the case, assume $\widetilde{\lambda}_j = \lambda_j(1+e_j)$ and $|e_j| \leq \frac{\epsilon}{4} \leq \frac{1}{2}$. The unnormalized solution satisfies

(19.15)
$$\left\| |\widetilde{x}\rangle - \kappa^{-1}x \right\| = \kappa^{-1} \left\| \sum_j c_j \left(\frac{1}{\widetilde{\lambda}_j} - \frac{1}{\lambda_j} \right) |v_j\rangle \right\| \leq \kappa^{-1} \left\| \sum_j \frac{c_j}{\lambda_j} \left(\frac{-e_j}{1+e_j} \right) |v_j\rangle \right\| \leq \kappa^{-1} \frac{\epsilon}{2} \|x\| .$$

Hence

$$\left| 1 - \frac{\| |\widetilde{x}\rangle \|}{\kappa^{-1} \|x\|} \right| \leq \frac{\epsilon}{2}. \tag{19.16}$$

By the triangle inequality

(19.17)
$$\| |\widetilde{x}\rangle - |x\rangle \| = \left\| \frac{|\widetilde{x}\rangle}{\| |\widetilde{x}\rangle \|} - \frac{x}{\|x\|} \right\| \leq \left\| \frac{|\widetilde{x}\rangle}{\| |\widetilde{x}\rangle \|} - \frac{|\widetilde{x}\rangle - (|\widetilde{x}\rangle - \kappa^{-1}x)}{\kappa^{-1}\|x\|} \right\| \leq \left| 1 - \frac{\| |\widetilde{x}\rangle \|}{\kappa^{-1}\|x\|} \right| + \frac{\left\| |\widetilde{x}\rangle - \kappa^{-1}x \right\|}{\kappa^{-1}\|x\|} \leq \epsilon.$$

◇

Let T_{QPE} denote the runtime for a single round of QPE. Since $\lambda_0 = \Theta(\kappa^{-1})$, estimating λ_0 to multiplicative precision ϵ (equivalently, additive precision $\epsilon' := \epsilon/\kappa$) requires $T_{\mathrm{QPE}} = \Omega(\kappa/\epsilon)$, without counting other factors such as failure probabilities.

Let us study the success probability of the HHL algorithm in more detail. Let $\xi = \left\| A^{-1} |b\rangle \right\|$ denote the norm of the unnormalized true solution. Under the choice $C = \kappa^{-1}$ discussed above, the success probability of the above procedure is

$$p(1) = \| |\widetilde{x}\rangle \|^2 \approx \left(\frac{\xi}{\kappa} \right)^2 . \tag{19.18}$$

We consider the following two cases for the magnitude of ξ.

1. In general if no further promise is given, then we only have the trivial bound $\xi \geq 1$. Taking $\xi = 1$ as the most pessimistic estimate, we find that $p(1) = \Omega(\kappa^{-2})$.
2. If $|b\rangle$ has a $\Omega(1)$ overlap with an eigenvector of A corresponding to the smallest eigenvalue, then $\xi = \Omega(\kappa)$. This is the best case scenario, and $p(1) = \Omega(1)$ and is independent of the condition number.

So the total runtime of a direct implementation of the HHL algorithm is

$$T_{\mathrm{QPE}} \frac{\kappa^2}{\xi^2} = \mathcal{O}\left(\frac{\kappa^3}{\xi^2 \epsilon} \right). \tag{19.19}$$

Here we emphasize that this is an informal use of the big-O notation, because the time complexity T_{QPE} may be worse than $\mathcal{O}(\kappa/\epsilon)$ in the HHL algorithm according to the discussion above. Thus the total runtime is $\mathcal{O}(\kappa/\epsilon)$ in the best case scenario, and $\mathcal{O}(\kappa^3/\epsilon)$ in the worst case. With amplitude amplification, the worst case complexity can be improved to $\mathcal{O}(\kappa^2/\epsilon)$.

Remark 19.2 (Query complexity lower bound)**.** The cost of a quantum algorithm for solving a generic QLSP scales at least as $\Omega(\kappa(A))$, where $\kappa(A) := \|A\| \left\|A^{-1}\right\|$ is the condition number of A. The proof is based on converting the QLSP into a Hamiltonian simulation problem, and the

lower bound with respect to κ is proved via the "no-fast-forwarding" theorem for simulating generic Hamiltonians [HHL09]. Nonetheless, for specific classes of Hamiltonians, it may still be possible to develop fast algorithms to overcome this lower bound. ◇

19.3. Quantum singular value transformation

When the eigenvalues of A do not have an exact d-bit representation, a direct implementation of HHL requires high-precision quantum phase estimation, and the complexity can scale polynomially in ϵ^{-1}. QSVT improves the dependence on precision and yields a simpler implementation of the required eigenvalue/singular-value transformation.

From the SVD $A = W\Sigma V^\dagger$, the matrix inverse can be expressed as

$$A^{-1} = V\Sigma^{-1}W^\dagger = f^\diamond(A^\dagger), \tag{19.20}$$

where $f(x) = x^{-1}$ is an odd function. We again assume $\|A\| = 1$, and the singular values of A are in the interval $[\kappa^{-1}, 1]$. Since $f(\cdot)$ is unbounded and singular at $x = 0$, we do not approximate it uniformly on $[-1, 1]$. Instead, we construct an odd polynomial $p(x)$ such that

$$\left| p(x) - \frac{1}{\beta\kappa x} \right| \leq \epsilon', \quad \forall x \in [\kappa^{-1}, 1]. \tag{19.21}$$

Here β is chosen so that $|p(x)| \leq 1$ for all $x \in [-1, 1]$, as required by condition (2) in Theorem 12.2. One way to obtain such an odd extension is to start from a smooth odd function on $[-1, 1]$ that agrees with x^{-1} away from the origin and then truncate its Chebyshev expansion. Consider the following smooth and odd extension of x^{-1} to $[-1, 1]$ [CKS17]:

$$f(x) := \frac{1 - (1 - x^2)^b}{x}. \tag{19.22}$$

To obtain an ϵ-close approximation to $1/x$ on $[\kappa^{-1}, 1]$, it is sufficient to choose $b = \lceil \kappa^2 \log(\frac{\kappa}{\epsilon}) \rceil$ and truncate the Chebyshev expansion to degree $d = \left\lceil \sqrt{b \log(\frac{4b}{\epsilon})} \right\rceil = \mathcal{O}(\kappa \log(\kappa/\epsilon))$.

[CKS17] also provides an analytic expression for the truncated sum of Chebyshev polynomials

$$f(x) = 4 \sum_{j=0}^{d} (-1)^j \frac{\sum_{i=j+1}^{b} \binom{2b}{b+i}}{2^{2b}} T_{2j+1}(x). \tag{19.23}$$

Special care should be taken when implementing such Chebyshev coefficients to avoid overflow/underflow issues, and in general it is better to evaluate the Chebyshev coefficients numerically using function values given in Eq. (19.22).

We may also use the convex optimization approach to directly construct an odd approximation. Fig. 19.2 compares the performance of the two approaches for $\kappa = 5$. The error in the convex optimization approach exhibits an equioscillation property on $[\kappa^{-1}, 1]$, while the analytic construction typically requires a slightly larger polynomial degree, with the error larger near $x = 0$ and decreasing towards $x = 1$.

Fig. 19.3 gives a concrete construction of an odd polynomial obtained via numerical optimization, and the phase factors are obtained via QSPPACK.

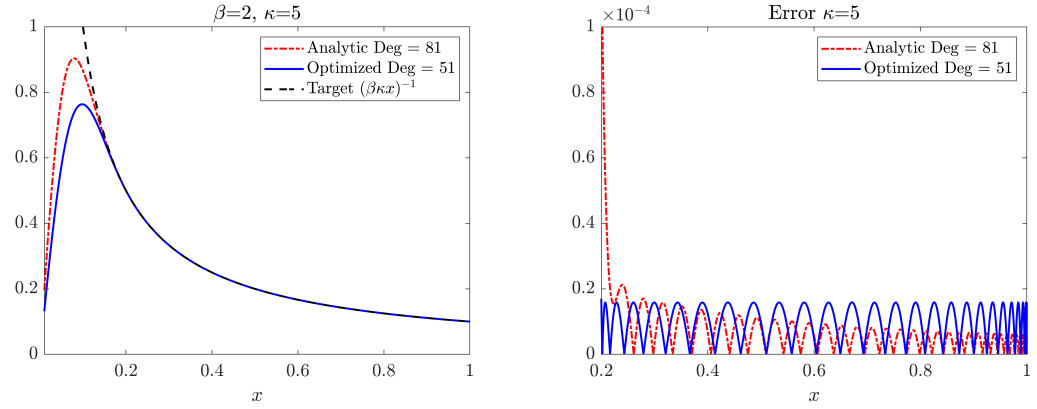


FIGURE 19.2. Comparison between polynomial approximations to $(\beta\kappa x)^{-1}$ on $[\kappa^{-1}, 1]$ using the analytic construction and convex optimization. Here $\kappa = 5, \beta = 2$, and $b = 200$ is chosen in the analytic odd extension in Eq. (19.22).

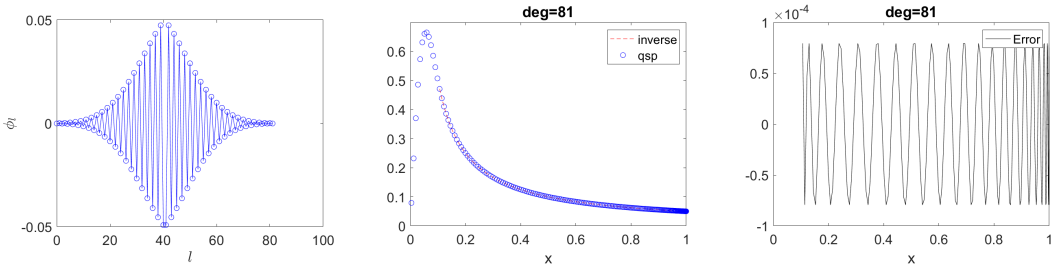


FIGURE 19.3. QSP representation of an odd polynomial approximating the inverse function on $[\kappa^{-1}, 1]$ with $\kappa = 10$. The phase factors plotted remove a factor of $\pi/4$ on both ends (see **??**).

Using QSVT, the circuit in Fig. 13.2 implements a $(1, m+1)$-block-encoding of $p^\diamond(A^\dagger) = Vp(\Sigma)W^\dagger$, denoted by U_Φ. Moreover,

$$\|p^\diamond(A^\dagger) - (\beta\kappa)^{-1}A^{-1}\| = \|p(\Sigma) - (\beta\kappa)^{-1}\Sigma^{-1}\| \leq \epsilon'. \tag{19.24}$$

The total number of queries to U_A and $U_A^\dagger$ is $\mathcal{O}\left(\kappa \log\left(\frac{\kappa}{\epsilon'}\right)\right)$.

Now let $|\widetilde{x}\rangle\!\rangle = \langle 0^{m+1}| U_\Phi |0^{m+1}\rangle |b\rangle = p^\diamond(A^\dagger)|b\rangle$, then

$$\left\| |\widetilde{x}\rangle\!\rangle - (\beta\kappa)^{-1}A^{-1}|b\rangle \right\| \leq \epsilon'. \tag{19.25}$$

Let $\xi = \left\|A^{-1}|b\rangle\right\|$ denote the norm of the unnormalized true solution. Since $|\widetilde{x}\rangle\!\rangle$ approximates $(\beta\kappa)^{-1}A^{-1}|b\rangle$, to ensure $\||\widetilde{x}\rangle\!\rangle - |x\rangle\| \leq \epsilon$ it suffices to set $\epsilon' = \epsilon\xi/(2\beta\kappa)$.

The discussion of the success probability is similar to that of the HHL algorithm. The success probability of the above procedure is $\||\widetilde{x}\rangle\!\rangle\|^2 \approx (\xi/\beta\kappa)^2$. With amplitude amplification, we can boost the success probability to be greater than $1/2$, using $\mathcal{O}(\beta\kappa/\xi)$ rounds of amplitude amplification, i.e., using $U_\Phi^\dagger$, U_Φ, U_b, and $U_b^\dagger$ for $\mathcal{O}(\beta\kappa/\xi)$ times. Therefore the total number of queries to

U_A and $U_A^\dagger$ is

$$\mathcal{O}\left(\frac{\beta\kappa^2}{\xi}\log\left(\frac{\kappa}{\epsilon'}\right)\right). \tag{19.26}$$

The number of queries to U_b and $U_b^\dagger$ is $\mathcal{O}(\beta\kappa/\xi)$.

We consider the following two cases for the magnitude of ξ.

(1) In general if no further promise is given, then $\xi \geq 1$. Taking $\xi = 1$ as the most pessimistic estimate, the total query complexity of U_A is therefore $\mathcal{O}(\kappa^2\log(\kappa/\epsilon))$ (using that $\beta = \Theta(1)$). This is the worst case scenario of using QSVT to solve QLSP.
(2) If $|b\rangle$ has a $\Omega(1)$ overlap with the left-singular vector of A with the smallest singular value, then $\xi = \Omega(\kappa)$. This is the best case scenario, and the total query complexity of U_A is $\mathcal{O}(\kappa\log(\kappa/\epsilon))$, and the number of queries to the right hand side vector $|b\rangle$ is $\mathcal{O}(1)$ (again using $\beta = \Theta(1)$).

In practice, we may not know the precise value of $\|A\|$, and the block encoding factor α may exceed $\|A\|$. We provide a refined version of the statement for using QSVT to solve the QLSP as follows.

THEOREM 19.3 (QSVT based linear system solver). *Let U_A be an $(\alpha, m, 0)$-block-encoding of A with condition number κ, U_b be the oracle preparing the right hand side vector $|b\rangle$, and $\xi = \left\|A^{-1}|b\rangle\right\| \in [1/\|A\|, \|A^{-1}\|]$. Then we can prepare a state $|\widetilde{x}\rangle$ so that $\||\widetilde{x}\rangle - |x\rangle\| \leq \epsilon$ and with constant success probability, using $\mathcal{O}\left(\alpha\kappa^2/(\|A\|^2\xi)\log\left(\kappa/(\|A\|\xi\epsilon)\right)\right)$ queries to U_A and $U_A^\dagger$, and $\mathcal{O}(\kappa/(\|A\|\xi))$ queries to U_b.*

Exercise 19.1. Design a LCU based algorithm for solving QLSP and analyze its complexity in terms of the number of queries to U_A, U_b.

Remark 19.4 (Comparison with classical iterative linear system solvers)**.** Let us now compare the cost of the QLSP solver to that of classical iterative algorithms. If A is n-qubit Hermitian positive definite with condition number κ, and is d-sparse (i.e., each row/column of A has at most d nonzero entries), then each matrix vector multiplication Ax costs $\mathcal{O}(dN)$ floating point operations. The number of iterations for the steepest descent (SD) algorithm is $\mathcal{O}(\kappa\log\epsilon^{-1})$, and the this number can be significantly reduced to $\mathcal{O}(\sqrt{\kappa}\log\epsilon^{-1})$ by the renowned conjugate gradient (CG) method. Therefore the total cost (or wall clock time) of SD and CG is $\mathcal{O}(dN\kappa\log\epsilon^{-1})$ and $\mathcal{O}(dN\sqrt{\kappa}\log\epsilon^{-1})$, respectively.

On the other hand, the query complexity of the QSVT based linear system solver is still $\widetilde{\mathcal{O}}(\kappa^2\log\epsilon^{-1})$ in the worst case. The potential power of QLSP solvers is based on that each application of A (in this case, using the unitary U) can be much faster. In particular, if U can be implemented with $\mathrm{poly}(n)$ gate complexity (also can be measured by the wall clock time), then the total gate complexity becomes $\widetilde{\mathcal{O}}(\mathrm{poly}(n)\kappa^2\log(\epsilon^{-1}))$.

◇

19.4. Example: Poisson's equation

As an application of the QLSP solvers, let us consider a toy problem of solving the **Poisson's equation** in one dimension with Dirichlet boundary conditions

$$-u''(r) = b(r), \quad r \in \Omega = [0,1], \quad u(0) = u(1) = 0. \tag{19.27}$$

We use the central finite difference formula to discretize the Laplacian operator on a uniform grid $r_i = ih$, $i \in [N]$, and $h = 1/(N+1)$, so that the boundary points are $r_0 = 0$ and $r_{N+1} = 1$. Let $u_i = u(r_i), b_i = b(r_i)$, then Poisson's equation is discretized into a linear system of equations $Au = b$, with a tridiagonal matrix

$$A = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & & & & \vdots & & \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}. \tag{19.28}$$

Our goal here is not to address the quality of the spatial discretization, but to study the cost of solving the resulting linear system. To this end we need to compute the condition number of A. We also assume the right hand vector b is already normalized so that $|b\rangle = b$.

Proposition 19.5 (Diagonalization of tridiagonal matrices)**.** *A Hermitian Toeplitz tridiagonal matrix*

$$A = \begin{pmatrix} a & \overline{b} & 0 & \cdots & 0 & 0 & 0 \\ b & a & \overline{b} & \cdots & 0 & 0 & 0 \\ \vdots & & & & \vdots & & \\ 0 & 0 & 0 & \cdots & b & a & \overline{b} \\ 0 & 0 & 0 & \cdots & 0 & b & a \end{pmatrix} \in \mathbb{C}^{N\times N} \tag{19.29}$$

can be analytically diagonalized as

$$Av_k = \lambda_k v_k, \quad k = 1, \ldots, N. \tag{19.30}$$

where $(v_k)_j = v_{j,k}, j = 1, \ldots, N$, $b = |b| e^{i\theta}$, *and*

$$\lambda_k = a + 2|b| \cos\frac{k\pi}{N+1}, \quad v_{j,k} = \sin\frac{jk\pi}{N+1} e^{ij\theta}. \tag{19.31}$$

Proof. Note that formally $v_{0,k} = v_{N+1,k} = 0$. Then direct matrix vector multiplication shows that for any $j = 1, \ldots, N$,

$$(Av_k)_j = a \sin\frac{jk\pi}{N+1} e^{ij\theta} + 2|b| \sin\frac{jk\pi}{N+1} \cos\frac{k\pi}{N+1} e^{ij\theta} = \lambda_k (v_k)_j. \tag{19.32}$$

□

Using Proposition 19.5 with $a = 2/h^2, b = -1/h^2$, the largest eigenvalue of A is $\lambda_{\max} = \|A\| \approx 4/h^2$, and the smallest eigenvalue $\lambda_{\min} = \left\|A^{-1}\right\|^{-1} \approx \pi^2$. So

$$\kappa(A) \approx \frac{4}{h^2\pi^2} = \mathcal{O}(N^2). \tag{19.33}$$

The circuit depth of the HHL algorithm is $\mathcal{O}(N^2/\epsilon)$, and the total worst case query complexity (using amplitude amplification) is $\mathcal{O}(N^4/\epsilon)$. The use of more advanced QLSP solvers such as QSVT only improves the scaling with respect to the precision to $\log(1/\epsilon)$. So there is no quantum advantage so far even when N is very large.

Let us now consider solving a d-dimensional Poisson's equation with Dirichlet boundary conditions

$$-\Delta u(\mathbf{r}) = b(\mathbf{r}), \quad \mathbf{r} \in \Omega = [0,1]^d, \quad u|_{\partial\Omega} = 0. \tag{19.34}$$

The grid is the Cartesian product of the uniform grid in 1D with N grid points per dimension and $h = 1/(N+1)$. The total number of grid points is $\mathcal{N} = N^d$. After discretization, we obtain a linear system $\mathcal{A}u = b$, where

$$\mathcal{A} = A \otimes I \otimes \cdots I + \cdots + I \otimes \cdots I \otimes A, \tag{19.35}$$

where I is an identity matrix of size N. Since $\mathcal{A}$ is Hermitian and positive definite, we have $\|\mathcal{A}\| \approx 4d/h^2$, and $\left\|\mathcal{A}^{-1}\right\|^{-1} \approx d\pi^2$. So $\kappa(\mathcal{A}) \approx 4/(h^2\pi^2) \approx \kappa(A)$. Therefore the condition number is independent of the spatial dimension d. Consequently, when the number of grid points per dimension N is fixed and the spatial dimension d increases, if $U = e^{i\mathcal{A}\tau}$ can be implemented efficiently for some $\tau \|\mathcal{A}\| < 1$ with poly(d) cost, then QLSP solvers can have an advantage over classical iterative methods, for which each matrix-vector multiplication costs $\mathcal{O}(\mathcal{N})$ operations and can therefore be exponential in d.

19.5. Example: Green's function of fermionic systems

For fermionic systems on N sites, let us denote the creation and annihilation operators by $\{\hat{a}_i^\dagger, \hat{a}_i\}_{i\in[N]}$. The Hamiltonian is a polynomial of these creation and annihilation operators. For instance, many Hamiltonians in quantum chemistry take the form

$$\hat{H} = \sum_{i,j\in[N]} T_{ij}\hat{a}_i^\dagger\hat{a}_j + \sum_{i,j,k,l\in[N]} V_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_l\hat{a}_k. \tag{19.36}$$

Let $(E_0, |\Psi_0\rangle)$ be the non-degenerate ground state eigenpair of $\hat{H}$. **Green's functions** contain the spectroscopic information due to excitations from the ground state. The single-particle Green's function[1], denoted by $G(z)$, is a matrix valued function with entries

$$G_{ij}(z) = \left\langle \Psi_0 \middle| \hat{a}_i \left(z + E_0 - \hat{H}\right)^{-1} \hat{a}_j^\dagger \middle| \Psi_0 \right\rangle, \quad i,j \in [N]. \tag{19.37}$$

In other words, G can be viewed as a mapping $\mathbb{C} \mapsto \mathbb{C}^{N\times N}$. Here the input $z = E - i\eta$ can be interpreted as a complex energy shift, and $\eta > 0$ is called the broadening parameter, and determines the resolution of Green's functions along the energy spectrum. Then $G(z)$ is well-defined since $E_0 + z$ is not an eigenvalue of $\hat{H}$. Also note that the dimension of the underlying Hilbert space for the problem is 2^N. Hence the dimension of the matrix G is much smaller compared to that of the Hamiltonian.

Now suppose we have an (α, m, ϵ)-block-encoding of the matrix inverse $\left(z + E_0 - \hat{H}\right)^{-1}$ denoted by U, obtained from a QLSP solver (for instance, by applying a Hermitian dilation to the generally non-Hermitian shifted operator). Then, using products of block encodings, we can construct an $(\alpha, m+2, \epsilon)$ block-encoding of $\hat{a}_i \left(z + E_0 - \hat{H}\right)^{-1} \hat{a}_j^\dagger$. The value of each entry $G_{ij}(z)$ can be estimated using the Hadamard test circuit.

[1]Strictly speaking, this is only the "advanced" Green's function (corresponding to the prescription $E - i\eta$ with $\eta > 0$). The "retarded" Green's function, which corresponds to $E + i\eta$, is omitted here.

The problem becomes even simpler if we are only interested in

$$\Gamma(z) = \frac{1}{2i}\left(G(z) - (G(z))^\dagger\right), \tag{19.38}$$

which is a Hermitian matrix encoding the imaginary part of $G(z)$. This component is frequently used since it determines the spectral density. Using the fact that $\hat{H}$ is a Hermitian operator,

$$\overline{G_{ji}(z)} = \overline{\left\langle \Psi_0 \middle| \hat{a}_j \left(z + E_0 - \hat{H}\right)^{-1} \hat{a}_i^\dagger \middle| \Psi_0 \right\rangle} = \left\langle \Psi_0 \middle| \hat{a}_i \left(\overline{z} + E_0 - \hat{H}\right)^{-1} \hat{a}_j^\dagger \middle| \Psi_0 \right\rangle. \tag{19.39}$$

For $z = E - i\eta$ with $E, \eta \in \mathbb{R}$, we have

$$\Gamma_{ij}(z) = \eta \left\langle \Psi_0 \middle| \hat{a}_i \left((E + E_0 - \hat{H})^2 + \eta^2\right)^{-1} \hat{a}_j^\dagger \middle| \Psi_0 \right\rangle. \tag{19.40}$$

Therefore Γ is a real symmetric matrix provided all coefficients of $\hat{H}$ are real.

Note that the diagonal entries are

$$\Gamma_{ii}(z) = \eta \left\langle \Psi_0 \middle| \hat{a}_i \left((E + E_0 - \hat{H})^2 + \eta^2\right)^{-1} \hat{a}_i^\dagger \middle| \Psi_0 \right\rangle = \eta \left\| \left(z + E_0 - \hat{H}\right)^{-1} \hat{a}_i^\dagger |\Psi_0\rangle \right\|_2^2 \tag{19.41}$$

If we solve the QLSP

$$(z + E_0 - \hat{H}) |y_i\rangle = \hat{a}_i^\dagger |\Psi_0\rangle, \tag{19.42}$$

then the computation of the norm of the solution can be readily obtained from the success probability of finding the normalized solution in the system register, without using the Hadamard test.

In the above real-coefficient setting in which $\Gamma(z)$ is real symmetric, the off-diagonal entries of $\Gamma(z)$ can be obtained from the polarization identity

$$\begin{aligned} \Gamma_{ij}(z) =& \frac{\eta}{2}\Bigg(\left\langle \Psi_0 \middle| (\hat{a}_i + \hat{a}_j) \left((E + E_0 - \hat{H})^2 + \eta^2\right)^{-1} (\hat{a}_i^\dagger + \hat{a}_j^\dagger) \middle| \Psi_0 \right\rangle \\ & - \left\langle \Psi_0 \middle| \hat{a}_i \left((E + E_0 - \hat{H})^2 + \eta^2\right)^{-1} \hat{a}_i^\dagger \middle| \Psi_0 \right\rangle \\ & - \left\langle \Psi_0 \middle| \hat{a}_j \left((E + E_0 - \hat{H})^2 + \eta^2\right)^{-1} \hat{a}_j^\dagger \middle| \Psi_0 \right\rangle \Bigg), \end{aligned} \tag{19.43}$$

which can again be evaluated using success probabilities for separately solving three linear systems (two of them are already obtained from the diagonal entries $\Gamma_{ii}(z)$).

19.6. Quantum adiabatic algorithm and near-optimal linear system solver

For both the HHL algorithm and QSVT-based solvers, even after amplitude amplification, the worst-case complexity for QLSP retains at least a quadratic dependence on the condition number κ. This is because the norm of the final solution $\|A^{-1}|b\rangle\|$ can be much smaller than the subnormalization factor κ, leading to a large number of repetitions.

In Example 7.6, we showed that the quantum linear system problem can be solved as a Hermitian eigenvalue problem. It turns out that such a reformulation, together with a **quantum adiabatic algorithm** to solve the eigenvalue problem, can provide the QLSP solver with near-optimal complexities, i.e., the query complexity to the matrix A is $\mathcal{O}(\kappa \,\mathrm{polylog}(\kappa/\epsilon))$ even in the worst-case scenario. We will first briefly introduce the concept of quantum adiabatic theorem, and then construct a quantum adiabatic dynamics to solve QLSP.

19.6.1. Quantum adiabatic theorem. Adiabatic algorithms are characterized by their reliance on the slow evolution of a Hamiltonian to maintain a system in its eigenstate. Consider the linear time-dependent Schrödinger equation:

$$i\frac{1}{T}\partial_s |\psi(s)\rangle = H(s)|\psi(s)\rangle, \quad 0 \le s \le 1, \tag{19.44}$$

with the initial condition $|\psi(0)\rangle$ being a normalized eigenvector of $H(0)$ with eigenvalue $\lambda(H(0))$. Here s denotes the rescaled time. The parameter T can be interpreted as the evolution time, since rescaling $s \to t = sT$ gives

$$i\partial_t |\psi(t)\rangle = H(t/T)|\psi(t)\rangle, \quad 0 \le t \le T. \tag{19.45}$$

The main assumption for adiabatic dynamics is the gap condition, which ensures the existence of eigenpaths of the Hamiltonian $H(s)$ that are uniformly separated by a positive constant gap Δ_* from the rest of the spectrum. Specifically, there exists continuous functions $b_\pm(s)$ such that $b_-(s) < b_+(s)$ for all $s \in [0,1]$, $\lambda(H(0)) \in [b_-(0), b_+(0)]$, and

$$\operatorname{dist}\left(\{b_+(s), b_-(s)\}, \operatorname{Spec}(H(s))\right) =: \Delta(s)/2 \ge \Delta_*/2. \tag{19.46}$$

Here $\operatorname{Spec}(H(s))$ represents the spectrum of $H(s)$.

Let $P(s)$ denote the spectral projection operator associated with the band $\operatorname{Spec}(H(s)) \bigcap [b_-(s), b_+(s)]$. Under the gap condition and additional regularity assumptions for $H(s)$, the adiabatic theorem asserts that if the initial state $|\psi(0)\rangle$ is within the range of $P(0)$, then $|\psi(1)\rangle$ will be approximately within the range of $P(1)$. The adiabatic error, measured for instance by the leakage outside the range of $P(1)$, primarily depends on the evolution time T and the spectral gap Δ. The error decreases with increasing T and Δ. The following result is a restatement from [JRS07]:

THEOREM 19.6. *For $H(s) \in C^2([0,1])$, for any normalized vector $|\psi(0)\rangle = P(0)|\psi(0)\rangle$, we have*

$$\|(I - P(s))|\psi(s)\rangle\| \le C\gamma(s), \quad s \in [0,1]. \tag{19.47}$$

Here C is a constant independent of $\Delta(s), T$, and

$$\gamma(s) = \frac{\left\|\dot{H}(0)\right\|}{T\Delta(0)^2} + \frac{\left\|\dot{H}(s)\right\|}{T\Delta(s)^2} + \frac{1}{T}\int_0^s \left(\frac{\left\|\ddot{H}(\tau)\right\|}{\Delta(\tau)^2} + \frac{\left\|\dot{H}(\tau)\right\|^2}{\Delta(\tau)^3} \right) \mathrm{d}\tau. \tag{19.48}$$

Theorem 19.6 states that in the presence of a spectral gap, as $T \to \infty$, the instantaneous quantum state $|\psi(s)\rangle$ belongs to the range of the spectral projection $P(s)$. The error characterized by the leakage outside the range of $P(s)$ scales as T^{-1}. Thus, to achieve a precision ϵ, the complexity, measured by the evolution time, scales as ϵ^{-1}.

It turns out that under additional assumptions, the accuracy of the adiabatic theorem can be exponentially improved. Intuitively, let $H^{(k)}(s)$ denote the k-th order time derivative of $H(s)$. If $H(s)$ is a smooth function of s, using integration by parts, the adiabatic error at time T can be expressed as a linear combination of terms involving only the derivatives at the boundary such as

$$\frac{\left\|H^{(k)}(s)\right\|}{T^l}, \quad s = 0, 1, \tag{19.49}$$

together with a remainder term (here l depends on the term). Therefore, if we can choose the adiabatic path such that

$$H^{(k)}(0) = H^{(k)}(1) = 0, \quad \forall k \ge 1, \tag{19.50}$$

we may exponentially suppress the error at the final time $s = 1$. This is the idea behind the rapid adiabatic preparation algorithm (see, e.g., [Nen93, GMC16]). Somewhat counterintuitively, using such a strategy, the error at intermediate times $0 < s < 1$ can be much larger and only scales as $\mathcal{O}(T^{-1})$.

Another observation is that the error in Theorem 19.6 can scale as Δ^{-3}, which is costly when the gap is small. This represents the worst case for generic Hamiltonians. For QLSP, the Hamiltonian is much more structured than the worst case scenario. Specifically, in the constructions below, the gap stays open but becomes smallest near the end of the adiabatic path (scaling as $1/\kappa$). We make use of these ideas and tailor them for QLSP to reduce the gap dependence and obtain efficient QLSP solvers.

19.6.2. Quantum adiabatic algorithm based linear system solver. For simplicity, we will only discuss the case when A is a Hermitian positive definite matrix, and the eigenvalues of A are in the interval $[\kappa^{-1}, 1]$. The treatment of a general matrix A involves a dilation similar to that in Eq. (19.1). The problem of finding a normalized state $|x\rangle$ such that $A|x\rangle \propto |b\rangle$ can be reformulated as eigenvalue problem:

$$H_1 \begin{pmatrix} |x\rangle \\ 0 \end{pmatrix} = 0, \quad H_1 = \begin{pmatrix} 0 & AQ_b \\ Q_b A & 0 \end{pmatrix}, \quad Q_b = I - |b\rangle\langle b|. \tag{19.51}$$

We may readily verify that the 0-eigenspace, i.e., the null space, of H_1 is spanned by $|0\rangle|x\rangle = (x, 0)^\top$, where $|x\rangle$ is the solution vector, and $|1\rangle|b\rangle = (0, b)^\top$. The rest of the spectrum is separated from 0 by a gap of $1/\kappa$. We then define

$$H_0 = \begin{pmatrix} 0 & Q_b \\ Q_b & 0 \end{pmatrix}, \tag{19.52}$$

and the null space of H_0 is spanned by $|0\rangle|b\rangle = (b, 0)^\top$ and $|1\rangle|b\rangle = (0, b)^\top$.

To use adiabatic quantum computing, we first specify the eigenpath. We define

$$H(f(s)) = (1 - f(s))H_0 + f(s)H_1, \quad s \in [0, 1], \tag{19.53}$$

where $f(s) : [0, 1] \to [0, 1]$ satisfying $f(0) = 0, f(1) = 1$ is called the scheduling function.

Lemma 19.7. *Let $A \in \mathbb{C}^{N\times N}$ be a positive matrix satisfying $A \succeq \kappa^{-1} I$. Then the spectral gap $\Delta(f)$ associated with the 0 eigenvalue of $H(f)$ satisfies*

$$\Delta(f) \geq 1 - f + f/\kappa. \tag{19.54}$$

Proof. The Hamiltonian $H(f)$ can be written in the block matrix form as

$$H(f) = \begin{pmatrix} 0 & ((1-f)I + fA)Q_b \\ Q_b((1-f)I + fA) & 0 \end{pmatrix}. \tag{19.55}$$

Let λ be an eigenvalue of $H(f)$, then

$$\begin{aligned} 0 &= \det \begin{pmatrix} \lambda I & -((1-f)I + fA)Q_b \\ -Q_b((1-f)I + fA) & \lambda I \end{pmatrix} \\ &= \det\left(\lambda^2 I - Q_b((1-f)I + fA)^2 Q_b\right) \end{aligned} \tag{19.56}$$

where the second equality holds because λI commutes with either of the two off-diagonal blocks.

Note that $Q_b |b\rangle = 0$, hence $|b\rangle$ is a 0-eigenvector of $Q_b((1-f)I+fA)^2Q_b$. Moreover, eigenvectors corresponding to non-zero eigenvalues are orthogonal to $|b\rangle$. Therefore

$$\begin{aligned}\Delta^2(f) &= \inf_{\langle b|\varphi\rangle=0,\,\langle\varphi|\varphi\rangle=1} \langle\varphi|Q_b((1-f)I+fA)^2Q_b|\varphi\rangle \\ &= \inf_{\langle b|\varphi\rangle=0,\,\langle\varphi|\varphi\rangle=1} \langle\varphi|((1-f)I+fA)^2|\varphi\rangle \\ &\geq \inf_{\langle\varphi|\varphi\rangle=1} \langle\varphi|((1-f)I+fA)^2|\varphi\rangle \\ &\geq (1-f+f/\kappa)^2.\end{aligned} \tag{19.57}$$

This proves the lemma. □

We start from an eigenstate of H_0, namely $|\psi(0)\rangle = |0\rangle |b\rangle$, and propagate the dynamics

$$\frac{i}{T}\partial_s |\psi_T(s)\rangle = H(f(s)) |\psi_T(s)\rangle, \quad s \in [0,1]. \tag{19.58}$$

Since $H(f(s))$ is uniformly gapped for all $s \in [0,1]$, we expect from the quantum adiabatic theorem that $\lim_{T\to\infty} |\psi_T(1)\rangle$ lies in the null space of $H(1) = H_1$, which encodes the desired solution vector. The choice of the scheduling function $f(s)$ is crucial for the efficiency. The AQC(exp) method proposed in [AL22] chooses

$$f(s) = c_e^{-1} \int_0^s \exp\left(-\frac{1}{\tau(1-\tau)}\right) \mathrm{d}\tau \tag{19.59}$$

where $c_e = \int_0^1 \exp\left(-1/(\tau(1-\tau))\right) \mathrm{d}\tau$ is a normalization constant such that $f(1) = 1$. In particular, this scheduling function ensures that $H^{(k)}(0) = H^{(k)}(1) = 0$ for all orders of derivatives $k \geq 1$. The following theorem is a restatement of the result in [AL22]:

THEOREM 19.8. *Consider a matrix $A \in \mathbb{C}^{N\times N}$ whose singular values are in the range $\left[\frac{1}{\kappa}, 1\right]$. For sufficiently large $T > 0$, the error of AQC(exp) at the final time $s = 1$, measured by the trace distance to the QLSP solution, is upper bounded, up to a constant factor, by*

$$\log(\kappa) \exp\left(-C\left(\frac{\kappa \log^2 \kappa}{T}\right)^{-\frac{1}{4}}\right). \tag{19.60}$$

Therefore we can prepare a state $|\widetilde{x}\rangle$ so that $|\langle\widetilde{x}|x\rangle| \geq 1-\epsilon$ and with constant success probability, by running a quantum adiabatic algorithm with runtime $T = \mathcal{O}\left(\kappa \log^2(\kappa) \log^4\left(\frac{\log\kappa}{\epsilon}\right)\right)$.

It is worth noting that Eq. (19.58) is a time-dependent Hamiltonian simulation problem. So after making the choice Eq. (19.59), the time-dependent Hamiltonian simulation problem still needs to be carefully discretized and implemented on the quantum computer, using e.g., the truncated Dyson series in Section 14.5.

19.7. Quantum Zeno effect and optimal linear system solver

Quantum Zeno effect (QZE) is the phenomenon in which frequent measurements hinder a quantum system's transition from its initial state to other states. It is closely related to the quantum adiabatic theorem. We first introduce QZE and then describe a QZE-based QLSP solver with the best asymptotic scaling to date. Specifically, the query complexity to the block encoding of A scales as $\mathcal{O}(\kappa \log(1/\epsilon))$.

19.7.1. Quantum Zeno effect. Specifically, given a Hamiltonian H and an initial state $|\psi\rangle$, if we evolve for time t and then perform a projective measurement with respect to $\{P = |\psi\rangle\langle\psi|, I-P\}$, then the probability of obtaining the outcome corresponding to P is $\left|\langle\psi|e^{-iHt}|\psi\rangle\right|^2$. However, if we evolve for time $\tau = t/M$, immediately measure $\{P, I-P\}$, and repeat this process M times, then the probability of obtaining P at every step is at least

$$\begin{aligned}\left(\left|\langle\psi|e^{-iH\tau}|\psi\rangle\right|^2\right)^M &= \left(\left|\langle\psi|I - iH\tau - \frac{H^2\tau^2}{2} + \mathcal{O}(\tau^3)|\psi\rangle\right|^2\right)^M \\ &= \left(1 - \tau^2\sigma^2 + \mathcal{O}(\tau^3)\right)^M \\ &\geq 1 - \tau t\sigma^2 + t\mathcal{O}(\tau^2).\end{aligned} \tag{19.61}$$

Here $\sigma^2 = \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2$. We have used $(1-x)^M \geq 1 - Mx$ for all $x \in [0,1]$, and $t = M\tau$. This lower bound converges to 1 when $\tau \to 0$. Therefore the state remains close to $|\psi\rangle$ despite the time evolution. One may also postselect and discard the state if $I - P$ is observed; conditioned on success at every step, the resulting state is the same (see the circuit in Fig. 19.4).

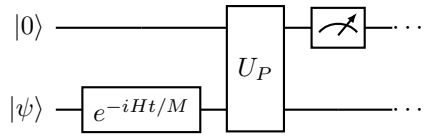


FIGURE 19.4. Circuit for quantum Zeno effect where the projection operator $P = |\psi\rangle\langle\psi|$ is implemented via a block encoding $U_P \in \mathrm{BE}_{1,1}(P)$, and success is indicated by measuring the ancilla qubit with outcome 0. The block above is repeated M times and the probability for all measurements to be 0 approaches 1 as $M \to \infty$.

Here we use a variant of QZE [BKS09], which can be viewed as a digital implementation of adiabatic quantum computing. The idea is to follow an adiabatic path through repeated measurements, which act as projections to the instantaneous eigenstate along the path. We choose a scheduling function $f(s)$, and discretize it on a uniform grid $f_j = f(s_j)$, $s_j = j/M$, $j = 0, \ldots, M$. Assume the 0 eigenvalue of $H(f(s))$ is uniformly gapped from all other eigenvalues for all $s \in [0,1]$. Starting from a state $|\psi(0)\rangle$ in the null space of $H(f_0)$, we consecutively apply projections to the null spaces of $H(f_1), H(f_2), \ldots, H(f_M)$, implemented via block encodings. For sufficiently large M, the probability that *all* projection operations succeed is $\Omega(1)$ (see Fig. 19.5). Moreover, the accuracy of the final state only depends on the last projection associated with $H(f_M)$; intermediate projections only affect the overall success probability. This procedure is inherently digital and does not require a further discretization of a continuous-time adiabatic evolution.

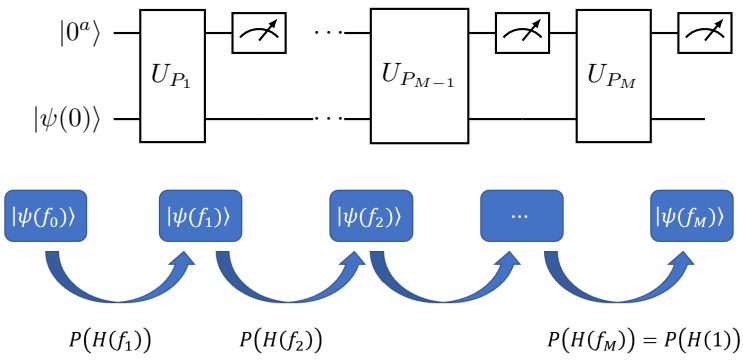


FIGURE 19.5. Circuit for quantum Zeno effect along an adiabatic path, which aims at achieving a consecutive set of M projections. Here P_j is the projection to the null space of $H(f_j)$, and $U_{P_j} \in \mathrm{BE}_{1,a}(P_j, \epsilon_j)$ is the block encoding for P_j. Upon successful application of U_{P_M}, the state in the system register is an approximate eigenstate of $H(1)$ to precision ϵ_M. The probability for all measurements to be successful approaches 1 as $M \to \infty$.

19.7.2. Quantum Zeno effect based QLSP solver. The first quantum algorithm that uses the quantum adiabatic theorem to solve linear systems of equations [SSO19] uses a randomized algorithm [BKS09] to traverse the eigenpath. Each step queries the time evolution under a fixed Hamiltonian $H(f(s))$ for a random amount of time, distributed uniformly on an interval whose range is specified by a bound on the spectral gap of $H(f(s))$. This algorithm is similar in spirit to the qDRIFT algorithm in Section 15.5. The cost is $\widetilde{\mathcal{O}}(\kappa/\epsilon)$, where ϵ is the target accuracy in trace distance. This provides a simple digital implementation of the adiabatic equation Eq. (19.58), but only achieves first-order accuracy.

We will now show that a QZE based algorithm also provides a simple digital implementation of the adiabatic evolution [LT20b], and the query complexity of this method is near-optimal, namely $\mathcal{O}(\kappa \log(1/\epsilon))$ up to $\log\log\kappa$ factors.

For any scheduling function f, let $|x(f)\rangle$ be a normalized vector such that

$$((1-f)I + fA)\,|x(f)\rangle \propto |b\rangle\,. \tag{19.62}$$

The null space of $H(f)$ is spanned by $|\psi(f)\rangle = |0\rangle\,|x(f)\rangle$ and $|1\rangle\,|b\rangle$. By adding the additional constraint

$$\langle x(f)|\partial_f x(f)\rangle = 0, \tag{19.63}$$

the eigenpath $\{|x(f)\rangle\}$ becomes uniquely defined with the initial condition $|x(0)\rangle = |b\rangle$. Lemma 19.7 states that the spectral gap associated with the 0 eigenvalue of $H(f)$ is lower bounded by $\Delta^*(f) = 1 - f + f/\kappa$. By the perturbation theory,

$$\|\partial_f\,|x(f)\rangle\,\| \le \frac{\|A - I\|}{\Delta^*(f)} \le \frac{2}{\Delta^*(f)}. \tag{19.64}$$

We will choose the scheduling function

$$f(s) = \frac{1-\kappa^{-s}}{1-\kappa^{-1}}, \tag{19.65}$$

which satisfies $f(0) = 0, f(1) = 1$. See Fig. 19.6. We also define the eigenpath length $L(a, b)$ between $0 < a < b < 1$ as

$$L(a,b) = \int_a^b \|\partial_f |x(f)\rangle\| \, \mathrm{d}f, \tag{19.66}$$

and it is upper bounded by

$$L(a,b) \le \int_a^b \frac{2}{\Delta^*(f)} \, \mathrm{d}f = \frac{2}{1-1/\kappa} \log\left(\frac{1-(1-1/\kappa)a}{1-(1-1/\kappa)b}\right) =: L_*(a,b). \tag{19.67}$$

In particular, the upper bound for the entire path is given by

$$L(0,1) \le L_*(0,1) = \frac{2\log(\kappa)}{1-1/\kappa}. \tag{19.68}$$

We then have

$$|\langle x(f_j)|x(f_{j-1})\rangle| \ge 1 - \frac{1}{2}\| |x(f_{j-1})\rangle - |x(f_j)\rangle \|^2 \ge 1 - \frac{1}{2}L_*(f_{j-1}, f_j)^2 \ge 1 - \frac{2\log^2(\kappa)}{M^2(1-1/\kappa)^2}. \tag{19.69}$$

To bound the success probability, for simplicity, we assume all block encodings are implemented exactly. Then if we choose $M \ge \frac{4\log^2(\kappa)}{(1-1/\kappa)^2}$, the success probability satisfies

$$\prod_{j=1}^{M} \|P_{f_j} |\psi(f_{j-1})\rangle\|^2 = \prod_{j=1}^{M} |\langle x(f_j)|x(f_{j-1})\rangle|^2 \ge \left(1 - \frac{2\log^2(\kappa)}{M^2(1-1/\kappa)^2}\right)^{2M} \ge \left(1 - \frac{2\log^2(\kappa)}{M(1-1/\kappa)^2}\right)^2 \ge \frac{1}{4}. \tag{19.70}$$

A more careful analysis shows that if the projection can only be approximately implemented, then it is sufficient to choose $\epsilon_1 = \cdots = \epsilon_{M-1} = \mathcal{O}(M^{-2})$, and $\epsilon_M = \epsilon$, so that the success probability is $\Omega(1)$, and the trace distance between the final state and $|0\rangle |x\rangle$ is $\mathcal{O}(\epsilon)$.

The spectral projector can be implemented using an even approximation to the rectangular function used in the proof of Lemma 12.9. The number of queries to A needed for implementing $U_{P_j} \in \mathrm{BE}_{1,a}(P_j, \epsilon_j)$ is $\mathcal{O}(\Delta^*(f_j)^{-1} \log \epsilon_j^{-1})$. Along the path, the number of queries for the first $M-1$ steps of the projection is of order

$$\begin{aligned} \log\left(\frac{1}{\epsilon'}\right) \sum_{j=1}^{M-1} \frac{1}{1 - f(s_j) + f(s_j)/\kappa} &\le \log\left(\frac{1}{\epsilon'}\right) M \int_0^1 \frac{1}{1 - f(s) + f(s)/\kappa} \, \mathrm{d}s \\ &= \log\left(\frac{1}{\epsilon'}\right) M \int_0^1 \kappa^s \, \mathrm{d}s \\ &\le \log\left(\frac{1}{\epsilon'}\right) M \frac{\kappa}{\log \kappa}. \end{aligned} \tag{19.71}$$

Plug in $M = \Theta(\log^2 \kappa), \epsilon' = \mathcal{O}(M^{-2}) = \mathcal{O}(\log^{-4} \kappa)$, we find that the number of queries to A is $\mathcal{O}(\kappa \log \kappa \log\log \kappa)$.

Finally, the last step of the projection should be implemented to precision ϵ, and the number of queries to A is $\mathcal{O}(\kappa \log(1/\epsilon))$.

The total cost of the algorithm is thus $\mathcal{O}(\kappa \log \kappa \log\log \kappa + \kappa \log(1/\epsilon))$.

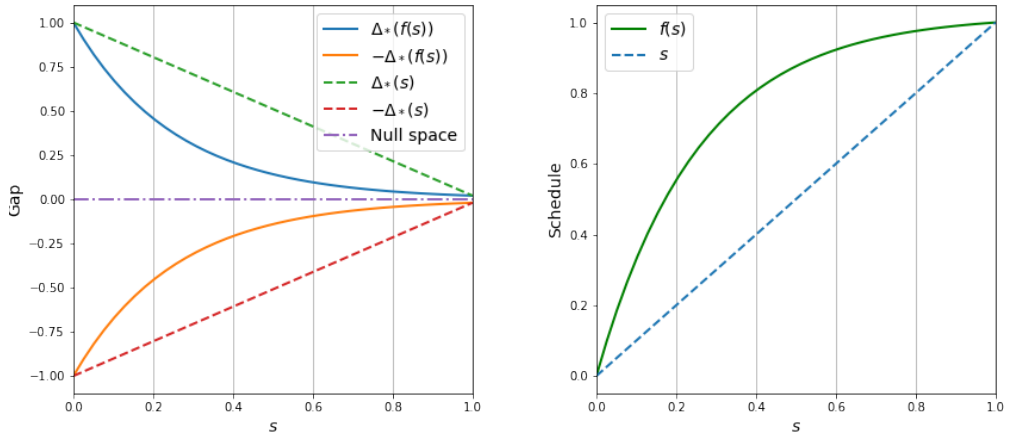


FIGURE 19.6. A lower bound of the spectral gap with the scheduling function $f(s)$ in Eq. (19.65) and a trivial scheduling function $f(s) = s$. Here $\kappa = 50$. To obtain the near-optimal scaling, it is important that the scheduling function increases rapidly when the gap is large, and slows down when the gap is small.

We have not discussed the construction of the block encoding for $H(f)$. This can be efficiently constructed if e.g., A is an s-sparse matrix, see Section 9.7. If $s = \mathcal{O}(1)$, then the QZE based algorithm can prepare a state $|\widetilde{x}\rangle$ with trace distance ϵ to the solution $|x\rangle \propto A^{-1}|b\rangle$, using $\widetilde{\mathcal{O}}(\kappa \log(1/\epsilon))$, and a constant number of ancilla qubits other than those used for constructing the block encoding of A.

We note that the query complexity of the algorithm above can still be slightly improved. Note that at each step of the algorithm, $\|P_{f_j}|\psi(f_{j-1})\rangle\|$ can be slightly smaller than 1. Therefore M needs to be chosen to be $\mathcal{O}(\log^2(\kappa))$ to ensure that the final success probability is $\Omega(1)$. However, by choosing $M = \Theta(\log(\kappa))$, it is already sufficient to guarantee

$$\|P_{f_j}|\psi(f_{j-1})\rangle\| = |\langle x(f_j)|x(f_{j-1})\rangle| \geq 1 - \frac{2\log^2(\kappa)}{M^2(1-1/\kappa)^2} = \Omega(1). \tag{19.72}$$

So we may use the fixed point amplitude amplification in Section 13.4 to prepare a state $|\widetilde{\psi}(f_j)\rangle$ so that

$$|\langle\widetilde{\psi}(f_j)|0, x(f_{j-1})\rangle| \geq 1 - \frac{1}{M}. \tag{19.73}$$

This process uses the block encoding of P_{f_j} for $\mathcal{O}(\log(M)) = \mathcal{O}(\log\log\kappa)$ times. The overall success probability after M steps is lower bounded by $(1 - M^{-1})^M \approx e^{-1}$.

Repeating the calculation in Eq. (19.71), we find that the number of queries for the first $M-1$ steps of the projection is proportional to

(19.74)
$$(\log M)\left(\log \epsilon'^{-1}\right) \sum_{j=1}^{M-1} \frac{1}{1-f(s_j)+f(s_j)/\kappa} \leq (\log M)\left(\log \epsilon'^{-1}\right) M \int_0^1 \frac{1}{1-f(s)+f(s)/\kappa}\,\mathrm{d}s$$
$$\leq (\log M)\left(\log \epsilon'^{-1}\right) \frac{M\kappa}{\log \kappa}.$$

Plug in $M = \Theta(\log \kappa), \epsilon' = \mathcal{O}(M^{-2}) = \mathcal{O}(\log^{-2} \kappa)$, we find that the number of queries to A is $\mathcal{O}(\kappa(\log\log \kappa)^2)$. For practical purposes, $\log\log \kappa$ can be treated as a constant (e.g., $\log\log 10^{12} \approx 3.3$).

We can now summarize the complexity of QZE based QLSP solver as follows, which is a variant of the results in [LT20b].

THEOREM 19.9. *Assume a matrix $A \in \mathbb{C}^{N\times N}$ whose singular values are in the range $\left[\frac{1}{\kappa}, 1\right]$ can be accessed using a block encoding $U_A \in \mathrm{BE}_{\alpha,m}(A)$, and the vector $|b\rangle$ can be prepared by a unitary U_B. Then we can prepare a state $|\widetilde{x}\rangle$ so that $|\langle\widetilde{x}|x\rangle| \geq 1-\epsilon$ and with constant success probability. The algorithm makes use of $\mathcal{O}(\kappa \log(1/\epsilon))$ queries to U_A and U_B, neglecting $\log\log \kappa$ factors.*

Notes and further reading

The HHL algorithm of [HHL09] can be combined with variable-time amplitude amplification (VTAA) [Amb12] to reduce the dependence on the condition number from quadratic to linear. Also using VTAA, the linear combination of unitaries (LCU) construction of [CKS17] gives the first polylogarithmic dependence on the target precision ϵ. Even so, the number of queries to the right hand side vector $|b\rangle$ is not optimal. This issue is addressed in the recent work of Low and Su [LS24] using a refined version of VTAA. This does not mean that they match the best classical iterative complexity in full generality: for positive definite matrices, classical conjugate gradient requires only $\mathcal{O}(\sqrt{\kappa})$ matrix-vector multiplications, whereas generic quantum algorithms do not generally achieve this scaling. There are, however, special settings in which one can recover analogous behavior [OD21]. For ill-conditioned problems, quantum preconditioning has been developed in a number of settings; see [CJS13, SX18, TAWL21, GOV22, DP24, JLMY25].

Compared to phase-estimation based approaches, QSVT-based linear system solvers provide a simpler route to implementing the inverse function. By casting the problem directly as a singular value transformation, QSVT avoids the associated arithmetic subroutines. Its analysis is also considerably simpler.

The Poisson example is included mainly as a pedagogical model for how a differential operator leads to a linear system with a large condition number after discretization. The same general viewpoint extends to more realistic discretizations, including finite element methods [MP16, DP24]. The main caveat is that a quantum speedup depends not only on the complexity of inverting the matrix, but also on the cost of implementing the oracle for A, preparing the right hand side, and extracting the relevant observable from the solution state. The Green's-function example is closer to applications in quantum many-body physics, where the goal is naturally phrased in terms of resolvents and matrix functions rather than a full classical description of the solution.

Adiabatic quantum computing (AQC) [JRS07, AL18] and the closely related randomization method (RM) [BKS09, SSO19] provide a different route to QLSP. The randomization method traverses the eigenpath through randomized short evolutions, while the adiabatic approach uses a

carefully chosen schedule to improve the precision dependence. In the form discussed here, RM gives complexity $\mathcal{O}(\kappa \log(\kappa)\epsilon^{-1})$ [SSO19], whereas the adiabatic construction of [AL22] improves this to $\mathcal{O}(\kappa \operatorname{polylog}(\kappa/\epsilon))$. The QZE-based algorithm of [LT20b] removes the continuous-time simulation step and achieves complexity $\mathcal{O}\left(\kappa \left(\log(1/\epsilon) + (\log\log\kappa)^2\right)\right)$.

The discrete adiabatic theorem leads to the optimal-scaling solver of [CAS+22], based on [DKS98], with complexity $\mathcal{O}\left(\kappa \log(1/\epsilon)\right)$. A different optimal-scaling construction based on augmentation and kernel reflection was proposed in [Dal24].

CHAPTER 20

Solving linear differential equations

In this chapter, we study quantum algorithms for solving linear differential equations, including ordinary differential equations and suitably discretized partial differential equations. The basic task resembles Hamiltonian simulation, but there is an immediate obstruction: a general linear evolution does not preserve norms. Consequently, the output model must keep track of both the direction and the magnitude of the solution, and a successful algorithm must control not only approximation error but also the probability of preparing the desired state. We begin by formulating the problem carefully and by isolating the quantities that govern this difficulty.

The chapter then introduces three types of algorithms to overcome this obstruction. The first rewrites the evolution as a linear system, which makes quantum linear system solvers available at the price of introducing a history state and its associated condition-number analysis. The second follows the more classical time-marching viewpoint, advancing the solution step by step and revealing a different growth parameter in the complexity. The third exploits additional dissipative structure to express the nonunitary evolution as a linear combination of unitary evolutions and thereby recover near-optimal complexity. We illustrate these methods on the heat equation and on certain non-Hermitian dynamics. We then prove a lower bound showing that the norm-growth dependence is intrinsically needed, due to a connection between linear differential equations and unstructured search.

20.1. Problem setup

The problem of solving a time-dependent linear ordinary differential equation can be formulated as

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = A(t)x(t) + b(t), \quad t \in [0,T], \quad x(0) = x_0. \tag{20.1}$$

Here $b(t), x(t) \in \mathbb{C}^d$ and $A(t) \in \mathbb{C}^{d\times d}$. The problem is called homogeneous if $b(t) = 0$ for all t, and inhomogeneous otherwise. It is called time-independent if $A(t) = A$ and $b(t) = b$ are independent of time. We assume that $A(t)$ and $b(t)$ are Lipschitz functions of t on $[0,T]$. By the Picard–Lindelöf theorem, this is sufficient to guarantee that the solution to Eq. (20.1) exists and is unique [HNW87]. A higher-order ordinary differential equation can always be rewritten as a system of first-order equations.

We have already introduced the Duhamel principle for time-independent Hamiltonian simulation in Proposition 3.22, and it can be generalized to arbitrary time-dependent linear differential equations.

Proposition 20.1 (Duhamel's principle for general time-dependent linear differential equations)**.** *Let $U(t,s) = \mathcal{T}e^{\int_s^t A(\tau)\,\mathrm{d}\tau}$ be the propagator for the homogeneous operator differential equation*

satisfying

$$\partial_t U(t,s) = A(t)U(t,s), \quad U(s,s) = I, \quad t \geq s. \tag{20.2}$$

Then the solution $x(t)$ to Eq. (20.1) *can be expressed as*

$$x(t) = U(t,0)x(0) + \int_0^t U(t,s)b(s)\,\mathrm{d}s. \tag{20.3}$$

Proof. Denote the right hand side by $R(t)$ and differentiate:

$$\begin{aligned} R'(t) &= A(t)U(t,0)x(0) + U(t,t)b(t) + \int_0^t \partial_t U(t,s)b(s)\ \mathrm{d}s \\ &= A(t)U(t,0)x(0) + b(t) + \int_0^t A(t)U(t,s)b(s)\ \mathrm{d}s = A(t)R(t) + b(t). \end{aligned} \tag{20.4}$$

Since $R(0) = x(0)$, the uniqueness of solutions implies that $R(t) = x(t)$. □

Remark 20.2 (Solving inhomogeneous differential equations)**.** Duhamel's principle expresses the inhomogeneous contribution as the integral $\int_0^t U(t,s)b(s)\ \mathrm{d}s$, which can then be approximated by numerical quadrature. Therefore, if we can efficiently construct a block encoding of $U(t,s)$, we can also prepare the contribution from the inhomogeneous term b using LCU. For this reason, we focus on the homogeneous case, namely the construction of a block encoding of $U(t,s)$. ◇

20.1.1. Input model. For the input model, without loss of generality, we assume the initial state is normalized and prepared by a unitary U_{x_0} such that

$$U_{x_0}\left|0\right\rangle_s = \left|x_0\right\rangle, \tag{20.5}$$

where $\left|0\right\rangle_s$ is in a d-dimensional system register.

The input matrix $A(t)$ at any time t is accessed via a block-encoding denoted by U_A that is analogous to the `HAM-T` oracle introduced for time-dependent Hamiltonian simulation. After discretizing time with a grid $\{t_k\}_{k=0}^{N_t-1}$, where $N_t = 2^{n_t}$, this oracle takes the form

$$\left(\left\langle 0^{m_A}\right| \otimes I_t \otimes I_s\right) U_A \left(\left|0^{m_A}\right\rangle \otimes I_t \otimes I_s\right) = \frac{1}{\alpha_A} \sum_{k=0}^{N_t-1} |k\rangle\langle k| \otimes A(t_k), \tag{20.6}$$

for some subnormalization factor α_A. Here, I_t denotes the identity matrix on the time register of dimension N_t, and I_s denotes the identity matrix on the system register of dimension d. This is essentially the same as `HAM-T` used in Definition 14.7 for encoding time-dependent Hamiltonians.

Similarly, the right-hand side vector $b(t)$ is accessed via a unitary U_b such that

$$\left(\left\langle 0^{m_b}\right| \otimes I_t \otimes I_s\right) U_b \left(\left|0^{m_b}\right\rangle \otimes I_t \otimes \left|0\right\rangle_s\right) = \frac{1}{\alpha_b} \sum_{k=0}^{N_t-1} |k\rangle\langle k| \otimes b(t_k), \tag{20.7}$$

for some subnormalization factor α_b. Here the vector $b(t_k)$ is understood to be represented as a block matrix wherein the first column of the matrix is $b(t_k)$.

20.1.2. Output model. The output of a linear differential equation solver is slightly subtler than the input, because the norm of the solution vector can vary substantially during the evolution. For example, consider the differential equation $\partial_t x(t) = -Zx(t)$ for $x \in \mathbb{C}^2$. The solution is

$$x(t) = \begin{bmatrix} x_0(0)e^{-t} \\ x_1(0)e^{t} \end{bmatrix}. \tag{20.8}$$

The corresponding normalized state is

$$|x(t)\rangle = \frac{x(t)}{\|x(t)\|} = \begin{bmatrix} x_0(0)e^{-t} \\ x_1(0)e^{t} \end{bmatrix} \Big/ \sqrt{|x_0(0)|^2 e^{-2t} + |x_1(0)|^2 e^{2t}}. \tag{20.9}$$

Unlike the Schrödinger equation, the normalization of the output vector is therefore an important part of the problem, because the magnitude of $x(t)$ may itself contain relevant information.

In full generality, we take a quantum "solution" to the differential equation to be given by a block encoding of the unnormalized vector $x(T)$. Then the solver can be viewed as a block encoding of the form

$$(\langle 0^{m_{\mathrm{sol}}}| \otimes I_s) U_{\mathrm{sol}} (|0^{m_{\mathrm{sol}}}\rangle |x_0\rangle) = \frac{1}{\alpha_{\mathrm{sol}}} x(T), \tag{20.10}$$

where α_{sol} denotes a known subnormalization factor. The magnitude of $\|x(T)\|$, if needed, can be inferred from the success probability associated with this block encoding. Consequently, we can calculate the average of observables as

$$x(T)^\dagger O x(T) = \langle x(T)|O|x(T)\rangle \, \|x(T)\|^2 . \tag{20.11}$$

Our aim is thus to produce a quantum state that block-encodes the solution of the differential equation. This is formalized in the following definition.

Definition 20.3 (Quantum linear differential equation problem)**.** *Let $A : \mathbb{R} \to \mathbb{C}^{N\times N}$ be a time-dependent operator and $b : \mathbb{R} \mapsto \mathbb{C}^N$ be a time-dependent inhomogeneity. Further, assume that we are provided an oracle U_{x_0} that prepares our initial state and oracles U_A and U_b that block encode $A(t)$ and $b(t)$. A quantum "solution" to the linear differential problem for evolution time T and error tolerance ϵ is to use the oracles U_A, U_b, U_{x_0} to construct a unitary U_{sol} that is an $(\alpha_{\mathrm{sol}}, m_{\mathrm{sol}}, \epsilon)$ block encoding of the vector $x(T)$ defined by Eq.* (20.1)*.*

The analysis of differential equation solvers can involve many polylogarithmic factors. To simplify the presentation, we use the notation $\widetilde{\mathcal{O}}$ to suppress such factors throughout this section. In particular, if the precision ϵ is not displayed explicitly in a cost estimate, its dependence is understood to be polylogarithmic.

It is tempting to imitate the strategy used for Hamiltonian simulation. That approach, however, is not efficient here unless A is anti-Hermitian. To see the obstruction, consider the simplest homogeneous problem, for which $b(t) = 0$ and hence $x(t) = e^{At}x(0)$. One might try to block encode e^{At} directly using LCU. If A admits a block encoding with normalization factor α, then a truncated Taylor expansion yields a block encoding of e^{At} with normalization factor $\alpha_{\mathrm{exp}} \approx e^{\alpha t}$, as discussed in Chapter 14. This normalization factor grows exponentially with t. In the anti-Hermitian case, the same issue is resolved by splitting the evolution into short segments of duration about $\ln(2)/\alpha$, for which the success probability is $1/4$, and then applying one round of oblivious amplitude amplification to boost the success probability to nearly 1.

This obstruction also reflects the distinction between eigenvalue transformations and singular value transformations. If $A = VDV^{-1}$ is diagonalizable, then $e^{At} = Ve^{Dt}V^{-1}$ is obtained by applying the scalar function $z \mapsto e^{tz}$ to the eigenvalues of A. By contrast, QSVT applied to a

block encoding of A directly controls the singular values of A, not its eigenvalues. Therefore, for a general non-Hermitian matrix A, a block encoding of A does not by itself give a direct QSVT implementation of e^{At}.

This argument breaks down for general linear differential equations because oblivious amplitude amplification requires the encoded operator to be close to unitary, which in this setting amounts to A being anti-Hermitian. Thus, except for very short times, the standard block-encoding strategy is ineffective. The next sections develop two ways around this obstruction. The first reduces the differential equation to a linear system and then applies a quantum linear system solver. The second rewrites the evolution as an integral of unitary dynamics and then applies Hamiltonian simulation methods.

20.2. Linear systems of equations method

In this section we introduce the linear systems method for solving Eq. (20.1). This was also the first quantum algorithm proposed for linear differential equations [Ber14]. The key idea is to rewrite the problem as a linear system by using the history-state formalism. History states are familiar from Hamiltonian complexity, where they are used, for example, in QMA-hardness constructions. In the present setting, the history vector stores the solution at all time steps in superposition. We use a uniform grid with spacing $\Delta t = T/N_t$, write $t_k = k\Delta t$, and denote $x_k = x(t_k)$ for $k = 0, \dots, N_t$. The **history state** vector, sometimes called the Feynman–Kitaev history state, is the unnormalized superposition

$$X(T) = \frac{1}{\sqrt{N_t}} \sum_{k=1}^{N_t} |t_k\rangle \otimes x_k. \tag{20.12}$$

Upon normalization, $|X(T)\rangle = \frac{X(T)}{\|X(T)\|}$, the solution can be produced by a unitary operation:

$$(\langle 0^{m_{\text{hist}}}| \otimes I_t \otimes I_s) U_{\text{hist}} (|0^{m_{\text{hist}}}\rangle |0\rangle_t |x_0\rangle) = \frac{1}{\alpha_{\text{hist}}} X(T). \tag{20.13}$$

Here $|0\rangle_t$ is the zero vector of size N_t for the time register, or of size $N_t + 1$ if the initial time t_0 is included, and α_{hist} is a known subnormalization factor. As before, the magnitude $\|X(T)\|$ can be inferred from the success probability of the block encoding. The history vector is therefore naturally obtained as the solution of a linear system of the form $\mathbf{x} = \mathcal{A}^{-1}\mathbf{b}$.

Note that x_{N_t}, which approximates the final value $x(T)$, appears in $X(T)$ with weight $1/\sqrt{N_t}$. Therefore, if our main interest is in observables at the final time, it is inefficient to estimate them directly from the history state. This can be remedied by introducing a **padded history state**, which appends N_t additional copies of the final vector at the cost of one ancilla qubit:

$$\widetilde{X}(T) = \frac{1}{\sqrt{N_t}} \sum_{k=1}^{N_t} |0, t_k\rangle \otimes x_k + \frac{1}{\sqrt{N_t}} \sum_{k=1}^{N_t} |1, t_k\rangle \otimes x_{N_t}. \tag{20.14}$$

Assume that we have already prepared the normalized padded history state $\widetilde{X}(T)/\left\|\widetilde{X}(T)\right\|$. To extract the final state, we measure the first qubit. The probability of obtaining the outcome 1 is

$$\frac{\|x_{N_t}\|^2}{\|x_{N_t}\|^2 + \frac{1}{N_t}\sum_{k=1}^{N_t} \|x_k\|^2} \approx \frac{1}{1+\chi^2}, \quad \chi^2 = \frac{\frac{1}{T}\int_0^T \|x(t)\|^2 \, \mathrm{d}t}{\|x(T)\|^2}. \tag{20.15}$$

We readily have

$$\chi \le q := \frac{\max_{0\le t\le T} \|x(t)\|}{\|x(T)\|}. \tag{20.16}$$

In particular, if $\|x(t)\| = 1$ for all t, we have $\chi = q = 1$, and the success probability is exactly $\frac{1}{2}$.

The history state is also convenient for computing time-averaged quantities, because it stores the solution on a dense time grid without collapsing the state at each intermediate time t_k. For instance, a time-averaged observable can be approximated by

$$\frac{1}{T}\int_0^T x(t)^\dagger O x(t)\ \mathrm{d}t = \frac{1}{N_t}\sum_{k=1}^{N_t} x_k^\dagger O x_k + \mathcal{O}\left(\frac{1}{N_t}\right), \tag{20.17}$$

provided that $t \mapsto x(t)^\dagger O x(t)$ is Lipschitz on $[0,T]$. Since $N_t = 2^{n_t}$, the quadrature error is exponentially small in the number of time-register qubits n_t. The discrete average can then be written as

$$\begin{aligned}\frac{1}{N_t}\sum_{k=1}^{N_t} x_k^\dagger O x_k &= X(T)^\dagger (I_{N_t}\otimes O) X(T) \\ &= \langle X(T)|(I_{N_t}\otimes O)|X(T)\rangle\ \|X(T)\|^2.\end{aligned} \tag{20.18}$$

which is precisely the discrete time average. Thus, although the quantum differential equation problem is defined in terms of the final vector $x(T)$, the history state also gives direct access to other observables of interest.

With the history state in place, we now explain how to rewrite the differential equation as a linear system. The simplest discretization is the forward Euler method on a uniform grid $t_k = k\Delta t$, where $\Delta t = T/N_t$ and $k = 0,\dots,N_t$. This discretization also incorporates the inhomogeneous term directly, without invoking Duhamel's principle. Let $A_k = A(t_k), b_k = b(t_k)$. The resulting discretized system becomes

$$x_{k+1} - x_k = \Delta t(A_k x_k + b_k), \quad k = 0,\dots,N_t - 1, \tag{20.19}$$

which can be rewritten as

$$\begin{pmatrix} I_s & 0 & 0 & \cdots & 0 & 0 \\ -(I_s+\Delta t A_1) & I_s & 0 & \cdots & 0 & 0 \\ 0 & -(I_s+\Delta t A_2) & I_s & \cdots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \cdots & -(I_s+\Delta t A_{N_t-1}) & I_s \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N_t} \end{pmatrix} = \begin{pmatrix} (I_s+\Delta t A_0)x_0 + \Delta t b_0 \\ \Delta t b_1 \\ \Delta t b_2 \\ \vdots \\ \Delta t b_{N_t-1} \end{pmatrix}, \tag{20.20}$$

or, more compactly, as the linear system

$$\mathcal{A}\mathbf{x} = \mathbf{b}. \tag{20.21}$$

Here I_s is the identity matrix of size d, and $\mathbf{x} \in \mathbb{C}^{N_t d}$ encodes the entire history of the states.

Remark 20.4 (Connection to matrix powers)**.** In Section 9.1, we discussed the challenges of constructing the block encoding of a matrix power A^L using products of block encodings. Notably, when $A(t) = A$ is a constant matrix and $b(t) = 0$, solving the linear differential equation is equivalent to constructing the block encoding of the matrix power $(I + \Delta t A)^{N_t}$, assuming the forward Euler method is used. If the block encoding of the matrix $I + \Delta t A$ is constructed using linear combination

of unitaries (LCU), the subnormalization factor will necessarily be greater than 1. Consequently, the cost of constructing the block encoding via repeated multiplication grows exponentially with N_t. We will see that the linear system method successfully avoids this issue. ⋄

20.2.1. Quantum linear system problem. To solve Eq. (20.20) with a quantum linear system solver, we need an efficient block encoding of the matrix $\mathcal{A}$. Observe that

$$\mathcal{A} = I_t \otimes I_s - \sum_{k=1}^{N_t-1} |t_{k+1}\rangle\langle t_k| \otimes (I_s + \Delta t A_k). \tag{20.22}$$

Here $\mathrm{ADD}\,|t_k\rangle = |t_{k+1}\rangle$ for $1 \le k \le N_t - 1$ is the adder circuit on the time register, with the convention that $\mathrm{ADD}\,|t_{N_t}\rangle = 0$. The term involving A_k is obtained by combining this shift with the block-encoding oracle U_A. Hence a block encoding of $\mathcal{A}$ can be prepared with LCU using one query to U_A, with subnormalization factor at most $2 + \alpha_A \Delta t$, which is constant when $\Delta t = \mathcal{O}(\alpha_A^{-1})$.

We also need to prepare the right hand side vector $\mathbf{b}$. Note that

$$\mathbf{b} = |t_1\rangle \otimes x_0 + \Delta t\ |t_1\rangle \otimes A_0 x_0 + \sqrt{T\Delta t}\frac{1}{\sqrt{N_t}} \sum_{k=1}^{N_t} |t_k\rangle \otimes b_{k-1}. \tag{20.23}$$

Here we use $\sqrt{N_t} = \sqrt{T/\Delta t}$. Thus the right hand side vector $\mathbf{b}$ can be prepared with LCU using one query each to U_A, U_b, and U_{x_0}, with subnormalization factor at most $1 + \alpha_A \Delta t + \sqrt{T\Delta t}\,\alpha_b$.

To evaluate observables associated with the final state more efficiently, we use the padded history state, which appends N_t copies of the final vector x_{N_t} to $\mathbf{x}$:

$$\mathbf{X} = |0\rangle \otimes \mathbf{x} + |1\rangle \otimes \mathbf{y}, \tag{20.24}$$

with the unnormalized vectors

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N_t} \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} x_{N_t+1} \\ x_{N_t+2} \\ \vdots \\ x_{2N_t} \end{pmatrix} := \begin{pmatrix} x_{N_t} \\ x_{N_t} \\ \vdots \\ x_{N_t} \end{pmatrix}. \tag{20.25}$$

The corresponding enlarged linear system becomes

$$\begin{pmatrix} I_s & & & & & & & \\ -(I_s + \Delta t A_1) & I_s & & & & & & \\ & \ddots & & & & & & \\ & & -(I_s + \Delta t A_{N_t-1}) & I_s & & & & \\ & & & -I_s & I_s & & & \\ & & & & -I_s & I_s & & \\ & & & & & \ddots & & \\ & & & & & & -I_s & I_s \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N_t} \\ x_{N_t+1} \\ x_{N_t+2} \\ \vdots \\ x_{2N_t} \end{pmatrix} = \begin{pmatrix} (I_s + \Delta t A_0)x_0 + \Delta t b_0 \\ \Delta t b_1 \\ \vdots \\ \Delta t b_{N_t-1} \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{20.26}$$

Passing from $\mathbf{x}$ to $\mathbf{X}$ introduces only one ancilla qubit. After solving the modified system Eq. (20.26) to precision ϵ, we can estimate $\langle x(T)|O|x(T)\rangle \,/\, \langle x(T)|x(T)\rangle$ by

$$\frac{\mathbf{y}^\dagger (I_t \otimes O)\mathbf{y}}{\mathbf{y}^\dagger \mathbf{y}} = \frac{\mathbf{X}^\dagger \left(|1\rangle\langle 1| \otimes I_t \otimes O\right)\mathbf{X}}{\mathbf{X}^\dagger \left(|1\rangle\langle 1| \otimes I_t \otimes I_s\right)\mathbf{X}}, \tag{20.27}$$

The size of this quantity does not scale with Δt. For example, if $\|x(t)\|$ is constant in time, then the success probability of measuring the ancilla qubit is

$$\frac{\mathbf{X}^\dagger \left(|1\rangle\langle 1| \otimes I_t \otimes I_s\right) \mathbf{X}}{\mathbf{X}^\dagger \mathbf{X}} = \frac{1}{2}. \tag{20.28}$$

The modified matrix $\mathcal{A}$ and the right hand side $\mathbf{b}$ can be constructed similarly.

20.2.2. Condition number analysis. To solve Eq. (20.20) or Eq. (20.26) with a QLSP solver, we need to estimate the condition number of $\mathcal{A}$. Note that $\mathcal{A}$ is a block-bidiagonal matrix and non-Hermitian.

For simplicity, consider the time-independent version of Eq. (20.20). Let $I = I_s$, and $B = (I + \Delta t A)$ with $\|B\| = \mathcal{O}(1)$. Then

$$\mathcal{A} = \begin{pmatrix} I & 0 & 0 & \cdots & 0 & 0 \\ -B & I & 0 & \cdots & 0 & 0 \\ 0 & -B & I & \cdots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \cdots & -B & I \end{pmatrix}. \tag{20.29}$$

Let S be the $N_t \times N_t$ lower-shift matrix with ones on the first subdiagonal. Then $\mathcal{A} = I_{N_t} \otimes I - S \otimes B$, so

$$\|\mathcal{A}\| \leq \|I_{N_t} \otimes I\| + \|S \otimes B\| \leq 1 + \|B\| = \mathcal{O}(1). \tag{20.30}$$

We may also explicitly evaluate $\mathcal{A}^{-1}$ as

$$\mathcal{A}^{-1} = \begin{pmatrix} I & 0 & 0 & \cdots & 0 & 0 \\ B & I & 0 & \cdots & 0 & 0 \\ B^2 & B & I & \cdots & 0 & 0 \\ \vdots & & & & & \vdots \\ B^{N_t-1} & B^{N_t-2} & \cdots & \cdots & B & I \end{pmatrix} = \sum_{j \in [N_t]} S^j \otimes B^j. \tag{20.31}$$

Then

$$\left\|\mathcal{A}^{-1}\right\| \leq \sum_{j \in [N_t]} \left\|S^j\right\| \left\|B^j\right\| = \sum_{j \in [N_t]} \left\|B^j\right\|. \tag{20.32}$$

Note that $B^j = (I + \Delta t A)^j \approx e^{j \Delta t A}$. In particular, we may choose a sufficiently small Δt so that the approximation is sufficiently accurate, and $B^j \approx e^{j \Delta t A}$ for any $j \in [N_t]$. Let

$$\zeta = \max_{0 \leq t \leq T} \left\|e^{At}\right\| \tag{20.33}$$

Then

$$\left\|\mathcal{A}^{-1}\right\| \leq \zeta N_t = \frac{T\zeta}{\Delta t}. \tag{20.34}$$

Remark 20.5. In practice, the choice of Δt and the target precision ϵ are not independent. For instance, the forward Euler method is first order, so its discretization error scales as $\epsilon = \mathcal{O}(\Delta t)$. Hence $\kappa(\mathcal{A}) = \mathcal{O}(\Delta t^{-1}) = \mathcal{O}(\epsilon^{-1})$. In addition, the region of absolute stability can impose further restrictions on the size of Δt, which again affects the condition number.

If we further have the information $\left\|e^{At}\right\| \leq C_1 e^{-C_2 t}$ for all $t \in [0,T]$ and for some $C_1, C_2 > 0$, and if the following multiplicative error bound holds $\left\|B^j - e^{j\Delta t A}\right\| \leq \epsilon \left\|e^{j\Delta t A}\right\|$, then

$$\left\|\mathcal{A}^{-1}\right\| \leq \sum_{j\in[N_t]} \left\|B^j\right\| \leq (1+\epsilon) C_1 \frac{1}{1-e^{-C_2\Delta t}} \approx \frac{C_1}{C_2 \Delta t} = \mathcal{O}(1/\Delta t), \tag{20.35}$$

which is independent of N_t. This gives an improved bound $\kappa(\mathcal{A}) = \mathcal{O}(\Delta t^{-1})$, which is independent of T unless C_2 is very small.

◇

Example 20.6 (Growth of the condition number)**.** If A has a positive eigenvalue, $\left\|e^{At}\right\|$ becomes unbounded as t grows, which implies that the upper bound for $\kappa(\mathcal{A})$ also becomes unbounded. This is the correct behavior. For instance, if $A = 1$ is a scalar and $b = 0$, the solution to the homogeneous equation grows exponentially as $x(T) = e^T$. See Fig. 20.1 for an illustration.

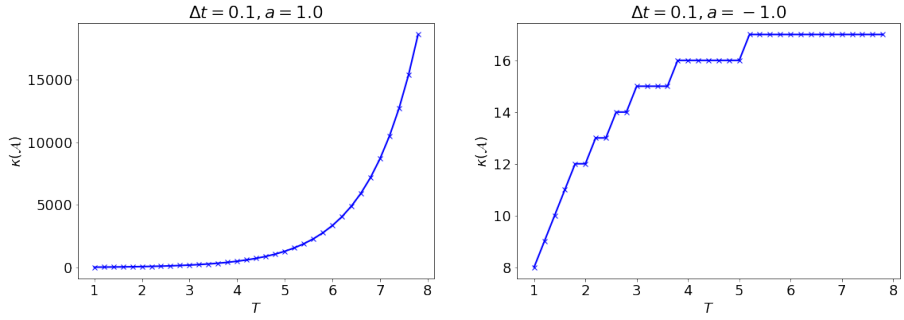


FIGURE 20.1. Growth of the condition number $\kappa(\mathcal{A})$ with respect to T with a fixed step size $\Delta t = 0.1$ for $a = 1.0$ and $a = -1.0$.

◇

The analysis of the condition number for the padded system in Eq. (20.26) is similar. We begin with a general bound for structured block lower bidiagonal matrices, which extends the preceding time-independent estimates.

Proposition 20.7. *Let $\{B_k\}_{k=1}^{m-1}$ be $n \times n$ matrices, and define the block lower bidiagonal matrix $\mathcal{A} \in \mathbb{C}^{mn\times mn}$ by*

$$\mathcal{A} = \begin{pmatrix} I & 0 & \cdots & 0 \\ -B_1 & I & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & -B_{m-1} & I \end{pmatrix}, \tag{20.36}$$

where I is the $n \times n$ identity matrix. Let

$$\zeta_0 = 1, \quad \zeta_k = \sup_{1\leq l\leq m-k} \|B_{l+k-1}\cdots B_l\|, \quad 1 \leq k \leq m-1. \tag{20.37}$$

Then

$$\kappa(\mathcal{A}) \leq (\zeta_0 + \zeta_1) \left(\sum_{k=0}^{m-1} \zeta_k \right). \tag{20.38}$$

PROOF. First, $\mathcal{A} = \mathcal{B}_0 - \mathcal{B}_1$, where $\mathcal{B}_0$ is the $mn \times mn$ identity matrix, and

$$\mathcal{B}_1 = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ B_1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & B_{m-1} & 0 \end{pmatrix}. \tag{20.39}$$

Note that

$$\mathcal{B}_1^\dagger \mathcal{B}_1 = \operatorname{diag}\left(B_1^\dagger B_1, \cdots, B_{m-1}^\dagger B_{m-1}, 0 \right), \tag{20.40}$$

where diag constructs a block diagonal matrix from the arguments and 0 is the $n \times n$ zero matrix. Then $\left\| \mathcal{B}_1^\dagger \mathcal{B}_1 \right\| \leq \sup_{1 \leq l \leq m-1} \|B_l\|^2 = \zeta_1^2$. This proves $\|\mathcal{B}_1\| \leq \zeta_1$, and

$$\|\mathcal{A}\| \leq \|\mathcal{B}_0\| + \|\mathcal{B}_1\| \leq \zeta_0 + \zeta_1. \tag{20.41}$$

To bound $\left\| \mathcal{A}^{-1} \right\|$, we first note that $\mathcal{A}^{-1}$ has the following analytic formula, which generalizes Eq. (20.31)

$$\mathcal{A}^{-1} = \begin{pmatrix} I & 0 & 0 & \cdots & 0 & 0 \\ B_1 & I & 0 & \cdots & 0 & 0 \\ B_2 B_1 & B_2 & I & \cdots & 0 & 0 \\ \vdots & & & & & \vdots \\ B_{m-1} \cdots B_1 & B_{m-1} \cdots B_2 & \cdots & \cdots & B_{m-1} & I \end{pmatrix} =: \sum_{k=0}^{m-1} \mathcal{B}_k. \tag{20.42}$$

Here $\mathcal{B}_k$ generalizes the definition of $\mathcal{B}_0, \mathcal{B}_1$ and refers to the k-th sub-block-diagonal of $\mathcal{A}^{-1}$. Then following the same calculation for $\mathcal{B}_1$, we find that

$$\left\| \mathcal{B}_k^\dagger \mathcal{B}_k \right\| \leq \sup_{1 \leq l \leq m-k} \left\| B_l^\dagger \cdots B_{l+k-1}^\dagger B_{l+k-1} \cdots B_l \right\| \leq \sup_{1 \leq l \leq m-k} \|B_{l+k-1} \cdots B_l\|^2 = \zeta_k^2, \tag{20.43}$$

or $\|\mathcal{B}_k\| \leq \zeta_k$. Then by the triangle inequality

$$\left\| \mathcal{A}^{-1} \right\| \leq \sum_{k=0}^{m-1} \zeta_k, \tag{20.44}$$

which implies the desired bound of the condition number. □

Consider again the time-independent problem for simplicity. Let $I = I_s$, $B = (I + \Delta t A)$. After padding, the enlarged matrix becomes

$$\mathcal{A}_e = \left(\begin{array}{ccccc|ccccc} I & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ -B & I & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -B & I & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & I & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & 0 & \cdots & -I & I & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & -I & I & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -I & I & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & I \end{array}\right). \tag{20.45}$$

We can then apply Proposition 20.7, and find that

$$\zeta_k = \begin{cases} \sup_{0\le l\le k} \|B^l\|, & 1 \le k \le N_t - 1, \\ \sup_{k-N_t\le l\le N_t-1} \|B^l\|, & N_t \le k \le 2N_t - 1. \end{cases} \tag{20.46}$$

Define $\zeta = \sup_{0\le l\le N_t-1} \left\|B^l\right\|$. This means that $\sum_{k=0}^{2N_t-1} \zeta_k \le 2N_t\zeta$, and the condition number satisfies

$$\kappa(\mathcal{A}_e) \le 2\max\{1, \|B\|\} \times 2\zeta N_t = \mathcal{O}(\zeta T/\Delta t). \tag{20.47}$$

20.2.3. Success probability. Recall the discussion in Chapter 19 that the performance of many QLSP solvers, such as HHL and QLSP, depend on the magnitude of unnormalized solution vector $\xi = \left\|\mathcal{A}_e^{-1}\mathbf{b}\right\|$ besides the condition number. However, for solvers with near-optimal complexity, there is no such dependence on ξ. Nonetheless, for linear differential equation solvers, the dependence on the success probability is still there because in order to prepare an approximation to the normalized final state $|x(T)\rangle = x(T)/\|x(T)\|$ we still need to measure the first qubit in the padded history state. According to Eq. (20.15), the success probability is $\frac{1}{1+\chi^2}$, and the number of repetition is $\mathcal{O}(1+\chi^2) = \mathcal{O}(q^2)$ where $q := \frac{\max_{0\le t\le T}\|x(t)\|}{\|x(T)\|}$. With amplitude amplification, the cost reduces to $\mathcal{O}(q)$.

20.2.4. Higher order algorithm and complexity. The preceding discussion extends to higher-order methods. According to Remark 20.2, we restrict attention to the homogeneous case for simplicity.

$$\frac{\mathrm{d}}{\mathrm{d}t}x(t) = A(t)x(t), \quad t \in [0,T], \quad x(0) = x_0. \tag{20.48}$$

A higher-order algorithm aims to construct a more accurate approximation to the exact propagator $U(t,s) = \mathcal{T}e^{\int_s^t A(\tau)\,\mathrm{d}\tau}$.

If A is time-independent, then a block encoding of the evolution operator $U(t+\Delta t, t) = e^{A\Delta t}$ can be constructed using the truncated Taylor series method, as discussed in Section 14.2.

For time-dependent problems, one additional ingredient is required. Higher-order algorithms, such as the truncated Dyson series method introduced in Section 14.5 for time-dependent Hamiltonian simulation, typically query the matrix $A(t)$ on a finer time grid. Concretely, for each interval $[t_k, t_{k+1}]$, we assume access to a unitary $U_{A,k}$ defined by

$$(\langle 0^{m_a}| \otimes I_{t_k} \otimes I_s)\, U_{A,[t_k,t_{k+1}]}\, (|0^{m_a}\rangle \otimes I_{t_k} \otimes I_s) = \frac{1}{\alpha_A} \sum_{l=0}^{2^{n_l}-1} |l\rangle\langle l| \otimes A\left(t_k + \frac{l(t_{k+1}-t_k)}{2^{n_l}}\right), \tag{20.49}$$

where I_{t_k} denotes the identity matrix of dimension 2^{n_l} for some integer n_l. These unitaries $U_{A,[t_k,t_{k+1}]}$ may be used sequentially, or combined into a single larger unitary U_A that simultaneously provides access to all intervals.

The following theorem, restated here for completeness, is nearly identical to the truncated Dyson simulation result for short time segments in Lemma 14.10.

Lemma 20.8 (Truncated Dyson Simulation for Short Segments)**.** *Let $A : [a, b] \to \mathbb{C}^{2^n \times 2^n}$ be a differentiable time-dependent matrix that can be accessed via a block encoding $U_{A,[a,b]}$ as in Eq.* (20.49) *using $m_a + n_l$ ancilla qubits, and assume $0 < b - a \le \ln(2)/\alpha_A$. Then for any $\epsilon' > 0$, there exists a quantum algorithm that constructs an (α', m', ϵ')-block encoding of $\Xi = \mathcal{T} e^{\int_a^b A(t)\,\mathrm{d}t}$, where*

$$\alpha' = 2 + \mathcal{O}(\epsilon'), \quad m' = \mathcal{O}((m_a + n_l)K), \quad K = \mathcal{O}(\log(1/\epsilon')/\log\log(1/\epsilon')), \tag{20.50}$$

and the algorithm uses $\mathcal{O}(K)$ queries to $U_{A,[a,b]}$.

We now use the same linear-systems framework to construct a block encoding of the long-time propagator. The linear system to be solved is

$$x_{k+1} = U(t_{k+1}, t_k) x_k, \quad k = 0, \dots, N_t - 1. \tag{20.51}$$

Let B_k be a short-time integrator approximating $\Xi_k := U(t_{k+1}, t_k)$. Then we arrive at the analogous linear system

$$\mathcal{A} = \begin{pmatrix} I & 0 & 0 & \cdots & 0 & 0 \\ -B_1 & I & 0 & \cdots & 0 & 0 \\ 0 & -B_2 & I & \cdots & 0 & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & \cdots & -B_{N_t-1} & I \end{pmatrix}. \tag{20.52}$$

The associated extended linear system after padding is

$$\mathcal{A}_e = \left(\begin{array}{ccccc|ccccc} I & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ -B_1 & I & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -B_2 & I & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & I & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & 0 & \cdots & -I & I & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & -I & I & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & -I & I & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & I \end{array}\right). \tag{20.53}$$

This leads to the following complexity bound.

THEOREM 20.9 (Linear system based solver). *Consider the homogeneous linear differential equation Eq.* (20.48)*, where the matrix function $A(t)$ is accessible via an oracle of the form Eq.* (20.49)*, and the initial state x_0 is prepared using an oracle U_{x_0}. Let $\{t_k\}_{k=0}^{N_t}$ be a time grid with $t_0 = 0$, $t_{N_t} = T$, and step sizes satisfying $0 < t_{k+1} - t_k \leq \ln(2)/\alpha_A$. Then, there exists a quantum algorithm that prepares a normalized quantum state $|x_{N_t}\rangle$ such that $\| |x_{N_t}\rangle - |x(T)\rangle \| \leq \epsilon$ with success probability $\Omega(1)$, using*

$$\widetilde{\mathcal{O}}(\alpha_A T \zeta q \operatorname{polylog}(1/\epsilon)) \tag{20.54}$$

queries to U_A, $U_A^\dagger$, U_{x_0}, and $U_{x_0}^\dagger$, where

$$\zeta = \sup_{0 \leq s < t \leq T} \left\| \mathcal{T} \exp\left(\int_s^t A(\tau)\, \mathrm{d}\tau \right) \right\|, \quad q = \frac{\max_{0 \leq t \leq T} \|x(t)\|}{\|x(T)\|}. \tag{20.55}$$

PROOF SKETCH. We first apply Proposition 20.7 to estimate the condition number of $\mathcal{A}$. Note that $\zeta_k \leq \zeta$ holds for all values of k. Then

$$\kappa(\mathcal{A}_e) = \mathcal{O}(N_t \zeta) = \mathcal{O}(T \alpha_A \zeta). \tag{20.56}$$

For the short-time propagator in Lemma 20.8, it is sufficient to take $\Delta t = \ln(2)/\alpha_A$, so the number of time steps is $N_t = T/\Delta t = \Theta(T\alpha_A)$. To choose the accuracy parameter ϵ', we use the perturbation theory for linear systems discussed in Section 7.2, which gives

$$\epsilon' = \mathcal{O}(\epsilon / T \alpha_A \zeta). \tag{20.57}$$

The number of queries to U_A and $U_A^\dagger$ needed to construct the block encoding of the propagator on each short time segment is $\mathcal{O}(\log(1/\epsilon')) = \mathcal{O}(\log(T\alpha_A\zeta/\epsilon))$. The cost of a near-optimal linear system solver, as discussed in Section 19.7, is $\mathcal{O}(\kappa \operatorname{polylog}(\kappa/\epsilon))$. The additional multiplicative factor q comes from amplitude amplification. □

20.3. Time marching method

At first glance, if we are mainly interested in the final state $x(T)$, the linear system based method (and approaches using the history state in general) may not seem natural for solving differential equations. Most classical differential equation solvers follow a **time-marching** procedure, which propagates a single copy of the state (or a handful of copies in the context of a multi-step method) from t_k to t_{k+1} until reaching the final time $t_{N_t} = T$. This time marching strategy, however, encounters significant difficulty for general linear differential equations.

To see this, consider the forward Euler discretization of the time-independent equation $\frac{\mathrm{d}}{\mathrm{d}t} x(t) = Ax(t)$ on a uniform grid with $t_k - t_{k-1} = \Delta t = T/N_t$, so that $x_k = (I + A\Delta t) x_{k-1}$. Given a block encoding of A, the approximate short-time propagator $B = I + A\Delta t$ can be implemented using LCU. The resulting block encoding, denoted by U, can be chosen to have subnormalization factor $1 + \alpha_A \Delta t$, where α_A is the subnormalization factor of the block encoding of A. Thus the probability of successfully preparing x_k from x_{k-1} is at most

$$\frac{1}{(1 + \alpha_A \Delta t)^2} \times \frac{\|x_k\|^2}{\|x_{k-1}\|^2}. \tag{20.58}$$

The probability of successfully implementing all N_t steps of evolution is thus at most

$$\frac{1}{(1+\alpha_A \Delta t)^{2N_t}} \times \prod_{k=1}^{N_t} \frac{\|x_k\|^2}{\|x_{k-1}\|^2} \approx e^{-2\alpha_A T} \frac{\|x(T)\|^2}{\|x_0\|^2}. \tag{20.59}$$

To see why this scaling is unsatisfactory, consider the Hamiltonian simulation problem with $A = -iH$, where H is Hermitian. Even though $\|x(T)\| = \|x(0)\|$, the success probability still decreases exponentially as $e^{-2\alpha_A T}$, and in particular as $e^{-2\|H\|T}$ if we take $\alpha_A = \|H\|$. Note that the subnormalization factor per step here still approaches 1 as $\Delta t \to 0$. The situation becomes even worse if the subnormalization factor per step is a constant $c > 1$. For instance, when approximating $e^{-iH\Delta t}$ using QSVT, we have $c = 2$. Then the overall success probability becomes $c^{-2N_t} = c^{-2T/\Delta t}$, which vanishes in the limit $\Delta t \to 0$ even for a finite simulation time T.

For Hamiltonian simulation, this difficulty can be overcome because $e^{-iH\Delta t}$ is unitary. A sufficiently accurate non-unitary approximation to $e^{-iH\Delta t}$ can therefore be boosted to success probability 1 using the oblivious amplitude amplification in Section 11.4. This is used, for example, in the truncated Taylor series method in Section 14.2.

We now explain how the same time-marching idea can be adapted to differential equations that are not Hamiltonian simulations. The main tool is the uniform singular value amplification (USVA) discussed in Section 13.4. According to Remark 20.2, it is enough to consider the homogeneous equation Eq. (20.48).

THEOREM 20.10 (Time-marching based differential equation solver [FLT23]). *Consider the homogeneous linear differential equation Eq.* (20.48)*, where the matrix function $A(t)$ is accessible via an oracle of the form Eq.* (20.49)*, and the initial state x_0 is prepared using an oracle U_{x_0}. Let $\{t_k\}_{k=0}^{N_t}$ be a time grid with $t_0 = 0$, $t_{N_t} = T$, and step sizes satisfying $0 < t_{k+1} - t_k \leq \ln(2)/\alpha_A$. Then, there exists a quantum algorithm that prepares a normalized quantum state $|x_{N_t}\rangle$ such that $\||x_{N_t}\rangle - |x(T)\rangle\| \leq \epsilon$ with success probability $\Omega(1)$, using*

$$\widetilde{\mathcal{O}}\left(Q\alpha_A^2 T^2 \operatorname{polylog}(\epsilon^{-1})\right) \tag{20.60}$$

queries to U_A and $U_A^\dagger$, and $\mathcal{O}(Q)$ applications of U_{x_0} and $U_{x_0}^\dagger$, where

$$Q = \frac{\prod_{k=0}^{N_t-1} \left\| \mathcal{T} \exp\left(\int_{t_k}^{t_{k+1}} A(s)\, \mathrm{d}s\right)\right\|}{\|x(T)\|}. \tag{20.61}$$

PROOF SKETCH. With the given time grid, we first use the truncated Dyson expansion in Lemma 20.8 to construct an (α', m', ϵ')-block encoding, denoted by V_k, of each short-time propagator

$$\Xi_k = \mathcal{T}\left[e^{\int_{t_k}^{t_{k+1}} A(s)\, \mathrm{d}s}\right]. \tag{20.62}$$

This requires $\mathcal{O}(\log(1/\epsilon'))$ queries to U_A, and the subnormalization factor satisfies $\alpha' = \Theta(1)$.

Next, we apply uniform singular value amplification (Proposition 13.7) to construct a unitary $V_{\Phi_k} \in \mathrm{BE}_{\|\Xi_k\|(1+\delta),m+1}(\Xi_k, \epsilon')$. This uses

$$\mathcal{O}\left(\delta^{-1} \log(1/\epsilon')\right) \tag{20.63}$$

applications of V_k and $V_k^\dagger$ for any $0 < \delta < 1$.

To implement this procedure for N_t steps, we can employ the product of block encodings in Example 9.11. The cumulative subnormalization factor is $\prod_k \|\Xi_k\|(1+\delta)^{N_t} \leq \prod_k \|\Xi_k\| e^{\delta N_t}$. By

setting $\delta N_t = \ln 2$, this subnormalization factor is upper bounded by $2\prod_k \|\Xi_k\| = 2Q\,\|x(T)\|$ using Eq. (20.61). Therefore, the overall success probability is $\Omega(Q^{-2})$.

Let us now set the accuracy parameter ϵ'. To prepare the normalized state $|x(T)\rangle$ to precision ϵ, it suffices to approximate the unnormalized solution $x(T)$ to precision $\epsilon\,\|x(T)\|$. Since the dynamics is not unitary, the local errors can be amplified by subsequent propagators. Thus it suffices to choose ϵ' so that

$$\epsilon' \sum_{j=0}^{N_t-1} \prod_{l=j+1}^{N_t-1} \|\mathcal{T} e^{\int_{t_l}^{t_{l+1}} A(t)\,\mathrm{d}t}\| \le \epsilon' N_t \prod_{l=0}^{N_t-1} \|\mathcal{T} e^{\int_{t_l}^{t_{l+1}} A(t)\,\mathrm{d}t}\| \le \epsilon\,\|x(T)\|\,, \tag{20.64}$$

which is achieved by taking

$$\epsilon' = \mathcal{O}(\epsilon/N_t Q). \tag{20.65}$$

The number of time steps is $N_t = \mathcal{O}(T\alpha_A)$.

Finally, choose $\delta = \Theta(N_t^{-1})$. The number of queries to U_A and $U_A^\dagger$ needed to construct each amplified unitary V_{Φ_k} is

$$\mathcal{O}\left(\delta^{-1}\log^2(1/\epsilon')\right) = \mathcal{O}\left(T\alpha_A \log^2(T\alpha_A Q/\epsilon)\right). \tag{20.66}$$

Hence the total number of queries for all V_{Φ_k} is

$$\mathcal{O}\left(T^2\alpha_A^2 \log^2(T\alpha_A Q/\epsilon)\right). \tag{20.67}$$

Taking the success probability into account and applying amplitude amplification, the number of queries to U_A and $U_A^\dagger$ becomes $\widetilde{\mathcal{O}}\left(Q\alpha_A^2 T^2 \log^2 \epsilon^{-1}\right)$. The initial-state preparation oracle U_{x_0} is used only during amplitude amplification, so the number of queries to U_{x_0} and $U_{x_0}^\dagger$ is $\mathcal{O}(Q)$. □

Compared to the linear-system-based solver, the time-marching method has a quadratic dependence on $\alpha_A T$, whereas the linear-system-based solver is linear in $\alpha_A T$. Moreover, its growth factor is governed by Q, whereas Eq. (20.16) only gives $q \ge \chi$; in general, Q and q may not be comparable.

Its main advantage is the dependence on the initial-state preparation oracle U_{x_0}, which is only $\mathcal{O}(Q)$. In the linear-system-based solver with near-optimal complexity, the matrix oracle and the right-hand side oracle are queried together, so the number of queries to U_{x_0} is of the same order as the number of queries to U_A. Consequently, the time-marching method can be advantageous when the initial state is expensive to prepare.

We may also combine this method with the compression gadget introduced in Example 11.10 to reduce the number of ancillas used in the time-marching procedure.

20.4. Linear combination of Hamiltonian simulation method

20.4.1. Problem setup and main result. In this section, we present a method that significantly simplifies the simulation of a class of homogeneous linear differential equations, achieving near-optimal complexity with respect to both the matrix oracle U_A and the initial state preparation oracle U_{x_0}. We consider the following homogeneous linear differential equation

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = -A(t)x(t), \quad x(0) = x_0. \tag{20.68}$$

Compared to Eq. (20.1), note that there is an additional minus sign in front of $A(t)$ to emphasize the dissipative nature of the dynamics, as will be seen below.

First, any matrix $A \in \mathbb{C}^{d\times d}$ can always be decomposed as

$$A = L + iH. \tag{20.69}$$

Here $L, H \in \mathbb{C}^{d\times d}$ are Hermitian matrices via the **Cartesian decomposition**

$$L = \frac{A + A^\dagger}{2}, \quad H = \frac{A - A^\dagger}{2i}, \tag{20.70}$$

which are called the matrix real part and the matrix imaginary part of A, respectively.

Exercise 20.1. ([Bha97, Theorem IX.3.1]) Assume $A = L+iH$ with $L = \frac{A+A^\dagger}{2}, \quad H = \frac{A-A^\dagger}{2i}$. Then for any $t \in \mathbb{R}$,

$$\left\|e^{-At}\right\| \le \left\|e^{-Lt}\right\|. \tag{20.71}$$

In particular, when $L \succeq 0$, we have $\left\|e^{-At}\right\| \le 1$ for any $t \ge 0$. Try to state and prove a similar result in the time-dependent setting. (Hint: Use the Trotter product formula $\left\|e^{-At}\right\| = \left\|(e^{-At/r})^r\right\|$.)

The dynamics of interest satisfy the condition that for all $t \in [0, T]$,

$$L(t) = \frac{A(t) + A^\dagger(t)}{2} \succeq 0. \tag{20.72}$$

For any $0 \le s \le t \le T$, the propagator satisfies

$$\left\|\mathcal{T} e^{-\int_s^t A(\tau)\ \mathrm{d}\tau}\right\| \le 1. \tag{20.73}$$

Hence $\|x(t)\| \le \|x(s)\|$ for $0 \le s \le t \le T$, so the solution norm is non-increasing and

$$\max_{0\le t\le T} \|x(t)\| = \|x_0\|. \tag{20.74}$$

An example where this condition arises naturally is given in Section 20.6. Such equations commonly appear in **non-Hermitian quantum dynamics** associated with open quantum systems, as discussed in Chapter 21.

We now introduce a method called the **linear combination of Hamiltonian simulation** (LCHS) algorithm [ALL23, ACL26], which uses tools from complex variable calculus. We first state the main result.

THEOREM 20.11 (LCHS-based differential equation solver). *Consider the homogeneous linear differential equation Eq.* (20.68)*, where the matrix function $A(t)$ satisfies the positivity condition Eq.* (20.72)*. Then, for any $\beta \in (0, 1)$, there exists a quantum algorithm that prepares a normalized quantum state $|x_{N_t}\rangle$ such that $\||x_{N_t}\rangle - |x(T)\rangle\| \le \epsilon$ with success probability $\Omega(1)$, using*

$$\widetilde{\mathcal{O}}\left(q\alpha_A T \left(\log(1/\epsilon)\right)^{1+1/\beta}\right) \tag{20.75}$$

queries to U_A and $U_A^\dagger$, and $\mathcal{O}(q)$ applications of U_{x_0} and $U_{x_0}^\dagger$, where

$$q = \frac{\max_{0\le t\le T} \|x(t)\|}{\|x(T)\|} = \frac{\|x_0\|}{\|x(T)\|}. \tag{20.76}$$

20.4.2. Linear combination of Hamiltonian simulation formula. To see how the LCHS method works, let us first consider two special cases, where $A(t) = A = L + iH$ is time independent and satisfies $L \succeq 0$.

(1) $L = 0$ and $A = iH$. This is the Hamiltonian simulation problem. Since the Cauchy density $\frac{1}{\pi(1+k^2)}$ satisfies

$$\int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} \, \mathrm{d}k = 1, \tag{20.77}$$

we have the identity

$$e^{-iHt} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-iHt} \, \mathrm{d}k. \tag{20.78}$$

(2) $H = 0$ and $A = L \succeq 0$. Using the Fourier representation of $e^{-|x|}$, we have

$$\int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-ikx} \, \mathrm{d}k = e^{-|x|}. \tag{20.79}$$

Applying the spectral mapping theorem, we obtain for a positive matrix L that

$$e^{-Lt} = \int_{\mathbb{R}} \frac{1}{\pi(1+k^2)} e^{-ikLt} \, \mathrm{d}k. \tag{20.80}$$

We can rewrite the Cauchy distribution as $\frac{1}{\pi(1+k^2)} = \frac{f(k)}{1-ik}$ with $f(k) = \frac{1}{\pi(1+ik)}$, which is an analytic function in the lower half of the complex plane $\{z : \mathrm{Im}(z) < 0\}$. A moment of thought reveals that using the residue theorem (by properly choosing a contour in the lower half plane), both Eq. (20.78) and Eq. (20.80) can be generalized to

$$\begin{aligned} e^{-iHt} &= \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-iHt} \, \mathrm{d}k = 2\pi f(-i) e^{-iHt} = e^{-iHt}, \\ e^{-iLt} &= \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-ikLt} \, \mathrm{d}k = 2\pi f(-i) e^{-iLt} = e^{-iLt}, \end{aligned} \tag{20.81}$$

as long as $2\pi f(-i) = \int_{\mathbb{R}} \frac{f(k)}{1-ik} \, \mathrm{d}k = 1$ and $f(z)$ satisfies some mild decay conditions. Indeed, viewed from the Fourier representation,

$$F(x) = \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-ikx} \, \mathrm{d}k, \tag{20.82}$$

the function $f(k) = \frac{1}{\pi(1+ik)}$ decays slowly to 0 as $|k| \to \infty$, and the Fourier transform $F(x)$ has a cusp at $x = 0$. If we consider another function,

$$f(k) = \frac{1}{2\pi e^{-2^\beta} e^{(1+ik)^\beta}}, \quad \beta \in (0,1). \tag{20.83}$$

which satisfies $2\pi f(-i) = 1$, then $f(k)$ decays to 0 faster than any polynomial of k, and $F(x)$ also becomes a smooth function (see Fig. 20.2).

The idea of the LCHS formula is that when $A = L + iH$, even though we may not apply the spectral mapping theorem, we may still be able to apply the residue theorem to obtain

$$\int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-i(H+kL)t} \, \mathrm{d}k = 2\pi f(-i) e^{-i(H-iL)t} = e^{-At}, \tag{20.84}$$

This expresses the time evolution as an integral of Hamiltonian evolution problems $e^{-i(H+kL)t}$, and hence the name of the method.

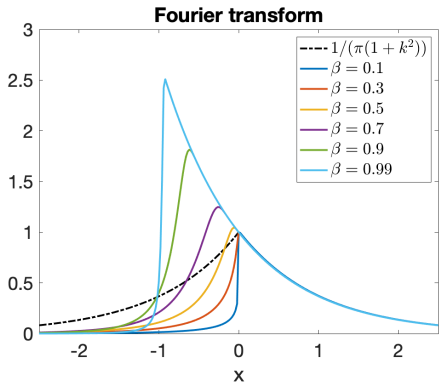


FIGURE 20.2. Fourier transform of the function $f(k)/(1-ik)$ where $f(k)$ is given in Eq. (20.83) for different values of β. Note that the values of all functions agree on $[0,\infty)$ and are equal to e^{-x}.

We now present the key identity used in the LCHS method, which is also valid in the time-dependent setting and is a restatement of the results in [ACL26]. In the time-independent case, this reduces to Eq. (20.84).

THEOREM 20.12 (Linear combination of Hamiltonian simulation). *Let $f(z)$ be a function of $z \in \mathbb{C}$, such that*

1. *$f(z)$ is analytic on the lower half plane $\{z : \mathrm{Im}(z) < 0\}$ and continuous on $\{z : \mathrm{Im}(z) \le 0\}$,*
2. *there exists a parameter $\alpha > 0$ such that $|z|^\alpha |f(z)| \le \widetilde{C}$ for a constant $\widetilde{C}$ when $\mathrm{Im}(z) \le 0$, and*
3. *$\int_{\mathbb{R}} \frac{f(k)}{1-ik}\,\mathrm{d}k = 1$.*

Let $A(t) \in \mathbb{C}^{N\times N}$ be decomposed as in Eqs. (20.69) and (20.70). If $L(s) \succeq 0$ for all $0 \le s \le t$, then

$$\mathcal{T} e^{-\int_0^t A(s)\,\mathrm{d}s} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} \mathcal{T} e^{-i\int_0^t (kL(s)+H(s))\,\mathrm{d}s}\,\mathrm{d}k. \tag{20.85}$$

PROOF SKETCH. Let $O_L(t) = \mathcal{T} e^{-\int_0^t A(s)\,\mathrm{d}s}$ and $O_R(t) = \int_{\mathbb{R}} \frac{f(k)}{1-ik} \mathcal{T} e^{-i\int_0^t (kL(s)+H(s))\,\mathrm{d}s}\,\mathrm{d}k$. By definition, $O_L(t)$ satisfies the ODE

$$\frac{\mathrm{d}O_L}{\mathrm{d}t} = -A(t)O_L(t), \quad O_L(0) = I. \tag{20.86}$$

We will show that $O_R(t)$ satisfies the same ODE.

First, for the initial condition, by plugging in $t = 0$ and using the normalization condition, we have

$$O_R(0) = \int_{\mathbb{R}} \frac{f(k)}{1-ik} I\,\mathrm{d}k = I. \tag{20.87}$$

Now, we choose a fixed $\delta > 0$ and consider $t \in [\delta, T]$. Differentiating $O_R(t)$ with respect to t yields

$$\begin{aligned}\frac{\mathrm{d}O_R(t)}{\mathrm{d}t} &= \mathcal{P}\int_{\mathbb{R}} \frac{f(k)}{1-ik}(-ikL(t) - iH(t))\mathcal{T}e^{-i\int_0^t (kL(s)+H(s))\,\mathrm{d}s}\,\mathrm{d}k \\ &= \mathcal{P}\int_{\mathbb{R}} \frac{f(k)}{1-ik}\left[(-L(t) - iH(t)) + (1-ik)L(t)\right]\mathcal{T}e^{-i\int_0^t (kL(s)+H(s))\,\mathrm{d}s}\,\mathrm{d}k \\ &= -A(t)O_R(t) + L(t)\left(\mathcal{P}\int_{\mathbb{R}} f(k)\mathcal{T}e^{-i\int_0^t (kL(s)+H(s))\,\mathrm{d}s}\,\mathrm{d}k\right).\end{aligned} \tag{20.88}$$

Here $\mathcal{P}\int_{\mathbb{R}}$ stands for the Cauchy principal values of the integrals, as the integrals may not converge absolutely. Note that the integrand of $\mathcal{P}\int_{\mathbb{R}} f(k)\mathcal{T}e^{-i\int_0^t (kL(s)+H(s))\,\mathrm{d}s}\,\mathrm{d}k$ is analytic in the lower half of the complex plane. We can prove that if $L(t) \succeq \lambda_0 > 0$ is a strictly positive matrix, then this term vanishes (this step is omitted for simplicity). So we obtain

$$\frac{\mathrm{d}O_R(t)}{\mathrm{d}t} = -A(t)O_R(t) \tag{20.89}$$

for all $t \in [\delta, T]$. As δ can be an arbitrary positive number, Eq. (20.89) holds for all $t \in (0, T]$. This proves that $O_R(t)$ satisfies the same ODE as $O_L(t)$ with the same initial condition, so $O_L(t) = O_R(t)$ by the uniqueness of the solution. We then take the limit $\lambda_0 \to 0$ and complete the proof. □

20.4.3. Proof sketch of Theorem 20.11. When using LCHS to simulate Eq. (20.68), the integral in k must be truncated to a finite interval $[-K, K]$. For the near-optimal kernel in Eq. (20.83), we have

$$\frac{f(k)}{1-ik} = \mathcal{O}(e^{-C|k|^\beta}) \tag{20.90}$$

as $k \to \infty$. Therefore it suffices to take $K = \mathcal{O}(\log^{1/\beta}(1/\epsilon))$. We may then apply a numerical quadrature to approximate the integral on this interval by a finite sum

$$\mathcal{T}e^{-\int_0^T A(s)\,\mathrm{d}s} \approx \sum_j \omega_j \mathcal{T}e^{-i\int_0^T (k_j L(s)+H(s))\,\mathrm{d}s}, \tag{20.91}$$

where $\{k_j, \omega_j\}$ are quadrature nodes and weights, respectively. This is a linear combination of Hamiltonian simulations. We can use a high-order numerical quadrature to discretize the integral in the LCHS formula, and the LCU cost is determined by the 1-norm of the coefficients, namely,

$$\sum_j |\omega_j| \approx \int_{\mathbb{R}} \frac{|f(k)|}{\sqrt{1+k^2}}\,\mathrm{d}k, \tag{20.92}$$

which is an $\mathcal{O}(1)$ constant independent of the simulation parameters T, α_A, and ϵ.

To solve each individual time-dependent Hamiltonian simulation problem $\mathcal{T}e^{-i\int_0^T (kL(s)+H(s))\,\mathrm{d}s}$, we can use the truncated Dyson series method. To this end, we need a query access model for the Hamiltonian $kL(t) + H(t)$ similar to that of $A(t)$ in Eq. (20.49). If possible, we may assume access to oracles encoding $L(t)$ and $H(t)$ separately, namely

$$\begin{aligned}(\langle 0^a| \otimes I_s)\text{HAM-T}_{L,k}(|0^a\rangle \otimes I_s) &= \frac{1}{\alpha_L}\sum_{l=0}^{2^{n_l}-1} |l\rangle\langle l| \otimes L(t_k + l(t_{k+1} - t_k)/2^{n_l}), \\ (\langle 0^a| \otimes I_s)\text{HAM-T}_{H,k}(|0^a\rangle \otimes I_s) &= \frac{1}{\alpha_H}\sum_{l=0}^{2^{n_l}-1} |l\rangle\langle l| \otimes H(t_k + l(t_{k+1} - t_k)/2^{n_l}).\end{aligned} \tag{20.93}$$

Here α_L and α_H are the block-encoding factors such that $\alpha_L \geq \max_t \|L(t)\|$, $\alpha_H \geq \max_t \|H(t)\|$. We may also directly construct HAM-$\mathrm{T}_{L,k}$ and HAM-$\mathrm{T}_{H,k}$ using LCU with $\mathcal{O}(1)$ applications of $U_{A,k}$. The resulting block-encoding factors satisfy $\alpha_L, \alpha_H = \mathcal{O}(\alpha_A)$. Then

$$\max_t K \|L(t)\| + \|H(t)\| = \mathcal{O}(\alpha_A \log^{1/\beta}(1/\epsilon)). \tag{20.94}$$

According to Theorem 14.11, the number of queries to U_A needed to construct a block encoding of $\mathcal{T} e^{-i\int_0^T (kL(s)+H(s))\,\mathrm{d}s}$ using the truncated Dyson series is

$$\widetilde{\mathcal{O}}\left(\alpha_A T \left(\log(1/\epsilon)\right)^{1+1/\beta}\right). \tag{20.95}$$

Taking the success probability into account and applying amplitude amplification, the total cost is

$$\widetilde{\mathcal{O}}\left(q\alpha_A T \left(\log(1/\epsilon)\right)^{1+1/\beta}\right). \tag{20.96}$$

The number of queries to U_{x_0} and $U_{x_0}^\dagger$ is $\mathcal{O}(q)$.

20.5. Example: Solving the heat equation

Let us consider a toy problem of solving the heat equation in one dimension with Dirichlet boundary conditions

$$\partial_t u(r,t) = u''(r), \quad r \in \Omega = [0,1], \quad u(0,t) = u(1,t) = 0. \tag{20.97}$$

This is the time-dependent version of the Poisson equation in Section 19.4. For simplicity, we use a central finite difference method to discretize the Laplacian operator with a uniform grid of N points. This gives a linear ODE system

$$\partial_t u = -Au, \tag{20.98}$$

where $A \in \mathbb{R}^{N\times N}$ is a Hermitian tridiagonal matrix with $\|A\| \approx 4N^2$.

Again for simplicity, we use the forward Euler method to discretize the simulation time interval $[0,T]$ into N_t sub-intervals with a uniform step size $\Delta t = T/N_t$. For numerical stability, the step size needs to be chosen so that $\Delta t = \mathcal{O}(\|A\|^{-1}) = \mathcal{O}(N^{-2})$. This gives rise to a linear system of size NN_t.

Using the linear system based method, according to Theorem 20.9, the query complexity of U_A for solving the heat equation, solved by the near-optimal linear system solver is $\widetilde{\mathcal{O}}\left(qN^2 T \operatorname{polylog}(\epsilon^{-1})\right)$, where $q = \|u_0\| / \|u(T)\|$. Since A is Hermitian, we can also apply the LCHS method to solve this problem as

$$e^{-At} = \int_{\mathbb{R}} \frac{f(k)}{1-ik} e^{-iktA}\,\mathrm{d}k. \tag{20.99}$$

The query complexity of U_A using the LCHS method is again $\widetilde{\mathcal{O}}\left(qN^2 T \operatorname{polylog}(\epsilon^{-1})\right)$. The query complexity of U_A using the time-marching method is $\widetilde{\mathcal{O}}\left(QN^4 T^2 \operatorname{polylog}(\epsilon^{-1})\right)$, where Q is the growth factor defined in Eq. (20.61).

With respect to the number of queries to the initial state oracle, the linear system based method is still $\widetilde{\mathcal{O}}\left(qN^2 T \operatorname{polylog}(\epsilon^{-1})\right)$. This is improved to $\mathcal{O}(q)$ in the time-marching and the LCHS method.

Similar to the situation of the Poisson equation, super-polynomial quantum advantage with respect to N in one dimension seems unlikely. However, there may be a potential quantum advantage in the higher-dimensional setting. When solving the d-dimensional heat equation

$$\partial_t u(\mathbf{r}, t) = \Delta u(\mathbf{r}, t), \quad \mathbf{r} \in \Omega = [0, 1]^d, \quad u(\cdot, t)|_{\partial\Omega} = 0. \tag{20.100}$$

This can be written as a linear system of equations

$$\partial_t u = -\mathcal{A}u, \tag{20.101}$$

where $\mathcal{A}$ is given in Eq. (19.35). The eigenvalues of $\mathcal{A}$ are all positive. Note that $\|\mathcal{A}\| = \Theta(dN^2)$, which only increases linearly in d and leads to a significant advantage over classical solvers. That being said, the input cost, output cost, together with the hardness of classical solvers need to be carefully scrutinized.

Exercise 20.2. Consider the initial value problem of the linear differential equation Eq. (20.1).

(1) Construct the linear system of equations similar to Eq. (20.20) using the backward Euler method.
(2) In the scalar case when $A(t) \equiv a \in \mathbb{C}$ is a constant satisfying $\mathrm{Re}(a) \leq 0$, estimate the query complexity of the QSVT algorithm applying to the linear system constructed in (1).

20.6. Example: Non-Hermitian quantum dynamics with complex absorbing potentials

Many problems in quantum dynamics, such as molecular scattering, photodissociation, and nanotransport are defined in an infinite space. Unlike solving the ground state of molecules in quantum chemistry, replacing the infinite space by a finite-sized box in these quantum dynamics problems may lead to significant errors at least along certain extended dimensions. Therefore boundary conditions need to be carefully designed and implemented to balance the accuracy of the simulation and the computational cost. One widely used method in quantum chemistry is the complex absorbing potential (also called the imaginary potential) method [Chi91, VBK92, MPNE04], which replaces the real potential by a complex one, and the time-dependent Schrödinger equation becomes

$$i\partial_t u(\mathbf{r}, t) = \left(-\frac{1}{2}\Delta_{\mathbf{r}} + V_R(\mathbf{r}, t) - iV_I(\mathbf{r})\right) u(\mathbf{r}, t), \quad u(\mathbf{r}, 0) = u_0(\mathbf{r}). \tag{20.102}$$

or equivalently,

$$\partial_t u(\mathbf{r}, t) = -\left(V_I(\mathbf{r}) + i\left(-\frac{1}{2}\Delta_{\mathbf{r}} + V_R(\mathbf{r}, t)\right)\right) u(\mathbf{r}, t) =: -A(t)u(\mathbf{r}, t), \quad u(\mathbf{r}, 0) = u_0(\mathbf{r}). \tag{20.103}$$

Here $V_R(\mathbf{r}, t)$ is the real time-dependent external potential, and $-iV_I(\mathbf{r})$ is the absorbing potential and can often be chosen to be time-independent. The minus sign reflects that this is a damping potential, and V_I can be chosen to be bounded and non-negative. These potentials can be accessed using oracles $U_{V_I} : |\mathbf{r}\rangle |0\rangle \to |\mathbf{r}\rangle |V_I(\mathbf{r})\rangle$, $U_{V_R} : |\mathbf{r}\rangle |s\rangle |0\rangle \to |\mathbf{r}\rangle |s\rangle |V_R(\mathbf{r}, s)\rangle$. For simplicity we will count the number of queries to a discretized version of $A(t)$.

In these applications, we are interested in the case before the scattering wave leaves the region of interest, i.e., $\|u(T)\|^2 = \int |u(\mathbf{r}, T)|^2 \, \mathrm{d}\mathbf{r}$ is not too small. Such a condition can also be satisfied if u_0 is a near-resonance state. Another widely used method for modeling open quantum system dynamics is the Lindblad equation, which will be discussed in more detail in Chapter 21. The non-Hermitian

quantum dynamics (20.103) is also related to a class of numerical methods for solving the Lindblad equation, known as the quantum jump or the Monte Carlo wavefunction method [DCM92, DZR92].

We now solve Eq. (20.103) using the LCHS algorithm. We first discretize the spatial variable $\mathbf{r}$ using N equidistant grid points, and the Laplace operator is discretized by, for example, a finite difference formula. In the equivalent equation $\partial_t u = -A(t)u$, the Hermitian part $H(t) = -\frac{1}{2}\Delta_{\mathbf{r}} + V_R(t)$ is the standard Hamiltonian with $\|H(t)\| = \mathcal{O}(N^2 + \max_t \|V_R(t)\|)$, and the non-Hermitian part $L = V_I$ is a time-independent positive semidefinite diagonal matrix with $\|L\| \le \max_t \|V_I(t)\|$. Therefore the block-encoding subnormalization factor satisfies $\alpha_A = \mathcal{O}(N^2 + \max_t \|V_R(t)\| + \|V_I(t)\|)$. Using LCHS, we can prepare an ϵ-approximation to the normalized state $u(T)/\|u(T)\|$ using $\widetilde{\mathcal{O}}\left(\frac{\|u_0\|}{\|u(T)\|}\alpha_A T \operatorname{polylog}(\epsilon^{-1})\right)$ applications of U_A and its inverse, and $\mathcal{O}(q)$ applications of the initial-state oracle and its inverse, where $q = \|u_0\| / \|u(T)\|$.

20.7. Lower bound of query complexity

In all methods, we show that the query complexity depends on norm-growth quantities such as χ, q, and Q. This is very different from the Hamiltonian simulation problem. In this section we show that a dependence of this kind cannot be removed in general by proving a lower bound in terms of Q. The strategy is to convert it into a Grover search problem.

THEOREM 20.13. *For any integer n, letting $N = 2^n$, there exists a matrix $A \in \mathbb{C}^{N\times N}$ that can be accessed through a $(1, m, 0)$-block encoding U_A, a target time $T = \mathcal{O}(n)$, and a normalized initial state $|u_0\rangle$ such that the following statement holds. Let $u(t)$ be the solution of the ODE $\frac{\mathrm{d}}{\mathrm{d}t}u(t) = Au(t)$ starting from $u(0) = |u_0\rangle$. Then for any $0 < \theta \le 1$, there is no quantum algorithm that can prepare a quantum state ρ (possibly mixed) satisfying*

$$D(|u(T)\rangle\langle u(T)|, \rho) \le \frac{1}{2}, \tag{20.104}$$

using $\mathcal{O}(Q^{1-\theta}\operatorname{poly}(T))$ queries to U_A. Here $D(\cdot,\cdot)$ denotes the trace distance between two quantum states, $|u(T)\rangle = u(T)/\|u(T)\|$ is the normalized final state, and

$$Q = \sup_L \sup_{0=t_0<t_1<\cdots<t_L=T} \frac{\prod_{l=0}^{L-1} \|e^{A(t_{l+1}-t_l)}\|}{\|u(T)\|}. \tag{20.105}$$

PROOF. We assume towards contradiction that such an algorithm exists. We use it to solve the unstructured search problem, in which we are asked to find a marked binary string of length n denoted by targ. Let O_{targ} be the standard bit oracle,

$$O_{\mathrm{targ}}|x, b\rangle = |x, b \oplus \mathbf{1}_{x=\mathrm{targ}}\rangle. \tag{20.106}$$

By phase kickback, one query to O_{targ} with the ancilla initialized to $|-\rangle$ implements the phase oracle

$$R_{\mathrm{targ}}|\mathrm{targ}\rangle = -|\mathrm{targ}\rangle, \quad R_{\mathrm{targ}}|x\rangle = |x\rangle, \quad x \ne \mathrm{targ}. \tag{20.107}$$

We let $A = -R_{\mathrm{targ}}$. Then $-R_{\mathrm{targ}}$ is a $(1, 0, 0)$-block encoding of A, and each query to U_A can be implemented using one query to O_{targ}. Starting from the uniform state

$$|u_0\rangle = \frac{1}{\sqrt{N}}\sum_x |x\rangle, \tag{20.108}$$

solving the ODE up to time T yields the unnormalized state

$$u(T) = \frac{1}{\sqrt{N}} \left(\sum_{x \neq \text{targ}} e^{-T} |x\rangle + e^{T} |\text{targ}\rangle \right). \tag{20.109}$$

In this state, the amplitude corresponding to the marked element targ is amplified, while the amplitudes corresponding to all other elements are suppressed. Consequently, the probability of obtaining targ when measuring the normalized state $|u(T)\rangle$ in the computational basis increases with time. At time T, this probability is

$$p_u = \frac{|\langle u(T)|\text{targ}\rangle|^2}{\langle u(T)|u(T)\rangle} = \frac{1}{(N-1)e^{-4T}+1}. \tag{20.110}$$

If we set $T = \frac{1}{4}\log(3(N-1)) = \mathcal{O}(n)$, then $p_u = 3/4$. Suppose we can prepare a state ρ with $D(\rho, |u(T)\rangle\langle u(T)|) \leq 1/2$. Then

$$p_\rho = \text{Tr}[\rho|\text{targ}\rangle\langle\text{targ}|] \geq p_u - D(\rho, |u(T)\rangle\langle u(T)|) \geq 3/4 - 1/2 = 1/4. \tag{20.111}$$

As a result, once we prepare a copy of ρ, we can measure in the computational basis, and with probability at least $1/4$ we obtain the marked element targ. We can verify whether the measurement outcome is targ using one query to the bit oracle O_{targ}. Therefore, to find targ with probability at least $2/3$, it suffices to prepare $\mathcal{O}(1)$ copies of ρ.

Now with the hypothetical algorithm for solving the ODE, we can prepare ρ using $\mathcal{O}(Q^{1-\theta}\,\text{poly}(T))$ queries to U_A. Here $T = \frac{1}{4}\log(3(N-1))$ as chosen above, and in this scenario

$$Q = \sup_{L} \sup_{0=t_0<t_1<\cdots<t_L=T} \frac{\prod_{l=0}^{L-1} \|e^{A(t_{l+1}-t_l)}\|}{\|u(T)\|}. \tag{20.112}$$

Since A is time-independent and $\left\|e^{A\Delta t}\right\| = e^{\Delta t}$ for every $\Delta t \geq 0$, the numerator is always equal to e^T. Hence

$$Q = \frac{\|e^{TA}\|}{\|u(T)\|} = \sqrt{\frac{N}{(N-1)e^{-4T}+1}} = \sqrt{\frac{3N}{4}}. \tag{20.113}$$

Therefore, we only need $\mathcal{O}(N^{\frac{1-\theta}{2}}\,\text{polylog}(N)) = o(\sqrt{N})$ queries to O_{targ} to prepare a single copy of ρ. Since only $\mathcal{O}(1)$ copies are needed, we would then be able to solve the unstructured search problem using only $o(\sqrt{N})$ queries to the search oracle. This contradicts the lower bound for the unstructured search problem in **??**. □

Notes and further reading

Classical background on consistency, stability, and higher-order integrators for ordinary differential equations may be found in [HNW87]; for composition methods and structure-preserving integrators, see also [HLW06]. The first quantum algorithm for linear differential equations is Berry's history-state construction with a high-order multistep discretization [Ber14]. The linear-system approach was later sharpened by spectral methods [CL20] and by Dyson-series based short-time propagators [BC22]. While the linear system-based method enables near-optimal query complexity in terms of U_A, it does not achieve optimal dependence on the cost of initial state preparation. This is resolved in [LS24] using an improved variable time amplitude amplification algorithm. The use of a history state for accessing observables over many times is closely related to dense-output constructions in quantum simulation; see [LL24].

The time-marching method of [FLT23] follows the classical one-step viewpoint more closely, and is the first algorithm to achieve optimal state preparation cost, but its complexity depends on the growth factor Q. The linear combination of Hamiltonian simulation method [ALL23, ACL26] can achieve both near-optimal query complexity in terms of U_A and optimal dependence on the initial state preparation cost. The LCHS method is closely related to Schrödingerization [JLY24], which maps a class of linear partial differential equations in d spatial dimensions to a Schrödinger equation in $d+1$ dimensions. There exists a broader class of linear differential equations that can be reformulated as unitary dynamics, including certain wave equations [CJO19] and classical Newtonian systems [BBK$^+$23].

The extension of quantum algorithms from linear to nonlinear differential equations is an active area of research. Although quantum mechanics is intrinsically linear, the development of quantum algorithms for nonlinear differential equations has attracted growing attention. We refer the reader to [LO08, LDPG$^+$20, KPE21, LKK$^+$21, Kro23, TLLM25, BW25] for various approaches to this problem.

CHAPTER 21

Solving open quantum systems

Open quantum systems interact with degrees of freedom that are not explicitly modeled. Consequently, their evolution is no longer described by unitary operators on the system register alone, but by quantum channels acting on density operators. In the Markovian regime, the natural continuous-time model is the Lindblad equation, which separates coherent Hamiltonian evolution from irreversible dissipative effects. This equation is standard in quantum statistical mechanics and quantum optics, and it also provides an algorithmic model for noise, equilibration, and engineered dissipation.

This shift from unitary dynamics to channel semigroups changes both the mathematical questions and the algorithmic ones. At the same time, dissipation is not merely a source of error: it can also be used to drive a system toward a desired fixed point, such as a thermal state or a ground state. We first develop the basic structural framework, and then discuss how these dynamics can be exploited and simulated using dilation-based, splitting-based, and truncated-Dyson methods.

21.1. Lindblad dynamics

The Gorini–Kossakowski–Sudarshan–Lindblad master equation, or **Lindblad equation** for short, has the form [Lin76, GKS76],

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \underbrace{-i[H,\rho]}_{\mathcal{L}_H(\rho)} + \underbrace{\sum_{j=1}^{J}\left(V_j\rho V_j^\dagger - \frac{1}{2}\{V_j^\dagger V_j,\rho\}\right)}_{\mathcal{L}_V(\rho)} =: \mathcal{L}(\rho). \tag{21.1}$$

Here $H \in \mathbb{C}^{d\times d}$ is the system Hamiltonian, and $V_j \in \mathbb{C}^{d\times d}$ are the jump operators arising from the interaction with the environment. Because exchange with an environment is typically an irreversible process, Lindblad evolution is often called **dissipative dynamics**. Accordingly, $\mathcal{L}_H$ is called the coherent part of the Lindbladian, while $\mathcal{L}_V$ is called the dissipative part. The brackets $[A,B]$ and $\{A,B\}$ denote the commutator and anticommutator of A and B, respectively. The generator $\mathcal{L}$ is called the Lindbladian. The solution to Eq. (21.1) can be written formally as

$$\rho(t) = e^{\mathcal{L}t}\rho(0). \tag{21.2}$$

It is convenient to denote the propagator by

$$\Phi_t := e^{\mathcal{L}t}, \qquad t \geq 0. \tag{21.3}$$

When $V_j = 0$ for all j, Eq. (21.1) reduces to the Liouville–von Neumann equation. In this sense, the Lindblad equation generalizes closed-system Hamiltonian evolution to open quantum systems.

A family $\{\Phi_t\}_{t\geq 0}$ of quantum channels is called a **norm-continuous semigroup of quantum channels** (or **quantum dynamical semigroups**) if

$$\Phi_0 = \mathcal{I}, \qquad \Phi_{t+s} = \Phi_t\Phi_s, \qquad t,s \geq 0, \tag{21.4}$$

and

$$\|\Phi_t - \Phi_s\|_\diamond \to 0 \qquad \text{as } t \to s. \tag{21.5}$$

It describes a continuous-time analogue of the discrete-time channels in Section 3.2. In the classical setting of Section 17.1, one studies a semigroup of stochastic matrices acting on probability vectors. The Lindblad equation plays the same role for density operators, with stochastic matrices replaced by quantum channels.

Before turning to structural results, it is useful to note that classical continuous-time Markov chains arise as a special case.

Example 21.1 (Classical Markov chains as Lindblad dynamics)**.** Let $\Sigma = [N]$, and let $q_{ij} \geq 0$ for all $i \neq j$. We interpret q_{ij} as the transition rate from state j to state i, consistent with the column-vector convention in Section 17.1. Set $H = 0$ and define jump operators

$$V_{ij} := \sqrt{q_{ij}}|i\rangle\langle j|, \qquad i \neq j. \tag{21.6}$$

Consider a classical state

$$\rho = \sum_{j \in [N]} p_j |j\rangle\langle j|, \tag{21.7}$$

where $p = (p_0, \ldots, p_{N-1})^\top$ is a probability vector. Then

$$V_{ij}\rho V_{ij}^\dagger = q_{ij} p_j |i\rangle\langle i|, \qquad V_{ij}^\dagger V_{ij} = q_{ij}|j\rangle\langle j|. \tag{21.8}$$

Substituting these identities into the Lindblad equation gives

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \sum_{i \neq j} q_{ij} p_j |i\rangle\langle i| - \sum_{j \in [N]} \left(\sum_{i \neq j} q_{ij} \right) p_j |j\rangle\langle j|. \tag{21.9}$$

Therefore the diagonal subspace is invariant, and the coefficients obey

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \sum_{j \neq i} q_{ij} p_j - \left(\sum_{k \neq i} q_{ki} \right) p_i. \tag{21.10}$$

Equivalently,

$$\frac{\mathrm{d}p}{\mathrm{d}t} = Qp, \tag{21.11}$$

where $Q \in \mathbb{R}^{N \times N}$ is the classical generator defined by

$$Q_{ij} = q_{ij} \quad (i \neq j), \qquad Q_{jj} = -\sum_{i \neq j} q_{ij}. \tag{21.12}$$

The matrix Q has nonnegative off-diagonal entries and each column sums to zero. Therefore it generates a classical continuous-time Markov semigroup, and $P_t := e^{Qt}$ is column stochastic for all $t \geq 0$. Hence, when restricted to diagonal density operators, the Lindblad semigroup $e^{\mathcal{L}t}$ is exactly the classical Markov semigroup P_t acting on probability distributions. $\diamond$

The Lindblad form is justified by two complementary statements. We first show constructively that every equation of the form Eq. (21.1) generates a semigroup of quantum channels. We then record the finite-dimensional characterization.

THEOREM 21.2. *For any $t \geq 0$, $e^{\mathcal{L}t} : \mathbb{C}^{d\times d} \to \mathbb{C}^{d\times d}$ is a completely positive trace preserving map, i.e., it is a quantum channel.*

PROOF. Let Δt be a small time step and write $t = N_t \Delta t$. Our strategy is to approximate the short-time propagator $e^{\mathcal{L}\Delta t}$ by a quantum channel Φ to precision $\mathcal{O}(\Delta t^2)$, that is,

$$\left\| e^{\mathcal{L}\Delta t} - \Phi \right\|_\diamond \leq C_1 \Delta t^2. \tag{21.13}$$

Since Φ is a quantum channel, we have $\|\Phi\|_\diamond = 1$. For any finite t, let $C_2 = \sup_{0\leq s\leq t} \left\| e^{\mathcal{L}s} \right\|_\diamond$. Since the diamond norm is an induced norm, we have $\|\mathcal{Q}_1\mathcal{Q}_2\|_\diamond \leq \|\mathcal{Q}_1\|_\diamond \|\mathcal{Q}_2\|_\diamond$, and can use the telescoping series

$$\begin{aligned} \left\| e^{\mathcal{L}t} - \Phi^{N_t} \right\|_\diamond \leq & \left\| e^{\mathcal{L}(N_t-1)\Delta t}(e^{\mathcal{L}\Delta t} - \Phi) \right\|_\diamond + \cdots + \left\| (e^{\mathcal{L}\Delta t} - \Phi)\Phi^{N_t-1} \right\|_\diamond \\ \leq & C_2 C_1 N_t \Delta t^2 = C_1 C_2 t \Delta t. \end{aligned} \tag{21.14}$$

Taking the limit $\Delta t \to 0$, we find that $e^{\mathcal{L}t}$ is the limit of a sequence of quantum channels as $N_t \to \infty$. Since the set of quantum channels is closed in the diamond norm, it follows that $e^{\mathcal{L}t}$ is itself a quantum channel.

One convenient construction of Φ starts from the dilated Hamiltonian

$$\widetilde{H} = |0\rangle\langle 0| \otimes H\sqrt{\Delta t} + \sum_j (|j\rangle\langle 0| \otimes V_j + \text{h.c.}) \tag{21.15}$$

whose matrix form is

$$\widetilde{H} = \begin{pmatrix} H\sqrt{\Delta t} & V_1^\dagger & \cdots & V_J^\dagger \\ V_1 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & 0 \\ V_J & 0 & \cdots & 0 \end{pmatrix}. \tag{21.16}$$

From this dilated Hamiltonian we define the channel Φ by

$$U = e^{-i\widetilde{H}\sqrt{\Delta t}}, \quad \Phi(\rho) = \mathrm{Tr}_a\, U\,(|0\rangle\langle 0| \otimes \rho)\, U^\dagger, \quad \forall \rho \in \mathcal{D}(\mathbb{C}^d). \tag{21.17}$$

Here Tr_a is the partial trace over the ancilla register with $a = \lceil \log_2(J+1) \rceil$ qubits.

We now prove Eq. (21.13) directly in diamond norm. Since the diamond norm is defined by taking a supremum over ancillary extensions and input operators of trace norm one, fix an ancilla register of dimension K and an operator $X \in L(\mathbb{C}^K \otimes \mathbb{C}^d)$ with $\|X\|_1 = 1$. Define

$$\widetilde{U} := I_k \otimes U. \tag{21.18}$$

Then, by linearity, the corresponding ancillary short-time channel is

$$(\mathcal{I}_k \otimes \Phi)(X) = \mathrm{Tr}_a \left[\widetilde{U}(|0\rangle\langle 0| \otimes X)\widetilde{U}^\dagger \right]. \tag{21.19}$$

The Taylor expansion of $e^{-i\widetilde{H}\sqrt{\Delta t}}$ to the third order gives

$$W = I - i\widetilde{H}(\Delta t)^{\frac{1}{2}} - \frac{1}{2}\widetilde{H}^2\Delta t + \frac{1}{6} i\widetilde{H}^3 (\Delta t)^{\frac{3}{2}}, \quad \|U - W\| = \mathcal{O}\left(\left\| \widetilde{H} \right\|^4 \Delta t^2 \right). \tag{21.20}$$

Set $\widetilde{W} := I_k \otimes W$. Using $\|AB\|_1 \le \|A\| \, \|B\|_1$, the fact that partial trace does not increase the Schatten 1-norm, and regarding $\left\|\widetilde{H}\right\|$ as a constant, we have

$$\begin{aligned} &\left\|(\mathcal{I}_k \otimes \Phi)(X) - \mathrm{Tr}_a \, \widetilde{W} \, (|0\rangle\langle 0| \otimes X) \, \widetilde{W}^\dagger\right\|_1 \\ \le &\left\|\mathrm{Tr}_a(\widetilde{U} - \widetilde{W}) \, (|0\rangle\langle 0| \otimes X) \, \widetilde{U}^\dagger\right\|_1 + \left\|\mathrm{Tr}_a \, \widetilde{U} \, (|0\rangle\langle 0| \otimes X) \, (\widetilde{W} - \widetilde{U})^\dagger\right\|_1 \\ \le &\left\|(\widetilde{U} - \widetilde{W}) \, (|0\rangle\langle 0| \otimes X) \, \widetilde{U}^\dagger\right\|_1 + \left\|\widetilde{U} \, (|0\rangle\langle 0| \otimes X) \, (\widetilde{W} - \widetilde{U})^\dagger\right\|_1 \\ \le &2 \left\|\widetilde{U} - \widetilde{W}\right\| = 2 \, \|U - W\| = \mathcal{O}(\Delta t^2). \end{aligned} \tag{21.21}$$

When calculating $\mathrm{Tr}_a \, \widetilde{W} \, (|0\rangle\langle 0| \otimes X) \, \widetilde{W}^\dagger$, we find that odd powers of $\sqrt{\Delta t}$ vanish after the partial trace. Then

$$\begin{aligned} \mathrm{Tr}_a \, \widetilde{W} \, (|0\rangle\langle 0| \otimes X) \, \widetilde{W}^\dagger =& X + \Delta t(\mathcal{I}_k \otimes \mathcal{L})(X) + \mathcal{O}(\Delta t^2) \\ =& (\mathcal{I}_k \otimes e^{\mathcal{L}\Delta t})(X) + \mathcal{O}(\Delta t^2). \end{aligned} \tag{21.22}$$

The $\mathcal{O}(\Delta t^2)$ term only involves products between bounded operators and X, with constants independent of K and X under the normalization $\|X\|_1 = 1$. Taking the supremum over all ancillary dimensions and all such X proves Eq. (21.13). □

We now record the converse structural statement: in finite dimensions, Lindblad generators are exactly the generators of norm-continuous semigroups of quantum channels.

Proposition 21.3 (Gorini–Kossakowski–Sudarshan–Lindblad characterization)**.** *Let $\{\Phi_t\}_{t \ge 0}$ be a norm-continuous semigroup of quantum channels on $L(\mathbb{C}^d)$, and let*

$$\mathcal{G}(\rho) := \lim_{t \to 0^+} \frac{\Phi_t(\rho) - \rho}{t} \tag{21.23}$$

be its generator. Then there exist a Hermitian matrix $H \in \mathbb{C}^{d \times d}$ and matrices $V_1, \dots, V_J \in \mathbb{C}^{d \times d}$ such that

$$\mathcal{G}(\rho) = -i[H, \rho] + \sum_{j=1}^{J} \left(V_j \rho V_j^\dagger - \frac{1}{2}\{V_j^\dagger V_j, \rho\} \right). \tag{21.24}$$

Proof sketch. For each sufficiently small $t > 0$, the map Φ_t is a quantum channel and hence admits a Kraus representation,

$$\Phi_t(\rho) = \sum_\alpha K_\alpha(t) \rho K_\alpha(t)^\dagger, \tag{21.25}$$

with $\sum_\alpha K_\alpha(t)^\dagger K_\alpha(t) = I$. A standard argument based on the first-order expansion of the Choi matrix near $t = 0$ allows one to choose the Kraus operators so that one term has the form

$$K_0(t) = I + tG + o(t), \tag{21.26}$$

while the remaining terms satisfy

$$K_j(t) = \sqrt{t} \, V_j + \mathcal{O}(t), \qquad j \ge 1. \tag{21.27}$$

Expanding the trace-preserving condition to first order shows that

$$G + G^\dagger + \sum_{j \ge 1} V_j^\dagger V_j = 0. \tag{21.28}$$

Therefore G can be written as

$$G = -iH - \frac{1}{2}\sum_{j\geq 1} V_j^\dagger V_j \tag{21.29}$$

for some Hermitian matrix H. Substituting these expansions into the Kraus form of Φ_t and collecting all first-order terms gives

$$\frac{\Phi_t(\rho)-\rho}{t} = -i[H,\rho] + \sum_{j\geq 1}\left(V_j\rho V_j^\dagger - \frac{1}{2}\{V_j^\dagger V_j,\rho\}\right) + o(1). \tag{21.30}$$

Taking $t \to 0^+$ yields the claim. □

If the short time propagator can be accurately approximated to precision ϵ', i.e., there is a quantum channel Φ such that

$$\left\|e^{\mathcal{L}\Delta t} - \Phi\right\|_\diamond \leq \epsilon', \tag{21.31}$$

then by the linear error growth property of quantum channels, we obtain the long time error estimate

$$\left\|e^{\mathcal{L}N_t\Delta t} - \Phi^{N_t}\right\|_\diamond \leq N_t \left\|e^{\mathcal{L}\Delta t} - \Phi\right\|_\diamond \leq N_t\epsilon'. \tag{21.32}$$

We next describe the dual evolution on observables.

For an observable O, the expectation value $\mathrm{Tr}[\rho(t)O]$ evolves under the Lindblad dynamics according to

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}[\rho(t)O] = \mathrm{Tr}[\rho(t)\mathcal{L}^\dagger(O)], \tag{21.33}$$

where $\mathcal{L}^\dagger$, called the adjoint of the Lindbladian $\mathcal{L}$, is defined as

$$\mathcal{L}^\dagger(O) = \underbrace{i[H,O]}_{\mathcal{L}_H^\dagger(O)} + \underbrace{\sum_{j=1}^{J}\left(V_j^\dagger O V_j - \frac{1}{2}\{V_j^\dagger V_j, O\}\right)}_{\mathcal{L}_V^\dagger(O)}. \tag{21.34}$$

From Eq. (21.33), we may also define the Heisenberg evolution of the observable O as

$$O(t) := e^{\mathcal{L}^\dagger t}(O). \tag{21.35}$$

Then $\mathrm{Tr}[\rho(t)O] = \mathrm{Tr}[\rho(0)O(t)]$.

Example 21.4 (Photon loss in an optical cavity)**.** Consider a single mode of an optical cavity with bosonic annihilation operator a. Photon loss in the cavity is modeled by a single jump operator $V = \sqrt{\kappa}\,a$, where κ is the decay rate.

The density operator ρ then evolves according to

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + \kappa\left(a\rho a^\dagger - \frac{1}{2}\{a^\dagger a,\rho\}\right), \tag{21.36}$$

where $H = \omega a^\dagger a$ is the Hamiltonian of the cavity mode with frequency ω. Using the adjoint Lindbladian introduced above, with number operator $n := a^\dagger a$, we compute

$$\begin{aligned}\mathcal{L}^\dagger(n) &= i[H,n] + \kappa\left(a^\dagger n a - \frac{1}{2}\{a^\dagger a, n\}\right)\\ &= \kappa\left(a^\dagger a^\dagger a a - n^2\right) = \kappa\left(n(n-1) - n^2\right) = -\kappa n.\end{aligned} \tag{21.37}$$

Here we used $[H, n] = 0$ and $a^\dagger a^\dagger aa = n(n-1)$. Therefore the mean photon number $\langle n\rangle = \mathrm{Tr}[n\rho]$ evolves according to

$$\frac{\mathrm{d}\langle n\rangle}{\mathrm{d}t} = -\kappa\langle n\rangle. \tag{21.38}$$

Therefore,

$$\langle n\rangle(t) = \langle n\rangle(0)e^{-\kappa t}, \tag{21.39}$$

so the mean photon number decays exponentially. As $t \to \infty$, the cavity loses all photons and the system relaxes to the vacuum state $|0\rangle$, which is the steady state. ◇

Exercise 21.1. Verify that $\mathcal{L}^\dagger$ is indeed the adjoint of $\mathcal{L}$ with respect to the Hilbert–Schmidt inner product $\langle X|Y\rangle := \mathrm{Tr}[X^\dagger Y]$.

The master equation describes the evolution of an ensemble state $\rho(t)$. For intuition and for numerical methods, it is often useful to represent the same semigroup as an average over stochastic pure-state trajectories, analogous to describing a classical Markov process through its sample paths. This representation is called an unraveling of the Lindblad equation. Consider the stochastic Schrödinger equation

$$\mathrm{d}\,|\psi_t\rangle = \left(-iH - \frac{1}{2}\sum_{j=1}^{J} V_j^\dagger V_j\right)|\psi_t\rangle\ \mathrm{d}t + \sum_{j=1}^{J} V_j\,|\psi_t\rangle\ \mathrm{d}W_t^j\,, \tag{21.40}$$

where $\{W_t^j\}_{j=1}^J$ are independent Wiener processes. This stochastic differential equation should be interpreted in the Itô sense. Applying Itô's formula to $|\psi_t\rangle\langle\psi_t|$ and taking expectations yields

$$\frac{\mathrm{d}\mathbb{E}\left[|\psi_t\rangle\langle\psi_t|\right]}{\mathrm{d}t} = -i\left[H, \mathbb{E}\left[|\psi_t\rangle\langle\psi_t|\right]\right] + \sum_{j=1}^{J} V_j \mathbb{E}\left[|\psi_t\rangle\langle\psi_t|\right] V_j^\dagger - \frac{1}{2}\sum_{j=1}^{J}\left\{V_j^\dagger V_j, \mathbb{E}\left[|\psi_t\rangle\langle\psi_t|\right]\right\}. \tag{21.41}$$

If the initial condition is $\mathbb{E}\left[|\psi_0\rangle\langle\psi_0|\right] = \rho(0)$, then Eq. (21.41) is equivalent to Eq. (21.1) with $\rho(t) = \mathbb{E}\left[|\psi_t\rangle\langle\psi_t|\right]$.

21.2. Example: Dissipative quantum thermal and ground state preparation

A useful feature of Lindblad dynamics is that certain states are stationary, or fixed points of the dynamics, satisfying

$$\partial_t\sigma = \mathcal{L}(\sigma) = 0. \tag{21.42}$$

Fixed points also appear in unitary dynamics, where a state σ satisfies $-i[H, \sigma] = 0$. However, in the unitary setting, any matrix that commutes with the Hamiltonian is a fixed point of the dynamics. This includes all eigenstates and convex combinations of eigenstates (as mixed states), making the set of fixed points too large to be algorithmically useful. In contrast, when dissipation is introduced through jump operators, certain Lindbladians can have a **unique** fixed point σ. In such cases, the dynamics is said to be **ergodic**. Ergodic Lindbladians thus offer a powerful framework for algorithm design, where the target state, such as a quantum thermal or ground state, is encoded as the unique fixed point of the dynamics. This approach is commonly referred to as **dissipative state engineering** or **dissipative state preparation**.

A common construction for dissipative state preparation starts from a family of coupling operators $\{A_a\}_{a\in\mathcal{A}}$, where each A_a may be simple, for example a Pauli operator, and does not depend explicitly on H. From these operators we define a family of jump operators by

$$V_a(\omega) := \int_{-\infty}^{\infty} f_\omega(s)\, e^{iHs} A_a e^{-iHs}\, \mathrm{d}s. \tag{21.43}$$

Because the jump operators are built from the Heisenberg evolution generated by H, they encode spectral information about the system. Here $f_\omega(s)$ is a filtering function, and ω may range over either a discrete or a continuous set. If $f_\omega(s)$ is smooth and decays rapidly as $|s| \to \infty$, then the integral in Eq. (21.43) can be truncated and discretized, and a block encoding of $V_a(\omega)$ can be constructed using the LCU method.

The resulting Lindbladian takes the form

$$\mathcal{L}(\rho) = -i[G,\rho] + \sum_a \int \left(V_a(\omega)\rho V_a(\omega)^\dagger - \frac{1}{2}\left\{ V_a(\omega)^\dagger V_a(\omega), \rho \right\} \right) \mathrm{d}\mu(\omega), \tag{21.44}$$

where G is the coherent term, constructed from H and the jump operators $V_a(\omega)$. The measure $\mu(\omega)$ determines how the parameter ω is sampled. If $\mu(\omega)$ is discrete, then the Lindbladian becomes

$$\mathcal{L}(\rho) = -i[G,\rho] + \sum_{a,\omega} \mu(\omega) \left(V_a(\omega)\rho V_a(\omega)^\dagger - \frac{1}{2}\left\{ V_a(\omega)^\dagger V_a(\omega), \rho \right\} \right), \tag{21.45}$$

which can be simulated using the methods discussed in previous chapters. If $\mu(\omega)$ is continuous, then the integral must first be discretized for simulation.

Despite this formal expression, the construction never requires explicitly diagonalizing H, which would be prohibitively expensive for large quantum systems.

To see how this framework can encode a target state, consider the simplest case of ground-state preparation. Let $\{\lambda_i, |\psi_i\rangle\}$ be the eigenpairs of H, ordered so that $\lambda_0 < \lambda_1 \leq \cdots$, and let $\Delta = \lambda_1 - \lambda_0$ be the spectral gap. For simplicity, take a single coupling operator A and define a single jump operator

$$V := \int_{-\infty}^{\infty} f(s)\, e^{iHs} A e^{-iHs}\, \mathrm{d}s. \tag{21.46}$$

This corresponds to choosing $\mu(\omega)$ as a discrete probability measure supported on a singleton set. Define the frequency-domain filter $\hat{f}(\omega)$ as the Fourier transform of the time-domain filter function:

$$\hat{f}(\nu) = \int_{\mathbb{R}} f(s) e^{i\nu s}\, \mathrm{d}s. \tag{21.47}$$

Inserting a resolution of the identity, we obtain

$$V = \sum_{i,j} \hat{f}(\lambda_i - \lambda_j)\, |\psi_i\rangle \langle\psi_i| A |\psi_j\rangle \langle\psi_j|. \tag{21.48}$$

As an idealized picture, suppose $\hat{f}$ satisfies

$$\hat{f}(\nu) = \begin{cases} 1, & \nu \leq -\Delta, \\ 0, & \nu \geq 0. \end{cases} \tag{21.49}$$

Then V only maps higher-energy states to lower-energy states, and never the reverse. In particular, $V|\psi_0\rangle = 0$. Moreover, for any $\lambda_j > \lambda_0$, if there exists some $\lambda_i \leq \lambda_j - \Delta$ such that $\langle\psi_i| A |\psi_j\rangle \neq 0$, then $V|\psi_j\rangle \neq 0$. This gives a mechanism by which the ground state can be selected as a dark state,

although uniqueness of the dark state and convergence to it require additional assumptions on the coupling structure.

Now choose $G = H$. The associated Lindblad dynamics is

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H,\rho] + \left(V\rho V^\dagger - \frac{1}{2}\{V^\dagger V, \rho\}\right). \tag{21.50}$$

Then $|\psi_0\rangle\langle\psi_0|$ is a fixed point of the dynamics. Under further assumptions one can prove convergence to the ground state and obtain quantitative mixing bounds; see, for example, [ZDH+26] for rigorous rapid-mixing results in a ground-state preparation setting.

These dissipative algorithms differ from most algorithms discussed in this book. For a given problem, the choice of coupling operators $\{A_a\}$ and filters can be highly system-dependent and offers a broad design space. They can be tailored to specific problems rather than relying only on coarse-grained parameters such as the spectral gap or the initial overlap with the target state. Preparing thermal states involves additional considerations, and proving ergodicity or quantitative mixing bounds typically requires problem-specific analysis.

In dissipative algorithms, assuming the dynamics converges to a fixed point σ, the time to reach σ from an initial state ρ_0 is characterized by the **mixing time**, defined in terms of the trace distance as

$$\tau_{\mathrm{mix}}(\eta) = \inf\left\{t \mid \left\|e^{\mathcal{L}t}(\rho_0) - \sigma\right\|_1 \le \eta, \quad \text{for all initial states } \rho_0\right\}. \tag{21.51}$$

The mixing time is often studied at a fixed precision, for example $\eta = \frac{1}{2}$. In quantum many-body systems on n sites, such as spin, bosonic, or fermionic systems, the dynamics is said to exhibit **fast mixing** if $\tau_{\mathrm{mix}} = \mathcal{O}(\mathrm{poly}(n))$, and **rapid mixing** if $\tau_{\mathrm{mix}} = \mathcal{O}(\mathrm{polylog}(n))$. Establishing such mixing bounds for a given class of quantum Hamiltonians is an active area of research.

21.3. Simulating a dilated Hamiltonian

The proof of Theorem 21.2 directly yields an algorithm for simulating Lindblad dynamics by repeatedly simulating a dilated Hamiltonian $\widetilde{H}$ and tracing out the ancilla register; see Fig. 21.1. More generally, the Stinespring dilation theorem (Theorem 3.20) states that any quantum channel can be represented as a unitary evolution on an extended Hilbert space that includes both the system and an ancillary register. This scheme is often called repeated interactions. Consequently, Hamiltonian simulation algorithms can be deployed directly to simulate Lindblad dynamics.

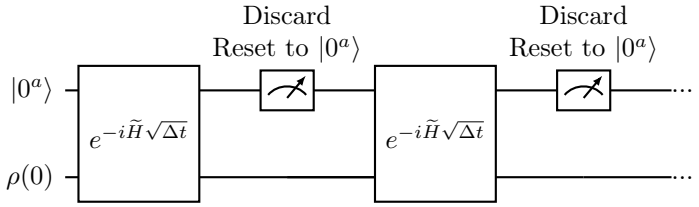


FIGURE 21.1. Simulating Lindblad dynamics by repeatedly simulating a dilated Hamiltonian $\widetilde{H}$ and tracing out the ancilla register.

Since $e^{\mathcal{L}t}$ is a quantum channel for every $t \ge 0$, we can refine Theorem 21.2 to obtain a more explicit error bound.

THEOREM 21.5. *Let* $\|\mathcal{L}\|_{\mathrm{be}} := 1+\|H\|+\sum_j \|V_j\|^2$, *and let* Φ *be defined in Eq.* (21.17). *Suppose* $\Delta t = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^{-1})$, *and write* $t = N_t \Delta t$. *Then*

$$\left\| e^{\mathcal{L}t} - \Phi^{N_t} \right\|_\diamond = \mathcal{O}\left(t \, \|\mathcal{L}\|_{\mathrm{be}}^2 \, \Delta t \right). \tag{21.52}$$

PROOF. We refine the proof of Theorem 21.2 by tracking the Δt-dependence of the dilated Hamiltonian

$$\widetilde{H} = |0\rangle\langle 0| \otimes H\sqrt{\Delta t} + \sum_j (|j\rangle\langle 0| \otimes V_j + \text{h.c.}). \tag{21.53}$$

Relative to the decomposition

$$\mathbb{C}^{J+1} = \mathrm{span}\{|0\rangle\} \oplus \mathrm{span}\{|1\rangle, \ldots, |J\rangle\}, \tag{21.54}$$

write $\widetilde{H}$ in block form as

$$\widetilde{H} = \begin{pmatrix} H\sqrt{\Delta t} & B^\dagger \\ B & 0 \end{pmatrix}, \tag{21.55}$$

where $B : \mathbb{C}^d \to \mathbb{C}^J \otimes \mathbb{C}^d$ is the column operator

$$B\,|\psi\rangle := \sum_{j=1}^{J} |j\rangle \otimes V_j \,|\psi\rangle\,. \tag{21.56}$$

Equivalently,

$$\widetilde{H} = |0\rangle\langle 0| \otimes H\sqrt{\Delta t} + R, \qquad R := \begin{pmatrix} 0 & B^\dagger \\ B & 0 \end{pmatrix}. \tag{21.57}$$

Since

$$R^2 = \begin{pmatrix} B^\dagger B & 0 \\ 0 & BB^\dagger \end{pmatrix}, \quad B^\dagger B = \sum_{j=1}^{J} V_j^\dagger V_j, \tag{21.58}$$

we have

$$\|R\|^2 = \left\| \sum_{j=1}^{J} V_j^\dagger V_j \right\| \le \sum_{j=1}^{J} \|V_j\|^2\,. \tag{21.59}$$

Therefore,

$$\left\| \widetilde{H} \right\| \le \|H\| \, \sqrt{\Delta t} + \|R\|\,, \tag{21.60}$$

and hence

$$\left\| \widetilde{H} \right\|^2 \le 2\,\|H\|^2\,\Delta t + 2\,\|R\|^2 \le 2\,\|H\|^2\,\Delta t + 2\sum_{j=1}^{J} \|V_j\|^2\,. \tag{21.61}$$

Since $\Delta t = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^{-1})$ and $\|\mathcal{L}\|_{\mathrm{be}} \ge 1 + \|H\|$, the first term is $\mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}})$. The second term is also $\mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}})$ by definition. Thus

$$\left\| \widetilde{H} \right\|^2 = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}). \tag{21.62}$$

Then by Eq. (21.20),

$$\|U - W\| = \mathcal{O}\left(\left\|\widetilde{H}\right\|^4 \Delta t^2\right) = \mathcal{O}\left(\|\mathcal{L}\|_{\mathrm{be}}^2 \Delta t^2\right). \tag{21.63}$$

Hence

$$\left\|\Phi - \widetilde{\Phi}\right\|_\diamond = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2 \Delta t^2), \tag{21.64}$$

where the quantum channel $\widetilde{\Phi}(\rho) = \mathrm{Tr}_a\, W\,(|0\rangle\langle 0| \otimes \rho)\, W^\dagger$.

A direct expansion gives

$$\widetilde{\Phi}(\rho) = \rho + \Delta t \mathcal{L}(\rho) + \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2 \Delta t^2). \tag{21.65}$$

Taylor expansion also gives

$$e^{\mathcal{L}\Delta t}(\rho) = \rho + \Delta t \mathcal{L}(\rho) + \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2 \Delta t^2). \tag{21.66}$$

Putting these estimates together, we obtain the refined approximation error bound from Eq. (21.13), namely,

$$\left\|e^{\mathcal{L}\Delta t} - \Phi\right\|_\diamond = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2 \Delta t^2). \tag{21.67}$$

The linear error growth property of quantum channels then yields the desired long-time estimate

$$\left\|e^{\mathcal{L}t} - \Phi^{N_t}\right\|_\diamond \leq N_t \left\|e^{\mathcal{L}\Delta t} - \Phi\right\|_\diamond = \mathcal{O}\left(t \|\mathcal{L}\|_{\mathrm{be}}^2 \Delta t\right). \tag{21.68}$$

□

Example 21.6 (Hamiltonian evolution with dephasing)**.** Consider the one-dimensional transverse-field Ising model (TFIM) on n sites with nearest-neighbor interactions,

$$H = -\sum_{j=1}^{n-1} Z_j Z_{j+1} - g \sum_{j=1}^{n} X_j, \tag{21.69}$$

where g is the coupling constant. We now apply a dephasing operation to each spin. This can be implemented by associating a jump operator $V_j = \sqrt{\gamma} Z_j$ to each spin, where γ is called the dephasing rate.

The Lindblad equation describing the time evolution of the density matrix ρ for this system is

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H, \rho] + \sum_{j=1}^{n} \left(V_j \rho V_j^\dagger - \frac{1}{2}\{V_j^\dagger V_j, \rho\}\right). \tag{21.70}$$

Substituting the expressions for H and V_j gives

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = i\left[\sum_{j=1}^{n-1} Z_j Z_{j+1} + g \sum_{j=1}^{n} X_j, \rho\right] + \gamma \sum_{j=1}^{n} \left(Z_j \rho Z_j - \rho\right). \tag{21.71}$$

Let us now apply the method based on simulating a dilated Hamiltonian to solve this problem. The dilated Hamiltonian takes the form

$$\widetilde{H} = |0\rangle\langle 0| \otimes H\sqrt{\Delta t} + \sum_{j=1}^{n} (|j\rangle\langle 0| \otimes \sqrt{\gamma} Z_j + \mathrm{h.c.}) \tag{21.72}$$

which uses $\lceil \log_2(n+1) \rceil$ ancilla qubits. The dilated Hamiltonian in its matrix form is

$$\widetilde{H} = \begin{pmatrix} H\sqrt{\Delta t} & \sqrt{\gamma} Z_1 & \cdots & \sqrt{\gamma} Z_n \\ \sqrt{\gamma} Z_1 & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & 0 \\ \sqrt{\gamma} Z_n & 0 & \cdots & 0 \end{pmatrix}. \tag{21.73}$$

We can then simulate the Lindblad equation by repeatedly simulating this dilated Hamiltonian $U = e^{-i\widetilde{H}\sqrt{\Delta t}}$ and tracing out the ancilla qubits. Assuming $g, \gamma = \mathcal{O}(1)$, we have

$$\|\mathcal{L}\|_{\mathrm{be}} = 1 + \|H\| + \gamma \sum_{j=1}^{n} \|Z_j\|^2 = \mathcal{O}(n). \tag{21.74}$$

To obtain trace-distance error at most ϵ at time T, it suffices to choose

$$\Delta t = \mathcal{O}(\epsilon / (T \|\mathcal{L}\|_{\mathrm{be}}^2)), \tag{21.75}$$

provided this choice also satisfies the step-size condition $\Delta t = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^{-1})$. The resulting number of channel steps is

$$N_t = T/\Delta t = \mathcal{O}(T^2 \|\mathcal{L}\|_{\mathrm{be}}^2 / \epsilon) = \mathcal{O}(T^2 n^2 / \epsilon), \tag{21.76}$$

which is also the number of queries to U. Note that we still need to construct the unitary $U = e^{-i\widetilde{H}\sqrt{\Delta t}}$ by solving a Hamiltonian simulation problem. ◇

21.4. Oblivious amplitude amplification of quantum channels

We follow the Kraus and Stinespring formalisms introduced in Section 3.2.

Let $\mathcal{Q} : L(\mathbb{C}^N) \to L(\mathbb{C}^N)$ be a quantum channel. Fix a Kraus representation

$$\mathcal{Q}(\rho) = \sum_{m \in [M]} K_m \rho K_m^\dagger, \tag{21.77}$$

where $K_m \in \mathbb{C}^{N \times N}$ and $\sum_{m \in [M]} K_m^\dagger K_m = I$. From Theorem 3.20, the associated Stinespring isometry $V : \mathbb{C}^N \to \mathbb{C}^M \otimes \mathbb{C}^N$ may be written as

$$V = \sum_{m \in [M]} |m\rangle \otimes K_m, \tag{21.78}$$

where the $|m\rangle$ register is the environment $A \cong \mathbb{C}^M$, so that $\mathcal{Q}(\rho) = \mathrm{Tr}_A[V \rho V^\dagger]$.

Assume without loss of generality that $M = 2^a$ (otherwise pad the Kraus family with zero operators), and that we have a coherent "select" oracle that applies a block encoding of the chosen Kraus operator. Concretely, suppose we can implement

$$U_{\mathrm{SELECT}} = \sum_m |m\rangle\langle m| \otimes U_{K_m}, \quad U_{K_m} \in \mathrm{BE}_{\alpha,b}(K_m), \tag{21.79}$$

so that, on input $|\psi\rangle |0^b\rangle$ and upon postselecting the b ancillas back to $|0^b\rangle$, U_{K_m} implements K_m/α on $|\psi\rangle$. Then we can construct a block encoding of the Stinespring isometry V as

$$W = U_{\mathrm{SELECT}} \left(\mathrm{H}^{\otimes a} \otimes I_{b+n} \right). \tag{21.80}$$

More precisely, for any n-qubit state $|\psi\rangle$, if the a-qubit register is initialized to $|0^a\rangle$ and we postselect the b ancillas to $|0^b\rangle$, then

$$(\langle 0^b| \otimes I)(W)(|0^a\rangle \otimes |\psi\rangle \otimes |0^b\rangle) = \frac{1}{\alpha\sqrt{M}} V |\psi\rangle . \tag{21.81}$$

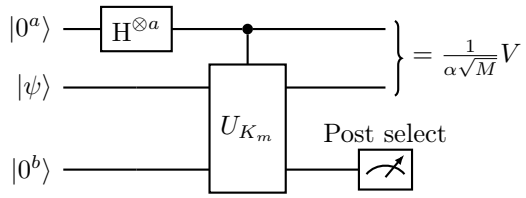


FIGURE 21.2. Circuit for implementing (a scaled version of) the Stinespring isometry of a quantum channel given the block encoding of its Kraus operators.

Recall the construction of the oblivious amplitude amplification in Section 11.4. If we can choose $\alpha\sqrt{M}$ to satisfy the condition

$$(\alpha\sqrt{M})^{-1} = \sin\frac{\pi}{2(2k+1)}, \tag{21.82}$$

for some $k \in \mathbb{N}$, then we can apply the same Chebyshev-based construction (interleaving $W, W^\dagger$ with the reflections Z_Π as in Section 11.4) to amplify the success probability. Although V is not unitary, this construction applies because V is an isometry, so all its nonzero singular values equal 1 and hence the nonzero singular values of $V/(\alpha\sqrt{M})$ are all equal to $(\alpha\sqrt{M})^{-1}$. With the choice above, the resulting transformation maps this singular value to ± 1, yielding a unitary $\mathcal{U}$ (up to an overall phase) such that, on input $|0^a\rangle |\psi\rangle |0^{b+1}\rangle$, the $b+1$ ancillas are returned to $|0^{b+1}\rangle$ and the induced map on the remaining registers is $V|\psi\rangle$. In particular, the postselection on the b ancillas is eliminated.

As a result, we obtain an efficient implementation of the quantum channel

$$\mathcal{Q}(\rho) = \mathrm{Tr}_{a'}\left[\mathcal{U}(|0^{a'}\rangle\langle 0^{a'}| \otimes \rho)\mathcal{U}^\dagger\right], \tag{21.83}$$

where the partial trace is over the $a' = a + b + 1$ ancillas. This construction is called the oblivious amplitude amplification of quantum channels.

Remark 21.7 (Implication for amplitude amplification)**.** Due to the close relation between unstructured search and amplitude amplification, it means that given a state $|\psi\rangle$ of which the probability of obtaining the "good" component is $p_0 1$, no quantum algorithms can amplify the amplitude to $\Omega(1)$ using $o\left(p_0^{-\frac{1}{2}}\right)$ queries to the reflection operators. ◇

Example 21.8 (Amplitude damping)**.** Assuming access to an oracle in Eq. (11.43), where p_0 is large, we can easily dampen the amplitude to any number $|\alpha| \le \sqrt{p_0}$.

We introduce an additional signal qubit. Then Eq. (11.43) becomes

$$(I \otimes U_{\psi_0})|0\rangle |0\rangle |0^n\rangle = |0\rangle \left(\sqrt{p_0}|0\rangle |\psi_0\rangle + \sqrt{1-p_0}|\perp\rangle\right). \tag{21.84}$$

Define a single qubit rotation operation as

$$R_\theta |0\rangle = \cos\theta |0\rangle + \sin\theta |1\rangle , \tag{21.85}$$

and we have

$$\begin{aligned} &(R_\theta \otimes I_{m+n})(I \otimes U_{\psi_0}) |0\rangle |0^m\rangle |0^n\rangle \\ =&\cos\theta |0\rangle (\sqrt{p_0} |0^m\rangle |\psi_0\rangle + \sqrt{1-p_0} |\perp\rangle) + \sin\theta |1\rangle (\sqrt{p_0} |0^m\rangle |\psi_0\rangle + \sqrt{1-p_0} |\perp\rangle) \\ :=&\sqrt{p_0}\cos\theta |0\rangle |0^m\rangle |\psi_0\rangle + \sqrt{1-p_0\cos^2\theta} |\perp'\rangle . \end{aligned} \tag{21.86}$$

Here $(|0^{m+1}\rangle\langle 0^{m+1}| \otimes I_n) |\perp'\rangle = 0$. We only need to choose $\sqrt{p_0}\cos\theta = \alpha$. ◇

21.5. Operator splitting method

Suppose the Lindbladian is decomposed as

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2, \tag{21.87}$$

where each semigroup $e^{\mathcal{L}_1 t}$ and $e^{\mathcal{L}_2 t}$ is a quantum channel for every $t \geq 0$. For example, one may take

$$\mathcal{L}_1 = \mathcal{L}_H, \qquad \mathcal{L}_2 = \mathcal{L}_V, \tag{21.88}$$

or refine the dissipative part further by splitting $\mathcal{L}_V$ into simpler channel generators.

If the factors $e^{\mathcal{L}_1 \Delta t}$ and $e^{\mathcal{L}_2 \Delta t}$ can be simulated efficiently, the natural first-order product formula is

$$\Phi(t) := e^{\mathcal{L}_1 t} e^{\mathcal{L}_2 t}. \tag{21.89}$$

As in the setting of Hamiltonian simulation, there are two useful ways to bound the error: a commutator bound, which captures near-commutativity, and a coarser operator norm bound that can be obtained from it as a corollary.

We directly prove the commutator type bound. Differentiating $\Phi(t)$ gives

$$\begin{aligned} \partial_t \Phi(t) &= \mathcal{L}_1 e^{t\mathcal{L}_1} e^{t\mathcal{L}_2} + e^{t\mathcal{L}_1} \mathcal{L}_2 e^{t\mathcal{L}_2} \\ &= (\mathcal{L}_1 + \mathcal{L}_2) e^{t\mathcal{L}_1} e^{t\mathcal{L}_2} + e^{t\mathcal{L}_1} \mathcal{L}_2 e^{t\mathcal{L}_2} - \mathcal{L}_2 e^{t\mathcal{L}_1} e^{t\mathcal{L}_2} \\ &= \mathcal{L}\Phi(t) + [e^{t\mathcal{L}_1}, \mathcal{L}_2] e^{t\mathcal{L}_2}, \end{aligned} \tag{21.90}$$

with initial condition $\Phi(0) = \mathcal{I}$. By the Duhamel principle,

$$\Phi(t) = e^{\mathcal{L}t} + \int_0^t e^{\mathcal{L}(t-s)} [e^{s\mathcal{L}_1}, \mathcal{L}_2] e^{s\mathcal{L}_2} \, \mathrm{d}s. \tag{21.91}$$

To rewrite the commutator term, define

$$G(s) := [e^{s\mathcal{L}_1}, \mathcal{L}_2] \tag{21.92}$$

and

$$\widetilde{G}(s) := \int_0^s e^{\tau\mathcal{L}_1} [\mathcal{L}_1, \mathcal{L}_2] e^{(s-\tau)\mathcal{L}_1} \, \mathrm{d}\tau. \tag{21.93}$$

Then $G(0) = \widetilde{G}(0) = 0$, and both satisfy the same inhomogeneous differential equation,

$$\partial_s G(s) = e^{s\mathcal{L}_1} [\mathcal{L}_1, \mathcal{L}_2] + G(s)\mathcal{L}_1, \tag{21.94}$$

$$\partial_s \widetilde{G}(s) = e^{s\mathcal{L}_1} [\mathcal{L}_1, \mathcal{L}_2] + \widetilde{G}(s)\mathcal{L}_1. \tag{21.95}$$

Therefore,

$$[e^{s\mathcal{L}_1}, \mathcal{L}_2] = \int_0^s e^{\tau\mathcal{L}_1}[\mathcal{L}_1, \mathcal{L}_2]e^{(s-\tau)\mathcal{L}_1}\,\mathrm{d}\tau. \tag{21.96}$$

Since $e^{\mathcal{L}(t-s)}$, $e^{\tau\mathcal{L}_1}$, $e^{(s-\tau)\mathcal{L}_1}$, and $e^{s\mathcal{L}_2}$ are quantum channels, their diamond norms are all equal to 1. Hence using $\|AB\|_\diamond \le \|A\|_\diamond \|B\|_\diamond$, we obtain

$$\left\|e^{\mathcal{L}t} - \Phi(t)\right\|_\diamond \le \int_0^t \int_0^s \|[\mathcal{L}_1, \mathcal{L}_2]\|_\diamond \,\mathrm{d}\tau\,\mathrm{d}s = \frac{t^2}{2}\,\|[\mathcal{L}_1, \mathcal{L}_2]\|_\diamond . \tag{21.97}$$

This is the direct analogue of the commutator Trotter bound in Section 15.4. In particular, if $[\mathcal{L}_1, \mathcal{L}_2] = 0$, then the first-order splitting is exact.

The commutator bound immediately implies a coarser norm bound. Indeed,

$$\|[\mathcal{L}_1, \mathcal{L}_2]\|_\diamond \le 2\,\|\mathcal{L}_1\|_\diamond \|\mathcal{L}_2\|_\diamond \le (\|\mathcal{L}_1\|_\diamond + \|\mathcal{L}_2\|_\diamond)^2. \tag{21.98}$$

To connect this with the Lindblad equation, note first that

$$\|\mathcal{L}_H\|_\diamond \le 2\,\|H\| . \tag{21.99}$$

Also, for a single jump operator V_j, the dissipative generator

$$\mathcal{D}_j(\rho) := V_j\rho V_j^\dagger - \frac{1}{2}\{V_j^\dagger V_j, \rho\} \tag{21.100}$$

satisfies

$$\|\mathcal{D}_j\|_\diamond \le 2\,\|V_j\|^2 . \tag{21.101}$$

Therefore, for any partition of the coherent part and dissipative terms into two groups defining $\mathcal{L}_1$ and $\mathcal{L}_2$, we have

$$\|\mathcal{L}_1\|_\diamond + \|\mathcal{L}_2\|_\diamond \le 2\left(\|H\| + \sum_j \|V_j\|^2\right) \le 2\,\|\mathcal{L}\|_{\mathrm{be}} . \tag{21.102}$$

Substituting into Eq. (21.97) yields the operator norm based error bound

$$\left\|e^{\mathcal{L}t} - \Phi(t)\right\|_\diamond \le 2t^2\,\|\mathcal{L}\|_{\mathrm{be}}^2 . \tag{21.103}$$

For long-time simulation, let $t = N_t\Delta t$. The linear error growth property of quantum channels gives

$$\left\|e^{\mathcal{L}t} - \Phi(\Delta t)^{N_t}\right\|_\diamond \le N_t\left\|e^{\mathcal{L}\Delta t} - \Phi(\Delta t)\right\|_\diamond = \mathcal{O}\left(t\,\|[\mathcal{L}_1, \mathcal{L}_2]\|_\diamond\,\Delta t\right). \tag{21.104}$$

Using the coarse norm bound above, this further implies

$$\left\|e^{\mathcal{L}t} - \Phi(\Delta t)^{N_t}\right\|_\diamond = \mathcal{O}\left(t\,\|\mathcal{L}\|_{\mathrm{be}}^2\,\Delta t\right). \tag{21.105}$$

As in the Hamiltonian setting, higher-order product formulas cannot be directly implemented since they typically require negative time steps, whereas $e^{-\mathcal{L}t}$ need not be a quantum channel.

Example 21.9 (Hamiltonian evolution with dephasing via operator splitting)**.** Consider again the one-dimensional transverse-field Ising model on n sites as in Example 21.6. Define the single-site dissipative generators by

$$\mathcal{D}_j(\rho) := V_j\rho V_j^\dagger - \frac{1}{2}\{V_j^\dagger V_j, \rho\} = \gamma(Z_j\rho Z_j - \rho). \tag{21.106}$$

Then

$$\mathcal{L} = \mathcal{L}_H + \sum_{j=1}^{n} \mathcal{D}_j. \tag{21.107}$$

Since Z_j and Z_k commute for all j, k, the superoperators $\mathcal{D}_j$ and $\mathcal{D}_k$ also commute. Hence the dissipative part can be exponentiated exactly as

$$e^{\left(\sum_{j=1}^{n} \mathcal{D}_j\right)\Delta t} = \prod_{j=1}^{n} e^{\mathcal{D}_j \Delta t}, \tag{21.108}$$

and the product may be applied in any order.

We therefore choose the first-order splitting step

$$\Phi(\Delta t) := e^{\mathcal{L}_H \Delta t} \prod_{j=1}^{n} e^{\mathcal{D}_j \Delta t}. \tag{21.109}$$

The coherent factor is simply

$$e^{\mathcal{L}_H \Delta t}(\rho) = e^{-iH\Delta t} \rho e^{iH\Delta t}, \tag{21.110}$$

while each dissipative factor is a single-qubit dephasing channel,

$$e^{\mathcal{D}_j \Delta t}(\rho) = \frac{1 + e^{-2\gamma \Delta t}}{2} \rho + \frac{1 - e^{-2\gamma \Delta t}}{2} Z_j \rho Z_j. \tag{21.111}$$

Thus each time step consists of one Hamiltonian evolution for time Δt together with n commuting one-site dephasing channels.

The only splitting error comes from separating the coherent part from the dissipative part. Writing

$$\mathcal{L}_1 = \mathcal{L}_H, \qquad \mathcal{L}_2 = \sum_{j=1}^{n} \mathcal{D}_j, \tag{21.112}$$

and the operator norm bound implies

$$\left\| e^{\mathcal{L}t} - \Phi(\Delta t)^{N_t} \right\|_\diamond = \mathcal{O}\left(t \left\| \mathcal{L} \right\|_{\mathrm{be}}^2 \Delta t \right). \tag{21.113}$$

Assuming $g, \gamma = \mathcal{O}(1)$, we have

$$\left\| \mathcal{L} \right\|_{\mathrm{be}} = 1 + \|H\| + \gamma \sum_{j=1}^{n} \|Z_j\|^2 = \mathcal{O}(n). \tag{21.114}$$

To achieve trace-distance error at most ϵ at time T, it is sufficient to choose

$$\Delta t = \mathcal{O}(\epsilon / (T \left\| \mathcal{L} \right\|_{\mathrm{be}}^2)), \tag{21.115}$$

which gives

$$N_t = T/\Delta t = \mathcal{O}(T^2 \left\| \mathcal{L} \right\|_{\mathrm{be}}^2 / \epsilon) = \mathcal{O}(T^2 n^2 / \epsilon). \tag{21.116}$$

Accordingly, the number of Hamiltonian-simulation steps is N_t, while the number of elementary dephasing-channel applications is $nN_t = \mathcal{O}(T^2 n^3 / \epsilon)$.

The commutator bound above is sharper in this example. Indeed, write

$$\mathcal{L}_H = \sum_{j=1}^{n-1} \mathcal{A}_j + \sum_{j=1}^{n} \mathcal{C}_j, \tag{21.117}$$

where

$$\mathcal{A}_j(\rho) := i[Z_jZ_{j+1}, \rho], \qquad \mathcal{C}_j(\rho) := -ig[X_j, \rho]. \tag{21.118}$$

Since Z_jZ_{j+1} commutes with every Z_k, each $\mathcal{A}_j$ commutes with every $\mathcal{D}_k$. Also, $\mathcal{C}_j$ commutes with $\mathcal{D}_k$ whenever $j \neq k$, because they act on different sites. Therefore

$$[\mathcal{L}_H, \sum_{j=1}^{n} \mathcal{D}_j] = \sum_{j=1}^{n} [\mathcal{C}_j, \mathcal{D}_j]. \tag{21.119}$$

Using $\|\mathcal{C}_j\|_\diamond \leq 2|g|\,\|X_j\| = 2|g|$ and $\|\mathcal{D}_j\|_\diamond \leq 2\gamma$, we obtain

$$\left\| [\mathcal{L}_H, \sum_{j=1}^{n} \mathcal{D}_j] \right\|_\diamond \leq |g| \sum_{j=1}^{n} 2\,\|\mathcal{C}_j\|_\diamond\,\|\mathcal{D}_j\|_\diamond \leq 8|g|\gamma n = \mathcal{O}(n), \tag{21.120}$$

assuming $g, \gamma = \mathcal{O}(1)$. Hence it is sufficient to choose

$$\Delta t = \mathcal{O}(\epsilon/(Tn)). \tag{21.121}$$

This gives the improved scaling

$$N_t = \mathcal{O}(T^2|g|\gamma n/\epsilon) = \mathcal{O}(T^2 n/\epsilon). \tag{21.122}$$

◇

21.6. Truncated Dyson method

We now describe a first-order truncated Dyson method for Lindblad dynamics. Suppose block encodings of H and V_j are available with subnormalization factors α_H and α_j, respectively. Define $\beta_J := \sum_{j=1}^{J} \alpha_j^2$. Since $\|H\| \leq \alpha_H$ and $\|V_j\| \leq \alpha_j$, we have

$$\|\mathcal{L}\|_{\mathrm{be}} = 1 + \|H\| + \sum_{j=1}^{J} \|V_j\|^2 \leq 1 + \alpha_H + \beta_J. \tag{21.123}$$

As before, we split the Lindbladian into a non-Hermitian part and a jump part,

$$\mathcal{L} = \mathcal{L}_{\mathrm{nh}} + \mathcal{L}_J, \tag{21.124}$$

where

$$\mathcal{L}_{\mathrm{nh}}(\rho) := -i(H_{\mathrm{eff}}\rho - \rho H_{\mathrm{eff}}^\dagger), \qquad \mathcal{L}_J(\rho) := \sum_{j=1}^{J} V_j \rho V_j^\dagger, \tag{21.125}$$

and

$$H_{\mathrm{eff}} := H - \frac{i}{2} \sum_{j=1}^{J} V_j^\dagger V_j. \tag{21.126}$$

The semigroup generated by $\mathcal{L}_{\mathrm{nh}}$ is

$$e^{\mathcal{L}_{\mathrm{nh}} t}(\rho) = e^{-iH_{\mathrm{eff}}t} \rho e^{iH_{\mathrm{eff}}^\dagger t}. \tag{21.127}$$

Applying the Duhamel principle over one short step gives

$$e^{\mathcal{L}\Delta t}(\rho) = e^{\mathcal{L}_{\mathrm{nh}}\Delta t}(\rho) + \int_0^{\Delta t} e^{\mathcal{L}_{\mathrm{nh}}(\Delta t - s)} \mathcal{L}_J\big(e^{\mathcal{L}s}(\rho)\big)\ \mathrm{d}s. \tag{21.128}$$

A first-order truncated Dyson approximation keeps only the zeroth-order term inside the integral. For the non-Hermitian branch, it is also sufficient at first order to replace the non-Hermitian evolution by its first-order Taylor expansion,

$$e^{-iH_{\mathrm{eff}}\Delta t} = I - iH_{\mathrm{eff}}\Delta t + \mathcal{O}(\|H_{\mathrm{eff}}\|^2\,\Delta t^2). \tag{21.129}$$

Accordingly, we define Kraus operators

$$Q_0 := I - iH_{\mathrm{eff}}\Delta t = I - iH\Delta t - \frac{1}{2}\left(\sum_{j=1}^{J} V_j^\dagger V_j\right)\Delta t, \qquad Q_j := \sqrt{\Delta t}\,V_j, \quad 1 \le j \le J, \tag{21.130}$$

and the short-time completely positive (but not trace preserving) map

$$\widetilde{\Phi}_{\Delta t}(\rho) := Q_0 \rho Q_0^\dagger + \sum_{j=1}^{J} Q_j \rho Q_j^\dagger. \tag{21.131}$$

A direct expansion shows that

$$\widetilde{\Phi}_{\Delta t}(\rho) = \rho + \Delta t\,\mathcal{L}(\rho) + \Delta t^2 H_{\mathrm{eff}} \rho H_{\mathrm{eff}}^\dagger. \tag{21.132}$$

Hence

$$\left\|\widetilde{\Phi}_{\Delta t} - (\mathcal{I} + \Delta t\,\mathcal{L})\right\|_\diamond \le \|H_{\mathrm{eff}}\|^2\,\Delta t^2 = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2\,\Delta t^2). \tag{21.133}$$

On the other hand, Taylor expansion of the exact evolution gives

$$e^{\mathcal{L}\Delta t} = \mathcal{I} + \Delta t\,\mathcal{L} + \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2\,\Delta t^2) \tag{21.134}$$

in diamond norm, and therefore

$$\left\|e^{\mathcal{L}\Delta t} - \widetilde{\Phi}_{\Delta t}\right\|_\diamond = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2\,\Delta t^2). \tag{21.135}$$

We now explain how to implement $\widetilde{\Phi}_{\Delta t}$ from the given block encodings. Since

$$Q_0 = I - iH\Delta t - \frac{1}{2}\left(\sum_{j=1}^{J} V_j^\dagger V_j\right)\Delta t, \tag{21.136}$$

a standard LCU construction using block encodings of I, H, and $\sum_{j=1}^{J} V_j^\dagger V_j$ yields a block encoding of Q_0 with subnormalization factor

$$\gamma_0 \le 1 + \alpha_H \Delta t + \frac{1}{2}\beta_J \Delta t = 1 + \mathcal{O}\left((1 + \alpha_H + \beta_J)\Delta t\right). \tag{21.137}$$

In particular, if $\Delta t = \mathcal{O}((1 + \alpha_H + \beta_J)^{-1})$, then γ_0 is bounded by a constant.

For the jump part, define the rectangular operator

$$W_J := \sum_{j=1}^{J} |j\rangle \otimes \frac{V_j}{\sqrt{\beta_J}}. \tag{21.138}$$

Then

$$W_J^\dagger W_J = \frac{\sum_{j=1}^{J} V_j^\dagger V_j}{\beta_J} \preceq I. \tag{21.139}$$

Using the standard select construction from the block encodings of the V_j, one obtains a block encoding of W_J with some constant subnormalization factor $\gamma_J = \mathcal{O}(1)$.

The Kraus family $\{Q_j\}_{j=1}^{J}$ is therefore implemented collectively with normalization $\gamma_J\sqrt{\beta_J\Delta t}$. Combining the non-Hermitian and jump branches via the usual LCU construction for channels yields an implementation of $\widetilde{\Phi}_{\Delta t}$ with overall subnormalization

$$\Gamma_{\Delta t} := \sqrt{\gamma_0^2 + \gamma_J^2\beta_J\Delta t}. \tag{21.140}$$

We choose the step size so that $\Gamma_{\Delta t}$ is bounded by a constant, say

$$\Gamma_{\Delta t} \le 2. \tag{21.141}$$

Equivalently, under the squared-normalization convention, one may require

$$\gamma_0^2 + \gamma_J^2\beta_J\Delta t \le 4. \tag{21.142}$$

This is achieved whenever $\Delta t = \mathcal{O}((1+\alpha_H+\beta_J)^{-1})$ with a sufficiently small constant.

At this point, the circuit has overall subnormalization at most 2. The channel version of oblivious amplitude amplification in Section 21.4 is stated for a Stinespring isometry with exact subnormalization 2, equivalently success amplitude exactly $1/2$. Therefore we first apply the standard one-qubit damping trick so that the success amplitude is exactly $1/2$, and then apply the channel oblivious amplitude amplification procedure. This only changes the cost by a constant factor.

Let $\Phi_{\Delta t}$ denote the resulting short-time quantum channel after this amplification step. Since both the local truncation error and the trace-preserving defect of $\widetilde{\Phi}_{\Delta t}$ are already of order Δt^2, the amplified channel still satisfies the same first-order accuracy bound,

$$\left\|e^{\mathcal{L}\Delta t} - \Phi_{\Delta t}\right\|_\diamond = \mathcal{O}(\|\mathcal{L}\|_{\mathrm{be}}^2\,\Delta t^2). \tag{21.143}$$

For long-time simulation, let $T = N_t\Delta t$. Since $\Phi_{\Delta t}$ is a quantum channel, the linear error growth property gives

$$\left\|e^{\mathcal{L}T} - \Phi_{\Delta t}^{N_t}\right\|_\diamond \le N_t\,\left\|e^{\mathcal{L}\Delta t} - \Phi_{\Delta t}\right\|_\diamond = \mathcal{O}(T\,\|\mathcal{L}\|_{\mathrm{be}}^2\,\Delta t). \tag{21.144}$$

Therefore, to achieve diamond-norm error at most ϵ at time T, it is sufficient to choose

$$\Delta t = \mathcal{O}\left(\min\left\{(1+\alpha_H+\beta_J)^{-1}, \frac{\epsilon}{T\,\|\mathcal{L}\|_{\mathrm{be}}^2}\right\}\right). \tag{21.145}$$

We remark that the operator $e^{-iH_{\mathrm{eff}}\Delta t}$ may also be viewed as the solution of a non-Hermitian differential equation, so one could approximate it using methods from Chapter 20, such as the LCHS method.

Notes and further reading

For background on open quantum systems, see [BP02]. In finite dimensions, the characterization of generators of quantum dynamical semigroups was obtained independently by Lindblad and by Gorini, Kossakowski, and Sudarshan in 1976 [Lin76, GKS76]; see also the short review [Man20]. In physical derivations from weak coupling to a bath, the Davies construction is the standard reference [Dav74, Dav76]; for a pedagogical discussion of the approximations behind the Markovian master equation, see [Lid19]. The chapter works entirely in finite dimensions, so it avoids the domain issues that arise for unbounded operators in infinite-dimensional settings.

For quantum algorithms, an early simulation result based on product formulas was given in [KBG$^+$11], and sparse Lindbladian simulation with higher-order product formulas was developed in [CL17]. The technical limitation is that higher-order splitting formulas usually require

negative time steps, whereas $e^{-\mathcal{L}t}$ need not be a quantum channel. This is one reason to pass to dilation-based and series-based constructions. The Stinespring-dilation viewpoint underlies the Hamiltonian-simulation approach in [CW17, DLL24c]. We refer readers to [DLL24c] for the high-order construction of this dilated Hamiltonian simulation method, while higher-order truncated Dyson constructions were developed in [LW23]. These methods are closely related to exponential-integrator ideas in numerical analysis, but the complete positivity constraint forces a different implementation strategy.

Ref. [VWC09] is a seminal paper on dissipative state preparation. Recent directions include dissipative preparation of structured many-body states [RCGG20, ZCL21, LLKH22, WSR$^+$23, Cub23], Lindbladian algorithms for thermal or ground-state preparation [TOV$^+$11, RWW23, SM21, GCDK24, DLL24a, DCL24, ZDH$^+$26], and rigorous analyses of mixing based on quantum logarithmic Sobolev inequalities and related tools [TKR$^+$10, KT13, BCG$^+$23, RFA24a, KACR25, RFA24b]. These mixing questions are the open-system analogue of convergence-rate questions for classical Markov chains, and they are central when Lindblad dynamics is used as an algorithm rather than as a physical model.

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