ABSTRACT

Title of dissertation: ADIABATIC QUANTUM COMPUTATION: NOISE IN THE ADIABATIC THEOREM AND USING THE JORDAN-WIGNER TRANSFORM TO FIND EFFECTIVE HAMILTONIANS

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This thesis explores two mathematical aspects of adiabatic quantum computation. Adiabatic quantum computation depends on the adiabatic theorem of quantum mechanics, and (a) we provide a rigorous formulation of the adiabatic theorem with explicit definitions of constants, and (b) we bound error in the adiabatic approximation under conditions of noise and experimental error. We apply the new results to a standard example of violation of the adiabatic approximation, and to a superconducting flux qubit.

Further, adiabatic quantum computation requires large ground-state energy gaps throughout a Hamiltonian evolution if it is to solve problems in polynomial time. We identify a class of random Hamiltonians with non-nearest-neighbor interactions and a ground-state energy gap of $\mathcal{O}(1/\sqrt{n})$, where n is the number of qubits. We also identify two classes of Hamiltonians with non-nearest-neighbor interactions whose ground state can be found in polynomial time with adiabatic quantum computing. We then

use the Jordan-Wigner transformation to derive equivalent results for Hamiltonians defined using Pauli operators.

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by

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Chapter 1

Introduction

Some combinatorial problems such as protein folding or algebraic problems such as factoring may require more logic operations than classical computers will be able to perform. However, quantum mechanics gives us the potential for massively-parallel computing, so that some of these problems may be within reach of future quantum computers.

The state of a classical register represents one number, and gate operations on that register may only operate on one number at a time. A quantum register may contain a superposition of all possible numbers of a fixed length, and a quantum gate operates on all those states at once. If that were the whole story, quantum computers could solve all problems in NP, namely those problems whose solution can be verified quickly, in polynomial time. Unfortunately, when measured, a quantum register reveals only one of the states contained in it, so quantum algorithms are carefully constructed to ensure the state likely to be measured is the solution. Two well-known quantum computing algorithms are Shor's algorithm for factoring numbers [50], which provides an exponential speedup over classical algorithms, and the Grover search algorithm, which searches N items in $\mathcal{O}(\sqrt{N})$ operations [23]. For a well-written introduction to quantum computing, see [38].

Adiabatic quantum computing (AQC) [18] is an approach to quantum computa-

tion where a problem is encoded as the ground state of some Hamiltonian $\mathcal{H}_P$, and then a physical system is evolved slowly from a simple Hamiltonian $\mathcal{H}_0$ to $\mathcal{H}_P$. It is assumed that it is feasible to prepare this system in the ground state of $\mathcal{H}_0$. Under the right conditions and if the evolution is done sufficiently slowly, then at the end of the evolution the state of the system will be the ground state of $\mathcal{H}_P$. Measurement of this final state reveals the solution to the original problem. There is an analogy between homotopy methods [56, p. 562] in numerical analysis and AQC, and a weaker analogy between classical simulated annealing [12, p. 55] and AQC.

As an approach to quantum computing, AQC is known to be equivalent to standard gated quantum computing, in that each can be efficiently simulated by the other [3, 62]. Also, a simple AQC evolution corresponds to the Grover search algorithm [42]. AQC has been implemented in NMR qubits [36, 54] and superconducting flux qubits [63]. Further, ground-state quantum adiabatic evolution has been used as a scheme for coupling superconducting flux qubits in a standard quantum computing experiment [39], and proposed as a method for realizing a cluster state [51], a prerequisite for measurement-based quantum computing, which is another formulation of quantum computing.

The biggest hurdles facing many potential implementations of a quantum computer are the errors due to interaction of the qubits with the environment. However, the effects of such errors are different in AQC than in standard quantum computing. AQC is robust against dephasing in the ground state, for instance [11], and some have suggested that noise in some regimes might actually assist adiabatic quantum computation [21].

The physical principle underlying AQC is the adiabatic approximation, whose error is established by the adiabatic theorem (AT). The AT bounds the run-time of the algorithm in terms of the minimum ground-state energy gap of the system during the evolution. The AT is often formulated imprecisely in the AQC literature, e.g. [42], and the existence of counterexamples to these imprecise formulations has stimulated recent controversy [35, 60, 64].

In Chapter 2, we prove a version of the AT that includes explicit definitions of constants, so that we may compare the predictions of theorems derived from it to example evolutions. Our version is based most closely on that of Reichardt [41], which is based on that by Avron [5] (with later corrections [6, 26, 31]). We chose this approach over others (e.g., [4, 24, 27, 61]) because it can be used to derive a specific and relatively tight error bound for finite τ. The differences between our theorem and Reichardt's theorem are

- Our version of the theorem includes an explicit definition of constants, necessary to obtain quantitative bounds.
- Our version of the theorem applies to subspaces rather than only a single non-degenerate state.
- We also present an integral formulation which provides better bounds when the energy gap is small for a very brief interval.

Unfortunately, rigorously-formulated adiabatic theorems cannot be applied directly to systems with noise or decoherence. There have been some numerical studies of AQC in the presence of noise [11, 21], and an analytic study using random matrix

theory [43]. Several recent studies have focused on the adiabatic approximation in open quantum systems using the density operator formalism [20, 46, 58, 59, 70]. However, it is difficult to derive rigorous bounds with this approach because the dynamics involve a non-Hermitian operator without a complete set of orthonormal eigenstates. Some progress has been made for the AQC equivalent of the Grover search algorithm, where (ideally) the dynamics are contained in a two-dimensional subspace of the Hilbert space [1, 2, 59].

Experimental error, including noise and decoherence, for quantum computing experiments can be conveniently divided into three categories [66]:

1. *Coherent* errors, due to a systematic implementation error such as miscalibration in a magnetic field generator.

2. *Incoherent* errors, due to deterministic qubit-level differences in the evolution such as those caused by manufacturing defects.

3. *Decoherent* errors, which are are random qubit-level errors due to coupling with the environment.

In Chapter 3, we prove several extensions of the AT to handle these different types of error. For coherent errors, we provide a theorem for perturbations in the initial state of the system and a theorem for systematic time-dependent perturbations in the Hamiltonian. In the case of decoherent errors, we provide two new theorems, one for open quantum systems and one for noise modeled as a time-dependent perturbation in the Hamiltonian. We apply the new theorems to the spin-1/2 particle in a rotating magnetic field, a standard example for controversy regarding the AT [10, 34, 60, 69].

We show our theorems make correct predictions about the error of the adiabatic approximation. Finally we apply the new theorems to the superconducting flux qubit [40], which has been proposed for AQC [28]. We use our theorems to determine a range of evolution times where the adiabatic approximation is guaranteed to perform well for a typical set of physical parameters and an apparently reasonable physical noise source. This provides the experimentalist with analytic tools for determining parameters to guarantee the adiabatic approximation works well, without the need to perform numerical simulations.

It is an open question whether the AQC approach will lead to the identification of *new* problems that can be solved efficiently by quantum computation. AQC succeeds in polynomial time only if the inverse of the ground-state energy gap is bounded by a polynomial in the problem size. A typical Hamiltonian must fit exponentially-many energy levels into a polynomial-sized energy range, so most energy gaps must be exponentially small, and it is not clear *a priori* why the ground-state energy gap should ever be larger than the rest. Since the dimension of the problem is exponentially large in the number of qubits, it is usually difficult to determine the minimum ground-state energy gap for large problems. Thus we examine when one might expect a large ground-state energy gap in an AQC evolution.

We expect an AQC evolution to undergo a quantum phase transition where the gap vanishes [32]. A quantum phase transition is a discontinuity in some derivative of the ground state energy in the limit as the number of qubits goes to infinity, which is usually accompanied by a qualitative change in the nature of the ground state. Perhaps the best-known example of a quantum phase transition is the one-

dimensional Ising model [44, p. 8]. If we define the matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \tag{1.1}$$

then the Pauli operator σ_j^α, for $\alpha = x, y, z$, has matrix representation

$$\overbrace{I_2 \otimes I_2 \otimes \cdots \otimes I_2}^{j-1} \otimes \sigma^\alpha \otimes \overbrace{I_2 \otimes \cdots \otimes I_2}^{n-j} , \tag{1.2}$$

where I_2 represents the 2×2 identity matrix and $\otimes$ represents the Kronecker product, in the basis where the operators $\{\sigma_k^z : k = 1 \ldots n\}$ are diagonal. Then the one-dimensional Ising model is

$$\mathcal{H}(s) = (1-s) \sum_{j=1}^{n} \sigma_j^z + s \sum_{j=1}^{n-1} \sigma_j^x \sigma_{j+1}^x . \tag{1.3}$$

A technique due to Lieb *et al.* [33] reveals the energy levels of $\mathcal{H}(s)$ for all $0 \leq s \leq 1$. This Hamiltonian evolution has been studied extensively. For instance, we know:

1. The minimum energy gap between the ground state and the first excited state scales as $\mathcal{O}(1/n)$ [49].

2. There is a second-order quantum phase transition at $s = 0.5$ [52].

3. The entanglement of the system has been studied, under various definitions of entanglement [13, 52].

The Hamiltonian evolution specified by Equation (1.3) is a useful example of an AQC evolution since $\mathcal{H}(0)$ is uncoupled and simple to analyze, and $\mathcal{H}(1)$ is coupled.

Further, it exhibits a ground-state energy gap that scales polynomially with the number of qubits. So we begin our search for Hamiltonians evolutions with large ground-state energy gaps with understanding the analysis of this example. In Chapter 4, we review facts about Clifford algebras, Fermionic commutation relations (FCRs), a theorem by Lieb *et al.* [33], and the Jordan-Wigner transform – all the tools necessary to analyze (1.3).

In Chapter 5, we identify a more general class of Hamiltonian evolutions whose ground-state energy gap can be found analytically. These Hamiltonian evolutions are more complex than (1.3) in that they allow terms with interactions between qubits with non-adjacent indices ("non-nearest-neighbor interactions"). We then identify a class of random Hamiltonians with $\mathcal{O}(1/\sqrt{n})$ ground-state energy gaps, where n is the number of qubits, and identify two large classes of Hamiltonians with non-nearest-neighbor interactions whose ground-state can be found in polynomial time with AQC. We use the Jordan-Wigner transformation [53] to derive equivalent results for Hamiltonians defined using Pauli operators.

Throughout the paper we will use the following notation. A Hamiltonian $\mathcal{H}$ is a Hermitian operator on a Hilbert space. We will use $\dagger$ to denote the Hermitian adjoint. The eigenfunctions of $\mathcal{H}$ we will call the eigenstates of the system, and the eigenvalues are their associated energies. States in the Hilbert space are denoted using Dirac bra-ket notation, e.g. $|\varphi\rangle$ and $\langle\varphi| = |\varphi\rangle^\dagger$.

Since we are interested in applications to quantum computing, we can assume the Hilbert space has countable degrees of freedom. For instance, a system of n qubits has 2^n degrees of freedom. Then we can represent the states as a linear combination

of some set of basis states. In this way we can represent states as complex column vectors with unit 2-norm, and operators as complex square matrices. In this work, every norm is the 2-norm.

Chapter 2

The Adiabatic Theorem

2.1 Introduction

Our proof of the AT follows closely those by Avron et al. [5] (later corrections exist [6, 31]), Reichardt [41], and Jansen et al. [26]. The purpose of revisiting the proof is to have explicit definitions of constants, so we can have quantitative bounds.

We begin with a Hamiltonian evolution $\mathcal{H}(s)$ parametrized by $s \in [0,1]$. If we define τ to be the total evolution time, then the Hamiltonian at time t is $\mathcal{H}(t/\tau)$. Thus, as τ grows, $\mathcal{H}(s)$ describes a slower evolution. Assume $\mathcal{H}(s)$ has countable eigenstates $\{|\psi_j(s)\rangle\}$ and eigenvalues $\lambda_0(s) \leq \lambda_1(s) \leq \ldots$, and consider the subspace

$$\Psi(s) = \text{Span}\left\{|\psi_m(s)\rangle, \ldots, |\psi_n(s)\rangle\right\} \ , \tag{2.1}$$

for some $0 \leq m \leq n$. Then the *adiabatic approximation* states that if the state of the system is contained in $\Psi(0)$ at $t = 0$, then at time $t = s/\tau$ the state is contained in $\Psi(s)$. The AT stated and proved in Section 2.5 makes this statement precise. Notice that while the ground state $|\psi_0(s)\rangle$ may be important for physical reasons, the definition above allows consideration of a more general set of states.

After reviewing some properties of projection operators, we will introduce the version of Schrödinger's equation that will be used and the assumptions that it requires. Then we will introduce some essential lemmas, and finally the AT and its proof.

2.2 Properties of projection operators

Before embarking on the proof, it will be helpful to review some properties of projection operators. First, we will enumerate some elementary properties. Then, we will introduce the resolvent formalism for rewriting projection operators as a contour integral.

Define the commutator $[A, B]$ as $[A, B] = AB - BA$, and $\dot{A} = dA/ds$. Let $\mathcal{H}(s)$ be some Hamiltonian with countable eigenstates $\{|\psi_j(s)\rangle\}$ and eigenvalues $\{\lambda_j(s) : j \geq 0\}$. Let $P(s)$ be the orthogonal projection operator onto the subspace

$$\Psi(s) = \text{Span}\left\{|\psi_m(s)\rangle, \ldots, |\psi_n(s)\rangle\right\} \ , \tag{2.2}$$

for some $0 \leq m \leq n$. Thus

$$P(s) = \sum_{i=m}^{n} |\psi_i(s)\rangle\langle\psi_i(s)| \ . \tag{2.3}$$

Let $Q(s) = I - P(s)$ be the projection onto the orthogonal complement of $\Psi(s)$. Then the following properties hold:

Property 1: $P(s) = P^2(s)$.

Property 2: $\dot{P}(s) = \dot{P}(s)P(s) + P(s)\dot{P}(s)$, obtained by differentiating both sides of Property 1.

Property 3: $P(s)\dot{P}(s)P(s) = 0$, obtained by multiplying Property 2 from the left by P.

Property 4: $Q(s)P(s) = 0$, using the definition of Q and Property 1.

Property 5: $P^\dagger(s) = P(s)$ and $Q^\dagger(s) = Q(s)$, where † indicates the conjugate transpose. This is evident from Equation (2.3).

Property 6: $||P(s)|| = ||Q(s)|| = 1$. Recall that the norm of an operator $P(s)$ is defined to be the maximum of $||P(s)|x\rangle||$ for choices of normalized states $|x\rangle$. For a projection operator, the maximal choice is a vector in the plane of projection, and in that case $P(s)|x\rangle = |x\rangle$. So $||P(s)|| = 1$. For $Q(s)$, choose $|x\rangle$ orthogonal to the plane of projection.

Property 7: $[\mathcal{H}(s), P(s)] = 0$. To prove this, take some state $|\phi\rangle$ and rewrite it as $|\phi\rangle = \sum_{j\geq 0} C_j|\psi_j(s)\rangle$. Then

$$\mathcal{H}(s)P(s)|\phi\rangle = \sum_{j\geq 0} C_j\mathcal{H}(s)P(s)|\psi_j(s)\rangle \tag{2.4}$$

$$= \sum_{j=m}^{n} C_j\mathcal{H}(s)|\psi_j(s)\rangle \tag{2.5}$$

$$= \sum_{j=m}^{n} C_j\lambda_j(s)|\psi_j(s)\rangle \ , \tag{2.6}$$

and

$$P(s)\mathcal{H}(s)|\phi\rangle = \sum_{j=m}^{n} P(s)\mathcal{H}(s)C_j|\psi_j(s)\rangle + \sum_{j\notin[m,n]} P(s)\mathcal{H}(s)C_j|\psi_j(s)\rangle \tag{2.7}$$

$$= \sum_{j=m}^{n} C_jP(s)\lambda_j(s)|\psi_j(s)\rangle + \sum_{j\notin[m,n]} C_jP(s)\lambda_j(s)|\psi_j(s)\rangle \tag{2.8}$$

$$= \sum_{j=m}^{n} C_j\lambda_j(s)|\psi_j(s)\rangle \ . \tag{2.9}$$

We will make use of the resolvent formalism to bound the projection operators. Define the *resolvent* of a Hamiltonian $\mathcal{H}(s)$ to be

$$R(z;\mathcal{H}(s)) = (\mathcal{H}(s) - zI)^{-1} \ . \tag{2.10}$$

Suppose we can draw a contour $\Gamma(s)$ in the complex plane whose enclosed region includes the eigenvalues corresponding to $\Psi(s)$ and excludes the rest of the spectrum of $\mathcal{H}(s)$. Then we can rewrite the projection operator $P(s)$ in terms of a line integral of the resolvent $R(s,z) = (\mathcal{H}(s) - zI)^{-1}$ around this contour:

$$P(s) = -\frac{1}{2\pi i} \oint_{\Gamma(s)} R(s,z)dz \ . \tag{2.11}$$

2.3 Schrödinger's equation

We rewrite Schrödinger's equation in terms of unitary evolution operators and the scaled time s, rather than using state vectors and real time t. Doing so will introduce the assumption that $\mathcal{H}(s)$ has a continuous, bounded second derivative.

The usual expression of the time-dependent Schrödinger's equation is

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \mathcal{H}(t)|\psi(t)\rangle \ . \tag{2.12}$$

Setting $t = s\tau$, $|\phi(s)\rangle = |\psi(s\tau)\rangle = |\psi(t)\rangle$, and $\mathcal{H}_\tau(s) = \mathcal{H}(s\tau) = \mathcal{H}(t)$, we can substitute and apply the chain rule for derivatives to get

$$\hbar|\dot{\phi}(s)\rangle = -i\tau\mathcal{H}_\tau(s)|\phi(s)\rangle \ , \tag{2.13}$$

where the dot indicates the s-derivative. Throughout the paper, we use units where $\hbar = 1$. Also we will assume that all subsequent state vectors, Hamiltonians, and time evolution operators are functions of the normalized time parameter s, so we can drop the subscript τ from $\mathcal{H}_\tau$. Thus we will write

$$|\dot{\phi}(s)\rangle = -i\tau\mathcal{H}(s)|\phi(s)\rangle \ . \tag{2.14}$$

Now define $U(s)$ so that for any $|\phi(0)\rangle$, we have $U(s)|\phi(0)\rangle = |\phi(s)\rangle$ where $|\phi(s)\rangle$ is the solution to this equation. Then we proceed as in [45, p. 68]. Assume that $\mathcal{H}(s)$ has a continuous bounded derivative; then $|\phi(s)\rangle$ has a continuous bounded second derivative. Thus the remainder for the first-order Taylor expansion is well-defined. For some point $s^* \in [s, s + \Delta s]$, we get

$$U(s + \Delta s)|\phi(0)\rangle = |\phi(s + \Delta s)\rangle \tag{2.15}$$

$$= |\phi(s)\rangle + |\dot{\phi}(s)\rangle \Delta s + |\ddot{\phi}(s^*)\rangle \frac{\Delta s^2}{2} \tag{2.16}$$

$$= |\phi(s)\rangle - i\tau \mathcal{H}(s)|\phi(s)\rangle \Delta s + \mathcal{O}(\Delta s^2) \tag{2.17}$$

$$= U(s)|\phi(0)\rangle - i\tau \mathcal{H}(s)U(s)|\phi(0)\rangle \Delta s + \mathcal{O}(\Delta s^2) \ . \tag{2.18}$$

Since this is true for any $|\phi(0)\rangle$ we can write

$$\lim_{\Delta s \to 0} \frac{U(s + \Delta s) - U(s)}{\Delta s} = -i\tau \mathcal{H}(s)U(s) \ , \tag{2.19}$$

or, equivalently,

$$\dot{U}(s) = -i\tau \mathcal{H}(s)U(s) \ . \tag{2.20}$$

Equation (2.20) is the form of Schrödinger's equation that we will rely on for the rest of the proof of the AT.

2.4 Essential lemmas

Recall that the adiabatic approximation states that a system with Hamiltonian $\mathcal{H}(s)$, initially in some state in $\Psi(0)$, evolves to approximately some state in $\Psi(s)$ at time $t = s\tau$. To compute bounds on the error of this approximation, we will identify a

Hamiltonian $\mathcal{H}_A(s)$ that has *exactly* this property. Define

$$\mathcal{H}_A(s) = \mathcal{H}(s) + \frac{i}{\tau}\left[\dot{P}(s), P(s)\right] , \tag{2.21}$$

where $P(s)$ is the projection operator onto $\Psi(s)$. Evidently $\mathcal{H}_A(s)$ is a $1/\tau$ perturbation of $\mathcal{H}(s)$, where τ is the scale factor between normalized time and unnormalized time. Define $U_A(s)$ to be the unitary evolution operator that is the solution to Schrödinger's equation for $\mathcal{H}_A(s)$, namely

$$\dot{U}_A(s) = -i\tau\mathcal{H}_A(s)U_A(s) . \tag{2.22}$$

The important property of $\mathcal{H}_A(s)$ can be restated as follows. If a system is initialized in $\Psi(0)$ at time $s = 0$, the state at time s under evolution by the Hamiltonian $\mathcal{H}_A(s)$ is entirely contained in $\Psi(s)$. We can write this property, known as the *intertwining property*, using $P(s)$ and $U_A(s)$ as defined in the previous paragraph.

Theorem 2.4.1 (The Intertwining Property)**.** *For $s \in [0, 1]$, let $\mathcal{H}(s)$ be Hermitian, twice differentiable, non-degenerate, and have a countable number of eigenstates. Let $U_A(s)$ and $P(s)$ be defined as previously. Then*

$$U_A(s)P(0) = P(s)U_A(s) . \tag{2.23}$$

Proof. Noticing that $U_A(s)$ is unitary, we can rewrite the claim as $P(0) = U_A^\dagger(s)P(s)U_A(s)$. Since $U_A(0) = I$ this is certainly true for $s = 0$. So it is sufficient to show that

$$\frac{d}{ds}\left[U_A^\dagger(s)P(s)U_A(s)\right] = 0 . \tag{2.24}$$

Applying the product rule for derivatives we get

$$\frac{d}{ds}\left[U_A^\dagger(s)P(s)U_A(s)\right] = \frac{d}{ds}\left[U_A^\dagger(s)P(s)\right]U_A(s) + U_A^\dagger(s)P(s)\dot{U}_A(s) \tag{2.25}$$

$$= \left(U_A^\dagger(s)\dot{P}(s) + \dot{U_A^\dagger}(s)P(s)\right)U_A(s) + U_A^\dagger(s)P(s)\dot{U}_A(s)\ . \tag{2.26}$$

Now observe that $\dot{U_A^\dagger}(s) = (\dot{U}_A(s))^\dagger$ since the derivative of a matrix operator is the derivative of its matrix entries. Further, recall that $\dot{U}_A(s) = -i\tau\mathcal{H}_A(s)U_A(s)$. So

$$\dot{U_A^\dagger}(s) = (\dot{U}_A(s))^\dagger \tag{2.27}$$

$$= (-i\tau\mathcal{H}_A(s)U_A(s))^\dagger \tag{2.28}$$

$$= +i\tau U_A^\dagger(s)\mathcal{H}_A^\dagger(s) \tag{2.29}$$

$$= i\tau U_A^\dagger(s)\mathcal{H}_A(s)\ , \tag{2.30}$$

since $\mathcal{H}_A(s)$ is Hermitian. Substituting, we get

$$\frac{d}{ds}\left[U_A^\dagger(s)P(s)U_A(s)\right] = \left(U_A^\dagger(s)\dot{P}(s) + i\tau U_A^\dagger(s)\mathcal{H}_A(s)P(s)\right)U_A(s)$$

$$+ U_A^\dagger(s)P(s)(-i)\tau\mathcal{H}_A(s)U_A(s) \tag{2.31}$$

$$= U_A^\dagger(s)\left(\dot{P}(s) + i\tau\mathcal{H}_A(s)P(s) - i\tau P(s)\mathcal{H}_A(s)\right)U_A(s) \tag{2.32}$$

$$= U_A^\dagger(s)\left(\dot{P}(s) + i\tau[\mathcal{H}_A(s), P(s)]\right)U_A(s)\ . \tag{2.33}$$

Now we will work on the inner term. We use the properties that $[H(s), P(s)] = 0$,

$P(s)\dot{P}(s)P(s) = 0$, $P^2(s) = P(s)$, and $\dot{P}(s) = \dot{P}(s)P(s) + P(s)\dot{P}(s)$.

$$
\begin{aligned}
[\mathcal{H}_A(s), P(s)] =& \mathcal{H}_A(s)P(s) - P(s)\mathcal{H}_A(s) && (2.34)\\
=& \left(\mathcal{H}(s) + \frac{i}{\tau}\left(\dot{P}(s)P(s) - P(s)\dot{P}(s)\right)\right)P(s) \\
& - P(s)\left(\mathcal{H}(s) + \frac{i}{\tau}\left(\dot{P}(s)P(s) - P(s)\dot{P}(s)\right)\right) && (2.35)\\
=& [\mathcal{H}(s), P(s)] + \frac{i}{\tau}\dot{P}(s)P^2(s) - \frac{i}{\tau}P(s)\dot{P}(s)P(s) \\
& - \frac{i}{\tau}P(s)\dot{P}(s)P(s) + \frac{i}{\tau}P^2(s)\dot{P}(s) && (2.36)\\
=& \frac{i}{\tau}\dot{P}(s)P^2(s) + \frac{i}{\tau}P^2(s)\dot{P}(s) && (2.37)\\
=& \frac{i}{\tau}\dot{P}(s)P(s) + \frac{i}{\tau}P(s)\dot{P}(s) && (2.38)\\
=& \frac{i}{\tau}\dot{P}(s)\ . && (2.39)
\end{aligned}
$$

We can substitute this into the original expression to get

$$
\begin{aligned}
\frac{d}{ds}\left[U_A^\dagger(s)P(s)U_A(s)\right] &= U_A^\dagger(s)\left(\dot{P}(s) + i\tau[\mathcal{H}_A(s), P(s)]\right)U_A(s) && (2.40)\\
&= U_A^\dagger(s)\left(\dot{P}(s) - \dot{P}(s)\right)U_A(s) && (2.41)\\
&= 0\ . && (2.42)
\end{aligned}
$$

□

Notice that this implies an intertwining property for the orthogonal complement:

$$U_A(s)Q(0) = Q(s)U_A(s)\ . \tag{2.43}$$

In the proof of the AT we will make use of the *twiddle* operation. Let $P(s)$ be a projection operator onto $\Psi(s)$, and assume the eigenvalues corresponding to $\Psi(s)$ are separated by a gap from the rest of the eigenvalues. Define

$$\tilde{X}(s) = \frac{1}{2\pi i}\oint_{\Gamma(s)} R(s,z)X(s)R(s,z)dz\ , \tag{2.44}$$

where $\Gamma(s)$ is a contour in the complex plane around the eigenvalues associated with the eigenstates onto which $P(s)$ projects, whose enclosed region excludes any other eigenvalues of $\mathcal{H}(s)$. We will need the following property of the twiddle operation.

Lemma 2.4.2 (The Twiddle Lemma)**.** *Assume $\hbar = 1$. For a fixed s, let P be a projection operator onto $\Psi(s)$, and assume the eigenvalues corresponding to $\Psi(s)$ are separated by a gap from the rest of the eigenvalues. Define $Q = I - P$, and let X be a bounded linear operator. Then*

$$QXP = -Q\left(\left[\mathcal{H}_A, \tilde{X}\right] - \frac{i}{\tau}\left[\dot{P}, \tilde{X}\right]\right)P\,. \tag{2.45}$$

Proof. We begin by observing that since $P^2 = P$ and $QP = 0$,

$$-Q[X,P]P = -Q(XP - PX)P \tag{2.46}$$

$$= -QXP\,. \tag{2.47}$$

Further, since the identity operator commutes with everything, $[zI, R(z)XR(z)] = 0$. Then

$$[\mathcal{H}, \tilde{X}] = \mathcal{H}\left(\frac{1}{2\pi i}\oint_\Gamma R(z)XR(z)dz\right) - \left(\frac{1}{2\pi i}\oint R(z)XR(z)dz\right)\mathcal{H} \tag{2.48}$$

$$= \frac{1}{2\pi i}\oint_\Gamma \left(\mathcal{H}R(z)XR(z) - R(z)XR(z)\mathcal{H}\right)dz \tag{2.49}$$

$$= \frac{1}{2\pi i}\oint_\Gamma [\mathcal{H}, R(z)XR(z)]dz \tag{2.50}$$

$$= \frac{1}{2\pi i}\oint_\Gamma [\mathcal{H} - zI, R(z)XR(z)]dz\,. \tag{2.51}$$

Now we use the fact that $(\mathcal{H} - zI)R = I$, that X does not depend on z, and Equa-

tion (2.11) to write

$$[\mathcal{H}, \tilde{X}] = \frac{1}{2\pi i} \oint_\Gamma (XR(z) - R(z)X)\, dz \tag{2.52}$$

$$= \frac{1}{2\pi i} \left[X, \oint_\Gamma R(z) dz \right] \tag{2.53}$$

$$= -[X, P] \, . \tag{2.54}$$

Also, using the definition of $\mathcal{H}_A$ in (2.21), we have

$$QXP = Q[X, P]P \tag{2.55}$$

$$= -Q[\mathcal{H}, \tilde{X}]P \tag{2.56}$$

$$= -Q \left(\left[\mathcal{H}_A, \tilde{X} \right] - \frac{i}{\tau} \left[\left[\dot{P}, P \right], \tilde{X} \right] \right) P \, . \tag{2.57}$$

All we need to finish the proof is to show

$$Q \left[\left[\dot{P}, P \right], \tilde{X} \right] P = Q \left[\dot{P}, \tilde{X} \right] P \, . \tag{2.58}$$

Using $P\dot{P}P = 0$, $P^2 = P$, and $\dot{P} = \dot{P}P + P\dot{P}$, we have

$$Q \left[\left[\dot{P}, P \right] \tilde{X} \right] P = Q \left[\dot{P}P - P\dot{P}, \tilde{X} \right] P \tag{2.59}$$

$$= Q \left(\dot{P}P - P\dot{P} \right) \tilde{X}P - Q\tilde{X} \left(\dot{P}P - P\dot{P} \right) P \tag{2.60}$$

$$= (I - P) \left(\dot{P}P - P\dot{P} \right) \tilde{X}P - (I - P)\tilde{X} \left(\dot{P}P - P\dot{P} \right) P \tag{2.61}$$

$$= \dot{P}P\tilde{X}P - P\dot{P}\tilde{X}P + P\dot{P}\tilde{X}P - \tilde{X}\dot{P}P + P\tilde{X}\dot{P}P \tag{2.62}$$

$$= \dot{P}\tilde{X}P - P\dot{P}\tilde{X}P - \tilde{X}\dot{P}P + P\tilde{X}\dot{P}P \tag{2.63}$$

$$= (I - P)\dot{P}\tilde{X}P - (I - P)\tilde{X}\dot{P}P \tag{2.64}$$

$$= Q\dot{P}\tilde{X}P - Q\tilde{X}\dot{P}P \tag{2.65}$$

$$= Q \left[\dot{P}, \tilde{X} \right] P \, . \tag{2.66}$$

□

2.5 The Adiabatic Theorem

Now we are ready to prove the AT. To compute the error of the adiabatic approximation, we apply $P(0)$ to obtain the component of the initial state contained in $\Psi(0)$, evolve it forward in time by applying $U(s)$, and then apply $I - P(s)$ to compute the component of the state outside $\Psi(s)$. For convenience, we define $Q(s) = I - P(s)$, so the error operator is $Q(s)U(s)P(0)$.

In fact it will be most useful to bound the 2-norm of this operator, denoted $||Q(s)U(s)P(0)||$. The 2-norm of an operator A is the square root of the largest eigenvalue of $A^\dagger A$, and in this case yields a bound on the magnitude of the output state, given a normalized input state. The AT guarantees an upper bound on $||Q(s)U(s)P(0)||$.

Theorem 2.5.1 (The Adiabatic Theorem)**.** *Assume for $s \in [0,1]$ that $\mathcal{H}(s)$ is twice differentiable, and let*

$$\left|\left|\dot{\mathcal{H}}(s)\right|\right| \leq b_1(s) \;, \qquad\qquad \left|\left|\ddot{\mathcal{H}}(s)\right|\right| \leq b_2(s) \;. \tag{2.67}$$

Further assume that $\mathcal{H}(s)$ has a countable number of eigenstates, with eigenvalues $\lambda_0(s) \leq \lambda_1(s) \leq \ldots$, and that $P(s)$ projects onto the eigenspace associated with the eigenvalues $\{\lambda_m(s), \lambda_{m+1}(s), \ldots \lambda_n(s)\}$. Define

$$w(s) = \lambda_n(s) - \lambda_m(s) \;, \quad \gamma(s) = \begin{cases} \min\{\lambda_{n+1}(s) - \lambda_n(s),\ \lambda_m(s) - \lambda_{m-1}(s)\} & m > 0 \\ \lambda_{n+1}(s) - \lambda_n(s) & m = 0 \end{cases} \;,$$

$$D(s) = 1 + \frac{2w(s)}{\pi\gamma(s)} \;, \qquad Q(s) = I - P(s) \;. \tag{2.68}$$

Finally, assume $\gamma(s) > 0$ for $s \in [0,1]$. Then we have

$$||Q(s)U(s)P(0)|| \leq \frac{8D^2(0)b_1(0)}{\tau\gamma^2(0)} + \frac{8D^2(s)b_1(s)}{\tau\gamma^2(s)} + \int_0^s \frac{8D^2(r)}{\tau\gamma^2(r)} \left(\frac{8(1+D(r))b_1^2(r)}{\gamma(r)} + b_2(r) \right) dr \ . \tag{2.69}$$

Proof. By multiplying by the identity and applying Theorem 2.4.1 (the intertwining property), we can write

$$Q(s)U(s)P(0) = Q(s)U_A(s)U_A^\dagger(s)U(s)P(0) \tag{2.70}$$

$$= U_A(s)Q(0)U_A^\dagger(s)U(s)P(0) \ . \tag{2.71}$$

Since $||U_A(s)|| = 1$, if $\left|\left|Q(0)U_A^\dagger(s)U(s)P(0)\right|\right|$ is small the magnitude of the error in the adiabatic approximation is small. In fact, if we define

$$W(s) = U_A^\dagger(s)U(s) \ , \tag{2.72}$$

then $W(s)$ satisfies a useful integral equation, and we prove the AT by bounding $||Q(0)W(s)P(0)||$ instead of working directly on $Q(s)U(s)P(0)$. To find the integral equation, we need to compute $\dot{W}(s)$. Using the product rule for derivatives, Schrödinger's equation, and the definition of $\mathcal{H}_A(s)$ in (2.21), we have

$$\dot{W}(s) = U_A^\dagger(s)\dot{U}(s) + \dot{U}_A^\dagger(s)U(s) \tag{2.73}$$

$$= -i\tau U_A^\dagger(s)\mathcal{H}(s)U(s) + i\tau U_A^\dagger(s)\mathcal{H}_A(s)U(s) \tag{2.74}$$

$$= -U_A^\dagger(s)\left[\dot{P}(s), P(s)\right]U(s) \tag{2.75}$$

$$= -U_A^\dagger(s)\left[\dot{P}(s), P(s)\right]U_A(s)W(s) \ . \tag{2.76}$$

Clearly $W(0) = I$ and so

$$W(s) = I - \int_0^s U_A^\dagger(r)[\dot{P}(r), P(r)]U_A(r)W(r)dr \ . \tag{2.77}$$

It will be useful sometimes to refer to the kernel of this integral equation, so we define

$$K(r) = U_A^\dagger(r) \left[\dot{P}(r), P(r)\right] U_A(r) \ . \tag{2.78}$$

Now we can use Equation (2.77) to rewrite $||Q(0)W(s)P(0)||$. Using the fact that $Q(0)P(0) = 0$, we can write

$$Q(0)W(s)P(0) = -\int_0^s Q(0)K(r)W(r)P(0)dr \ . \tag{2.79}$$

Our plan is to rewrite the integrand to obtain an expression where all but one term has a $1/\tau$ factor. Integration by parts on the remaining term will ensure all terms have a $1/\tau$ factor. Then we can factor out the $1/\tau$ and bound the operators in each term to yield the AT.

To obtain this expression, we need to introduce a $P(0)$ in the middle of Equation (2.79) so that we can apply Lemma 2.4.2. To do so, we will use the fact that $Q(0) = Q(0)^2$ to introduce another $Q(0)$, and then use the fact that $Q(0)K(r) = K(r)P(0)$.

To show that $Q(0)K(r) = K(r)P(0)$, we use intertwining properties, the fact that

$Q(r)P(r) = 0$, and the properties $P^2(r) = P(r)$ and $P(r)\dot{P}(r)P(r) = 0$:

$$Q(0)K(r) = Q(0)U_A^\dagger(r)[\dot{P}(r), P(r)]U_A(r) \tag{2.80}$$

$$= U_A^\dagger(r)Q(r)[\dot{P}(r), P(r)]U_A(r) \tag{2.81}$$

$$= U_A^\dagger(r)\left(Q(r)\dot{P}(r)P(r) - Q(r)P(r)\dot{P}(r)\right)U_A(r) \tag{2.82}$$

$$= U_A^\dagger(r)Q(r)\dot{P}(r)P(r)U_A(r) \tag{2.83}$$

$$= U_A^\dagger(r)\left(\dot{P}(r)P^2(r) - P(r)\dot{P}(r)P(r)\right)U_A(r) \tag{2.84}$$

$$= U_A^\dagger(r)\left[\dot{P}(r), P(r)\right]P(r)U_A(r) \tag{2.85}$$

$$= U_A^\dagger(r)\left[\dot{P}(r), P(r)\right]U_A(r)P(0) \tag{2.86}$$

$$= K(r)P(0)\ . \tag{2.87}$$

Then we can rewrite

$$Q(0)W(s)P(0) = -\int_0^s Q(0)K(r)W(r)P(0)dr \tag{2.88}$$

$$= -\int_0^s Q(0)^2K(r)W(r)P(0)dr \tag{2.89}$$

$$= -\int_0^s Q(0)K(r)P(0)W(r)P(0)dr\ . \tag{2.90}$$

Now we use the definition of $K(r)$, the properties $P^2(r) = P(r)$ and $Q^2(r) = Q(r)$, and the intertwining property again:

$$Q(0)W(s)P(0) = -\int_0^s Q(0)^2U_A^\dagger(r)\left[\dot{P}(r), P(r)\right]U_A(r)P(0)^2W(r)P(0)dr \tag{2.91}$$

$$= -\int_0^s Q(0)U_A^\dagger(r)Q(r)\left[\dot{P}(r), P(r)\right]P(r)U_A(r)P(0)W(r)P(0)dr\ . \tag{2.92}$$

We would like to apply Lemma 2.4.2 with

$$X(r) = \left[\dot{P}(r), P(r)\right]\ . \tag{2.93}$$

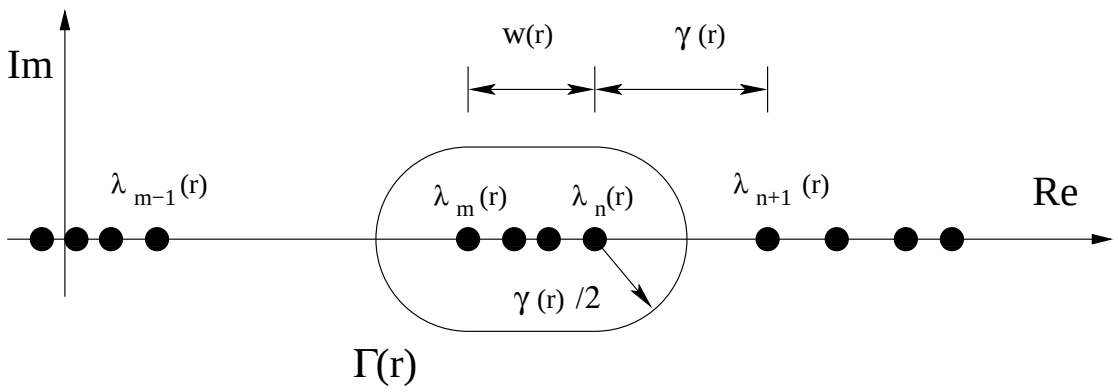

Figure 2.1: Visualization of the resolvent contour $\Gamma(r)$. The eigenvalues of $\mathcal{H}(r)$ (represented with black dots) all lie along the real axis since $\mathcal{H}(r)$ is Hermitian. Notice $\Gamma(r)$ lies at least $\gamma(r)/2$ from any eigenvalues. The length of $\Gamma(r)$ is $\pi\gamma(r) + 2w(r) = D(r)\pi\gamma(r)$. Observe that $D(r)$ is the ratio of the length of $\Gamma(r)$ to the circumference of a circle of radius $\gamma(r)/2$.

In order to apply the lemma, we need to show $X(r)$ is a bounded linear operator. Clearly $X(r)$ is linear, and since $P(r)$ has unit norm then it is sufficient to show that $\left|\left|\dot{P}(r)\right|\right|$ has a bound.

To bound the norm of $\dot{P}(r)$ we will use the resolvent formalism. We first need to bound the norm of the resolvent $R(r, z)$. Notice that if the eigenstates of $\mathcal{H}(r)$ are $\{|\psi_j(r)\rangle : j \geq 0\}$, then

$$R(r, z) = \sum_{j\geq 0} \frac{1}{\lambda_j(r) - z} |\psi_j(r)\rangle\langle\psi_j(r)| \,, \tag{2.94}$$

so the norm of $R(r, z)$ equals the inverse of the minimum distance of z to an eigenvalue of $\mathcal{H}(r)$. So we need to choose the contour $\Gamma(r)$ around the eigenvalues of $\Psi(r)$ to maximize the minimum distance of $\Gamma(r)$ to any eigenvalue. Also, to obtain the best bound on the path integral, we will want to minimize the length of $\Gamma(r)$, given that maximum minimum distance. We choose $\Gamma(r)$ consisting of two semicircles connected by lines, forming a pill-shape. The semicircles are centered at $\lambda_m(r)$ and $\lambda_n(r)$, and

they have radius $\gamma(r)/2$. Figure 2.1 illustrates this choice, which bounds the norm of $R(r,z)$ at $2/\gamma(r)$ and the length at $D(r)\pi\gamma(r)$.

We can check the tightness of this choice by using it to bound the norm of $P(r)$, which we know is unity. We have

$$||P(r)|| = \left|\left|-\frac{1}{2\pi i}\oint_{\Gamma(r)} R(r,z)dz\right|\right| \tag{2.95}$$

$$\leq \frac{1}{2\pi} D(r)\pi\gamma(r)\frac{2}{\gamma(r)} \tag{2.96}$$

$$= D(r) \ , \tag{2.97}$$

so the approximation is tight for $D(r) = 1$. When $D(r) > 1$, it is complicated by the fact that the closest eigenvalue is not always the same at different points on $\Gamma(r)$.

The elements of $R(r,z)$ are rational functions of the elements of $\mathcal{H}(r)$, which are assumed to be differentiable. So we can apply the quotient rule for derivatives to determine that $R(r,z)$ is differentiable for z not an eigenvalue of $\mathcal{H}(r)$.

We proceed by differentiating both sides of the equation

$$R(r,z)(\mathcal{H}(r) - zI) = I \ , \tag{2.98}$$

and multiplying both sides by $R(r,z)$ on the right. We thus obtain

$$\dot{R}(r,z) = -R(r,z)\dot{\mathcal{H}}(r)R(r,z) \ . \tag{2.99}$$

So by Equation (2.11)

$$\dot{P}(r) = \frac{1}{2\pi i}\oint_{\Gamma(r)} R(r,z)\dot{\mathcal{H}}(r)R(r,z)dz \ . \tag{2.100}$$

Also, recall that $\left|\left|\dot{\mathcal{H}}(r)\right|\right| \leq b_1(r)$, so we can bound the norm of the integral in Equation (2.100) with a rectangle approximation. Using our formula for the length

of $\Gamma(r)$, we get

$$\left|\left|\dot{P}(r)\right|\right| \leq \frac{1}{2\pi} D(r)\pi\gamma(r)\frac{4b_1(r)}{\gamma(r)^2} \tag{2.101}$$

$$= \frac{2D(r)b_1(r)}{\gamma(r)} \ . \tag{2.102}$$

Finally, we can bound $||X(r)||$. Using the definition of X we have

$$||X(r)|| = \left|\left|[\dot{P}(r), P(r)]\right|\right| \tag{2.103}$$

$$\leq 2\left|\left|\dot{P}(r)\right|\right| \ ||P(r)|| \tag{2.104}$$

$$= \frac{4D(r)b_1(r)}{\gamma(r)} \ . \tag{2.105}$$

Thus we can apply Lemma 2.4.2. We remove the extra $Q(r)$ and $P(r)$ the same way they were introduced, and use Schrödinger's equation.

$$Q(0)W(s)P(0) = \int_0^s Q(0)U_A^\dagger(r)\left(\left[\mathcal{H}_A(r), \tilde{X}(r)\right] - \frac{i}{\tau}\left[\dot{P}(r), \tilde{X}(r)\right]\right)$$
$$\times U_A(r)P(0)W(r)P(0)dr \tag{2.106}$$

$$= \int_0^s Q(0)U_A^\dagger(r)\mathcal{H}_A(r)\tilde{X}(r)U_A(r)P(0)W(r)P(0)dr$$
$$- \int_0^s Q(0)U_A^\dagger(r)\tilde{X}(r)\mathcal{H}_A(r)U_A(r)P(0)W(r)P(0)dr$$
$$- \frac{i}{\tau}\int_0^s Q(0)U_A^\dagger(r)\left[\dot{P}(r), \tilde{X}(r)\right]U_A(r)P(0)W(r)P(0)dr \tag{2.107}$$

$$= \int_0^s Q(0)U_A^\dagger(r)\mathcal{H}_A(r)\tilde{X}(r)U_A(r)P(0)W(r)P(0)dr$$
$$- \frac{i}{\tau}\int_0^s Q(0)U_A^\dagger(r)\tilde{X}(r)\dot{U}_A(r)P(0)W(r)P(0)dr$$
$$- \frac{i}{\tau}\int_0^s Q(0)U_A^\dagger(r)\left[\dot{P}(r), \tilde{X}(r)\right]U_A(r)P(0)W(r)P(0)dr \ . \tag{2.108}$$

Evidently the last two integrals have a $1/\tau$ factor, and we only need to work on

the first integral. We will integrate it by parts, using

$$A(r) = \tilde{X}(r)U_A(r)P(0)W(r) \ , \tag{2.109}$$

$$dA = \tilde{X}(r)U_A(r)P(0)\dot{W}(r)dr + \left(\dot{\tilde{X}}(r)U_A(r) + \tilde{X}(r)\dot{U}_A(r)\right)P(0)W(r)dr \ , \tag{2.110}$$

$$B(r) = U_A^\dagger(r) \ , \tag{2.111}$$

$$dB = i\tau U_A^\dagger(r)\mathcal{H}_A(r)dr \ . \tag{2.112}$$

Applying the integration by parts to $\int dBA$ yields

$$\begin{aligned}\int_0^s U_A^\dagger(r)\mathcal{H}_A(r)\tilde{X}(r)U_A(r)P(0)W(r)dr = &-\frac{i}{\tau}U_A^\dagger(r)\tilde{X}(r)U_A(r)P(0)W(r)\Big|_{r=0}^{s} \\ &+ \frac{i}{\tau}\int_0^s U_A^\dagger(r)\tilde{X}(r)U_A(r)P(0)\dot{W}(r)dr \\ &+ \frac{i}{\tau}\int_0^s U_A^\dagger(r)\dot{\tilde{X}}(r)U_A(r)P(0)W(r)dr \\ &+ \frac{i}{\tau}\int_0^s U_A^\dagger(r)\tilde{X}(r)\dot{U}_A(r)P(0)W(r)dr \ .\end{aligned} \tag{2.113}$$

When we substitute, we see that the last integral cancels with the second integral in Equation (2.108), so we obtain

$$\begin{aligned}Q(0)W(s)P(0) = &-\frac{i}{\tau}Q(0)U_A^\dagger(r)\tilde{X}(r)U_A(r)P(0)W(r)P(0)\Big|_{r=0}^{s} \\ &+ \frac{i}{\tau}Q(0)\int_0^s U_A^\dagger(r)\tilde{X}(r)U_A(r)P(0)\dot{W}(r)P(0)dr \\ &+ \frac{i}{\tau}Q(0)\int_0^s U_A^\dagger(r)\left(\dot{\tilde{X}}(r) - [\dot{P}(r), \tilde{X}(r)]\right)U_A(r)P(0)W(r)P(0)dr \ .\end{aligned} \tag{2.114}$$

To finish the proof, we need to bound each of the three terms on the right. We will do this by applying the triangle inequality to all the operators in Equation (2.114). Unitary operators and projection operators have unit norm, and we have bounded

$\dot{P}(r)$ already, so it remains to bound the norms of $\tilde{X}(r)$, $\dot{\tilde{X}}(r)$, and $\dot{W}(r)$. As dependencies we will also need to find the norms of $\ddot{P}(r)$ and $\dot{X}(r)$.

1. $\left|\left|\ddot{P}(r)\right|\right|$: To bound $\ddot{P}(r)$ we need to compute $\ddot{R}(r,z)$. Using the product rule for derivatives,

$$-\ddot{R}(r,z) = \frac{d}{dr}R(r,z)\dot{\mathcal{H}}(r)R(r,z) \tag{2.115}$$

$$= \frac{d}{dr}\left(R(r,z)\dot{\mathcal{H}}(r)\right)R(r,z) + R(r,z)\dot{\mathcal{H}}(r)\dot{R}(r,z) \tag{2.116}$$

$$= \left(\dot{R}(r,z)\dot{\mathcal{H}}(r) + R(r,z)\ddot{\mathcal{H}}(r)\right)R(r,z) + R(r,z)\dot{\mathcal{H}}(r)\dot{R}(r,z) \tag{2.117}$$

$$= \dot{R}(r,z)\dot{\mathcal{H}}(r)R(r,z) + R(r,z)\ddot{\mathcal{H}}(r)R(r,z) + R(r,z)\dot{\mathcal{H}}(r)\dot{R}(r,z)\ . \tag{2.118}$$

Since $\left|\left|\dot{R}(r)\right|\right| \leq ||R(r)||^2 \left|\left|\dot{\mathcal{H}}(r)\right|\right| \leq 4b_1(r)/\gamma(r)^2$, we have

$$\left|\left|\ddot{R}(r,z)\right|\right| \leq \frac{16b_1(r)^2}{\gamma(r)^3} + \frac{4b_2(r)}{\gamma(r)^2} \tag{2.119}$$

$$= \frac{4}{\gamma(r)^2}\left(\frac{4b_1(r)^2}{\gamma(r)} + b_2(r)\right)\ . \tag{2.120}$$

So, following the reasoning used to bound $\left|\left|\dot{P}(r)\right|\right|$,

$$\left|\left|\ddot{P}(r)\right|\right| = \left|\left|-\frac{1}{2\pi i}\oint_{\Gamma(r)}\ddot{R}(r,z)dz\right|\right| \tag{2.121}$$

$$\leq \frac{1}{2\pi}\pi\gamma(r)D(r)\frac{4}{\gamma(r)^2}\left(\frac{4b_1(r)^2}{\gamma(r)} + b_2(r)\right) \tag{2.122}$$

$$= \frac{2D(r)}{\gamma(r)}\left(\frac{4b_1(r)^2}{\gamma(r)} + b_2(r)\right)\ . \tag{2.123}$$

2. $\left|\left|\tilde{X}(r)\right|\right|$: By Equation (2.44), we have

$$\left|\left|\tilde{X}(r)\right|\right| \leq \frac{1}{2\pi}\oint_{\Gamma(r)} ||R(r,z)||\ ||X(r)||\ ||R(r,z)||\, dz \tag{2.124}$$

$$\leq \frac{1}{2\pi}\pi\gamma(r)D(r)\frac{2}{\gamma(r)}\frac{4D(r)b_1(r)}{\gamma(r)}\frac{2}{\gamma(r)} \tag{2.125}$$

$$= \frac{8D(r)^2 b_1(r)}{\gamma(r)^2}\,. \tag{2.126}$$

3. $\left|\left|\dot{X}\right|\right|$: Notice $\dot{X}(r) = \left[\ddot{P}(r), P(r)\right]$, so

$$\left|\left|\dot{X}(r)\right|\right| = \left|\left|[\ddot{P}(r), P(r)]\right|\right| \tag{2.127}$$

$$\leq 2\left|\left|\ddot{P}(r)\right|\right|\ ||P(r)|| \tag{2.128}$$

$$= \frac{4D(r)}{\gamma(r)}\left(\frac{4b_1(r)^2}{\gamma(r)} + b_2(r)\right)\,. \tag{2.129}$$

4. $\left|\left|\dot{\tilde{X}}(r)\right|\right|$: We have

$$\left|\left|\dot{\tilde{X}}(r)\right|\right| = \frac{1}{2\pi}\left|\left|\frac{d}{dr}\oint_{\Gamma(r)} R(r,z)X(r)R(r,z)dz\right|\right| \tag{2.130}$$

$$= \frac{1}{2\pi}\left|\left|\oint_{\Gamma(r)} \frac{d}{dr}R(r,z)X(r)R(r,z)dz\right|\right| \tag{2.131}$$

$$= \frac{1}{2\pi}\left|\left|\oint_{\Gamma(r)} R(r,z)X(r)\dot{R}(r,z)\right.\right. \tag{2.132}$$

$$\left.\left. + \left(\dot{R}(r,z)X(r) + R(r,z)\dot{X}(r)\right)R(r,z)dz\right|\right| \tag{2.133}$$

$$= \frac{1}{2\pi}\left|\left|\oint_{\Gamma(r)} -R(r,z)X(r)R(r,z)\dot{\mathcal{H}}(r)R(r,z)\right.\right.$$

$$\left.\left. -R(r,z)\dot{\mathcal{H}}(r)R(r,z)X(r)R(r,z) + R(r,z)\dot{X}(r))R(r,z)dz\right|\right|\,.$$

Now since $||R(r,z)|| \leq 2/\gamma(r)$, we get

$$\left|\left|\dot{\tilde{X}}(r)\right|\right| \leq \frac{1}{2\pi}\pi\gamma(r)D(r)\left(\frac{16b_1(r)}{\gamma(r)^3}||X(r)|| + \frac{4}{\gamma(r)^2}\left|\left|\dot{X}(r)\right|\right|\right) \tag{2.134}$$

$$= \frac{8D(r)^2}{\gamma(r)^2}\left(\frac{8b_1(r)^2}{\gamma(r)} + b_2(r)\right)\,. \tag{2.135}$$

5. $\left|\left|\dot{W}(r)\right|\right|$: Recall from Equation (2.76) that

$$\dot{W}(r) = -\, U_A^\dagger(r) \left[\dot{P}(r), P(r)\right] U(r)W(r)\ . \tag{2.136}$$

We know that $||W(r)|| = \left|\left|U_A^\dagger(r)\right|\right| = ||U(r)|| = 1$, and remember that $X(r) = \left[\dot{P}(r), P(r)\right]$. So we can apply the triangle inequality to get

$$\left|\left|\dot{W}(r)\right|\right| \leq ||X(r)|| \tag{2.137}$$

$$\leq \frac{4D(r)b_1(r)}{\gamma(r)}\ . \tag{2.138}$$

The resulting bounds are

$$\left|\left|\dot{P}(r)\right|\right| \leq \frac{2D(r)b_1(r)}{\gamma(r)}\ , \qquad \left|\left|\tilde{X}(r)\right|\right| \leq \frac{8D(r)^2 b_1(r)}{\gamma(r)^2}\ , \tag{2.139}$$

$$\left|\left|\dot{W}(r)\right|\right| \leq \frac{4D(r)b_1(r)}{\gamma(r)}\ , \qquad \left|\left|\dot{\tilde{X}}(r)\right|\right| \leq \frac{8D(r)^2}{\gamma(r)^2}\left(\frac{8b_1(r)^2}{\gamma(r)} + b_2(r)\right)\ . \tag{2.140}$$

Now let us apply these bounds to Equation (2.114) by taking the norm of both sides:

$$\begin{aligned} ||Q(0)W(s)P(0)|| \leq\ & \frac{1}{\tau}\left|\left|Q(0)U_A^\dagger(r)\tilde{X}(r)U_A(r)P(0)W(r)P(0)\Big|_{r=0}^{s}\right|\right| \\ & + \frac{1}{\tau}\left|\left|Q(0)\int_0^s U_A^\dagger(r)\tilde{X}(r)U_A(r)P(0)\dot{W}(r)P(0)dr\right|\right| \\ & + \frac{1}{\tau}\left|\left|Q(0)\int_0^s U_A^\dagger(r)\left(\dot{\tilde{X}}(r) + [\dot{P}(r), \tilde{X}(r)]\right)U_A(r)P(0)W(r)P(0)dr\right|\right|\ . \end{aligned} \tag{2.141}$$

We can further simplify this by noting that the norm of each integral is less than the integral of the norm of its integrand. Further, we use the triangle inequality and

the fact that the norm of unitary operators and projection operators are unity:

$$\begin{aligned}||Q(0)W(s)P(0)|| \leq & \frac{1}{\tau}\left[\left|\left|\tilde{X}(0)\right|\right| + \left|\left|\tilde{X}(s)\right|\right| \right. \\ & \left. + \int_0^s \left(\left|\left|\tilde{X}(r)\right|\right|\left|\left|\dot{W}(r)\right|\right| + \left|\left|\dot{\tilde{X}}(r)\right|\right| + \left|\left|[\dot{P}(r), \tilde{X}(r)]\right|\right|\right) dr\right] \\ \leq & \frac{8D^2(0)b_1(0)}{\tau\gamma^2(0)} + \frac{8D^2(s)b_1(s)}{\tau\gamma^2(s)} \\ & + \int_0^s \frac{8D^2(r)}{\tau\gamma^2(r)}\left(\frac{8(1+D(r))b_1^2(r)}{\gamma(r)} + b_2(r)\right) dr \ . \end{aligned} \tag{2.142}$$

Finally, from Equation (2.71), we get

$$||Q(s)U(s)P(0)|| \leq ||Q(0)W(s)P(0)|| \tag{2.143}$$

$$\begin{aligned} \leq & \frac{8D^2(0)b_1(0)}{\tau\gamma^2(0)} + \frac{8D^2(s)b_1(s)}{\tau\gamma^2(s)} \\ & + \int_0^s \frac{8D^2(r)}{\tau\gamma^2(r)}\left(\frac{8(1+D(r))b_1^2(r)}{\gamma(r)} + b_2(r)\right) dr \ . \end{aligned} \tag{2.144}$$

We also know that $||Q(s)U(s)P(0)|| \leq 1$ by the triangle inequality. □

Notice that the first two terms in Equation (2.144) do not go to zero as $s \to 0$, which is a consequence of simplifications that were made to determine this bound. However, since AQC is the intended application of our results, we are only interested in the error bound at the end of the evolution, namely $s = 1$. Also, we will usually assume there are $\bar{b}_1 \geq b_1(s)$, $\bar{b}_2 \geq b_2(s)$, $\bar{\gamma} \leq \gamma(s)$, and $\bar{D} \geq D(s)$ for $s \in [0, 1]$. Then we can find a constant upper bound for the integrand in Equation (2.144) and thus bound the integral, resulting in the simpler expression

$$||Q(s)U(s)P(0)|| \leq \frac{8\bar{D}^2}{\tau\bar{\gamma}^2}\left(2\bar{b}_1 + s\bar{b}_2 + s\frac{8(1+\bar{D})\bar{b}_1^2}{\bar{\gamma}}\right) \ . \tag{2.145}$$

In fact, we will usually be interested in the AT for non-degenerate ground states, in

which case $m = n = 0$ and $\bar{D} = 1$, and we can use the inequality

$$||Q(s)U(s)P(0)|| \leq \frac{8}{\tau\bar{\gamma}^2}\left(2\bar{b}_1 + s\bar{b}_2 + s\frac{16\bar{b}_1^2}{\bar{\gamma}}\right) . \tag{2.146}$$

Also notice our statement of the AT is consistent with the common interpretation of the theorem: if $\tau \gg 1/\bar{\gamma}^2$ then the error in the adiabatic approximation is small.

Having derived the AT with explicit definitions of constants, we are ready to bound the error of the adiabatic approximation under various conditions of experimental error.

Chapter 3

Adiabatic Theorems for Noisy Hamiltonian Evolutions

Now we provide new variants of the adiabatic theorem that apply under conditions of experimental error, and demonstrate their usefulness in examples. In Section 3.1, we provide an AT for perturbations in the initial state of the system and an AT for systematic time-dependent perturbations in the Hamiltonian. In Section 3.2, we provide an AT for certain open quantum systems and an AT for noise modeled as a time-dependent perturbation in the Hamiltonian. The rest of the chapter is dedicated to two examples. The spin-1/2 particle in a rotating magnetic field, a standard example for controversy regarding the AT [10, 60, 69, 34], is discussed in Section 3.3. Finally in Section 3.4, we consider an adiabatic evolution of the superconducting flux qubit [40].

3.1 Coherent or incoherent errors

Coherent or incoherent errors, due to systematic or deterministic perturbations, may occur in one of two ways: either as a perturbation in the initial condition or as a smooth perturbation in the Hamiltonian. Let us explore how such errors affect the adiabatic approximation for a non-degenerate ground state.

Let us first consider a perturbation in the initial state,

$$|\phi(0)\rangle = \eta\left(|\psi_0(0)\rangle + \delta|\phi_\perp\rangle\right) \ , \tag{3.1}$$

where $\eta^{-2} = 1 + |\delta|^2$ is a normalization factor, $|\psi_0(0)\rangle$ is the ground state of $\mathcal{H}(0)$, and $|\phi_\perp\rangle$ is some state orthogonal to $|\psi_0(0)\rangle$. It is not sufficient here to define the error of the adiabatic approximation as the norm of the operator $Q(s)U(s)P(0)$, where $P(s)$ is the projection onto $|\psi_0(s)\rangle$, since this does not depend on the initial state. The component of the final state which lies outside the ground state at normalized time s is $Q(s)U(s)|\phi(0)\rangle$, and so here we take this as the error.

Theorem 3.1.1 (AT for Error in the Initial State (AT-Initial))**.** *Let $\mathcal{H}(s)$ have the properties required by the AT, and let the initial state $|\phi(0)\rangle$ be as in Equation (3.1). Then the error is bounded as*

$$||Q(s)U(s)|\phi(0)\rangle|| \leq |\eta| \left(|\delta| + \frac{8}{\tau \bar{\gamma}^2} \left(2\bar{b}_1 + s\bar{b}_2 + s\frac{16\bar{b}_1^2}{\bar{\gamma}} \right) \right) . \tag{3.2}$$

Proof. Using the AT and the triangle inequality for operator norms, and noting that the norm of unitary and projection operators is unity, we have

$$\begin{aligned} ||Q(s)U(s)|\phi(0)\rangle|| &= ||Q(s)U(s)\eta\left(|\psi_0(0)\rangle + \delta|\phi_\perp\rangle\right)|| && (3.3)\\ &= ||\eta\left(Q(s)U(s)P(0)|\psi_0(0)\rangle + \delta Q(s)U(s)|\phi_\perp\rangle\right)|| && (3.4)\\ &\leq |\eta|\left(||Q(s)U(s)P(0)|| + |\delta|\right) && (3.5)\\ &\leq |\eta| \left(|\delta| + \frac{8}{\tau \bar{\gamma}^2} \left(2\bar{b}_1 + s\bar{b}_2 + s\frac{16\bar{b}_1^2}{\bar{\gamma}} \right) \right) . && (3.6) \end{aligned}$$

□

Now suppose there is a smooth perturbation in the Hamiltonian caused by a systematic error, so that

$$\mathcal{H}_\epsilon(s) = \mathcal{H}(s) + \epsilon\Delta(s) , \tag{3.7}$$

where $\epsilon > 0$. Then we can use the AT on $\mathcal{H}_\epsilon$ by observing that

$$\left|\left|\dot{\mathcal{H}}_\epsilon(s)\right|\right| \leq \left|\left|\dot{\mathcal{H}}(s)\right|\right| + \epsilon \left|\left|\dot{\Delta}(s)\right|\right| , \tag{3.8}$$

$$\left|\left|\ddot{\mathcal{H}}_\epsilon(s)\right|\right| \leq \left|\left|\ddot{\mathcal{H}}(s)\right|\right| + \epsilon \left|\left|\ddot{\Delta}(s)\right|\right| . \tag{3.9}$$

However, we must account for the difference in ground state between $\mathcal{H}_\epsilon(s)$ and $\mathcal{H}(s)$. Since we want to measure error from the intended eigenstates of the system, not the perturbed eigenstates, the error operator is $Q(s)U_\epsilon(s)P(0)$, where we introduce the following notation:

$U_\epsilon(s)$	The solution to $\dot{U}_\epsilon(s) = -i\tau\mathcal{H}_\epsilon(s)U_\epsilon(s)$.
$P_\epsilon(s)$	The projection operator onto the ground state of $\mathcal{H}_\epsilon(s)$.
$Q_\epsilon(s)$	$I - P_\epsilon(s)$.
$\bar{\gamma}_\epsilon$	The minimum energy gap between the ground state and first excited state of $\mathcal{H}_\epsilon(s)$.

Theorem 3.1.2 (AT for Systematic Error (AT-Error))**.** *Assume that $\mathcal{H}_\epsilon(s)$ has the properties required by the AT, and let*

$$\left|\left|\dot{\mathcal{H}}_\epsilon(s)\right|\right| \leq \bar{b}_1 , \qquad \left|\left|\ddot{\mathcal{H}}_\epsilon(s)\right|\right| \leq \bar{b}_2 , \tag{3.10}$$

$$\sqrt{1 - |\langle\psi_0(0)|\phi_0(0)\rangle|^2} = \delta_0 , \qquad \sqrt{1 - |\langle\psi_0(1)|\phi_0(1)\rangle|^2} = \delta_1 , \tag{3.11}$$

where $|\psi_0(s)\rangle$ is the ground state of $\mathcal{H}_\epsilon(s)$ and $|\phi_0(s)\rangle$ is the ground state of $\mathcal{H}(s)$. If $\bar{\gamma}_\epsilon > 0$, then we have

$$||Q(1)U_\epsilon(1)P(0)|| \leq \frac{8}{\tau\bar{\gamma}_\epsilon^2}\left(2\bar{b}_1 + \bar{b}_2 + \frac{16\bar{b}_1^2}{\bar{\gamma}_\epsilon}\right) + \delta_0 + \delta_1 + \delta_0\delta_1 . \tag{3.12}$$

Proof. We know from AT that

$$||Q_\epsilon(1)U_\epsilon(1)P_\epsilon(0)|| \leq \frac{8}{\tau\bar{\gamma}_\epsilon^2}\left(2\bar{b}_1 + \bar{b}_2 + \frac{16\bar{b}_1^2}{\bar{\gamma}_\epsilon}\right) , \tag{3.13}$$

but we want to find $||Q(1)U_\epsilon(1)P(0)||$. So define

$$\Delta P(s) = P_\epsilon(s) - P(s) \ . \tag{3.14}$$

Then we have

$$\begin{aligned} Q(1)U_\epsilon(1)P(0) =& \left(Q_\epsilon(1) + \Delta P(1)\right) U_\epsilon(1) \left(P_\epsilon(0) - \Delta P(0)\right) && (3.15) \\ =& Q_\epsilon(1)U_\epsilon(1)P_\epsilon(0) - Q_\epsilon(1)U_\epsilon(1)\Delta P(0) + \Delta P(1)U_\epsilon(1)P_\epsilon(0) \\ & - \Delta P(1)U_\epsilon(1)\Delta P(0) \ . && (3.16) \end{aligned}$$

Now, the 2-norm of unitary and projection operators is unity, so

$$\begin{aligned} ||Q(1)U_\epsilon(1)P(0)|| \leq & \frac{8}{\tau\bar{\gamma}_\epsilon^2}\left(2\bar{b}_1 + \bar{b}_2 + \frac{16\bar{b}_1^2}{\bar{\gamma}_\epsilon}\right) \\ & + ||\Delta P(0)|| + ||\Delta P(1)|| + ||\Delta P(0)||\,||\Delta P(1)|| \ . \end{aligned} \tag{3.17}$$

It remains to find $||\Delta P(s)||$. We hope to write

$$|\phi_0(s)\rangle = M(s)|\psi_0(s)\rangle \ , \tag{3.18}$$

for some unitary transformation $M(s)$ that is close to the identity provided $\psi_0(s)$ and $\phi_0(s)$ are close to each other. We use the Givens rotation, where the first basis state is $|\phi_0(s)\rangle$ and the second is the complement of the projection of $|\psi_0(s)\rangle$ onto the first basis state:

$$\hat{e}_1 = |\phi_0(s)\rangle \ , \qquad \hat{e}_2 = \frac{\left(1 - |\phi_0(s)\rangle\langle\phi_0(s)|\ \right)\ |\psi_0(s)\rangle}{\sqrt{1 - |\langle\phi_0(s)|\psi_0(s)\rangle|^2}} \ . \tag{3.19}$$

The remaining basis states are chosen arbitrarily so long as the resulting basis is orthonormal and spans the Hilbert space. In that basis, Equation (3.18) is realized

by

$$\begin{pmatrix} C^*(s) & S(s) & & & & & \\ -S(s) & C(s) & & & & & \\ & & 1 & & & & \\ & & & 1 & & & \\ & & & & \ddots & & \\ & & & & & 1 & \end{pmatrix} \begin{pmatrix} C(s) \\ S(s) \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} , \tag{3.20}$$

where we define

$$C(s) = \langle \phi_0(s) | \psi_0(s) \rangle \, , \tag{3.21}$$

$$S(s) = \sqrt{1 - |\langle \phi_0(s) | \psi_0(s) \rangle|^2} \, . \tag{3.22}$$

We see that

$$M(s) P_\epsilon(s) M^\dagger(s) = M(s) |\psi_0(s)\rangle\langle\psi_0(s)| M^\dagger(s) \tag{3.23}$$

$$= |\phi_0(s)\rangle\langle\phi_0(s)| \tag{3.24}$$

$$= P(s) \, . \tag{3.25}$$

Letting $E(s) = I - M(s)$, we have

$$\Delta P(s) = P_\epsilon(s) - P(s) \tag{3.26}$$

$$= M^\dagger(s) P(s) M(s) - M^\dagger(s) M(s) P(s) \tag{3.27}$$

$$= M^\dagger(s) \left[P(s), M(s) \right] \tag{3.28}$$

$$= M^\dagger(s) \left[E(s), P(s) \right] \, . \tag{3.29}$$

But we know $E(s)$ and $P(s)$:

$$E(s) = \begin{pmatrix} 1 - C^*(s) & -S(s) & & & & \\ S(s) & 1 - C(s) & & & & \\ & & 0 & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}, \quad P(s) = \begin{pmatrix} 1 & 0 & & & & \\ 0 & 0 & & & & \\ & & 0 & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}, \tag{3.30}$$

so

$$[E(s), P(s)] = \begin{pmatrix} 0 & S(s) & & & & \\ S(s) & 0 & & & & \\ & & 0 & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix}. \tag{3.31}$$

Finally,

$$||\Delta P(s)|| = ||P_\epsilon(s) - P(s)|| \tag{3.32}$$

$$= || \, [E(s), P(s)] \, || \tag{3.33}$$

$$= S(s) \, . \tag{3.34}$$

Combining Equations (3.34) and (3.17) yields the theorem. □

When it is inconvenient to compute δ_0 and δ_1 exactly, they can be bounded using

the "sin(Θ) theorem" [55, p. 251]:

$$\delta_0 \leq \frac{\epsilon\,||\Delta(0)||}{\lambda_1(0) - \lambda_0^\epsilon(0)}\,, \qquad\qquad \delta_1 \leq \frac{\epsilon\,||\Delta(1)||}{\lambda_1(1) - \lambda_0^\epsilon(1)}\,, \tag{3.35}$$

where $\lambda_0^\epsilon(s)$ is the energy of the ground state of $\mathcal{H}_\epsilon(s)$. If $\lambda_0^\epsilon(s)$ is difficult to find, we can use the Bauer-Fike theorem [55, p. 192] to get

$$\delta_0 \leq \frac{\epsilon\,||\Delta(0)||}{\gamma(0) - \epsilon\,||\Delta(0)||}\,, \qquad\qquad \delta_1 \leq \frac{\epsilon\,||\Delta(1)||}{\gamma(1) - \epsilon\,||\Delta(1)||}\,, \tag{3.36}$$

where $\gamma(s)$ is the energy gap of the unperturbed Hamiltonian $\mathcal{H}(s)$.

A remarkable feature of AT-Error is that it does not depend directly on the magnitude of the perturbation term $\epsilon\Delta(s)$ except at the endpoints. It does not matter which path we take through state space, so long as we begin and end near the correct Hamiltonians and do not accumulate too much error along the way.

3.2 Decoherent errors

Now we consider decoherent errors induced, perhaps, by noise in the environment. We first consider noise modeled as a coupled quantum system where the environment Hamiltonian is independent of time, and then as a classical time-dependent perturbation in the Hamiltonian.

For the environment Hamiltonian $\mathcal{H}_{env}$ and interaction Hamiltonian $\epsilon\Delta(s)$, we can write the combined Hamiltonian $\mathcal{H}_\epsilon(s)$ as

$$\mathcal{H}_\epsilon(s) = \mathcal{H}(s) \otimes I + I \otimes \mathcal{H}_{env} + \epsilon\Delta(s)\,. \tag{3.37}$$

Direct application of the AT yields a very pessimistic result because the ground state of the composite system has, in the weak coupling limit, both the target system

and the environment in the ground state of their respective Hamiltonians. The target system remaining in the ground state and the environment tunneling to its first excited state will be considered a failure of the adiabatic approximation. An experimentalist probably cannot achieve the environmental ground state, and the energy gap between environment states is likely quite small so that the AT produces a very large error bound.

One way to resolve this problem in the interpretation of the adiabatic approximation is to work with the density operator that results from the partial trace [46]:

$$\rho(s) = \mathrm{Tr}_{env}(\rho_\epsilon(s)) \ , \tag{3.38}$$

where $\rho_\epsilon(s)$ is the density operator associated with the state of the composite system $\mathcal{H}_\epsilon(s)$. Usually we can write

$$\dot{\rho}(s) = \mathcal{L}(s)\rho(s) \ , \tag{3.39}$$

where $\mathcal{L}(s)$ is a linear operator but not generally Hermitian. We might try to use this differential equation to prove an adiabatic theorem restated in terms of the expectation $\langle\phi_0(s)|\rho(s)|\phi_0(s)\rangle$, where $|\phi_0(s)\rangle$ is the ground state of $\mathcal{H}(s)$. The problem is that $\mathcal{L}(s)$ does not have a complete set of orthonormal eigenstates, which is of great assistance in proving the AT. A rigorous bound on the error of the adiabatic approximation has yet to be found using this approach [20, 46, 58, 59, 70].

The density operator approach sums together the set of states in the composite system whose measurement on the system of interest yields the ground state. Instead, below we will simply consider that set of states a subspace, and identify conditions where the usual AT for evolution of a subspace applies.

For adiabatic quantum computation, we expect the energy gap $\bar{\gamma}$ to be significantly larger than the temperature $k_B T$. When the system is significantly coupled to only a small number N of nearby particles, then the range of relevant environmental energy levels is on the order of $N k_B T$, so $||\mathcal{H}_{env}||$ is also order $N k_B T$. If $||\mathcal{H}_{env}|| < \bar{\gamma}$, we may use the AT.

More generally, we must determine the error operator for evolution in the composite system. The projection operator of interest projects states in the composite system onto those states whose measurement reveals the original system to be in the ground state. If $P(s)$ is the projection onto the ground state of $\mathcal{H}(s)$, then this operator is $P(s) \otimes I$. Its complement is $Q(s) \otimes I = I \otimes I - P(s) \otimes I$, since Kronecker products distribute. Then the error operator is $(Q(s) \otimes I)\, U_\epsilon(s)\, (P(0) \otimes I)$.

Theorem 3.2.1 (AT for Coupling to Low-Temperature Environment (AT-Env))**.** *Suppose we are given*

$$\mathcal{H}_\epsilon(s) = \mathcal{H}(s) \otimes I + I \otimes \mathcal{H}_{env} + \epsilon \Delta(s) \;, \tag{3.40}$$

and suppose we can choose w so that

$$||\mathcal{H}_{env}|| + 2\epsilon\, ||\Delta(s)|| \leq w < \bar{\gamma} \;, \tag{3.41}$$

where $\bar{\gamma}$ is the minimum energy gap between the ground state and first excited state of $\mathcal{H}(s)$. Assume that $\mathcal{H}_\epsilon(s)$ has the properties required by the AT, and assume that $\mathcal{H}_{env}$ has M states and its ground state has zero energy. Let

$$\left|\left|\dot{\mathcal{H}}_\epsilon(s)\right|\right| \leq \bar{b}_1 \;, \qquad\qquad \left|\left|\ddot{\mathcal{H}}_\epsilon(s)\right|\right| \leq \bar{b}_2 \;, \tag{3.42}$$

$$\delta_0 = \frac{\epsilon\,||\Delta(0)||}{\bar{\gamma} - ||\mathcal{H}_{env}|| - \epsilon\,||\Delta(0)||}\,, \qquad \delta_1 = \frac{\epsilon\,||\Delta(1)||}{\bar{\gamma} - ||\mathcal{H}_{env}|| - \epsilon\,||\Delta(1)||}\,, \tag{3.43}$$

$$\bar{\gamma}_\epsilon = \begin{cases} \bar{\gamma} - w & : \epsilon > 0 \\ \\ \bar{\gamma} & : \epsilon = 0 \end{cases}, \qquad \bar{D} = \begin{cases} 1 + \frac{2w}{\pi\bar{\gamma}_\epsilon} & : \epsilon > 0 \\ \\ 1 & : \epsilon = 0 \end{cases}. \tag{3.44}$$

Then we have

$$||(Q(1)\otimes I)\,U_\epsilon(1)\,(P(0)\otimes I)|| \leq \frac{8\bar{D}^2}{\tau\bar{\gamma}_\epsilon^2}\left(2\bar{b}_1 + \bar{b}_2 + \frac{8(1+\bar{D})\bar{b}_1^2}{\bar{\gamma}_\epsilon}\right) + \delta_0 + \delta_1 + \delta_0\delta_1\,, \tag{3.45}$$

where τ is the total evolution time.

Proof. For $\epsilon = 0$, we can ignore $\mathcal{H}_{env}$ and this theorem is simply the AT. So let us consider $\epsilon > 0$. We will do this by considering $\epsilon > 0$ as a perturbation of the $\epsilon = 0$ case.

For $\epsilon = 0$, the eigenstates of $\mathcal{H}_\epsilon(s)$ are simply the eigenstates of $\mathcal{H}(s)$ tensored to the eigenstates of $\mathcal{H}_{env}$, and the energy of those states is the sum of the energy of the state in $\mathcal{H}(s)$ and the energy of the state in $\mathcal{H}_{env}$.

Define the ground state energy of $\mathcal{H}(s)$ as $\lambda_0(s)$, the energy of the first excited state as $\lambda_1(s)$, and $\gamma(s) = \lambda_1(s) - \lambda_0(s)$. Recall that the M energies of the $\mathcal{H}_{env}$ states are non-negative and less than $\bar{\gamma}$. Then the first M eigenstates of $\mathcal{H}_\epsilon(s)$ are the ground state of $\mathcal{H}(s)$ tensored with different eigenstates of $\mathcal{H}_{env}$, and the rest of the states are some excited state of $\mathcal{H}(s)$ tensored with an environment state.

In particular, the M^{th} state of $\mathcal{H}_\epsilon$ is the ground state of $\mathcal{H}$ tensored with the most energetic state of $\mathcal{H}_{env}$, and thus has energy $\lambda_0(s) + ||\mathcal{H}_{env}||$. The $M+1$ state is the first excited state of $\mathcal{H}$ tensored with the ground state of $\mathcal{H}_{env}$, and has energy $\lambda_1(s)$.

So the energy gap between the first M states and the rest of the spectrum is exactly $\gamma(s) - ||\mathcal{H}_{env}||$.

For positive ϵ, these eigenstates are perturbed. Using the Bauer-Fike theorem [55, p. 192], we see that the gap is reduced by at most $2\epsilon\,||\Delta(s)||$ in the presence of coupling, so the gap is still at least $\bar{\gamma}_\epsilon$.

What we want is the adiabatic approximation of the evolution of the subspace formed by these M eigenstates, with a spectral width at most w and an energy gap of $\bar{\gamma}_\epsilon$. Following the proof of AT-Error, define

$$\Delta P(s) = P_\epsilon(s) - P(s) \otimes I \ . \tag{3.46}$$

Then we have

$$\begin{aligned}(Q(1) \otimes I)\, U_\epsilon(1)\, (P(0) \otimes I) &= (Q_\epsilon(1) + \Delta P(1))\, U_\epsilon(1)\, (P_\epsilon(0) - \Delta P(0)) &(3.47)\\ &= Q_\epsilon(1)U_\epsilon(1)P_\epsilon(0) - Q_\epsilon(1)U_\epsilon(1)\Delta P(0) + \Delta P(1)U_\epsilon(1)P_\epsilon(0)\\ &\quad - \Delta P(1)U_\epsilon(1)\Delta P(0)\ . &(3.48)\end{aligned}$$

We can bound $||\Delta P(s)||$ using the fact that the singular values of $\Delta P(s)$ are given by the sines of the canonical angles between $P_\epsilon(s)$ and $P(s) \otimes I$ [55, p. 43], the "sin(Θ) theorem" [55, p. 251], and the Bauer-Fike theorem [55, p. 192]:

$$\Delta P(s) \leq \frac{\epsilon\,||\Delta(s)||}{\gamma(s) - ||\mathcal{H}_{env}|| - \epsilon\,||\Delta(s)||}\ , \tag{3.49}$$

so

$$\Delta P(0) \leq \delta_0\ , \qquad\qquad \Delta P(1) \leq \delta_1\ . \tag{3.50}$$

Now we are ready to apply the AT:

$$||(Q(1)\otimes I)\,U_\epsilon(1)\,(P(0)\otimes I)|| \leq ||Q_\epsilon(1)U_\epsilon(1)P_\epsilon(0)|| + \delta_0 + \delta_1 + \delta_0\delta_1 \tag{3.51}$$

$$\leq \frac{8\bar{D}^2}{\tau\bar{\gamma}_\epsilon^2}\left(2\bar{b}_1 + \bar{b}_2 + \frac{8(1+\bar{D})\bar{b}_1^2}{\bar{\gamma}_\epsilon}\right) + \delta_0 + \delta_1 + \delta_0\delta_1\ . \tag{3.52}$$

□

Now let us consider another model of decoherent noise, namely a time-dependent perturbation in the Hamiltonian. There is a problem applying the AT directly, because the time-dependent perturbation is a function of true time t, not the unitless evolution parameter s. So as τ grows, more noise fluctuations are packed into the interval $s \in [0,1]$, causing $||d\mathcal{H}/ds||$ to diverge. Then there is no bound $\bar{b}_1$ greater than $||d\mathcal{H}/ds||$ that is independent of τ. In fact this problem was the source of confusion in the recent controversy surrounding the adiabatic theorem [35, 60, 64].

We will need to consider Hamiltonians $\mathcal{H}_\tau(s)$ that depend on both s and t. We define the following notation:

$U_\tau(s)$ The solution to $\dot{U}_\tau(s) = -i\tau\mathcal{H}_\tau(s)U_\tau(s)$ for a fixed τ.

$P_\tau(s)$ The projection operator onto the ground state of $\mathcal{H}_\tau(s)$.

$Q_\tau(s)$ $I - P_\tau(s)$.

$\gamma_\tau(s)$ The energy difference between the ground state and first excited state of $\mathcal{H}_\tau(s)$.

Theorem 3.2.2 (Adiabatic Theorem for Hamiltonian Evolutions on Two Time Scales (AT-2))**.** *Suppose, for any fixed τ, that $\mathcal{H}_\tau(s)$ has the properties required by the AT. Further assume there are real functions $g_1(\tau)$ and $g_2(\tau)$ such that*

$$\left|\left|\dot{\mathcal{H}}_\tau(s)\right|\right| \leq g_1(\tau)\ , \qquad\qquad \left|\left|\ddot{\mathcal{H}}_\tau(s)\right|\right| \leq g_2(\tau)\ , \tag{3.53}$$

for all τ. If there is a $\bar{\gamma}_{min}$ so that

$$0 < \bar{\gamma}_{min} \leq \gamma_\tau(s) \tag{3.54}$$

for $s \in [0,1]$ and τ, then we have

$$||Q_\tau(s)U_\tau(s)P_\tau(0)|| \leq \frac{8}{\tau\bar{\gamma}_{min}^2}\left(2g_1(\tau) + sg_2(\tau) + s\frac{16g_1^2(\tau)}{\bar{\gamma}_{min}}\right) . \tag{3.55}$$

Proof. The theorem we are trying to prove is the union of special cases of the AT, when the AT is applied to one-parameter projections of the original Hamiltonian.

For fixed τ, we consider $\mathcal{H}_\tau(s)$ as a one-parameter Hamiltonian to which the usual AT will apply. Then by the AT, we can write

$$||Q_\tau(s)U_\tau(s)P_\tau(0)|| \leq \frac{8}{\tau\bar{\gamma}_{min}^2}\left(2g_1(\tau) + sg_2(\tau) + s\frac{16g_1^2(\tau)}{\bar{\gamma}_{min}}\right) . \tag{3.56}$$

But we can do this for any τ, so the result holds. □

Now we can apply AT-2 to the case where there is an evolution performed on some scaled time s, with an additive noise Hamiltonian $\mathcal{H}_{noise}(t)$ that is a function of real time $t = s\tau$:

$$\mathcal{H}_\tau(s) = \mathcal{H}(s) + \mathcal{H}_{noise}(s\tau) . \tag{3.57}$$

We define the error operator for the noisy Hamiltonian as $Q(s)U_\tau(s)P(0)$. The projection operators refer to the unperturbed Hamiltonian because success should be defined in terms of the intended states.

Theorem 3.2.3 (Adiabatic Theorem for Noisy Hamiltonian Evolutions (AT-Noise))**.** *Suppose for any fixed τ, that $\mathcal{H}_\tau(s) = \mathcal{H}(s) + \mathcal{H}_{noise}(s\tau)$ has the properties required*

by the AT. Assume

$$\left|\left|\frac{d}{ds}\mathcal{H}(s)\right|\right| \leq c_1 \ , \qquad \left|\left|\frac{d^2}{ds^2}\mathcal{H}(s)\right|\right| \leq c_2 \ , \tag{3.58}$$

$$\left|\left|\frac{d}{dt}\mathcal{H}_{noise}(t)\right|\right| \leq d_1 \ , \qquad \left|\left|\frac{d^2}{dt^2}\mathcal{H}_{noise}(t)\right|\right| \leq d_2 \ , \tag{3.59}$$

$$\sqrt{1-|\langle\psi_0(0)|\phi_0(0)\rangle|^2} = \delta_0 \ , \qquad \sqrt{1-|\langle\psi_0(1)|\phi_0(1)\rangle|^2} = \delta_1 \ , \tag{3.60}$$

where $|\psi_0(s)\rangle$ *is the ground state of* $\mathcal{H}_\tau(s)$ *and* $|\phi_0(s)\rangle$ *is the ground state of* $\mathcal{H}(s)$. *Further assume that there is a* $\bar{\gamma}_{noise}$ *so that*

$$0 < \bar{\gamma}_{noise} \leq \gamma_\tau(s) \tag{3.61}$$

for $s \in [0,1]$ *and* τ. *Then we have*

$$||Q(1)U_\tau(1)P(0)|| \leq \frac{8}{\bar{\gamma}_{noise}^2}\left[\left(d_2+\frac{16d_1^2}{\bar{\gamma}_{noise}}\right)\tau + 2d_1\left(1+\frac{16c_1}{\bar{\gamma}_{noise}}\right)+\left(2c_1+c_2+\frac{16c_1^2}{\bar{\gamma}_{noise}}\right)\frac{1}{\tau}\right] + \delta_0+\delta_1+\delta_0\delta_1 \ . \tag{3.62}$$

Proof. Evidently

$$\frac{d}{ds}\mathcal{H}_\tau(s) = \frac{d}{ds}\mathcal{H}(s) + \tau\frac{d}{dt}\mathcal{H}_{noise}(t) \ , \tag{3.63}$$

$$\left|\left|\frac{d}{ds}\mathcal{H}_\tau(s)\right|\right| \leq c_1 + \tau d_1 \ , \tag{3.64}$$

$$\frac{d^2}{ds^2}\mathcal{H}_\tau(s) = \frac{d^2}{ds^2}\mathcal{H}(s) + \tau^2\frac{d^2}{dt^2}\mathcal{H}_{noise}(t) \ , \tag{3.65}$$

$$\left|\left|\frac{d^2}{ds^2}\mathcal{H}_\tau(s)\right|\right| \leq c_2 + \tau^2 d_2 \ . \tag{3.66}$$

Substitution of Equation (3.64) and Equation (3.66) into AT-2 yields, for $s \in [0,1]$ and τ,

$$||Q_\tau(s)U_\tau(s)P_\tau(0)|| \leq \frac{8}{\bar{\gamma}_{noise}^2}\left[\left(d_2+\frac{16d_1^2}{\bar{\gamma}_{noise}}\right)\tau + 2d_1\left(1+\frac{16c_1}{\bar{\gamma}_{noise}}\right)+\left(2c_1+c_2+\frac{16c_1^2}{\bar{\gamma}_{noise}}\right)\frac{1}{\tau}\right] \ . \tag{3.67}$$

As in the proof of AT-Error, we define

$$\Delta P(0) = P_\tau(0) - P(0) \,, \qquad\qquad \Delta P(1) = P_\tau(1) - P(1) \,. \tag{3.68}$$

Then for $s = 1$ we have

$$\begin{aligned} Q(1)U_\tau(1)P(0) =& \left(Q_\tau(1) + \Delta P(1)\right) U_\tau(1) \left(P_\tau(0) - \Delta P(0)\right) && (3.69) \\ =& Q_\tau(1)U_\tau(1)P_\tau(0) - Q_\tau(1)U_\tau(1)\Delta P(0) + \Delta P(1)U_\tau(1)P_\tau(0) \\ & - \Delta P(1)U_\tau(1)\Delta P(0) \,. && (3.70) \end{aligned}$$

Now we bound the norm of the error:

$$\begin{aligned} ||Q(1)U_\tau(1)P(0)|| \leq \frac{8}{\bar{\gamma}_{noise}^2} \left[\left(d_2 + \frac{16 d_1^2}{\bar{\gamma}_{noise}} \right) \tau + 2 d_1 \left(1 + \frac{16 c_1}{\bar{\gamma}_{noise}} \right) + \left(2c_1 + c_2 + \frac{16 c_1^2}{\bar{\gamma}_{noise}} \right) \frac{1}{\tau} \right] \\ + ||\Delta P(0)|| + ||\Delta P(1)|| + ||\Delta P(0)||\,||\Delta P(1)|| \,. \end{aligned} \tag{3.71}$$

Using the Givens rotation just as in the proof of AT-Error, we have

$$||\Delta P(0)|| = \delta_0 \,, \qquad\qquad ||\Delta P(1)|| = \delta_1 \,, \tag{3.72}$$

which, when substituted into Equation (3.71), completes the proof. □

Several observations can be made about this result:

1. As with AT-Error, if it is inconvenient to compute δ_0 and δ_1 exactly, they can be bounded using the "sin(Θ) theorem" combined with the Bauer-Fike theorem [55, p. 192]:

$$\delta_0 \leq \frac{||\mathcal{H}_{noise}(0)||}{\gamma(0) - ||\mathcal{H}_{noise}(0)||} \,, \qquad \delta_1 \leq \frac{||\mathcal{H}_{noise}(1)||}{\gamma(1) - ||\mathcal{H}_{noise}(1)||} \,, \tag{3.73}$$

where $\gamma(s)$ is the energy gap between the ground state and first excited state of $\mathcal{H}(s)$. Also, δ_0 and δ_1 can be taken as zero if $\mathcal{H}_{noise}(0) = \mathcal{H}_{noise}(\tau) = 0$.

In general, we expect them to be quite small if $\mathcal{H}_{noise}(t)$ is several orders of magnitude smaller than $\mathcal{H}(s)$.

2. When τ is small, the $1/\tau$ term dominates. This term is exactly the bound from the (noiseless) AT. It shows there is always a positive lower bound on the running time of the adiabatic algorithm to guarantee a particular error tolerance.

3. When τ is large, the first term dominates. In fact, we can see that in the presence of noise, there is *always* some sufficiently large τ beyond which the adiabatic approximation may perform poorly. So given an error tolerance, there is always an upper bound on the running time for the adiabatic algorithm, beyond which the theorem cannot guarantee the tolerance to be met. This observation has also been made in studies of open systems in, for example, [46, 47, 48, 58].

4. If there is a great deal of noise, and thus d_1 is large, the constant term (with respect to τ) could become as large as $\mathcal{O}(1)$ and there could be *no* running time for the adiabatic algorithm which results in an accurate calculation.

We are also interested in a lower bound on the error of the adiabatic approximation in the presence of noise. A lower bound could be used to prove that a certain amount of noise was unacceptable for AQC, because it would guarantee failure of the algorithm for some level of noise. However, it will be difficult to get a non-trivial lower bound, since there are time-dependent perturbations which yield *zero* error in the adiabatic

approximation, better than might exist without the perturbation. To see this, define

$$\mathcal{H}_A(s) = \mathcal{H}(s) + i/\tau[\dot{P}(s), P(s)] \,, \tag{3.74}$$

where the term $i/\tau[\dot{P}(s), P(s)]$ is the perturbation. We proved in Theorem 2.4.1 that the evolution of $\mathcal{H}_A(s)$ satisfies

$$U_A(s)P(0) = P(s)U_A(s) \,, \tag{3.75}$$

where $U_A(s)$ is the unitary operator associated with $\mathcal{H}_A(s)$, and $P(s)$ is the projection onto the ground state of $\mathcal{H}(s)$. Then

$$\begin{aligned} Q(s)U_A(s)P(0) &= Q(s)U_A(s)P(0) & (3.76)\\ &= Q(s)P(s)U_A(s) & (3.77)\\ &= 0 \,, & (3.78) \end{aligned}$$

since $Q(s)P(s) = 0$, so the adiabatic approximation is perfect for $\mathcal{H}(s)$ if the perturbation term $i/\tau[\dot{P}(s), P(s)]$ is added to it. Notice further that the perturbation gets arbitrarily small as τ grows.

Finally, we also observe that noise that commutes with the Hamiltonian does not cause any state transitions, because it has no effect on the eigenstates - in other words, it causes no coupling between states. For instance, consider the Hamiltonian on N particles

$$\mathcal{H}(s) = M(s) \sum_{j=1}^{N} \sigma_j^z \,, \tag{3.79}$$

where $M(s)$ is a real scalar function representing a time-dependent applied magnetic field. Noise in the magnetic field $M(s)$ results in a perturbation that commutes with $\mathcal{H}(s)$, and has no effect on the error of the adiabatic approximation.

3.3 Application to the spin-1/2 particle in a rotating magnetic field

Recently Tong *et al.* [60] presented an example of a Hamiltonian evolution for which the adiabatic approximation performs poorly. The Hamiltonian is for a spin-1/2 particle in a rotating magnetic field. Here we apply AT-Noise to their example. Their evolving Hamiltonian is

$$\mathcal{H}(t) = -\frac{\omega_0}{2}\left(\sigma^x \sin\theta\cos\omega t + \sigma^y \sin\theta \sin\omega t + \sigma^z \cos\theta\right) \ , \tag{3.80}$$

which we represent in the basis where σ^z is diagonal as

$$\mathcal{H}(t) = -\frac{\omega_0}{2}\begin{pmatrix} \cos\theta & e^{-i\omega t}\sin\theta \\ e^{i\omega t}\sin\theta & -\cos\theta \end{pmatrix} \ . \tag{3.81}$$

Suppose θ is small. We can think of the time-independent diagonal component of the Hamiltonian as the intended Hamiltonian, and the wobbling off-diagonal component as a noise term operating on an independent timescale.

The eigenstates of $\mathcal{H}(t)$ depend on t, but the eigenvalues do not. So the energy gap is constant and in fact equal to ω_0. Thus one might think that the adiabatic approximation works well, predicting that a particle starting out in the spin-down state stays in the spin-down state under this Hamiltonian evolution.

We will see below that if the wobble is at a resonant frequency with respect to the energy difference between the spin-up and spin-down states, the wobble induces a complete transition from the spin-down to spin-up state. So the adiabatic approximation eventually fails in the most complete sense possible in this example. However, we will also see that the AT-Noise correctly provides an *increasing* error bound with time, because the s-derivatives in this example increase with τ.

We can rewrite the Hamiltonian using $t = s\tau$ as

$$\mathcal{H}_\tau(s) = -\frac{\omega_0}{2}\begin{pmatrix} \cos\theta & e^{-i\omega s\tau}\sin\theta \\ e^{i\omega s\tau}\sin\theta & -\cos\theta \end{pmatrix} . \tag{3.82}$$

We can also compute the first two derivatives:

$$\frac{d}{ds}\mathcal{H}_\tau(s) = -\frac{\omega\omega_0\tau\sin\theta}{2}\begin{pmatrix} 0 & -ie^{-i\omega s\tau} \\ ie^{i\omega s\tau} & 0 \end{pmatrix} , \tag{3.83}$$

and

$$\frac{d^2}{ds^2}\mathcal{H}_\tau(s) = \frac{\omega^2\omega_0\tau^2\sin\theta}{2}\begin{pmatrix} 0 & -e^{-i\omega s\tau} \\ e^{i\omega s\tau} & 0 \end{pmatrix} . \tag{3.84}$$

We can compute the norms of these matrices exactly, giving

$$\mathcal{H}_\tau^\dagger(s)\mathcal{H}_\tau(s) = \frac{\omega_0^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \tag{3.85}$$

$$\left(\frac{d\mathcal{H}_\tau(s)}{ds}\right)^\dagger\left(\frac{d\mathcal{H}_\tau(s)}{ds}\right) = -\frac{\omega^2\omega_0^2\tau^2\sin^2\theta}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \tag{3.86}$$

and

$$\left(\frac{d^2\mathcal{H}_\tau(s)}{ds^2}\right)^\dagger\left(\frac{d^2\mathcal{H}_\tau(s)}{ds^2}\right) = -\frac{\omega^4\omega_0^2\tau^4\sin^2\theta}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{3.87}$$

Thus we can write

$$\left|\left|\frac{d^k}{ds^k}\mathcal{H}_\tau(s)\right|\right| \leq \frac{|\omega_0|}{2}\left(1 + |\omega\sin\theta|\,\tau + \omega^2\,|\sin\theta|\,\tau^2\right) , \tag{3.88}$$

for $s \in [0,1]$ and for $k = 0, 1, 2$. Also, $\gamma_\tau(s) = \omega_0$ for any s, τ [60], so we let $\bar{\gamma}_{noise} = \omega_0$.

Schrödinger's equation can also be solved exactly for the Hamiltonian in Equation (3.82). Define $\bar{\omega} = \sqrt{\omega_0^2 + \omega^2 + 2\omega_0\omega\cos\theta}$. From Tong *et al.* [60] the unitary time evolution operator for this system is

$$U_\tau(t) = \begin{pmatrix} \left(\cos\left(\frac{\bar{\omega}t}{2}\right) + i\frac{\omega+\omega_0\cos\theta}{\bar{\omega}}\sin\left(\frac{\bar{\omega}t}{2}\right)\right)e^{-i\omega t/2} & i\frac{\omega_0\sin\theta}{\bar{\omega}}\sin\left(\frac{\bar{\omega}t}{2}\right)e^{-i\omega t/2} \\ i\frac{\omega_0\sin\theta}{\bar{\omega}}\sin\left(\frac{\bar{\omega}t}{2}\right)e^{i\omega t/2} & \left(\cos\left(\frac{\bar{\omega}t}{2}\right) - i\frac{\omega+\omega_0\cos\theta}{\bar{\omega}}\sin\left(\frac{\bar{\omega}t}{2}\right)\right)e^{i\omega t/2} \end{pmatrix}. \tag{3.89}$$

Therefore the error operator for the adiabatic approximation is

$$Q(t)U_\tau(t)P(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} U_\tau(t) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{3.90}$$

$$= \begin{pmatrix} 0 & 0 \\ i\frac{\omega_0\sin\theta}{\bar{\omega}}\sin\left(\frac{\bar{\omega}t}{2}\right)e^{i\omega t/2} & 0 \end{pmatrix}, \tag{3.91}$$

so

$$||Q(t)U_\tau(t)P(0)|| = \left|\frac{\omega_0\sin\theta}{\bar{\omega}}\sin\left(\frac{\bar{\omega}t}{2}\right)\right|. \tag{3.92}$$

If the perturbation is resonant, then $\omega = -\omega_0\cos\theta$ so $\bar{\omega} = |\omega_0|\sin\theta$. Then we have

$$||Q(t)U_\tau(t)P(0)|| = \left|\sin\left(\frac{\omega_0\sin(\theta)t}{2}\right)\right|. \tag{3.93}$$

As an example, assume that $\theta = 0.001$, $\omega = 10\ \mu\text{s}^{-1}$, $\omega_0 = -10\ \mu\text{s}^{-1}$. Let $\chi(\tau)$ be the error bound defined by the adiabatic theorem. Then we can calculate $||P_\tau(s) - P(s)||$ exactly to get $\delta_0 = \delta_1 = 0.0005$, and so we have

$$\chi(\tau) = 0.00900025 + (0.04\ \mu\text{s}^{-1})\cdot\tau \tag{3.94}$$

and

$$||Q(s)U_\tau(s)P(0)|| = \left|\sin((0.005\ \mu\text{s}^{-1})\cdot s\tau)\right|. \tag{3.95}$$

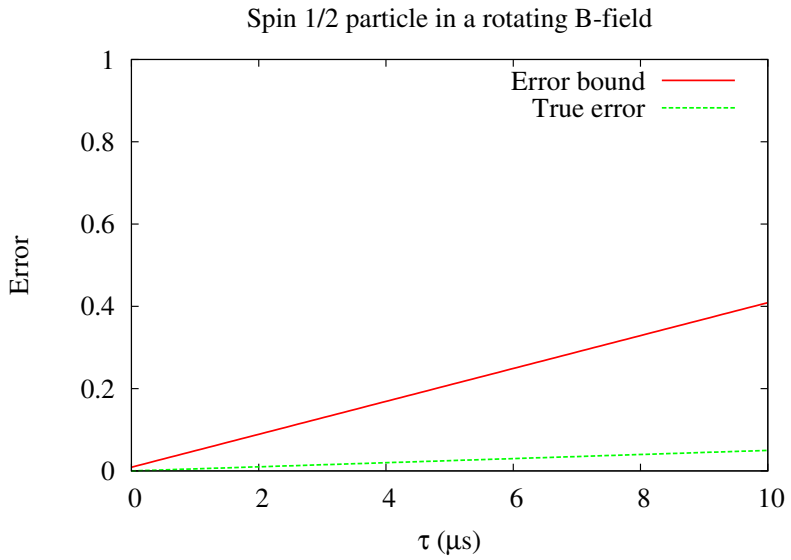

Figure 3.1: A plot of the error bound $\chi(\tau)$ for parameters $\theta = 0.001$, $\omega = 10\ \mu\text{s}^{-1}$, and $\omega_0 = -10\ \mu\text{s}^{-1}$, compared to the true error for the Tong *et al.* [60] example. We can see that the adiabatic approximation gets worse as τ gets larger, as observed by Tong *et al.* [60]. However, our error bound from AT-Noise remains valid.

Figure 3.1 illustrates our result. Not only is the bound consistent with the true error, it has the same qualitative behavior, increasing linearly with τ.

3.4 Application to a superconducting flux qubit

Next we apply AT-Noise to the superconducting flux qubit of Orlando et al. [40], proposed for use in adiabatic quantum computation [28]. With this qubit, the adiabatic evolution may be as simple as monotonically varying an applied magnetic field.

Consider the four-junction qubit shown in Figure 3.2. We will follow the analysis of Orlando *et al.* [40]. The dynamical variables are the phases ϕ_i across the four Josephson junctions, however flux quantization in each loop gives us two constraints: $\phi_1 - \phi_2 + \phi_3 = -2\pi f_1$ and $\phi_4 - \phi_3 = -2\pi f_2$, where f_1 and f_2 are the magnetic

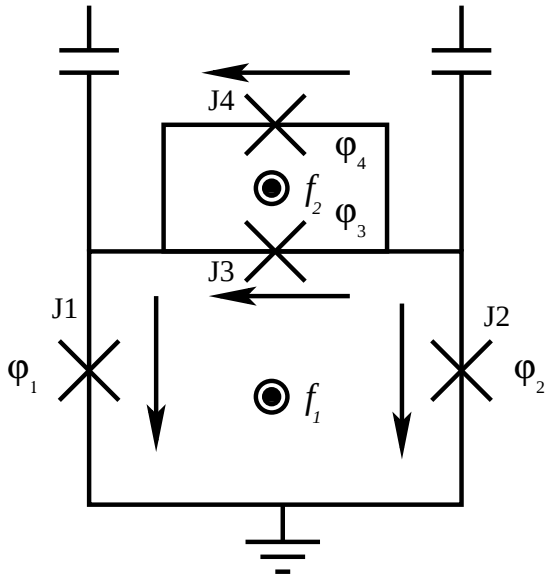

Figure 3.2: (Adapted from Orlando *et al.* [40]) The circuit schematic for the superconducting flux qubit. The X's represent Josephson junctions, and the main qubit loop is formed by junctions J1, J2, and J3. Junction J4 allows tuning of the effective properties of junction J2 through control of the frustration f_2.

frustrations in each loop. So there are two degrees of freedom, which we define as $\phi_p = (\phi_1 + \phi_2)/2$ and $\phi_m = (\phi_1 - \phi_2)/2$, where $f_a = f_2$, and $f_b = f_1 + f_2/2$. Then the Hamiltonian can be written as

$$\mathcal{H} = -\frac{\hbar^2}{2M_p}\frac{\partial^2}{\partial\phi_p^2} - \frac{\hbar^2}{2M_m}\frac{\partial^2}{\partial\phi_m^2} + U(\phi_p, \phi_m) \ , \tag{3.96}$$

where M_p and M_m are constants, and the potential $U(\phi_p, \phi_m)$ is defined as

$$U(\phi_p, \phi_m) = E_J \left[2 + 2\beta - 2\cos(\phi_p)\cos(\phi_m) - 2\beta\cos(\pi f_a)\cos(2\pi f_b + 2\phi_m)\right] \ , \tag{3.97}$$

where E_J and β are constants.

At $f_1 = f_2 = 1/3$, we have $f_b = 1/2$ and $f_a = 1/3$, and $U(\phi_p, \phi_m)$ has minima, or *wells*, at $\phi_p = 0$ and $\phi_m = \pm\cos^{-1}(\beta/2)$, symmetric about the ϕ_p axis. By varying f_1 and f_2, we can tilt the potential so that one well is deeper than the other, and we can adjust the barrier height. We can approximate the Hamiltonian with a two-state

system. A Hamiltonian evolution that begins at the degeneracy point and varies f_1 can can be written:

$$\mathcal{H}(s) = -t_1\sigma^x + s\epsilon r_1\sigma^z \ , \tag{3.98}$$

where t_1 and r_1 are parameters that can be estimated with the WKB approximation. For the qubit parameters recommended by Orlando et al. [40], $r_1 = 4.8E_J$ and $t_1 = 10^{-3}E_J$, where E_J is a constant. A typical value for E_J is $(200\text{ GHz}) \cdot h = (1.256 \cdot 10^6\ \mu\text{s}^{-1}) \cdot \hbar$. We choose $\epsilon = -.0002$, so that the Hamiltonian changes from proportional to σ^x at $s = 0$ to equally-weighted σ^x and σ^z terms at $s = 1$, because this seems a natural milestone in the evolution to the σ^z-dominated final Hamiltonian.

There are a couple of sources of noise in this qubit. One source of noise in a superconducting flux qubit is noise in the critical current of the Josephson junctions [67], which decreases as $1/T$ where T is temperature. Such noise would result in variations in the weights of the terms in Equation (3.97). Another source is noise in the magnetic flux bias generated by nearby current-carrying wires on the chip. Current carrying wires could be used for nearby measurement devices or to perform a gate operation on the qubit with an RF pulse. Since we have from above a two-state Hamiltonian parametrized by flux bias, we consider this latter noise. Orlando *et al.* [40] estimated that a nearby wire of typical dimensions and carrying 100nA current would cause a difference in either f_1 or f_2 of $\Delta f = 10^{-7}$. Let us assume that there is there is approximately 0.5 nA of noise on the wire introduced by the current source. Further suppose the power of the noise scales as inverse frequency $1/\nu$ from $\nu_{min} = 2.5$ GHz to $\nu_{max} = 3.5$ GHz, so that we include the qubit frequencies

throughout the evolution.

There are clever means of simulating $1/\nu$ noise with discrete models, such as by summing independent bistable fluctuators (a.k.a. Random Telegraph Noise) [17]. However, this results in non-differentiable Hamiltonians so is not appropriate for us. Instead, suppose we want to write down a formula for a noise source with $1/\nu$ power spectrum in the range ν_{min} to ν_{max}. Let n be an integer, with $n = 100$ in the following example. Define $\Delta\nu = (\nu_{max} - \nu_{min})/n$ and $\nu_j = \nu_{min} + j\Delta\nu$ for $j = 1 \ldots n$. Then we can define two independent noise functions, representing variation in the magnetic frustration in our qubit, as

$$\mathcal{N}_1(t) = C \sum_{j=1}^{n} \frac{\cos(2\pi\nu_j t + \xi_{1,j})\Delta\nu}{\sqrt{\nu_j}} \,, \tag{3.99}$$

$$\mathcal{N}_2(t) = C \sum_{j=1}^{n} \frac{\cos(2\pi\nu_j t + \xi_{2,j})\Delta\nu}{\sqrt{\nu_j}} \,, \tag{3.100}$$

where $\xi_{1,j}$ and $\xi_{2,j}$ are phase factors chosen uniformly at random and $C = 10^{-10}$ MHz$^{-1/2}$, chosen to agree with the 0.5 nA noise. The Hamiltonian for noise in the magnetic frustration is

$$\mathcal{H}_{noise}(t) = \mathcal{N}_1(t) r_1 \sigma^z + N_2(t)(r_2\sigma^z - w\sigma^x) \,, \tag{3.101}$$

where $w = 2.4E_J$ for the chosen qubit parameters.

Evaluating the functions numerically over an interval much larger than the longest wavelength reveals the bounds $|\mathcal{N}_i(t)| \leq 4.9100 \cdot 10^{-10}$, $\left|\dot{\mathcal{N}}_i(t)\right| \leq 9.1100 \cdot 10^{-6}$ μs^{-1}, and $\left|\ddot{\mathcal{N}}_i(t)\right| \leq 0.1667$ μs^{-2}.

Recalling that $t = s\tau$, where s is unitless, we are ready to compute derivatives

and norms of the whole Hamiltonian:

$$\mathcal{H}_\tau(s) = \mathcal{H}(s) + \mathcal{H}_{noise}(s\tau) \tag{3.102}$$

$$= -t_1\sigma^x + sr_1\epsilon\sigma^z + \mathcal{N}_1(t)r_1\sigma^z + \mathcal{N}_2(t)\left(r_2\sigma^z - w\sigma^x\right) \ , \tag{3.103}$$

$$\left|\left|\dot{\mathcal{H}}_\tau(s)\right|\right| = \left|\left|r_1\epsilon\sigma^z + \tau\frac{d}{dt}\mathcal{N}_1(t)r_1\sigma^z + \tau\frac{d}{dt}\mathcal{N}_2(t)(r_2\sigma^z - w\sigma^x)\right|\right| \tag{3.104}$$

$$\leq (1206.4\ \mu\text{s}^{-1}) + \tau\cdot(84.7149\ \mu\text{s}^{-2}) \ , \tag{3.105}$$

$$\left|\left|\ddot{\mathcal{H}}_\tau(s)\right|\right| = \left|\left|\tau^2\frac{d^2}{dt^2}\mathcal{N}_1(t)r_1\sigma^z + \tau^2\frac{d^2}{dt^2}\mathcal{N}_2(t)(r_2\sigma^z - w\sigma^x)\right|\right| \tag{3.106}$$

$$\leq \tau^2\ (1.5502\cdot 10^6\ \mu\text{s}^{-3}) \ . \tag{3.107}$$

Observe that since s is unitless, $\mathcal{H}(s)$ and its s-derivatives all have units of energy, but since $\hbar = 1$, energy units are inverse time units.

We also need to compute the minimum energy gap. In this case, it occurs at $s = 0$, and the energy gap is $\bar{\gamma}_{noise} = 2t_1 = 2513\ \mu\text{s}^{-1}$.

Finally, we need to find δ_0 and δ_1. We compute the projection operators directly and obtain the bounds $\delta_0 = 1.800\cdot 10^{-6}$ and $\delta_1 = 9.117\cdot 10^{-7}$. From AT-Noise, we have

$$||Q_\tau(s)U_\tau(s)P(0,\tau)|| \leq (1.9634\ \mu\text{s}^{-1})\cdot\tau + 0.0019 + \frac{(0.0148\ \mu\text{s})}{\tau} \ . \tag{3.108}$$

This generates a hyperbolic curve with a vertical asymptote at $\tau = 0$ and a linear asymptote for large τ, shown in Figure 3.3. Recall this curve represents the norm of the error operator and its square represents the probability of error in this system.

To check our results, we would like to compute the error of the adiabatic approximation numerically. However efficient numerical simulation of this system requires

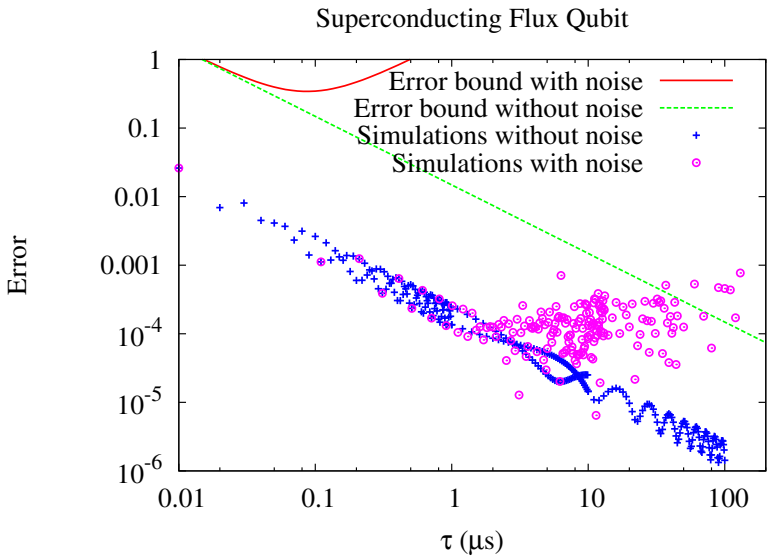

Figure 3.3: A plot of the error bound $\chi(\tau)$ for the superconducting flux qubit example. The crosses represent results of numerical simulations of the error. Since the noise commutes with the dominant term in the final Hamiltonian, the bound is a substantial overestimate. Nonetheless the qualitative shape between the bound curve and the simulation data agree.

some care. A straightforward solution to Schrödinger's equation

$$i\frac{d}{dt}|\psi(t)\rangle = \mathcal{H}_\tau(t/\tau)|\psi(t)\rangle \tag{3.109}$$

will have rapidly oscillating phases that make the solutions very unstable and time-consuming to compute. Instead, we will rewrite Schrödinger's equation for this system in a basis whose phase rotates with time.

To begin, we choose a time-dependent eigenbasis of $\mathcal{H}_\tau(t/\tau)$ with the property $\langle\phi_n(t)|\dot{\phi}_n(t)\rangle = 0$.

Lemma 3.4.1. *There is a time dependent eigenbasis* $\{|\phi_n(t)\rangle\}$ *with the property that* $\langle\phi_n(t)|\dot{\phi}_n(t)\rangle = 0$ *for all* n *[10].*

Proof. Suppose $\{|\phi_n(t)\rangle\}$ does not have this property. Then for each n, define the

variable $\xi_n(t)$ as follows:

$$\xi_n(t) = i \int_0^t \langle \phi_n(w) | \dot{\phi}_n(w) \rangle dw \ , \tag{3.110}$$

and let

$$|\alpha_n(t)\rangle = e^{i\xi_n(t)} |\phi_n(t)\rangle \ . \tag{3.111}$$

Then $\{|\alpha_n(t)\rangle\}$ has the desired property. To see this, we simply compute it:

$$\langle \alpha_n(t) | \dot{\alpha_n}(t) \rangle = \langle \phi_n(t) | e^{-i\xi_n(t)} \left[i\dot{\xi}_n(t) e^{i\xi_n(t)} |\phi_n(t)\rangle + e^{i\xi_n(t)} |\dot{\phi}_n(t)\rangle \right] \tag{3.112}$$

$$= i\dot{\xi}_n(t) + \langle \phi_n(t) | \dot{\phi}_n(t) \rangle \tag{3.113}$$

$$= i \cdot i \langle \phi_n(t) | \dot{\phi}_n(t) \rangle + \langle \phi_n(t) | \dot{\phi}_n(t) \rangle \tag{3.114}$$

$$= 0 \ . \tag{3.115}$$

□

Let us write the solution $|\psi(t)\rangle$ in terms of the basis states $|\phi_n(t)\rangle$ with energies $E_n(t)$ as follows:

$$|\psi(t)\rangle = \sum_n c_n(t) e^{-i\int_0^t E_n(w)dw} |\phi_n(t)\rangle \ . \tag{3.116}$$

Then in the case of two states, assuming the eigenstates are labeled in increasing order with respect to their eigenvalues, the norm of the adiabatic error operator is simply $|c_1(t)|$.

Let us substitute the representation in Equation (3.116) into Schrödinger's equation (Equation (3.109)), and left multiply by $\langle \phi_m(t)|$. After simplification, this yields

$$\dot{c}_m(t) = -\sum_n c_n(t) e^{-i\int_0^t (E_n(w) - E_m(w))dw} \langle \phi_m(t) | \dot{\phi}_n(t) \rangle \ . \tag{3.117}$$

Evidently the $n = m$ term in the sum is zero in the chosen basis.

Since we have

$$\mathcal{H}_\tau(t/\tau) = (-t_1 - \mathcal{N}_2(t)s_2)\,\sigma^x + \left(\frac{t\ r_1\ \epsilon}{\tau} + \mathcal{N}_1(t)r_1 + \mathcal{N}_2(t)r_2\right)\sigma^z\ , \tag{3.118}$$

if we define

$$a(t) = -t_1 - \mathcal{N}_2(t)s_2\ , \tag{3.119}$$

$$b(t) = \frac{t\ r_1\ \epsilon}{\tau} + \mathcal{N}_1(t)r_1 + \mathcal{N}_2(t)r_2\ , \tag{3.120}$$

$$\theta(t) = \cot^{-1}\left(\frac{b(t)}{a(t)}\right)\ , \tag{3.121}$$

then we can diagonalize the Hamiltonian easily in terms of $a(t)$ and $b(t)$. We choose the cotangent for numerical stability because $b(0) \approx 0$. Then

$$E_0(t) = -\sqrt{a^2(t) + b^2(t)}\ , \qquad E_1(t) = \sqrt{a^2(t) + b^2(t)}\ , \tag{3.122}$$

$$|\phi_0(t)\rangle = \begin{pmatrix} -\sin\left(\frac{\theta(t)}{2}\right) \\ \cos\left(\frac{\theta(t)}{2}\right) \end{pmatrix}\ , \qquad |\phi_1(t)\rangle = \begin{pmatrix} \cos\left(\frac{\theta(t)}{2}\right) \\ \sin\left(\frac{\theta(t)}{2}\right) \end{pmatrix}\ . \tag{3.123}$$

It is easy to check that $\langle\phi_0(t)|\dot{\phi}_0(t)\rangle = \langle\phi_1(t)|\dot{\phi}_1(t)\rangle = 0$. Now, we would like to compute $\langle\phi_0(t)|\dot{\phi}_1(t)\rangle$ and $\langle\phi_1(t)|\dot{\phi}_0(t)\rangle$:

$$\langle\phi_0(t)|\dot{\phi}_1(t)\rangle = \begin{pmatrix} -\sin\left(\frac{\theta(t)}{2}\right) \\ \cos\left(\frac{\theta(t)}{2}\right) \end{pmatrix}^\dagger \begin{pmatrix} -\frac{1}{2}\sin\left(\frac{\theta(t)}{2}\right)\dot{\theta}(t) \\ \frac{1}{2}\cos\left(\frac{\theta(t)}{2}\right)\dot{\theta}(t) \end{pmatrix} \tag{3.124}$$

$$= \frac{\dot{\theta}(t)}{2}\ , \tag{3.125}$$

$$\langle\phi_1(t)|\dot{\phi}_0(t)\rangle = \begin{pmatrix} \cos\left(\frac{\theta(t)}{2}\right) \\ \sin\left(\frac{\theta(t)}{2}\right) \end{pmatrix}^\dagger \begin{pmatrix} -\frac{1}{2}\cos\left(\frac{\theta(t)}{2}\right)\dot{\theta}(t) \\ -\frac{1}{2}\sin\left(\frac{\theta(t)}{2}\right)\dot{\theta}(t) \end{pmatrix} \tag{3.126}$$

$$= -\frac{\dot{\theta}(t)}{2}\ . \tag{3.127}$$

It remains to compute $\dot{\theta}(t)$, which can be done with implicit differentiation:

$$\cot(\theta(t)) = \frac{b(t)}{a(t)} \,, \tag{3.128}$$

$$-\csc^2(\theta(t))\dot{\theta}(t) = \frac{\dot{b}(t)a(t) - b(t)\dot{a}(t)}{a^2(t)} \,, \tag{3.129}$$

$$\dot{\theta}(t) = \sin^2(\theta(t))\frac{\dot{a}(t)b(t) - a(t)\dot{b}(t)}{a^2(t)} \tag{3.130}$$

$$= \frac{a^2(t)}{a^2(t) + b^2(t)}\frac{\dot{a}(t)b(t) - a(t)\dot{b}(t)}{a^2(t)} \tag{3.131}$$

$$= \frac{\dot{a}(t)b(t) - a(t)\dot{b}(t)}{a^2(t) + b^2(t)} \,. \tag{3.132}$$

Finally, the equations of motion are

$$\dot{c}_0(t) = -c_1(t)e^{-2i\int_0^t \sqrt{a^2(w)+b^2(w)}dw}\frac{\dot{\theta}(t)}{2} \,, \tag{3.133}$$

$$\dot{c}_1(t) = c_0(t)e^{2i\int_0^t \sqrt{a^2(w)+b^2(w)}dw}\frac{\dot{\theta}(t)}{2} \,. \tag{3.134}$$

We provide these equations to a differential equation solver, ode23, in Matlab. Care must be taken with the integral in the exponent. We need not recompute the integral entirely at each time; rather we cache the intermediate values of this integral. Thus at each evaluation we only integrate on the interval from the last cached time to the current time.

This method was used to produce the numeric results in Figure 3.3. The parameters of the system are those previously described in the example. There are 571 noiseless data points and 125 noisy data points. A new set of random phases was generated for each noisy point, and each point took up to 5.5 CPU hours to compute. The workstation used had dual Xeon 3.06 GHZ processors with hyperthreading enabled (thus four effective CPUs) and 6GB of RAM, running Red Hat Enterprise 3.

The simulation data in Figure 3.3 is several orders of magnitude less than the bound. The fact that the bound is an overestimate is not surprising since the noise term commutes with the dominant term in the final Hamiltonian of the evolution. However the qualitative shape between the bound curve and the simulation data is the same, and the bound does provide a simulation-free guarantee of error for an interval of τ.

In the bounds on the error of the adiabatic approximation in the preceding sections, the minimum evolution time τ required to guarantee a given error tolerance, if any evolution time achieves the tolerance, is a polynomial in $1/\gamma$, where γ is the minimum ground-state energy gap. Evidently if γ is exponentially small in the number of qubits, then the required evolution time is exponentially long.

Since a typical Hamiltonian of n qubits must fit 2^n energy levels into a polynomial-sized energy range, most energy gaps must be exponentially small, and it is not clear *a priori* why the ground-state energy gap should ever be larger than the rest. In the following chapters we identify new classes of Hamiltonians and Hamiltonian evolutions with large ground-state energy gaps.

Chapter 4

Clifford Algebras and the Jordan-Wigner Transformation

We begin our search for Hamiltonians evolutions with large ground-state energy gaps with understanding the analysis of the one-dimensional Ising model. In Section 4.1, we review facts about Clifford algebras, which we use as a framework to understand Pauli operators in Section 4.2. Also in that framework we introduce the Fermionic commutation relations (FCRs) and their properties in Section 4.3, and the Jordan-Wigner transform in Section 4.4. Finally, in Section 4.5 we show how to use the tools developed in this chapter to analyze the one-dimensional Ising model.

4.1 Clifford algebras

Operators on two-state interacting particles, or qubits, can be described using Clifford algebras. We begin with an introduction to Clifford algebras, closely following [25, p. 179]. Let $\{g_1, \ldots, g_L\}$ be a set of L elements, which we identify as generators, satisfying the following anti-commutation relation:

$$\{g_i, g_j\} = g_i g_j + g_j g_i = 2Q_{i,j} \ , \tag{4.1}$$

where Q is an $L \times L$ matrix. Usually we will take $Q = I_L$ but sometimes, if $L = 2n$, we consider

$$Q = Q_n^F \equiv \frac{1}{2} \begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix} \ . \tag{4.2}$$

We can take products of these generators, and for either choice of Q we can use Equation (4.1) to simplify the results so that in each product, the generators appear in order of increasing index, and no generator occurs twice in any product. Evidently there are 2^L linearly-independent products; let us label them $\{e_1, \ldots, e_{2^L}\}$. The usual *Clifford algebra* C_L is the 2^L-dimensional vector space

$$C_L(Q) = \left\{ \sum_{j=1}^{2^L} A_j e_j \ : \ A_j \in \mathbf{R} \right\} . \tag{4.3}$$

It is an algebra as well as a vector space, because we can multiply elements. However, in this setting, it will be easier to instead consider the complexification:

$$Cl_L(Q) = \left\{ \sum_{j=1}^{2^L} A_j e_j \ : \ A_j \in \mathbf{C} \right\} , \tag{4.4}$$

as in [65].

4.2 Pauli operators and the standard model

Define the *Pauli operators* σ^x and σ^y by their standard matrix representation:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad\qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} . \tag{4.5}$$

If we take these as generators, $g_1 = \sigma^x$ and $g_2 = \sigma^y$, then Equation (4.1) is satisfied with $Q = I_2$. There are 2^2 linearly independent products of g_1 and g_2, namely I, σ^x, σ^y, and $\sigma^x\sigma^y$, thus defining a four-dimensional vector space. Let us define $\sigma^z = -i\sigma^x\sigma^y$, with matrix representation

$$\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{4.6}$$

Since we are working in a complex vector space, we could instead use I, σ^x, σ^y, and σ^z as a basis for the vector space.

One consequence of Equation (4.1) and the definition of σ^z that we will need frequently is

$$(\sigma^z)^2 = (-i\sigma^x\sigma^y)(-i\sigma^x\sigma^y) \tag{4.7}$$

$$= -\sigma^x\sigma^y\sigma^x\sigma^y \tag{4.8}$$

$$= (\sigma^x\sigma^x)(\sigma^y\sigma^y) \tag{4.9}$$

$$= I\ . \tag{4.10}$$

A more general identity that we can derive from Equation (4.1) and the definition of σ^z is, for α, β, and γ distinct,

$$\sigma^\alpha\sigma^\beta = i\epsilon_{\alpha\beta\gamma}\sigma^\gamma\ , \tag{4.11}$$

where $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol defined here as

$$\epsilon_{\alpha\beta\gamma} = \begin{cases} +1 & \text{when } (\alpha,\beta,\gamma) \text{ is a cyclic permutation of } (x,y,z) \\ -1 & \text{otherwise} \end{cases}\ . \tag{4.12}$$

Referring to (4.4), we then define the *standard model*, or the algebra of Pauli operators on n qubits, as $Cl_2(I_2)^{\otimes n}$, and label the generators σ_j^x, σ_j^y, etc. for $j = 1 \ldots n$. Because of the basic properties of Kronecker products, we have the useful fact that Pauli operators on different qubits commute:

$$\left[\sigma_j^\alpha, \sigma_k^\beta\right] = 0\ , \tag{4.13}$$

for $j \neq k$ and $\alpha, \beta \in \{x, y, z\}$. The algebra of Pauli operators is a common algebra used to describe Hamiltonians or gate operations in quantum computing.

4.3 Fermi operators

Another kind of particle operators, *Fermi operators*, generate $Cl_{2n}(Q_n^F)$. The first n generators we will label $\{c_j : \ j = 1 \ldots n\}$, and for the remaining generators we will take $\{c_j^\dagger : \ j = 1 \ldots n\}$. Equation 4.1 with $Q = Q_n^F$ represents a set of equations known as the the *Fermionic commutation relations* (FCRs), which can be written:

$$\{c_j, c_k^\dagger\} = \delta_{j,k} \ , \qquad\qquad \{c_j, c_k\} = 0 \ . \tag{4.14}$$

Operators obeying the FCRs have many useful properties. Our presentation is inspired by an excellent posting in Michael Nielsen's blog [37]; see also [9].

The following observations about Fermi operators are essential to the rest of the discussion and follow from (4.14):

Property 1: $(c_j^\dagger c_j)^2 = c_j^\dagger c_j$, and so the only eigenvalues of $c_j^\dagger c_j$ are zero and one.

Property 2: $c_j^\dagger$ is a "raising" operator for $c_j^\dagger c_j$, since if $|\psi\rangle$ is an eigenstate of $c_j^\dagger c_j$ with zero eigenvalue, then $c_j^\dagger|\psi\rangle$ is an eigenstate of $c_j^\dagger c_j$ with unit eigenvalue.

Property 3: For *any* state $|\psi\rangle$, the state $c_j|\psi\rangle$ is an eigenstate of $c_j^\dagger c_j$ with zero eigenvalue, since $c_j^2 = 0$. Thus c_j is a "lowering" operator for $c_j^\dagger c_j$.

Property 4: If $k \neq j$ and $|\psi\rangle$ is an eigenstate of $c_j^\dagger c_j$, then $c_k|\psi\rangle$ and $c_k^\dagger|\psi\rangle$ are also eigenstates of $c_j^\dagger c_j$ with the same eigenvalue.

Property 5: If $c_j^\dagger c_j|\psi\rangle = 0$, then using $c_j^2 = 0$ we can show $c_j|\psi\rangle = 0$.

Property 6: If $c_j^\dagger c_j|\psi\rangle = |\psi\rangle$, then using $(c_j^\dagger)^2 = 0$ it is clear $c_j^\dagger|\psi\rangle = 0$.

Property 7: $[c_j^\dagger c_j, c_k^\dagger c_k] = 0$, where the bracket notation indicates the commutator: $[a, b] = ab - ba$. Thus there is a basis for the Hilbert space on which these operate where each basis state is an eigenstate of $c_j^\dagger c_j$ for all j.

Property 8: By Property 7, we can find a state $|\psi\rangle$ that is an eigenstate of $c_j^\dagger c_j$ for all j. Suppose $c_j^\dagger c_j|\psi\rangle = |\psi\rangle$, and define $|\psi'\rangle = c_j|\psi\rangle$. By Property 4, $|\psi'\rangle$ has the same eigenvalue as $|\psi\rangle$ for $c_k^\dagger c_k$ for $k \neq j$, but by Property 3, $c_j^\dagger c_j|\psi'\rangle = 0$. Now, pick a subset of indices $\{k_1, k_2, k_3 \dots\}$, and define

$$|\phi\rangle = c_{k_1}^{(\dagger)} c_{k_2}^{(\dagger)} c_{k_3}^{(\dagger)} \dots |\psi\rangle \ , \tag{4.15}$$

where there is a † on c_{k_l} if and only if $c_{k_l}^\dagger c_{k_l}|\psi\rangle = 0$. Then, using Properties 2, 3, and 4, we conclude that $|\phi\rangle$ is also an eigenstate of $c_j^\dagger c_j$ for all j, but it has different eigenvalues than $|\psi\rangle$ for $c_{k_1}^\dagger c_{k_1}$, $c_{k_2}^\dagger c_{k_2}$, etc. We could have picked any of the 2^n subsets of indices, and each subset results in a state with different combinations of eigenvalues.

Sometimes it is convenient to think of these states as representing a binary configuration with n sites, where site j is "occupied" in state $|\phi\rangle$ if $c_j^\dagger c_j|\phi\rangle = |\phi\rangle$, and site j is "unoccupied" if $c_j^\dagger c_j|\phi\rangle = 0$. Therefore we call this basis the Fermi occupation basis. It is a complete basis if there are no other quantum particles in the system, and in that case it is unique up to phase.

Suppose we have a Hamiltonian of the form

$$\mathcal{H} = \sum_{j=1}^{n} C_j c_j^\dagger c_j \ , \tag{4.16}$$

where the coefficients C_j are real. Evidently the 2^n states in the Fermi occupation basis are all eigenstates of $\mathcal{H}$. The eigenvalue of $\mathcal{H}$ corresponding to a state $|\phi\rangle$ can be obtained by summing a subset of the coefficients, where C_j is included in the sum provided site j is "occupied" in $|\phi\rangle$. Further, if $C_j \geq 0$ for all j, then the ground-state energy of $\mathcal{H}$ is zero, and the first excited state energy is the least positive coefficient. To decide whether an arbitrary value is an eigenvalue of $\mathcal{H}$ for arbitrary coefficients is NP-complete however, as it is equivalent to the subset-sum problem (also known as the knapsack problem) [37].

A critical property of FCRs that will help us shoehorn Hamiltonians of interest into Equation (4.16) is that the FCRs are preserved through certain unitary transformations. We can think of these transformations as the symmetries of the bilinear form Q_n^F.

Theorem 4.3.1 (Unitary transformations)**.** *Suppose the operators* $\{c_j : \ j = 1, \ldots, n\}$ *obey the FCRs. Let*

$$T = \begin{pmatrix} U & V \\ V & U \end{pmatrix}, \tag{4.17}$$

where U *and* V *are real* $n \times n$ *matrices, and suppose* T *is unitary. Define the set of*

operators $\{\eta_j : \ j = 1, \ldots, n\}$ *by*

$$\begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_n \\ \eta_1^\dagger \\ \eta_2^\dagger \\ \vdots \\ \eta_n^\dagger \end{pmatrix} = T \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ c_1^\dagger \\ c_2^\dagger \\ \vdots \\ c_n^\dagger \end{pmatrix} , \tag{4.18}$$

where Equation (4.18) is interpreted as

$$\left.\begin{array}{ll} \eta_j & = \sum_{k=1}^n U_{jk} c_k + V_{jk} c_k^\dagger \\ \eta_j^\dagger & = \sum_{k=1}^n V_{jk} c_k + U_{jk} c_k^\dagger \end{array}\right\} \ j = 1 \ldots n \ . \tag{4.19}$$

Then $\{\eta_j : \ j = 1, \ldots, n\}$ *also obey the FCRs.*

Proof. First observe that the j^{th} equation from Equation (4.18) is

$$\eta_j = \sum_{k=1}^n U_{jk} c_k + V_{jk} c_k^\dagger \ , \tag{4.20}$$

which is indeed the Hermitian adjoint of the $(n+j)^{th}$ equation. Therefore our use of the notation η_j and $\eta_j^\dagger$ is justified.

Let us verify the first FCR:

$$\{\eta_k, \eta_m^\dagger\} = \eta_k \eta_m^\dagger + \eta_m^\dagger \eta_k \tag{4.21}$$

$$= \left(\sum_{i=1}^{n} U_{ki} c_i + V_{ki} c_i^\dagger\right)\left(\sum_{j=1}^{n} U_{mj} c_j^\dagger + V_{mj} c_j\right) + \left(\sum_{r=1}^{n} U_{mr} c_r^\dagger + V_{mr} c_r\right)\left(\sum_{s=1}^{n} U_{ks} c_s + V_{ks} c_s^\dagger\right) \tag{4.22}$$

$$= \sum_{i,j=1}^{n} U_{ki} U_{mj} c_i c_j^\dagger + U_{ki} V_{mj} c_i c_j + V_{ki} U_{mj} c_i^\dagger c_j^\dagger + V_{ki} V_{mj} c_i^\dagger c_j + \sum_{r,s=1}^{n} U_{mr} U_{ks} c_r^\dagger c_s + U_{mr} V_{ks} c_r^\dagger c_s^\dagger + V_{mr} U_{ks} c_r c_s + V_{mr} V_{ks} c_r c_s^\dagger \ . \tag{4.23}$$

First, we apply the FCRs to all the terms in the second sum:

$$\{\eta_k, \eta_m^\dagger\} = \sum_{i,j=1}^{n} U_{ki} U_{mj} c_i c_j^\dagger + U_{ki} V_{mj} c_i c_j + V_{ki} U_{mj} c_i^\dagger c_j^\dagger + V_{ki} V_{mj} c_i^\dagger c_j + \sum_{r,s=1}^{n} -U_{mr} U_{ks} c_s^\dagger c_r - U_{mr} V_{ks} c_s^\dagger c_r^\dagger - V_{mr} U_{ks} c_s c_r - V_{mr} V_{ks} c_s c_r^\dagger + \sum_{s=1}^{n} U_{ms} U_{ks} + V_{ms} V_{ks} \ . \tag{4.24}$$

Then we can combine the sums, ordering terms so that $r = j$ and $s = i$. Most terms cancel, leaving us with:

$$\{\eta_k, \eta_m^\dagger\} = \sum_{i=1}^{n} U_{ki} U_{mi} + V_{ki} V_{mi} \ . \tag{4.25}$$

This equals the entry in the k^{th} row and m^{th} column of the real $n \times n$ matrix $UU^\dagger + VV^\dagger$. Since T is unitary we know $TT^\dagger = I_{2n}$, and in particular

$$UU^\dagger + VV^\dagger = I_n \ , \tag{4.26}$$

so we have

$$\{\eta_k, \eta_m^\dagger\} = \delta_{k,m} \ , \tag{4.27}$$

yielding the first FCR. For the second FCR, an identical procedure yields

$$\{\eta_k, \eta_m\} = \sum_{i=1}^{n} V_{ki}U_{mi} + V_{mi}U_{ki} \ . \tag{4.28}$$

This is the entry in the k^{th} row and m^{th} column of the real $n \times n$ matrix $VU^\dagger + UV^\dagger$. But T is unitary, so

$$UV^\dagger + VU^\dagger = 0 \ ; \tag{4.29}$$

thus we conclude $\{\eta_k, \eta_m\} = 0$. □

Using Theorem 4.3.1, we can find a unitary transformation to convert more general Hamiltonians into the form of (4.16). Suppose we have a Hamiltonian $\mathcal{H}$ defined as

$$\mathcal{H} = \sum_{j,k=1}^{n} A_{j,k}\left(c_j^\dagger c_k - c_j c_k^\dagger\right) + B_{j,k}\left(c_j^\dagger c_k^\dagger - c_j c_k\right) \ , \tag{4.30}$$

for some set of real coefficients $A_{j,k}$ and $B_{j,k}$. For convenience, sometimes we will gather these coefficients into real $n \times n$ matrices that we label A and B. It can be quickly verified using the FCRs that $\mathcal{H}$ is Hermitian for any choice of real A and B, and if A and B are *not* real, then $\mathcal{H}$ is not necessarily Hermitian.

It is also clear, using the FCRs, that different choices of A and B may represent the same Hamiltonian. However, we will establish that for any given Hamiltonian in this form, A can be chosen to be symmetric and B anti-symmetric.

Lemma 4.3.2 (Choice of A and B)**.** *For any Hamiltonian in the form of (4.30), A can be chosen to be symmetric and B can be chosen to be anti-symmetric.*

Proof. Define

$$\Psi = \left\{c_j^\dagger c_k - c_j c_k^\dagger \ , \ c_j^\dagger c_k^\dagger - c_j c_k \ : \quad j,k = 1 \ldots n\right\} \ . \tag{4.31}$$

Then the span of Ψ is the set of Hamiltonians represented by Equation (4.30). Now define

$$\Phi = \left\{ c_j^\dagger c_k - c_j c_k^\dagger + c_k^\dagger c_j - c_k c_j^\dagger \ , \ c_j^\dagger c_k^\dagger - c_j c_k - c_k^\dagger c_j^\dagger + c_k c_j \ : \quad j \leq k \right\} \ . \tag{4.32}$$

The span of Φ is the subset of Hamiltonians represented by Equation (4.30) where A is restricted to be symmetric and B is restricted to be anti-symmetric, since

$$\begin{aligned} A_{j,k}\left(c_j^\dagger c_k - c_j c_k^\dagger\right) + A_{k,j}\left(c_k^\dagger c_j - c_k c_j^\dagger\right) &= \left(\frac{A_{j,k} + A_{k,j}}{2}\right)\left(c_j^\dagger c_k - c_j c_k^\dagger + c_k^\dagger c_j - c_k c_j^\dagger\right) \ , \\ B_{j,k}\left(c_j^\dagger c_k^\dagger - c_j c_k\right) + B_{k,j}\left(c_k^\dagger c_j^\dagger - c_k c_j\right) &= \left(\frac{B_{j,k} - B_{k,j}}{2}\right)\left(c_j^\dagger c_k^\dagger - c_j c_k - c_k^\dagger c_j^\dagger + c_k c_j\right) \ , \end{aligned} \tag{4.33}$$

for any $A_{j,k}$, $A_{k,j}$, $B_{j,k}$, and $B_{k,j}$. These two identities show that Span(Φ) is identical to Span(Ψ). □

Theorem 4.3.3 establishes the unitary transformation that puts the Hamiltonian in (4.30) into the form of (4.16), and is due to Lieb *et al.* [33].

Theorem 4.3.3 (Principal axis transformation on Fermi operators)**.** *Consider the Hamiltonian in (4.30) where A is an $n \times n$ real symmetric matrix, B is an $n \times n$ real anti-symmetric matrix, and the operators $\{c_k : k = 1, \ldots, n\}$ satisfy the FCRs. Then we can find non-negative diagonal Λ and unitary X so that $X(A-B)(A+B) = \Lambda^2 X$, and unitary Y so that $Y(A+B)(A-B) = \Lambda^2 Y$. Define the operators $\{\eta_k : k =$*

$1, \ldots, n\}$ *by*

$$\begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_n \\ \eta_1^\dagger \\ \eta_2^\dagger \\ \vdots \\ \eta_n^\dagger \end{pmatrix} = \frac{1}{2} \begin{pmatrix} X+Y & X-Y \\ X-Y & X+Y \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ c_1^\dagger \\ c_2^\dagger \\ \vdots \\ c_n^\dagger \end{pmatrix} . \tag{4.34}$$

Then $\{\eta_j : \ j = 1, \ldots, n\}$ *satisfy the FCRs, and*

$$\mathcal{H} = \sum_{j=1}^{n} 2\Lambda_j \eta_j^\dagger \eta_j - \left(\sum_{j=1}^{n} \Lambda_j \right) I_{2^n} , \tag{4.35}$$

where Λ_j *denotes the* j^{th} *entry on the diagonal of the matrix* Λ*.*

Proof. We write Equation (4.30) as

$$\mathcal{H} = \begin{pmatrix} c_1^\dagger & c_2^\dagger & \ldots & c_n^\dagger & c_1 & c_2 & \ldots & c_n \end{pmatrix} \begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ c_1^\dagger \\ c_2^\dagger \\ \vdots \\ c_n^\dagger \end{pmatrix} , \tag{4.36}$$

The theorem is equivalent to showing there are solutions to

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} = \frac{1}{2}\begin{pmatrix} (X+Y) & (X-Y) \\ (X-Y) & (X+Y) \end{pmatrix}^{\dagger} \begin{pmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{pmatrix} \frac{1}{2}\begin{pmatrix} (X+Y) & (X-Y) \\ (X-Y) & (X+Y) \end{pmatrix} , \tag{4.37}$$

for some non-negative real $n \times n$ diagonal matrix Λ, where X and Y are unitary. If so, then substituting Equation (4.37) into Equation (4.36) and using the definition of η_k, we get

$$\mathcal{H} = \sum_{k=1}^{n} \left(\Lambda_k \eta_k^{\dagger} \eta_k - \Lambda_k \eta_k \eta_k^{\dagger} \right) . \tag{4.38}$$

Further, by Theorem 4.3.1, $\{\eta_k : k = 1 \ldots n\}$ satisfy the FCRs. So we can apply the FCRs to the second term in each summand to get Equation (4.35).

Now we set about finding solutions to Equation (4.37). We rewrite it for convenience as:

$$\begin{pmatrix} X+Y & X-Y \\ X-Y & X+Y \end{pmatrix} \begin{pmatrix} A & B \\ -B & -A \end{pmatrix} = \begin{pmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{pmatrix} \begin{pmatrix} X+Y & X-Y \\ X-Y & X+Y \end{pmatrix} . \tag{4.39}$$

Equation (4.39) is equivalent to the following four equations:

$$(X+Y)A - (X-Y)B = \Lambda(X+Y) , \tag{4.40}$$

$$(X+Y)B - (X-Y)A = \Lambda(X-Y) , \tag{4.41}$$

$$(X-Y)A - (X+Y)B = -\Lambda(X-Y) , \tag{4.42}$$

$$(X-Y)B - (X+Y)A = -\Lambda(X+Y) . \tag{4.43}$$

Evidently only two of the equations are independent. Adding and subtracting Equations (4.40) and (4.42) yields

$$X(A - B) = \Lambda Y \ , \tag{4.44}$$

$$Y(A + B) = \Lambda X \ . \tag{4.45}$$

We can left-multiply by Λ to get

$$\Lambda X(A - B) = \Lambda^2 Y \ , \tag{4.46}$$

$$\Lambda Y(A + B) = \Lambda^2 X \ , \tag{4.47}$$

and then substitute Equation (4.45) into Equation (4.46) and Equation (4.44) into Equation (4.47) to get the pair of eigen-decomposition equations

$$Y(A + B)(A - B) = \Lambda^2 Y \ , \tag{4.48}$$

$$X(A - B)(A + B) = \Lambda^2 X \ . \tag{4.49}$$

Since A is real symmetric and B is real anti-symmetric, $(A + B)^\dagger = A - B$ and so $(A-B)(A+B)$ and $(A+B)(A-B)$ are symmetric positive semi-definite. So there is always a unitary X and Y with non-negative diagonal Λ^2 satisfying Equations (4.48) and (4.49).

As a final comment, we could negate entries of Λ and recover the same energies of $\mathcal{H}$, but this is more confusing than enlightening. So we will take Λ as non-negative. $\square$

Note that since $(A + B)^\dagger = A - B$, Λ_j is a singular value of $A + B$, and $2\Lambda_j$ corresponds to the coefficient C_j in (4.16). If $A + B$ is non-singular, then twice the least singular value is the ground-state energy gap of $\mathcal{H}$. If $A + B$ is singular, then

$\mathcal{H}$ has a degenerate ground state, and twice the least non-zero singular value is the energy gap between the ground-state subspace and the higher energy levels of the Hamiltonian.

We can efficiently compute the ground-state energy gap of the Hamiltonian in (4.30), but what can we say about the ground state itself? It is the eigenstate with zero eigenvalue on $\{\eta_j^\dagger \eta_j : \ j = 1 \dots n\}$, but what is that state in the original basis? We now show that it can be constructed.

Consider the operator

$$\hat{\eta} = \eta_1 \eta_2 \dots \eta_n \ . \tag{4.50}$$

We will show that $\hat{\eta}$ applied to a random state yields a ground state of $\mathcal{H}$ almost surely. Using Properties 3 and 4, we can see that if we apply $\hat{\eta}$ to the most excited state of $\mathcal{H}$, which is the state with unit eigenvalue on all the operators $\{\eta_j^\dagger \eta_j : \ j = 1 \dots n\}$, then we will get a ground state of $\mathcal{H}$, namely the state with zero eigenvalue on all the operators $\{\eta_j^\dagger \eta_j : \ j = 1 \dots n\}$.

Further, suppose $|\varphi\rangle$ is an eigenstate of $\mathcal{H}$, not the most excited state. Then for some k we have $\eta_k^\dagger \eta_k |\varphi\rangle = 0$. Using Property 5 in conjunction with the FCRs, we see

$$\hat{\eta}|\varphi\rangle = \eta_1 \eta_2 \dots \eta_n |\varphi\rangle \tag{4.51}$$

$$= (-1)^{n-k} \overbrace{\eta_1 \eta_2 \dots \eta_n}^{\text{except } \eta_k} \eta_k |\varphi\rangle \tag{4.52}$$

$$= 0 \ . \tag{4.53}$$

So the algorithm to find the ground state is the following: pick a random state $|\psi\rangle$, and compute $\hat{\eta}|\psi\rangle$. Define $|\phi\rangle$ to be the most excited state, in particular the (unknown) state with unit eigenvalue on all of $\{\eta_j^\dagger \eta_j : \ j = 1 \dots n\}$. Then since $|\psi\rangle$

is random, almost surely $\langle\psi|\phi\rangle \neq 0$. So $|\psi\rangle = \alpha|\phi\rangle + \beta|\phi^\perp\rangle$ for some $\langle\phi^\perp|\phi\rangle = 0$ and $\alpha \neq 0$. Then compute

$$\hat{\eta}|\psi\rangle = \hat{\eta}\left(\alpha|\phi\rangle + \beta|\phi^\perp\rangle\right) \tag{4.54}$$

$$= \alpha|\bar{\phi}\rangle \ , \tag{4.55}$$

where $|\bar{\phi}\rangle$ is a ground state of $\mathcal{H}$, in particular the state with zero eigenvalue on all of $\{\eta_j^\dagger\eta_j : \ j = 1 \ldots n\}$.

If the ground state is degenerate, then $\Lambda_k = 0$ for some k. Let $|\bar{\phi}_k\rangle = \eta_k^\dagger|\bar{\phi}\rangle$. Then using Property 2 and Property 4, $|\bar{\phi}_k\rangle$ has zero eigenvalue on $\eta_j^\dagger\eta_j$ for $j \neq k$, and unit eigenvalue on $\eta_k^\dagger\eta_k$. While $|\bar{\phi}_k\rangle$ is orthogonal to $|\bar{\phi}\rangle$, it has the same energy since $\Lambda_k = 0$. Extending this reasoning, we can recover a basis for the whole ground state subspace.

In general, an n-qubit quantum state requires 2^n space to store, and 2^n work to operate on. So it takes exponential space to represent the random state $|\psi\rangle$ and exponential work to compute $\hat{\eta}|\psi\rangle$, unless there is some special structure in the problem that we may leverage.

4.4 The Jordan-Wigner transformation

Now we explore the Jordan-Wigner transformation, which relates Fermi operators to Pauli operators. We begin with the *Brauer-Weyl* construction, which constructs generators for $Cl_{2n}(I_{2n})$ using elements of $Cl_2(I_2)^{\otimes n}$.

Theorem 4.4.1 (Brauer-Weyl construction)**.** *Define the generators* $\{\bar{g}_j : \ j = 1, \ldots, 2n\}$

by

$$\left\{\begin{array}{ll} \bar{g}_1 = \sigma_1^x & \bar{g}_2 = \sigma_1^y \\ \bar{g}_3 = \sigma_1^z\sigma_2^x & \bar{g}_4 = \sigma_1^z\sigma_2^y \\ \bar{g}_5 = \sigma_1^z\sigma_2^z\sigma_3^x & \bar{g}_6 = \sigma_1^z\sigma_2^z\sigma_3^y \\ \vdots & \vdots \end{array}\right\} . \tag{4.56}$$

Then the elements $\bar{g}_j$ satisfy (4.1) with $Q = I_{2n}$.

The proof splits into 12 cases of (4.1), taking j and k odd and even and $j < k$, $j = k$, and $j > k$. To verify each of the twelve cases, the properties needed are (4.10), (4.11), and (4.13). Here we simply work out an example:

$$\{\bar{g}_3, \bar{g}_4\} = \bar{g}_3\bar{g}_4 + \bar{g}_4\bar{g}_3 \tag{4.57}$$

$$= \sigma_1^z\sigma_2^x\sigma_1^z\sigma_2^y + \sigma_1^z\sigma_2^y\sigma_1^z\sigma_2^x \tag{4.58}$$

$$= (\sigma_1^z)^2\sigma_2^x\sigma_2^y + (\sigma_1^z)^2\sigma_2^y\sigma_2^x \tag{4.59}$$

$$= \sigma_2^x\sigma_2^y + \sigma_2^y\sigma_2^x \tag{4.60}$$

$$= \sigma_2^x\sigma_2^y - \sigma_2^x\sigma_2^y \tag{4.61}$$

$$= 0 . \tag{4.62}$$

We can use the Brauer-Weyl construction to establish an isomorphism between $Cl_2(I_2)^{\otimes n}$ and $Cl_{2n}(I_{2n})$.

Theorem 4.4.2 (Isomorphism of algebras)**.** *The algebra $Cl_2(I_2)^{\otimes n}$ is isomorphic to $Cl_{2n}(I_{2n})$.*

Proof. The outline of the proof is the following:

1. We use the Brauer-Weyl construction to define a complete map F from $Cl_{2n}(I_{2n})$ to $Cl_2(I_2)^{\otimes n}$.

2. We show that F is an homomorphism, i.e. it respects addition and multiplication.

3. Finally, we show that F is invertible.

First, define F on the generators g_j of $Cl_{2n}(I_{2n})$ by $F(g_j) = \bar{g}_j$. Then, by construction, F respects Equation (4.1) with $Q = I_{2n}$ in the sense

$$\{F(g_i), F(g_j)\} = F(g_i)F(g_j) + F(g_j)F(g_i) = 2\delta_{ij} \ . \tag{4.63}$$

Next, we extend F to the linearly independent products of generators $\{e_j : \ j = 1 \dots 2^{2n}\}$ in the following way. Suppose $e_j = g_{j_1} g_{j_2} \dots$ in the canonical form where the indices of the generators are increasing and non-repeating. Then define

$$F(e_j) = F(g_{j_1})F(g_{j_2}) \dots \tag{4.64}$$

For any e_j, e_k, we can use (4.1) for $Q = I_{2n}$ to simplify the product $e_j e_k$ into the form

$$e_j e_k = \pm e_l \ , \tag{4.65}$$

for some other product of generators e_l. The sign is determined by the number of swaps required to sort the generators in e_j and e_k into canonical form. We can see using (4.64) and (4.63) that the same simplification may be performed for F to achieve

$$F(e_j)F(e_k) = \pm F(e_l) \ . \tag{4.66}$$

Finally, we extend F to the rest of $Cl_{2n}(I_{2n})$ by asserting that it is linear on the basis vectors e_k:

$$F\left(\sum_{j=1}^{2^{2n}} A_j e_j\right) = \sum_{j=1}^{2^{2n}} A_j F(e_j) \ . \tag{4.67}$$

Now we can check that F is an algebra homomorphism. F is an algebra homomorphism if the following three properties hold:

- $F(kx) = kF(x)$, for a scalar k.
- $F(x+y) = F(x) + F(y)$.
- $F(xy) = F(x)F(y)$.

It is obvious that F satisfies the first two properties, because we defined it to be linear. To check that F respects multiplication, we only need to write x and y as linear combinations of basis elements $\{e_j\}$, and apply (4.67) and (4.66).

Finally, we check that F is invertible. First, observe using (4.56) that

$$\sigma_j^z = -i\bar{g}_{2j-1}\bar{g}_{2j} \ . \tag{4.68}$$

Then, using this fact and $(\sigma_j^z)^2 = I$, we can invert the left equations in (4.56):

$$\sigma_j^x = \sigma_{j-1}^z \sigma_{j-2}^z \dots \sigma_1^z \bar{g}_{2j-1} \tag{4.69}$$

$$= (-i)^{j-1}(\bar{g}_{2j-3}\bar{g}_{2j-2})(\bar{g}_{2j-5}\bar{g}_{2j-4}) \dots (\bar{g}_1\bar{g}_2)\ \bar{g}_{2j-1} \ . \tag{4.70}$$

Similarly, we can invert the right equations in (4.56):

$$\sigma_j^y = \sigma_{j-1}^z \sigma_{j-2}^z \dots \sigma_1^z \bar{g}_{2j} \tag{4.71}$$

$$= (-i)^{j-1}(\bar{g}_{2j-3}\bar{g}_{2j-2})(\bar{g}_{2j-5}\bar{g}_{2j-4}) \dots (\bar{g}_1\bar{g}_2)\ \bar{g}_{2j} \ . \tag{4.72}$$

Now we can construct F^{-1}. First, define

$$F^{-1}(\sigma_j^x) = (-i)^{j-1}(g_{2j-3}g_{2j-2})(g_{2j-5}g_{2j-4})\dots(g_1g_2)\ g_{2j-1}\ , \tag{4.73}$$

$$F^{-1}(\sigma_j^y) = (-i)^{j-1}(g_{2j-3}g_{2j-2})(g_{2j-5}g_{2j-4})\dots(g_1g_2)\ g_{2j}\ . \tag{4.74}$$

We can use a similar procedure to extend F^{-1} to the whole Pauli algebra: first extending to products of Pauli operators, and then linear combinations of such products. □

We can identify generators $\{c_j,\ d_j : j = 1\dots n\}$ for $Cl_{2n}(Q_n^F)$ using $\{\bar{g}_j : j = 1\dots 2n\}$ by a simple change of basis:

$$\begin{aligned} c_j &= \frac{(-1)^{j-1}}{2}\left(\bar{g}_{2j-1} - i\bar{g}_{2j}\right)\ , \\ d_j &= \frac{(-1)^{j-1}}{2}\left(\bar{g}_{2j-1} + i\bar{g}_{2j}\right)\ . \end{aligned} \tag{4.75}$$

We can verify that $\{c_j,\ d_j : j = 1\dots n\}$ satisfy (4.1) with $Q = Q_n^F$, using the fact that $\{\bar{g}_j : j = 1\dots 2n\}$ satisfy (4.1) with $Q = I_{2n}$. Since $\bar{g}_j$ is Hermitian, we can take $d_j = c_j^\dagger$, and then c_j and $c_j^\dagger$ satisfy the FCRs. Substituting (4.56) into (4.75) and setting $d_j = c_j^\dagger$ yields the Jordan-Wigner transformation, e.g. [53]:

$$\begin{aligned} c_j &= (-1)^{j-1}\sigma_1^z\sigma_2^z\dots\sigma_{j-1}^z\left(\frac{\sigma_j^x - i\sigma_j^y}{2}\right)\ , \\ c_j^\dagger &= (-1)^{j-1}\sigma_1^z\sigma_2^z\dots\sigma_{j-1}^z\left(\frac{\sigma_j^x + i\sigma_j^y}{2}\right)\ , \end{aligned} \tag{4.76}$$

or, defining

$$a_j = \frac{\sigma_j^x - i\sigma_j^y}{2}\ , \tag{4.77}$$

we can write

$$\begin{aligned} c_j &= (-1)^{j-1}\sigma_1^z\sigma_2^z\dots\sigma_{j-1}^z a_j\ , \\ c_j^\dagger &= (-1)^{j-1}\sigma_1^z\sigma_2^z\dots\sigma_{j-1}^z a_j^\dagger\ . \end{aligned} \tag{4.78}$$

4.5 One-dimensional Ising model

Now we are ready to analyze the Hamiltonian

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n}\sigma_j^z + s\sum_{j=1}^{n-1}\sigma_j^x\sigma_{j+1}^x \ , \tag{4.79}$$

that defines the one-dimensional Ising model. We can verify from (4.77) the following transformation:

$$\begin{aligned} \sigma_j^x &= a_j + a_j^\dagger \ , & \sigma_j^y &= i\left(a_j - a_j^\dagger\right) \ , \\ \sigma_j^z &= 2a_j^\dagger a_j - I_{2^n} \ . \end{aligned} \tag{4.80}$$

Then (4.79) can be expressed with the operators a_j and $a_j^\dagger$ as

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n}\left(2a_j^\dagger a_j - I_{2^n}\right) + s\sum_{j=1}^{n-1}(a_j + a_j^\dagger)(a_{j+1} + a_{j+1}^\dagger) \tag{4.81}$$

$$= (1-s)\sum_{j=1}^{n}\left(2a_j^\dagger a_j - I_{2^n}\right) + s\sum_{j=1}^{n-1}\left(a_j^\dagger a_{j+1} + a_j a_{j+1}^\dagger + a_j^\dagger a_{j+1}^\dagger + a_j a_{j+1}\right) \ . \tag{4.82}$$

Now we apply the Jordan-Wigner transformation (4.78). We make use of the following identities:

$$\begin{aligned} c_j^\dagger c_j &= a_j^\dagger a_j \ , & c_j c_{j+1} &= -a_j a_{j+1} \ , \\ c_j^\dagger c_{j+1} &= a_j^\dagger a_{j+1} \ , & c_j c_{j+1}^\dagger &= -a_j a_{j+1}^\dagger \ , \\ c_j^\dagger c_{j+1}^\dagger &= a_j^\dagger a_{j+1}^\dagger \ . \end{aligned} \tag{4.83}$$

These identities can be checked using the same properties that we used to verify the Brauer-Weyl construction. So we have

$$\begin{aligned}\mathcal{H}(s) =&(1-s)\sum_{j=1}^{n}\left(2c_j^\dagger c_j - I_{2^n}\right) + s\sum_{j=1}^{n-1}\left(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger + c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}\right) \quad (4.84)\\ =&(1-s)\sum_{j=1}^{n}\left(c_j^\dagger c_j - c_j c_j^\dagger\right) + \frac{s}{2}\sum_{j=1}^{n-1}\left(c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger + c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}\right.\\ &\left.+c_{j+1}^\dagger c_j - c_{j+1} c_j^\dagger - c_{j+1}^\dagger c_j^\dagger + c_{j+1} c_j\right) . \quad (4.85)\end{aligned}$$

Taking $A_{j,j} = (1-s)$, $B_{j,j+1} = -B_{j+1,j} = A_{j,j+1} = A_{j+1,j} = s/2$, and setting the rest of A and B to zero, then we have

$$\mathcal{H} = \sum_{j,k=1}^{n} A_{j,k}\left(c_j^\dagger c_k - c_j c_k^\dagger\right) + B_{j,k}\left(c_j^\dagger c_k^\dagger - c_j c_k\right) . \quad (4.86)$$

Now, by finding the singular values of $A+B$, we can use Theorem 4.3.3 to find the ground-state energy and the ground-state energy gap. Since $(A+B)(A-B)$ is Toeplitz (constant diagonal elements) tri-diagonal, we can even find these singular values analytically. What is remarkable about this technique, though, is that $\mathcal{H}(s)$ is 2^n dimensional, and yet to apply Theorem 4.3.3 we only had to diagonalize an $n \times n$ matrix.

The reason this technique does not obviously extend past nearest-neighbor interactions is that we depend on the simple relationships in (4.83) to apply the Jordan-Wigner transformation. Those relationships are not so simple for non-nearest-neighbor interactions. If our Hamiltonian has a term such as $\sigma_j^x \sigma_{j+2}^x$, then after we substitute a_j and $a_j^\dagger$ we will have terms such as $a_j^\dagger a_{j+2}$. Now, instead of Equation (4.83) we have to use the relationship

$$a_j^\dagger a_{j+2} = -c_j^\dagger \sigma_{j+1}^z c_{j+2} . \quad (4.87)$$

But when we make this substitution, our Hamiltonian will not be in the necessary form to apply Theorem 4.3.3.

We have developed the tools necessary to analyze the one-dimensional Ising model. Now we are ready to identify new classes of Hamiltonians and Hamiltonian evolutions with large ground-state energy gaps.

Chapter 5

Finding Effective Hamiltonians for Adiabatic Quantum Computing

Now we use the tools developed in Chapter 4 to identify some classes of Hamiltonian evolutions with large ground-state energy gaps. Section 5.1 focuses on such Hamiltonians defined with Fermi operators, and Section 5.2 considers those Hamiltonians represented with Pauli operators.

5.1 A class of Hamiltonians with a large ground-state energy gap

In this section, we consider Hamiltonian evolutions with a simple starting Hamiltonian and whose final Hamiltonian is in the form of (4.30). We prove that certain random Hamiltonians in the form of (4.30) have an $\mathcal{O}(1/\sqrt{n})$ ground-state energy gap, where n is the number of qubits. We also identify two classes of Hamiltonians whose ground state can be found in polynomial time with AQC.

Suppose $\{c_j : \ j = 1 \ldots n\}$ satisfy the FCRs, and consider the Hamiltonian evolution

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n}(2c_j^\dagger c_j - I_{2^n}) + s\sum_{j,k=1}^{n}\left(A_{j,k}\left(c_j^\dagger c_k - c_j c_k^\dagger\right) + B_{j,k}\left(c_j^\dagger c_k^\dagger - c_j c_k\right)\right) , \tag{5.1}$$

or equivalently,

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n}(c_j^\dagger c_j - c_j c_j^\dagger) + s\sum_{j,k=1}^{n}\left(A_{j,k}\left(c_j^\dagger c_k - c_j c_k^\dagger\right) + B_{j,k}\left(c_j^\dagger c_k^\dagger - c_j c_k\right)\right) . \tag{5.2}$$

At $s = 0$, the Hamiltonian is uncoupled and easy to analyze. At $s = 1$, there are interactions between qubits, and the ground state is not so obvious. If A and B are tri-diagonal, then $\mathcal{H}(1)$ is the Hamiltonian for a one-dimensional chain of interacting spin 1/2 particles [33]; we considered a special case of this in Section 4.5, namely the one-dimensional Ising model. If $B = 0$ and the non-zero entries of A correspond to the adjacency matrix for a lattice, then $\mathcal{H}(1)$ is the Hamiltonian for free non-interacting electrons tunneling on a lattice [14, p. 251], namely a Hubbard model with no on-site interaction terms, e.g. terms such as $c_j^\dagger c_j c_k^\dagger c_k$. However, our purpose here is not to model physical phenomena, but rather exhibit Hamiltonians and Hamiltonian evolutions with many degrees of freedom and large ground-state energy gaps, that have potential applications in AQC.

Let us define

$$\breve{A}(s) = (1-s)I_{2^n} + sA$$
$$\breve{B}(s) = sB \ . \tag{5.3}$$

Then we can rewrite Equation (5.1) as

$$\mathcal{H}(s) = \sum_{j,k=1}^{n} \left(\breve{A}_{j,k}(s) \left(c_j^\dagger c_k - c_j c_k^\dagger \right) + \breve{B}_{j,k}(s) \left(c_j^\dagger c_k^\dagger - c_j c_k \right) \right) \ . \tag{5.4}$$

Let $\{\Lambda_j(s) : \ j = 1 \ldots n\}$ be the singular values of $\breve{A}(s) + \breve{B}(s)$. By Theorem 4.3.3, there is a set of time-dependent operators $\{\eta_j(s) : j = 1 \ldots n, s \in [0,1]\}$ satisfying the FCRs so that

$$\mathcal{H}(s) = \sum_{j=1}^{n} 2\Lambda_j(s)\eta_j^\dagger(s)\eta_j(s) - \left(\sum_{j=1}^{n} \Lambda_j(s) \right) I_{2^n} \ . \tag{5.5}$$

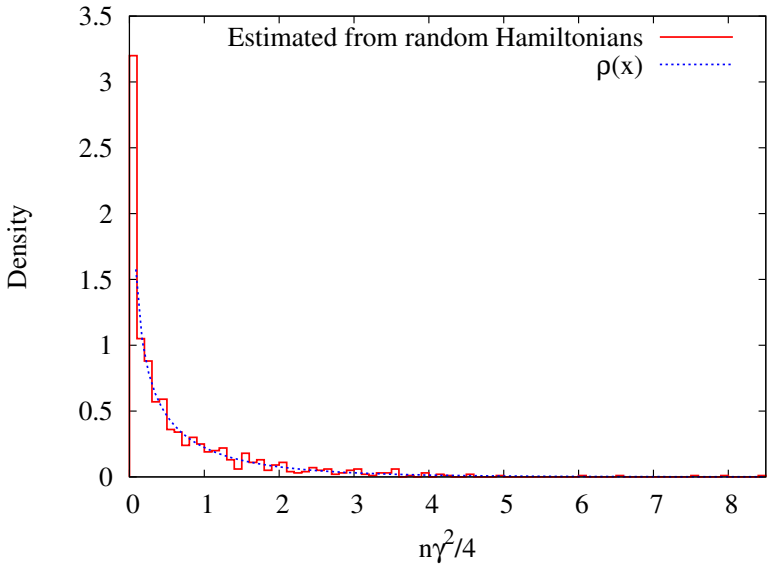

Figure 5.1: The ground-state energy gap γ is computed for 1000 random $n = 10$ (10-qubit) Hamiltonians. Each Hamiltonian was chosen randomly as in Theorem 5.1.1. The resulting estimated probability density function for $n\gamma^2/4$ is compared with $\rho(x)$. Even with only $n = 10$, the numerical gaps have a distribution very close to $\rho(x)$.

Note that $\mathcal{H}(s)$ must fit 2^n eigenvalues in a range polynomial in n. Even so, we have reason to be optimistic that the ground-state energy gap is not exponentially small, because the ground state energy gap is twice the smallest non-zero singular value of the matrix $\breve{A}(s) + \breve{B}(s)$, which is only $n \times n$. We now show that for certain random Hamiltonians of the form of (4.30), the ground-state energy gap is $\mathcal{O}(1/\sqrt{n})$.

Theorem 5.1.1 (Ground-state energy gap for random Hamiltonians)**.** *Let C be an $n \times n$ matrix with independent N(0,1) coefficients, and let A be the symmetric part of C, and B be the anti-symmetric part of C, so*

$$A = \frac{C + C^\dagger}{2} \qquad\qquad B = \frac{C - C^\dagger}{2}\,, \tag{5.6}$$

and $C = A + B$. Define

$$\mathcal{H} = \sum_{j,k=1}^{n} \left(A_{j,k} \left(c_j^\dagger c_k - c_j c_k^\dagger \right) + B_{j,k} \left(c_j^\dagger c_k^\dagger - c_j c_k \right) \right) , \tag{5.7}$$

and let γ be the ground-state energy gap of $\mathcal{H}$. Then, for large n, $n\gamma^2/4$ converges in distribution to the probability density function

$$\rho(x) = \frac{1 + \sqrt{x}}{2\sqrt{x}} e^{-(x/2+\sqrt{x})} . \tag{5.8}$$

Proof. From [16, Corollary 3.1], if $\gamma/2$ is the least singular value of C, then $n\gamma^2/4$ converges in distribution to $\rho(x)$ for large n. This means that C is non-singular with probability one and thus γ is the ground-state energy gap. □

Note that in Theorem 5.1.1, A and B have independent Gaussian upper-triangular entries since $C_{j,k} + C_{k,j}$ and $C_{j,k} - C_{k,j}$ are independent and Gaussian. In particular, the diagonal of A has unit variance, and the off-diagonal entries of A and B have variance of one-half.

Figure 5.1 compares the ground-state energy gap computed for 1000 randomly-generated 10-qubit Hamiltonians with the distribution predicted by $\rho(x)$. Even with only $n = 10$, the energy gaps found numerically are very close to those predicted by $\rho(x)$.

Since there must be 2^n distinct energy levels in an energy range of $\mathcal{O}(n^2)$, most of the energy gaps must be exponentially small. In fact it can be shown that the Hamiltonians in Theorem 5.1.1 are almost surely non-degenerate, so these exponentially small gaps are also non-zero. Figure 5.2 illustrates the difference between the distribution of the ground-state energy gaps and the rest of the gaps for 1000 randomly-generated

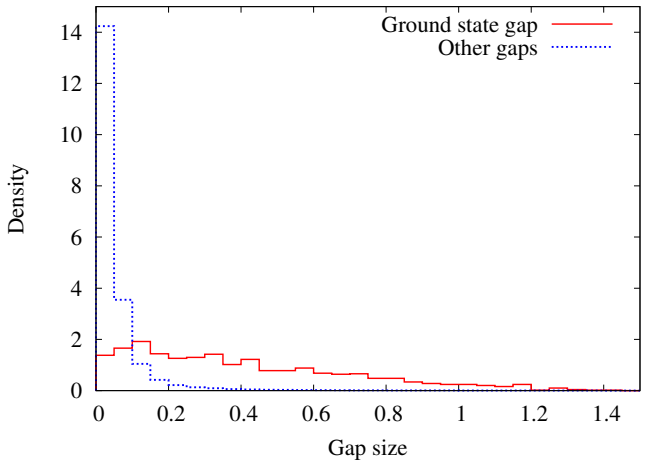

Figure 5.2: All the energy levels are computed for 1000 random $n = 10$ (10-qubit) Hamiltonians. Each Hamiltonian was chosen randomly as described in Theorem 5.1.1. The ground-state energy gap distribution is compared to the distribution for the other energy gaps. As predicted by Theorem 5.1.1, the ground-state energy gaps are much larger than the other gaps.

10-qubit Hamiltonians, and indeed the ground-state energy gaps are typically much larger than the other gaps.

We may be interested in the case where $B = 0$ and A is a random symmetric matrix. That case may be interpreted as a disordered Hubbard model with no on-site interactions. We can immediately derive a class of random Hamiltonians with random symmetric A and $B = 0$, for whom AQC evolution has a minimum ground-state energy gap of $\mathcal{O}(1/n)$.

Theorem 5.1.2 (Ground-state energy gap for random Hamiltonian evolutions)**.** *Let C be an $n \times n$ matrix with independent N(0,1) coefficients, and let $A = CC^\dagger$. Define*

$$\mathcal{H}_P = \sum_{j,k=1}^{n} A_{j,k} \left(c_j^\dagger c_k - c_j c_k^\dagger \right) \ , \tag{5.9}$$

and

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n}(2c_j^\dagger c_j - I_{2^n}) + s\mathcal{H}_P \ . \tag{5.10}$$

Then the ground-state energy gap for $\mathcal{H}(s)$ *is*

$$\breve{\gamma}(s) = 2(1-s) + s\gamma \ , \tag{5.11}$$

where $n\gamma/2$ *converges in distribution to* $\rho(x)$ *(see Equation (5.8)) for large* n*.*

Proof. Since $A = CC^\dagger$, if $\sqrt{\gamma/2}$ is the least singular value of C then by [16, Corollary 3.1], for large n, $n\gamma/2$ converges in distribution to the density function $\rho(x)$, and is non-zero with probability one. Since A is symmetric positive semi-definite, $\gamma/2$ is also its least singular value. Thus γ is the ground-state energy gap of $\mathcal{H}_P$.

Define

$$\breve{A}(s) = (1-s)I_n + sA \ , \tag{5.12}$$

then the ground-state energy gap $\breve{\gamma}(s)$ of $\mathcal{H}(s)$ is twice the least non-zero singular value of $\breve{A}(s)$. Since A and I are symmetric positive semi-definite, and $(1-s)$ and s are non-negative, $\breve{A}(s)$ is symmetric and positive semi-definite. So the singular values of $\breve{A}(s)$ are the eigenvalues of $\breve{A}(s)$. Since $\gamma/2$ is the least eigenvalue of A, the least eigenvalue of $\breve{A}$ is

$$\frac{\breve{\gamma}(s)}{2} = (1-s) + s\left(\frac{\gamma}{2}\right) \ . \tag{5.13}$$

□

Figure 5.3 illustrates the energy levels for an 8-qubit instance of a random evolution as in (5.10). To generate the figure we actually took $A = CC^\dagger/n$, so that

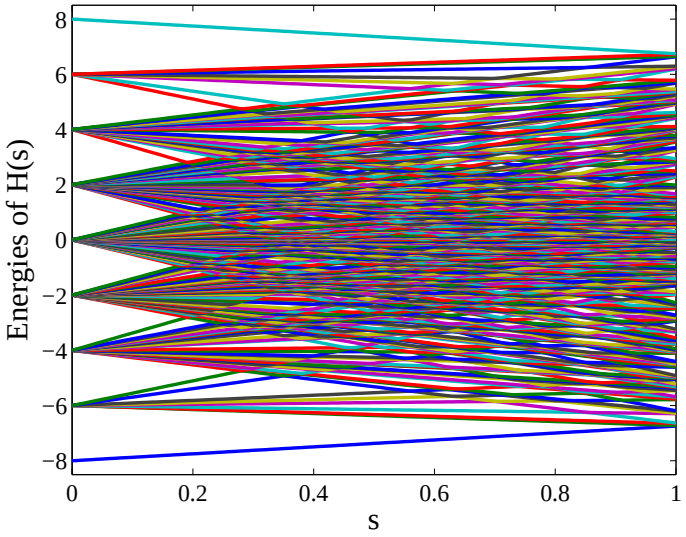

Figure 5.3: Eigenvalues of $\mathcal{H}(s)$ as a function of s, where $\mathcal{H}(s)$ was defined as in (5.10) with $A = CC^\dagger/n$ for $n = 8$. The division by n is so that $||\mathcal{H}(0)|| \approx ||\mathcal{H}(1)||$, resulting in a better visualization although making the ground-state energy gap $\mathcal{O}(1/n^2)$ instead of $\mathcal{O}(1/n)$. We can see that the ground-state energy gap is linearly decreasing with s as predicted by Theorem 5.1.2, and is much larger than most of the other energy gaps.

$||\mathcal{H}(0)|| \approx ||\mathcal{H}(1)||$. It is easy to check that the same proof holds, although the ground-state energy gap is then $\mathcal{O}(1/n^2)$ instead of $\mathcal{O}(1/n)$.

Now, we consider the special case where A and B are *circulant*. A circulant matrix is a matrix where each row is a cyclic shift of the previous row, such as these A and B matrices:

$$A = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & 1/2 & -1/2 \\ -1/2 & 0 & 1/2 \\ 1/2 & -1/2 & 0 \end{pmatrix}. \tag{5.14}$$

In general, for n qubits, there are n degrees of freedom in choosing Hamiltonians of the form of Equation (4.30) such that A and B are circulant.

Theorem 5.1.3 (Ground-state energy gap for Hamiltonians with circulant A and B matrices)**.** *Let*

$$\mathcal{H} = \sum_{j,k=1}^{n} \left(A_{j,k} \left(c_j^\dagger c_k - c_j c_k^\dagger \right) + B_{j,k} \left(c_j^\dagger c_k^\dagger - c_j c_k \right) \right) , \tag{5.15}$$

where A is a real circulant $n \times n$ symmetric matrix, and B is a real circulant anti-symmetric $n \times n$ matrix. Then the ground-state energy gap of $\mathcal{H}$ is bounded below by a polynomial in n^{-1}.

Proof. Circulant matrices form a commutative ring [22, p. 201], so if A and B are circulant, then so is $G = (A-B)(A+B)$. Also, G is symmetric positive semi-definite, and the ground-state energy gap of $\mathcal{H}$ is twice the square root of the least non-zero eigenvalue of G.

Circulant matrices also have the nice property that their eigenvalues are given by the discrete Fourier transform of their first column. Recall we label the eigenvalues of G as Λ_k^2. Labeling the entries in the first column of G as g_k, we can write:

$$\begin{pmatrix} \Lambda_1^2 \\ \Lambda_2^2 \\ \Lambda_3^2 \\ \dots \\ \Lambda_n^2 \end{pmatrix} = \frac{1}{\sqrt{n}} \begin{pmatrix} e^{(0\cdot 0)2\pi i/n} & e^{(0\cdot 1)2\pi i/n} & e^{(0\cdot 2)2\pi i/n} & \dots \\ e^{(1\cdot 0)2\pi i/n} & e^{(1\cdot 1)2\pi i/n} & e^{(1\cdot 2)2\pi i/n} & \dots \\ e^{(2\cdot 0)2\pi i/n} & e^{(2\cdot 1)2\pi i/n} & e^{(2\cdot 2)2\pi i/n} & \dots \\ \dots & & & \\ e^{((n-1)1\cdot 0)2\pi i/n} & e^{((n-1)\cdot 1)2\pi i/n} & e^{((n-1)\cdot 2)2\pi i/n} & \dots \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ \dots \\ g_n \end{pmatrix} \tag{5.16}$$

Also, G is symmetric so $g_k = g_{n+2-k}$ for $k \geq 2$. Then we have, for n odd:

$$\Lambda_k^2 = \frac{1}{\sqrt{n}} \left(g_1 + \sum_{j=2}^{(n+1)/2} g_j \left(e^{((j-1)\cdot(k-1))2\pi i/n} + e^{((n-j+1)\cdot(k-1))2\pi i/n} \right) \right) \tag{5.17}$$

$$= \frac{1}{\sqrt{n}} \left(g_1 + \sum_{j=2}^{(n+1)/2} g_j \left(e^{((j-1)\cdot(k-1))2\pi i/n} + e^{-((j-1)\cdot(k-1))2\pi i/n} \right) \right) \tag{5.18}$$

$$= \frac{1}{\sqrt{n}} \left(g_1 + \sum_{j=2}^{(n+1)/2} g_j \cos\left(2\pi(j-1)(k-1)/n\right) \right) . \tag{5.19}$$

For n even we have a leftover term, but it simplifies:

$$\Lambda_k^2 = \frac{1}{\sqrt{n}} \left(g_1 + g_{n/2+1} e^{((n/2)\cdot(k-1))2\pi i/n} + \sum_{j=2}^{n/2} g_j \cos\left(2\pi(j-1)(k-1)/n\right) \right) \tag{5.20}$$

$$= \frac{1}{\sqrt{n}} \left(g_1 + (-1)^{(k-1)} g_{n/2+1} + \sum_{j=2}^{n/2} g_j \cos\left(2\pi(j-1)(k-1)/n\right) \right) . \tag{5.21}$$

For $n \geq 1$, we have $1/n \leq 1/\sqrt{n}$. So whether n is even or odd, Taylor expansion on cosine makes it clear that if $\Lambda_k \neq 0$ then Λ_k is bounded below by a polynomial in n^{-1}. So the ground-state energy gap of $\mathcal{H}$ is bounded below by a polynomial in n^{-1}. □

We can extend this result to a whole Hamiltonian evolution:

Corollary 5.1.4 (Hamiltonian evolutions with circulant A and B matrices)**.** *Let*

$$\mathcal{H}(s) = (1-s) \sum_{j=1}^{n} (2c_j^\dagger c_j - I_{2^n}) + s \sum_{j,k=1}^{n} \left(A_{j,k} \left(c_j^\dagger c_k - c_j c_k^\dagger \right) + B_{j,k} \left(c_j^\dagger c_k^\dagger - c_j c_k \right) \right) , \tag{5.22}$$

where A is a real circulant $n \times n$ symmetric matrix, and B is a real circulant anti-symmetric $n \times n$ matrix. Then the ground-state energy gap of $\mathcal{H}(s)$ is bounded below by a polynomial in n^{-1} and s.

Proof. First rewrite $\mathcal{H}(s)$ as in (5.4). The elements of the matrix

$$\breve{G}(s) = \left(\breve{A}(s) - \breve{B}(s) \right) \left(\breve{A}(s) + \breve{B}(s) \right) \tag{5.23}$$

are quadratic functions of s. Then we can follow the proof of Theorem 5.1.3 to see that the eigenvalues of $\breve{G}(s)$ are bounded by a polynomial in s and n^{-1}, and so the ground-state energy gap of $\mathcal{H}(s)$ is bounded below by a polynomial in n^{-1} and s. $\square$

5.2 Hamiltonians in the standard Pauli model with large ground-state gaps

It is well known that the Hamiltonians in the previous section include those describing nearest-neighbor interactions, but the class is considerably larger than that. In this section we study one subclass of these Hamiltonians, related to a specific definition of $\{c_j\}$. Theorem 5.2.1 is equivalent to the result in [65, p. 4], but using a different basis representation.

Theorem 5.2.1 (Representation with Pauli operators of quadratic forms in Fermi operators)**.** *There is a bijection between Hamiltonians on n qubits of the form*

$$\begin{aligned}\mathcal{H} = &\sum_{j=1}^{n} W_{j,j}\sigma_j^z + \sum_{j=1}^{n-1}\left(W_{j,j+1}\sigma_j^x\sigma_{j+1}^x + W_{j+1,j}\sigma_j^y\sigma_{j+1}^y\right)\\ &+ \sum_{j=1}^{n-2}\left(W_{j,j+2}\sigma_j^x\sigma_{j+1}^z\sigma_{j+2}^x + W_{j+2,j}\sigma_j^y\sigma_{j+1}^z\sigma_{j+2}^y\right)\\ &+ \sum_{j=1}^{n-3}\left(W_{j,j+3}\sigma_j^x\sigma_{j+1}^z\sigma_{j+2}^z\sigma_{j+3}^x + W_{j+3,j}\sigma_j^y\sigma_{j+1}^z\sigma_{j+2}^z\sigma_{j+3}^y\right) + \ldots\\ &+ W_{1,n}\sigma_1^x\sigma_2^z\ldots\sigma_{n-1}^z\sigma_n^x + W_{n,1}\sigma_1^y\sigma_2^z\ldots\sigma_{n-1}^z\sigma_n^y\,, \end{aligned} \tag{5.24}$$

where the coefficients $W_{j,k}$ are real, and Hamiltonians of the form

$$\mathcal{H} = \sum_{j,k=1}^{n} A_{j,k}\left(c_j^\dagger c_k - c_j c_k^\dagger\right) + B_{j,k}\left(c_j^\dagger c_k^\dagger - c_j c_k\right)\,, \tag{5.25}$$

where $\{c_j : \ j = 1, \ldots, n\}$*, defined by (4.76), satisfy the FCRs,* A *is a real symmetric* $n \times n$ *matrix, and* B *is a real anti-symmetric matrix. The bijection is given by the invertible transformation*

$$\begin{aligned} A_{j,j} &= W_{j,j} \ , \\ A_{j,j+m} = A_{j,j+m} &= \frac{(-1)^{m+1}}{2} \left(W_{j,j+m} + W_{j+m,j} \right) \ , \\ B_{j,j+m} = -B_{j,j+m} &= \frac{(-1)^{m+1}}{2} \left(W_{j,j+m} - W_{j+m,j} \right) \ . \end{aligned} \tag{5.26}$$

Proof. It will be helpful to rewrite Equation (5.25) so that we only have to consider terms with $j \leq k$. Using the FCRs, we get

$$\begin{aligned} \mathcal{H} = \sum_{j=1}^{n} A_{j,j} \left(2c_j^\dagger c_j - I_{2^n} \right) + \sum_{1 \leq j < k \leq n} 2 \Big[A_{j,k} \left(c_j^\dagger c_k - c_j c_k^\dagger \right) \\ + B_{j,k} \left(c_j^\dagger c_k^\dagger - c_j c_k \right) \Big] \ . \end{aligned} \tag{5.27}$$

Now we apply the Jordan-Wigner transformation from Equation (4.76). Let us simplify each term in (5.27) separately. Using the fact that $(\sigma_j^z)^2 = I_{2^n}$, we get

$$2c_j^\dagger c_j - I_{2^n} = 2 \left(\frac{\sigma_j^x + i\sigma_j^y}{2} \right) \left(\frac{\sigma_j^x - i\sigma_j^y}{2} \right) - I_{2^n} \ . \tag{5.28}$$

Since $(\sigma_j^x)^2 = (\sigma_j^y)^2 = I_{2^n}$ and $-i\sigma_j^x \sigma_j^y = i\sigma_j^y \sigma_j^x = \sigma_j^z$, Equation (5.28) simplifies to

$$2c_j^\dagger c_j - I_{2^n} = \sigma_j^z \ . \tag{5.29}$$

Now for $j < k$, using commutativity and the fact that $(\sigma_j^z)^2 = I_{2^n}$, we get:

$$c_j^\dagger c_k = (-1)^{j+k} \left(\frac{\sigma_j^x + i\sigma_j^y}{2}\right) \sigma_j^z \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x - i\sigma_k^y}{2}\right) , \tag{5.30}$$

$$c_j c_k^\dagger = (-1)^{j+k} \left(\frac{\sigma_j^x - i\sigma_j^y}{2}\right) \sigma_j^z \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x + i\sigma_k^y}{2}\right) , \tag{5.31}$$

$$c_j^\dagger c_k^\dagger = (-1)^{j+k} \left(\frac{\sigma_j^x + i\sigma_j^y}{2}\right) \sigma_j^z \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x + i\sigma_k^y}{2}\right) , \tag{5.32}$$

$$c_j c_k = (-1)^{j+k} \left(\frac{\sigma_j^x - i\sigma_j^y}{2}\right) \sigma_j^z \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x - i\sigma_k^y}{2}\right) . \tag{5.33}$$

Now, we eliminate σ_j^z using the identities $\sigma_j^x \sigma_j^z = -i\sigma_j^y$ and $\sigma_j^y \sigma_j^z = i\sigma_j^x$:

$$c_j^\dagger c_k = (-1)^{j+k} \left(\frac{-i\sigma_j^y - \sigma_j^x}{2}\right) \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x - i\sigma_k^y}{2}\right) , \tag{5.34}$$

$$c_j c_k^\dagger = (-1)^{j+k} \left(\frac{-i\sigma_j^y + \sigma_j^x}{2}\right) \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x + i\sigma_k^y}{2}\right) , \tag{5.35}$$

$$c_j^\dagger c_k^\dagger = (-1)^{j+k} \left(\frac{-i\sigma_j^y - \sigma_j^x}{2}\right) \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x + i\sigma_k^y}{2}\right) , \tag{5.36}$$

$$c_j c_k = (-1)^{j+k} \left(\frac{-i\sigma_j^y + \sigma_j^x}{2}\right) \sigma_{j+1}^z \dots \sigma_{k-1}^z \left(\frac{\sigma_k^x - i\sigma_k^y}{2}\right) . \tag{5.37}$$

When we subtract (5.35) from (5.34) and (5.37) from (5.36), the imaginary terms cancel, and factoring out a minus we get:

$$c_j^\dagger c_k - c_j c_k^\dagger = \frac{(-1)^{j+k+1}}{2} \left(\sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^x + \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^y\right) , \tag{5.38}$$

$$c_j^\dagger c_k^\dagger - c_j c_k = \frac{(-1)^{j+k+1}}{2} \left(\sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^x - \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^y\right) . \tag{5.39}$$

Observing that $(-1)^{k+j+1} = (-1)^{k-j+1}$, we are ready to rewrite the Hamiltonian in (5.27):

$$\begin{aligned}\mathcal{H} = \sum_{j=1}^{n} A_{j,j} \sigma_j^z + \sum_{1 \le j < k \le n} (-1)^{j-k+1} A_{j,k} \left(\sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^x + \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^y\right) \\ + \sum_{1 \le j < k \le n} (-1)^{j-k+1} B_{j,k} \left(\sigma_j^x \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^x - \sigma_j^y \sigma_{j+1}^z \sigma_{j+2}^z \dots \sigma_{k-1}^z \sigma_k^y\right) .\end{aligned} \tag{5.40}$$

It is evident we can set, for $j \leq k$,

$$W_{j,j} = A_{j,j} \tag{5.41}$$

$$W_{j,k} = (-1)^{k-j+1}\,(A_{j,k} + B_{j,k}) \qquad W_{k,j} = (-1)^{k-j+1}\,(A_{j,k} - B_{j,k})\ , \tag{5.42}$$

and that all values of W are possible through appropriate choices of A and B. Now we invert the transformation to obtain:

$$A_{j,j} = W_{j,j} \tag{5.43}$$

$$A_{j,j+m} = \frac{(-1)^{m+1}}{2}\,(W_{j,j+m} + W_{j+m,j}) \quad B_{j,j+m} = \frac{(-1)^{m+1}}{2}\,(W_{j,j+m} - W_{j+m,j})\ . \tag{5.44}$$

Through appropriate choice of W we can realize any real symmetric A and real anti-symmetric B. □

Observe that, up to sign, the elements of the matrix W are the same those of $A+B$. So to find the ground-state energy gap for a Hamiltonian that can be written in the form of (5.24), we only need to arrange the W coefficients into an $n \times n$ matrix, apply the necessary sign changes, and find twice the least non-zero singular value of the resulting matrix.

Let us now work out a simple example to demonstrate Theorem 5.2.1. Consider

$$\mathcal{H} = \sigma_1^x \sigma_2^z \sigma_3^x - \sigma_2^z\ . \tag{5.45}$$

To find the spectrum of $\mathcal{H}$, normally we must diagonalize its 8×8 matrix represen-

tation

$$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} . \tag{5.46}$$

Instead, we will demonstrate how to find the eigenvalues by diagonalizing a 3×3 matrix. The W matrix for $\mathcal{H}$ is

$$W = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \tag{5.47}$$

and by Theorem 5.2.1, the associated A and B matrices are

$$A = \begin{pmatrix} 0 & 0 & -1/2 \\ 0 & -1 & 0 \\ -1/2 & 0 & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 0 & 0 & -1/2 \\ 0 & 0 & 0 \\ 1/2 & 0 & 0 \end{pmatrix} . \tag{5.48}$$

To apply Theorem 4.3.3, we need to find the singular values of $A+B$, which turn out to be $\Lambda_1 = 0$, $\Lambda_2 = 1$, and $\Lambda_3 = 1$. Table 5.1 illustrates how to find the energy levels of $\mathcal{H}$ using these values.

If $\mathcal{H}_P$ is in the form of (5.24), then so is the Hamiltonian evolution

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n} \sigma_j^z + s\mathcal{H}_P , \tag{5.49}$$

$\Lambda_1 = 0$	$\Lambda_2 = 1$	$\Lambda_3 = 1$	Energy
-1	-1	-1	-2
-1	-1	1	0
-1	1	-1	0
-1	1	1	+2
1	-1	-1	-2
1	-1	1	0
1	1	-1	0
1	1	1	+2

Table 5.1: Table of the different Fermi occupations with their corresponding energies, computed from the application of Theorem 5.2.1 and Theorem 4.3.3 to $\mathcal{H} = \sigma_1^x \sigma_2^z \sigma_3^x - \sigma_2^z$. Each row represents a different occupation configuration for sites 1, 2, and 3. To compute the energy of a row, start with zero, and for each site j, if site j is occupied (a "1" entry) add Λ_j to the energy; otherwise subtract Λ_j. There is perfect correspondence between the energy levels computed this way and the energy levels computed directly from the matrix representation of $\mathcal{H}$.

for $0 \leq s \leq 1$. As in the previous section, we have reason to expect the ground-state energy gap to be polynomial in n. We can use Theorem 5.2.1 to restate Theorem 5.1.1, to show that the ground-state energy gap is $\mathcal{O}(1/\sqrt{n})$ for certain random Hamiltonians on n qubits:

Theorem 5.2.2 (Random Hamiltonians using Pauli operators)**.** *Let $\mathcal{H}$ be defined by (5.24), where the elements of W are N(0,1) and independent. Let γ be the ground-state energy gap of $\mathcal{H}$. Then, for large n, $n\gamma^2/4$ converges in distribution to the probability density function*

$$\rho(x) = \frac{1 + \sqrt{x}}{2\sqrt{x}} e^{-(x/2+\sqrt{x})} \ . \tag{5.50}$$

Proof. Observe that the entries of W are, up to sign, those of $A + B$ as defined by Theorem 5.2.1. Thus $A + B$ has independent N(0,1) entries, so we have the same proof as Theorem 5.1.1. □

We can also restate Theorem 5.1.2:

Theorem 5.2.3 (Random Hamiltonian evolutions using Pauli operators)**.** *Let C be an $n \times n$ matrix with independent N(0,1) elements, and let $A = CC^\dagger$. Let $\mathcal{H}_P$ be defined by (5.24), where $W_{j,k} = (-1)^{k-j+1} A_{j,k}$ for $j \neq k$ and $W_{j,j} = A_{j,j}$, and define the Hamiltonian evolution*

$$\mathcal{H}(s) = (1-s) \sum_{j=1}^{n} \sigma_j^z + s\mathcal{H}_P \; . \tag{5.51}$$

Then the ground-state energy gap of $\mathcal{H}(s)$ is

$$\breve{\gamma}(s) = 2(1-s) + \gamma \; , \tag{5.52}$$

where $n\gamma/2$ converges in distribution to the probability density function

$$\rho(x) = \frac{1+\sqrt{x}}{2\sqrt{x}} e^{-(x/2+\sqrt{x})} \tag{5.53}$$

for large n.

Proof. Apply Theorem 5.2.1 to Theorem 5.1.2. □

Further, if the A and B matrices of $\mathcal{H}_P$, as defined by Theorem 5.2.1, are circulant, then we can use Theorem 5.1.3 to conclude that the ground-state energy gap is bounded below by a polynomial in n^{-1} and s for the whole evolution specified by Equation (5.49). For instance, suppose

$$\mathcal{H}_P = \sigma_1^x \sigma_2^x + \sigma_2^x \sigma_3^x - \sigma_1^y \sigma_2^z \sigma_3^y \; . \tag{5.54}$$

Then, by Theorem 5.2.1, $\mathcal{H}_P$ has the A and B matrices given in (5.14) which are circulant, and Theorem 5.1.3 tells us that AQC finds the ground state of $\mathcal{H}_P$ in polynomial time, using the evolution specified by (5.49).

Theorem 5.2.4 (Hamiltonian evolutions with circulant matrices using Pauli operators)**.** *Let $\tilde{W}$ be circulant, and let $\mathcal{H}_P$ be defined by (5.24), where $W_{j,k} = (-1)^{k-j+1}\tilde{W}_{j,k}$ for $j \neq k$, and $W_{j,j} = \tilde{W}_{j,j}$. Define the Hamiltonian evolution*

$$\mathcal{H}(s) = (1-s)\sum_{j=1}^{n}\sigma_j^z + s\mathcal{H}_P\ . \tag{5.55}$$

Then the ground-state energy gap of $\mathcal{H}(s)$ is bounded below by a polynomial in n^{-1} and s.

Proof. If $\tilde{W}$ is circulant then so is $\tilde{W}^\dagger$. By Theorem 5.2.1, $\tilde{W} = A + B$, and since A is symmetric and B is anti-symmetric, $\tilde{W}^\dagger = A - B$, so we have $A = (\tilde{W} + \tilde{W}^\dagger)/2$ and $B = (\tilde{W} - \tilde{W}^\dagger)/2$. Since circulant matrices form a closed algebra, A and B are circulant. Then we can apply Corollary 5.1.4 to $\mathcal{H}(s)$ to conclude the whole evolution has a minimum energy gap bounded below by a polynomial in n^{-1} and s. □

Chapter 6

Conclusions and Future Work

We proved a version of the Adiabatic Theorem that includes explicit definitions of constants, so that we could compare the predictions of theorems derived from it to examples, and we provided rigorous bounds for the adiabatic approximation under four sources of experimental error: perturbations in the initial condition, systematic time-dependent perturbations in the Hamiltonian, coupling to low-energy quantum systems, and decoherent time-dependent perturbations in the Hamiltonian. We applied the new results to the spin-1/2 particle in a rotating magnetic field, which is a standard example for discussing controversy in the adiabatic theorem [10, 60, 69]. We showed that our theorem makes correct predictions about the error of the adiabatic approximation as a function of time. We also applied the new results to the superconducting flux qubit proposed by Orlando *et al.* [40], with time-dependent perturbations in the applied magnetic field. This qubit has properties that make it a candidate for quantum adiabatic computation [28]. Because our version of the adiabatic theorem does not have unspecified constants, we are able to make numerical predictions about this qubit. We showed that for a particular amount of noise on superconducting wires near a qubit with ideal physical parameters, we could guarantee a small error in the adiabatic approximation provided that the evolution time was set within a particular interval.

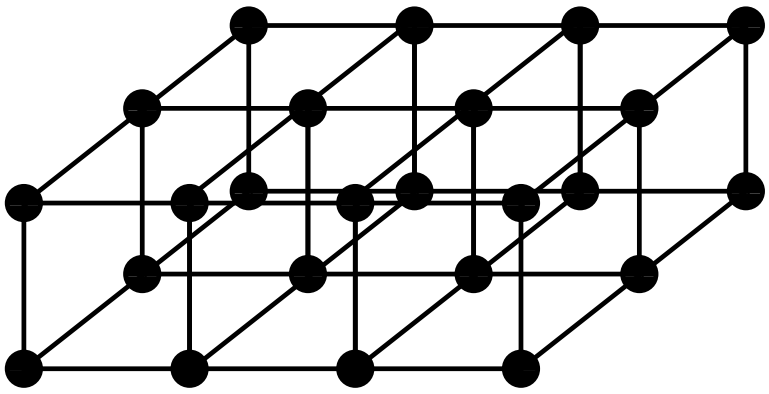

Figure 6.1: A two-level grid with n nodes representing spins $\{S_j : j = 1 \ldots n\}$. Non-zero interaction coefficients $J_{j,k} \in \{-1, 1\}$ are permitted only if there is an edge between S_j and S_k in the grid. Then minimizing the cost function $E(S_1, \ldots, S_n) = \sum_{j,k=1}^{n} J_{j,k} S_j S_k$ over inputs $S_j \in \{\pm 1\}$ is NP-complete.

We used the technique developed by Lieb *et al.* [33] for analyzing the one-dimensional XY model to identify a class of random Hamiltonians with non-nearest-neighbor interactions whose ground-state energy gap is $\mathcal{O}(1/\sqrt{n})$, where n is the number of qubits, and two classes of Hamiltonians with non-nearest-neighbor interactions whose ground state can be found in polynomial time with AQC. We used the Jordan-Wigner transformation to derive equivalent results for Hamiltonians defined using Pauli operators.

On the subject of the adiabatic theorem under noisy conditions, it remains to determine a bound on the error of the adiabatic approximation, for finite τ and with explicit definitions of constants, for general open quantum systems. Also, it may be possible to develop tighter bounds on AT-Noise, that take advantage of additional information about the Hamiltonian evolution, e.g., if the commutator between the noise term and the intended Hamiltonian is small.

For the purposes of AQC, it would be useful to know how to use the Hamiltonians

in Chapter 5 to model known classical problems. One possible starting point may be the relationship between the Hubbard model and the graph coloring problem [68]. Another is the relationship of the Hamiltonians in Chapter 5 to the knapsack problem [37].

It may be possible to analyze classical spin-glass models [7] by approximating their energy functions using Hamiltonians from Chapter 5. The classical spin-glass problem is to minimize the cost function

$$E(S_1, \ldots, S_n) = \sum_{j,k=1}^{n} J_{j,k} S_j S_k \ , \tag{6.1}$$

over all possible inputs $S_j \in \{\pm 1\}$, where $J_{j,k} \in \{-1, 0, 1\}$ are coefficients. Under the restrictions on $J_{j,k}$ illustrated in Figure 6.1, this problem is known to be NP-complete [7]. So solutions to this problem can be used to solve any problem whose solution can be efficiently verified, and even approximate solutions may be useful. It can be shown that minimizing E is equivalent to finding the ground state of

$$\mathcal{H}_E = \sum_{j,k=1}^{n} J_{j,k} \sigma_j^x \sigma_k^x \ . \tag{6.2}$$

Through a combination of approximations to various terms and use of ancillary qubits [29] we hope to approximate the ground state of $\mathcal{H}_E$ and thus the solution to the corresponding classical problem.

It is likely that we could extend the class of Hamiltonians whose ground-state energy gap can be determined efficiently, by considering other ways to construct Fermi operators. One alternative generalizes the Jordan-Wigner transform from a chain-like construction to a tree-like construction, thus facilitating analysis of multi-dimensional

lattices instead of one-dimensional systems [57]. Another alternative generalizes the Jordan-Wigner transformation to larger-spin operators, e.g. qudits [8, 15, 19, 30].

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