

The Quantum Adiabatic Optimization Algorithm and Local Minima

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ABSTRACT

The quantum adiabatic optimization algorithm uses the adiabatic theorem from quantum physics to minimize a function by interpolation between two Hamiltonians. The quantum wave function can sometimes tunnel through significant obstacles. However it can also sometimes get stuck in local minima, even for fairly simple problems. An initial Hamiltonian which insufficiently mixes computational basis states is analogous to a poorly mixing Markov transition rule.

We study a physical system – the Ising quantum chain with alternating sector interaction defects, but constant transverse field – which is equivalent to applying the quantum adiabatic algorithm to a particular SAT problem. We prove that for a constant range of values for the transverse field, the spectral gap is exponentially small in the sector length. Indeed, we prove that there are exponentially many eigenvalues all exponentially close to the ground state energy. Applying the adiabatic theorem therefore takes exponential time, even for this simple problem.

Categories and Subject Descriptors

F.2 [Theory of Computation]: Analysis of Algorithms and Problem Complexity

General Terms

Algorithms, Theory

Keywords

quantum adiabatic optimization, Ising quantum chain

1. INTRODUCTION

1.1 Quantum Adiabatic Optimization Algorithm

The quantum adiabatic optimization algorithm provides a general method for minimizing a function $f : \{0, 1\}^n \rightarrow \mathcal{R}$ [4]. Working in \mathcal{C}^{2^n} , define a final, problem Hamiltonian H_1 to be diagonal in the computational basis with f along its diagonal:

$$H_1 = \sum_{x \in \{0,1\}^n} f(x) |x\rangle\langle x|. \quad (1)$$

Choose an initial Hamiltonian H_0 . For $s \in [0, 1]$, let $H(s) = (1-s)H_0 + sH_1$ an interpolation between the two Hamiltonians. Choose a timing schedule $t(s)$ a strictly increasing function with $t(0) = 0$, $t(1) = \tau$. Starting with $|\psi(0)\rangle$ in the ground state of H_0 evolve the system according to Schrödinger's equation:

$$\frac{d}{ds} |\psi(s)\rangle = -\frac{i}{\hbar} t'(s) H(s) |\psi(s)\rangle. \quad (2)$$

The adiabatic theorem states that if the timing schedule is slow enough, then $|\psi\rangle$ will closely track the ground state of H_s , and the system will end up near the ground state of H_1 . How slow is “slow enough”? It has become almost a folk theorem in quantum computing that

$$\tau \gg \int_0^1 \frac{\| \frac{d}{ds} H \|}{\gamma(s)^2} ds \quad (3)$$

suffices, where γ is the eigenvalue gap of H away from the ground state energy. Measuring the final state in the computational basis will therefore give the minimum of f with good probability.

By quantum adiabatic *optimization* algorithm, we refer to the above prescription for minimizing a function f . More general quantum adiabatic computation also uses the adiabatic theorem to track the ground state between two Hamiltonians, but does not prescribe a specific form for H_1 as in Eq. (1). Quantum adiabatic computation is universal for quantum computing [1], even with linear interpolation between local Hamiltonians (in which each qudit interacts with only a constant number of neighbors).

1.2 This Paper

One reason for studying quantum adiabatic computation is that it can give physical insights into how quantum algorithms really work. The goal of this paper is to increase our

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understanding of this important model for quantum computing, and especially of quantum adiabatic optimization.

To start with, we are not aware of any paper using the quantum adiabatic algorithm that includes a rigorous statement of the quantum adiabatic theorem itself, nor even a citation to a rigorous proof of the theorem. So in Sect. 2 we give a rigorous statement of the theorem, and the necessary details for a proof, based on [2], are in Appendix A. Roughly, the theorem says that for any k , there is a constant $c(k)$ such that

$$\tau \geq c(k) \min_s \frac{\left\| \frac{d}{ds} H \right\|^{1+1/k}}{\gamma^{2+1/k}} \quad (4)$$

suffices to give small error.

In Sect. 3 we give a problem which displays some of the adiabatic algorithm's power. We prove a result, originally suggested by Farhi et al [7], that the adiabatic algorithm tunnels through an obstacle that a classical algorithm like simulated annealing could not overcome. This shows that the possibility of tunneling is one way in which quantum algorithms are more powerful than classical counterparts.

The requirement " $\tau \gtrsim 1/\gamma^2$ " is sufficient for the quantum adiabatic algorithm to work, but not generally necessary. Ideally, one would like a necessary lower bound on τ for the adiabatic algorithm to succeed. A continuous-time hybrid argument seems to be the most natural way to prove lower bounds. However, all previous attempts have essentially encountered the difficulty that the error allowed by the adiabatic theorem can accumulate in just the wrong places. In Sect. 4 we give an example of a highly symmetric problem for which a hybrid argument applies to give necessity of the adiabatic condition.

Finally in Sect. 5 we give the main result of this paper. Previously, a highly-nonlocal 3-SAT formula was known with an exponentially small eigenvalue gap [5]. Here the function to be minimized is the number of unsatisfied formula clauses of a particular truth assignment. The f -query complexity of SAT is only $O(n^3)$ [4], so exponential lower bounds of the type for black-box search do not apply. In fact, Farhi et al [8] have given numerical evidence that the quantum adiabatic optimization algorithm might be very efficient on random, hard SAT instances, possibly for locality reasons.

We consider a certain local – and quite physically natural – SAT formula with a natural choice of initial Hamiltonian H_0 . Our same Hamiltonian had been studied in a more physical context, where it was only argued that the minimum eigenvalue gap should be polynomially small [16]. We show that the minimum eigenvalue gap is in fact exponentially small. Moreover, we can choose parameters so there are exponentially many eigenvalues exponentially close to the ground state energy. This implies that applying the adiabatic theorem requires exponential time. Intuitively, the algorithm gets stuck in a local minimum because the initial Hamiltonian does not generate sufficiently nonlocal transitions, in analogy to poorly mixing Markov transition rules.

The technique for this proof draws from quantum statistical mechanics. We are trying to analyze an exponentially large matrix for which it is hard to even find the ground state or ground state energy. The first step of our analysis is to apply a Jordan-Wigner transformation to reduce the problem down to an $N \times N$ matrix whose eigenvalues are the squares of the eigenvalue gaps of the original Hamiltonian.

This much smaller matrix turns out to be tridiagonal, so we can study its Sturm sequence to bound its eigenvalues.

2. RIGOROUS STATEMENT OF A QUANTUM ADIABATIC THEOREM FOR COMPUTER SCIENCE

In this section, we give a rigorous statement of an adiabatic theorem for matrices, the case most interesting from a computer science perspective. We include an exact, computable error upper bound, confirming the “folk theorem” that the time required to prevent transitions out of an eigenspace is (arbitrarily close to) inverse quadratic in the minimum eigenvalue gap.

Consider the evolution from time $t = 0$ to $t = \tau$ of a quantum system under the Hamiltonian $H = H(s = t/\tau)$. We can solve for $U(s)$ the unitary evolution operator with Schrödinger's equation

$$\frac{d}{ds} U = -i \frac{\tau}{h} H U, \quad U(0) = I. \quad (5)$$

ADIABATIC THEOREM. *Let $H(s)$, $s \in [0, 1]$, be a finite-dimensional, $(k+1)$ -times differentiable, Hermitian matrix, $k \geq 1$. Let $U(s)$ be the solution to Schrödinger's equation Eq. (5). Let P_0 be a projection onto an eigenstate of $H(0)$, with corresponding eigenvalue λ_0 . Assume that λ_0 can be defined continuously for all $s \in [0, 1]$, $\lambda_0(s)$, and is always nondegenerate. Let $P(s)$ be the projection onto the spectral subspace corresponding to $\lambda_0(s)$ for $H(s)$. Then there is a constant $c(k)$ such that, assuming $\|(\frac{d}{ds})^l H(s)\| \leq h(s)$ for all $l \leq k$,*

$$\|(I - P) U P_0\| \leq c(k) \left(\frac{1}{\tau} \frac{1}{\gamma^2} h \Big|_{b.c.} + \max_{0 \leq \sigma \leq s} \frac{1}{\tau^k} \frac{1}{\gamma^{2k+1}} h^{k+1} \right), \quad (6)$$

where $\gamma(s)$ is defined to be the minimum eigenvalue gap away from λ_0 , i.e., labeling the eigenvalues of $H(s)$ by λ_i , $\gamma \equiv \min_{i \neq 0} |\lambda_i - \lambda_0|$. The matrix norm $\|\cdot\|$ is that induced by the l_2 metric. The notation $|_{b.c.}$ is to indicate that we evaluate the expression at the boundaries 0 and s , and add these values.

The theorem states that if we start in an eigenvector $|\psi\rangle$ of $H(0)$ and evolve for a long enough time $\tau \geq \text{constant} \times h^{1+1/k} / \gamma^{2+1/k}$ for any constant k , then we will end up close to the corresponding eigenvector of $H(1)$. It is stated in terms of the projection operators, e.g. $P_0 = |\psi\rangle\langle\psi|$, because the phase is not nailed down.

This theorem is based on an adiabatic theorem due to Avron et al [2]. However, they do not estimate the dependence of the error on the eigenvalue gap γ or on h – only on τ . The key ingredient of our proof, given in Appendix A, is [2, Lemma 2.5], which we combine with explicit error estimates.

3. ADIABATIC TUNNELING

In this section and the next, we consider two variations on the simple and highly symmetric problem of trying to minimize the Hamming weight of a bit string.

3.1 Adiabatic Algorithm for the Hamming Weight Function

First we need to understand the unperturbed problem. Consider $f(x) = |x|$ the Hamming weight function. Let

$H_0 = \sum_{i=1}^n (H_0)_i$, and

$$H_1 = \sum_{x \in \{0,1\}^n} |x\rangle\langle x| = \sum_{i=1}^n (H_1)_i, \quad (7)$$

where

$$H_0 = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (8)$$

Letting $\Delta = \sqrt{1 - 2s + 2s^2}$, the eigenvalues and corresponding eigenvectors of $H(s) = (1-s)H_0 + sH_1$ are

$$E_{\pm} = \frac{1}{2}(1 \pm \Delta) \\ |v_{\pm}\rangle = \frac{1}{\sqrt{2\Delta(\Delta \pm s)}} (\pm(\Delta \pm s)|0\rangle + (1-s)|1\rangle). \quad (9)$$

The eigenvalue gap Δ is minimized at $s = \frac{1}{2}$, when $\Delta = \frac{1}{\sqrt{2}}$.

The ground state of $H(s)$ is

$$|v_{-}\rangle^{\otimes n} = \frac{1}{(2\Delta(\Delta + s))^{n/2}} \sum_{x \in \{0,1\}^n} (1-s)^{|x|} (\Delta + s)^{n-|x|} |x\rangle. \quad (10)$$

As the ground state is a tensor product, its measured Hamming weight has a binomial distribution with parameters $(1-s)^2$ and $(\Delta + s)^2$. Applying the adiabatic algorithm takes $O(n)$ time.

3.2 The Hamming Weight Function With a Barrier

We consider a perturbed Hamming weight function

$$f'(x) = \begin{cases} |x| + p(x) & \text{if } l < |x| < u \\ |x| & \text{o.w.} \end{cases}, \quad (11)$$

for some nonnegative perturbation p added between the bounds l and u .

Since the unperturbed ground state is distributed as a binomial, it has a width (standard deviation) of about \sqrt{m} when it is centered on strings of weight m . We therefore expect that it should be able to tunnel through obstacles of width about \sqrt{m} , so the gap should be inverse-polynomial for $u = l + \sqrt{l}$. Numerical experiments using symmetry to reduce the Hamiltonian down to an $n \times n$ tridiagonal matrix strongly suggest that this is indeed the case. We can prove a weaker tunneling bound, still very good compared to a classical local random search. This problem is similar to the Hamming weight function with a spike, studied numerically in [7] but we allow the barrier to be polynomially wide.

Let $h_k = \sup_{|x|=k} p(x)$ and $h = \sup_k h_k$.

LEMMA 1. For $u = O(l)$, $\lambda'_0 \leq \lambda_0 + O\left(\frac{h(u-l)}{\sqrt{l}}\right)$.

PROOF.

$$\begin{aligned} \lambda'_0 - \lambda_0 &\leq \langle (v_{-})^{\otimes n} | (H' - H) | (v_{-})^{\otimes n} \rangle \\ &\leq \frac{1}{(2\Delta(\Delta + s))^n} \sum_{k=0}^n \binom{n}{k} h_k (1-s)^{2k} (\Delta + s)^{2(n-k)} \\ &= O\left(h \frac{(u-l)}{\sqrt{l}}\right), \end{aligned} \quad (12)$$

since \sqrt{l} is the width of a binomial distribution centered at l , so $(u-l)/\sqrt{l}$ is approximately the fraction of the ground state binomial distribution covered by the perturbation. \square

LEMMA 2. If $(H' - H)$ is diagonal and nonnegative, then the spectrum of H' lies above that of H : $\lambda'_k \geq \lambda_k \forall k$.

This is a special case of Weyl's Monotonicity Theorem [3] and follows immediately from the minimax principle.

By Lemmas 1 and 2, $\lambda'_1 - \lambda'_0 \geq \lambda_1 - \lambda'_0 \geq \Delta - O\left(h \frac{(u-l)}{\sqrt{l}}\right)$. So for example, for l and u both $\Theta(n)$, the perturbation can have width and height $\Omega(n^{1/4})$ and there still be a constant eigenvalue gap above the ground state energy. This polynomially large perturbation does not impede the progress of the quantum adiabatic algorithm.

4. ADIABATIC HYBRID ARGUMENT FOR A PERTURBED HAMMING WEIGHT FUNCTION

Van Dam et al [4] consider a perturbed Hamming weight problem, in which the function along the diagonal of the final Hamiltonian is

$$f'(x) = \begin{cases} |x| & \text{if } |x| \leq (\frac{1}{2} + \epsilon)n \\ p(x) & \text{o.w.} \end{cases}, \quad (13)$$

for $\epsilon > 0$ constant and $p(x)$ a function decreasing in $|x|$ that achieves the global minimum $f'(x) = p(x) = -1$ in the $|x| > (\frac{1}{2} + \epsilon)n$ region. They show that H'_s has an exponentially small eigenvalue gap. By the adiabatic theorem, exponential time is sufficient to find the minimum of f' . We will show with a hybrid argument that an exponential amount of time is necessary.

THEOREM 3. If $f'(x) = |x|$ for $x \leq (\frac{1}{2} + \epsilon)n$, $\epsilon > 0$, and achieves its minimum in the $|x| > (\frac{1}{2} + \epsilon)n$ region, then the adiabatic algorithm run for sufficient time to track the ground state of the unperturbed problem, but using H' instead, requires exponential time to minimize f' successfully with nonnegligible probability.

PROOF. Let $|\varphi_s\rangle$ be the state from running the unperturbed adiabatic algorithm with timing schedule $t(\cdot)$, and $|\varphi'_s\rangle$ be that from running the perturbed problem. If the Hamiltonians change slowly enough, then $|\varphi_s\rangle$ and $|\varphi'_s\rangle$ will closely track the ground states of the corresponding Hamiltonians. Now

$$|\varphi'_s\rangle = |\varphi_s\rangle + \int_0^s U'(\sigma, s) |dE_\sigma\rangle, \quad (14)$$

where

$$\begin{aligned} |dE(\sigma)\rangle &= (dU'(\sigma) - dU(\sigma))|\varphi_\sigma\rangle \\ &= ((1 - it'(\sigma)H'(\sigma)) - (1 - it(\sigma)H(\sigma)))|\varphi_\sigma\rangle d\sigma \\ &= it'(\sigma)\sigma(H_1 - H'_1)|\varphi_\sigma\rangle d\sigma \end{aligned} \quad (15)$$

is the error accumulated from times σ to $\sigma + d\sigma$, which is then propagated forward by $U'(\sigma, s)$. For $t'(s) = \Omega(n)$, $|\varphi_s\rangle$ tracks the ground state of H_s , so

$$\begin{aligned} \sqrt{2} \approx \|\varphi'_1 - \varphi_1\| &\leq \int_0^1 \sigma \|U'(\sigma, s)\| \cdot \|(H_1 - H'_1)|\varphi_\sigma\rangle\| d\sigma \\ &\leq \frac{t(1)}{2^{\Omega(n)}}. \end{aligned} \quad (16)$$

The second inequality follows because $|\varphi\rangle$ is a tensor product state $(a|0\rangle + b|1\rangle)^{\otimes n}$ with $|b| \leq \frac{1}{\sqrt{2}} + \epsilon$, so has only exponentially small weight on strings with Hamming weight more than $(\frac{1}{2} + \epsilon)n$. Therefore the total time needed is $\tau = t(1) \geq 2^{\Omega(n)}$. \square

Note that $|\varphi\rangle$ is *not* the ground state of H ; it only lies close to the ground state, with an error of $\sim 1/\tau$. If this error were arbitrary, then the hybrid argument would fail, since it could lie exactly in the support of $H - H'$. However tensor product symmetry prevents this possibility.

5. THE SAT FORMULA

Farhi et al [9] consider applying the adiabatic algorithm to SAT formulas; the function f to be minimized is the number of unsatisfied clauses of a particular boolean truth assignment. They define the “2-bit agree” clause to have satisfying assignments by 00 and 11.

Consider the SAT formula on N bits which includes a number c_k of 2-bit agree clauses between bits x_k and x_{k+1} , $k = 1, \dots, N-1$, and assume the multiplicities c_k vary with period n :

$$c_k = \begin{cases} W & \text{if } [k/n] \text{ is odd} \\ 1 & \text{otherwise} \end{cases}, \quad (17)$$

with $W > 1$. Choose an initial Hamiltonian which generates local spin flips $H_0 = -\sum_k \sigma_k^x$, where σ_k^x is a Pauli matrix acting on the k th site. Intuitively, the adiabatic algorithm should have a difficult time with this problem, because the odd sectors will be forced to commit to being all zeros or all ones before the even sectors. But then two odd sectors separated by a low-weight even sector can’t coordinate with each other and have only probability one half of agreeing. With N/n sectors, the probability that they all agree can be made exponentially small.

The computational problem so defined corresponds exactly to a problem in physics: the Ising quantum chain in a transverse magnetic field has the Hamiltonian

$$H = -\Gamma \sum_{k=1}^N \sigma_k^x - \sum_{k=1}^{N-1} J_k \sigma_k^z \sigma_{k+1}^z, \quad (18)$$

with periodically alternating coupling constants $J_k > 0$:

$$J_k = \begin{cases} w_1 & \text{if } [k/n] \text{ is odd} \\ w_2 & \text{otherwise} \end{cases}. \quad (19)$$

The parameter correspondence with the SAT formula is $\Gamma = 1 - s$, $w_2 = s$ and $w_1 = sW$. If the period n is fixed, then it is known that in the thermodynamic limit $N \rightarrow \infty$, the spectral gap above the ground state energy goes like $1/(N \exp(\Theta(n)))$ [10].

Several authors have considered the case where the number of sectors N/n is fixed instead of the period [15, 11]. However, these authors required that the transverse field Γ also vary periodically so the ratio J_k/Γ_k is fixed – when this ratio is 1, the sectors simultaneously achieve criticality. [16] considered the case when different sectors could have different ratios J/Γ . They approximate, justified by conformal invariance, that the spectral gap decreases like $1/N$.

In fact, however, we will prove that the spectral gap is *exponentially* small in the period length n , when sectors alternate between being z -ordered ($\Gamma/J < 1$) and z -disordered

($\Gamma/J > 1$). Unlike [10], our argument does not require that n be fixed as $N \rightarrow \infty$.

Intuitively, if a disordered sector is bracketed by two ordered sectors, the ordered sectors can be biased in the same z direction or in different z directions. The ground state energy of a disordered chain with constant J and left, right boundary conditions 0,0 or 1,1 is exponentially close to the ground state energy of the same chain with boundary conditions 0,1 or 1,0. Since the initial Hamiltonian generates only local spin flips, the algorithm is likely to get stuck in a local minimum, like $0^n 0^m 1^{n-m} 1^n$, if run for less than exponential time. In this case we can correct this by choosing H_0 so the different sectors achieve criticality simultaneously. Or we might allow sector spin flips, of the type $\sigma_k^x \sigma_{k+1}^x \cdots \sigma_N^x$ so in the dual basis the Hamiltonian decouples into the sum of single-qubit Hamiltonians (as for the unperturbed Hamming weight problem).

5.1 Theorem Statement and Overview of Proof

Take H as in (18), (19), with $(N-1)/n = (2b+1)$ alternating sectors¹. By scaling, assume $\Gamma = 1 - s$, $w_2 = s$ and $w_1 = sW$, for $s \in [0, 1]$, with $W > 1$ ($w_1 > w_2$). Formally, we’ll prove:

THEOREM 4. *For any fixed $s > \frac{1}{1+W}$, $H(s)$ has one eigenvalue only $O((\frac{1-s}{sW})^n)$ above the ground state energy. For $\frac{1}{1+W} < s \leq \frac{1}{1+\sqrt{W}}$ or $\frac{1}{1+\sqrt{W}} \leq s < 1/2$, $H(s)$ has $(2^{b+1} - 1)$ eigenvalues only $O(b(\frac{1-s}{sW})^n)$ or $O(b(\frac{s}{1-s})^n)$, respectively, above the ground state energy.*

Figure 1 shows two numerical examples. Loosely, the high-weight sectors have a critical point when the transverse field balances the coupling terms: $sW = 1 - s$, or $s = \frac{1}{1+W}$. For $s > \frac{1}{1+W}$, the couplings dominate the field, and the high-weight sectors are z -ordered. Similarly the critical point for the low-weight sectors is $s = \frac{1}{2}$; for $s > \frac{1}{2}$, the low-weight sectors are ordered. The whole system is critical, as $r \rightarrow \infty$, when the geometric mean of the weights balance the field [10], or $s = \frac{1}{1+\sqrt{W}}$.

The adiabatic algorithm consists of starting in the ground state at $s = 0$, $\frac{1}{2^{N/2}}(|0\rangle + |1\rangle)^{\otimes N}$, and slowly increasing s to 1. The ground state is nondegenerate when $s = 0$ ($w_1 = w_2 = 0$) and doubly degenerate at $s = 1$ ($\Gamma = 0$). The relevant eigenvalue gap for applying the adiabatic theorem is therefore the gap to the *second* eigenvalue above the ground state. Theorem 4 implies that this gap is exponentially small in n across a constant range $\frac{1}{1+W} < s < \frac{1}{2}$, so applying the adiabatic theorem requires exponential time². In fact, for n and b both $\Theta(\sqrt{N})$, there are exponentially many exponentially small excitations above the ground state.

There are two steps to the proof of Theorem 4. First, we write H as a quadratic form in fermion operators. By the classical techniques of [12], the spectral gaps of the $2^N \times 2^N$ matrix H are the square roots of the eigenvalues of an $N \times N$ symmetric, tridiagonal matrix. Next, we analyze the Sturm

¹Periodicity simplifies notation, but the sectors can have different lengths $n_1, n_2, \dots, n_{2b+1}$, $\sum_{k=1}^{2b+1} n_k = N-1$. Cyclic or anticyclic boundary conditions $\sigma_{N+1}^z = \pm \sigma_1^z$ can also be imposed.

²Since the gap is small across a constant range of s , a nonlinear timing schedule does not give a square root speedup, as one does for example in adiabatic Grover search [4].

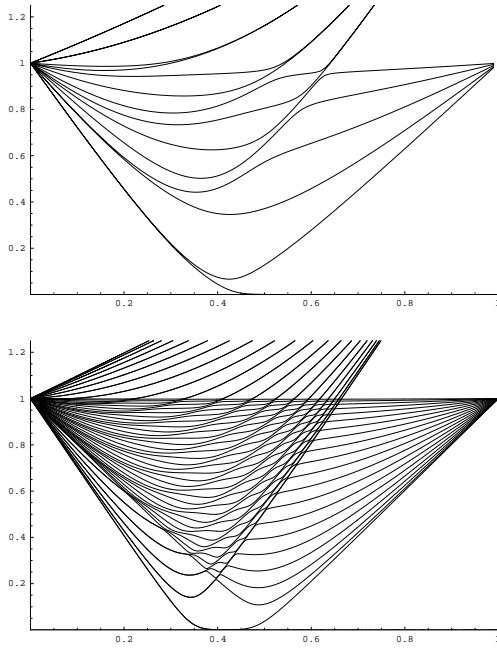


Figure 1: The eigenvalue *gaps* of $H(s)$ versus s , for three sectors of weights 2, 1 and 2, respectively ($b = 1, W = 2$). For the top graph, each sector has size $n = 5$. Of the two smallest gaps, only one approaches 0 as $s \rightarrow 1$. On the bottom, $n = 20$.

sequence of the principal leading minors of this matrix to bound the eigenvalue gaps of H .

5.2 Ising Model With Transverse Field as Quadratic Form in Fermion Operators

LEMMA 5. The eigenvalue gaps of H are the square roots of the eigenvalues of

$$4\Gamma^2 + 4 \begin{pmatrix} 0 & & & \\ & J_1^2 & & \\ & & \ddots & \\ & & & J_{N-1}^2 \end{pmatrix} - 4\Gamma \begin{pmatrix} 0 & J_1 \\ J_1 & 0 & & \\ & & \ddots & J_{N-1} \\ & & & 0 \end{pmatrix}. \quad (20)$$

Indeed, define fermion annihilation and creation operators a_k, a_k^\dagger by $a_k \equiv \sigma_1^x \sigma_2^x \dots \sigma_{k-1}^x \frac{1}{2} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}_k$ [13]. Then $\sigma_k^x = 1 - 2a_k^\dagger a_k$ and $\sigma_k^z \sigma_{k+1}^z = (a_k^\dagger - a_k)(a_{k+1}^\dagger + a_{k+1})$. Substituting into (18) and using the fermion anticommutation rules $\{a_j, a_k\} = 0, \{a_j, a_k^\dagger\} = \delta_{jk}$ ($\{a, c\} \equiv ac + ca$) gives

$$H = -N\Gamma + \sum_{ij} a_i^\dagger A_{ij} a_j + \frac{1}{2} (a_i^\dagger B_{ij} a_j^\dagger + a_i B_{ji} a_j), \quad (21)$$

where

$$A = 2\Gamma - \begin{pmatrix} 0 & J_1 & & \\ J_1 & 0 & J_2 & \\ & J_2 & \ddots & J_{N-1} \\ & & J_{N-1} & 0 \end{pmatrix}, \quad (22)$$

$$B = \begin{pmatrix} 0 & -J_1 & & \\ J_1 & 0 & -J_2 & \\ & J_2 & \ddots & -J_{N-1} \\ & & J_{N-1} & 0 \end{pmatrix}$$

are $N \times N$ matrices.

The Hamiltonian can then be written

$$H = E_g + \sum_{k=1}^N \sqrt{\lambda_k} \eta_k^\dagger \eta_k, \quad (23)$$

where the η_k, η_k^\dagger are fermion operators. The eigenvalues of H are $E_g + \sum_{k \in S} \sqrt{\lambda_k}$, where $S \subset \{1, \dots, N\}$. E_g is the ground state energy. The squared gaps λ_k are the eigenvalues of $(A - B)(A + B)$, given in (20) [12].

5.3 Bound Eigenvalues of $(A - B)(A + B)$ Using Sturm Sequence Property

LEMMA 6 ([14]). For C a symmetric, tridiagonal, irreducible matrix, let $m_i(\lambda)$ be the determinant of $C_i - \lambda I$, where C_i is the i th-order principal leading submatrix of C (i.e., the first i rows and i columns). The number of disagreements in sign between consecutive members of the sequence $m_0(\lambda) \equiv 1, m_1(\lambda), \dots, m_N(\lambda)$ is the number of eigenvalues of C which are at most λ .

The sequence $m_i(\lambda)$ can be computed recursively by $m_0(\lambda) = 1, m_1(\lambda) = \alpha_1 - \lambda$, and

$$m_i(\lambda) = (\alpha_i - \lambda)m_{i-1}(\lambda) - \beta_{i-1}^2 m_{i-2}(\lambda), \quad (24)$$

where $\alpha_i, i = 1, \dots, N$ are the diagonal entries of C , and $\beta_i, i = 1, \dots, N - 1$ the off-diagonal entries. This recursion implies that the eigenvalues of C_i and C_{i+1} are strictly separated if $\beta_i \neq 0$, from which Lemma 6 follows in [14, 5.38].

To prove Theorem 4, we solve the recursion (24) with $C = \frac{1}{4}(A - B)(A + B)$.

Fix the coupling weights of H to be w_1 in a sector of length n_1 , then w_2 in a sector of length n_2 , then w_1 again in a sector of length n_3 , with $w_1 > w_2$ different constants (for H normalized, $w_1 = sW, w_2 = s$). Let p_1, \dots, p_{n_1} be the Sturm sequence within the first sector, q_1, \dots, q_{n_2} the sequence within the second sector, and r_1, \dots, r_{n_3} the sequence within the third sector. Initial conditions for the recursions are $p_{-1} = 1, p_0 = \Gamma^2 - \lambda, q_{-1} = p_{n_1-1}, q_0 = p_{n_1}, r_{-1} = q_{n_2-1}, r_0 = q_{n_2}$.

5.3.1 Recursion (24) Within a Constant Weight Sector

Within a sector where the coupling weights are constant at w, α and β are also constant; from (20),

$$\alpha = \Gamma^2 + w^2$$

$$\beta = -\Gamma w. \quad (25)$$

Then (24) has solution $m_i = a_+ x_+^{i+1} + a_- x_-^{i+1}$, where x_\pm are the (distinct) roots of $x^2 - (\alpha - \lambda)x + \beta^2 = 0$:

$$\begin{aligned} x_\pm &= \frac{1}{2}(\sigma \pm \sqrt{\delta}) \\ \sigma &= \Gamma^2 + w^2 - \lambda \\ \delta &= (\Gamma^2 - w^2)^2 - 2(\Gamma^2 + w^2)\lambda + \lambda^2. \end{aligned} \quad (26)$$

For Γ bounded away from w (i.e., s bounded from $\frac{1}{1+w/s}$), δ is bounded above zero, so the roots are bounded away from each other and indeed distinct. Then we may write, if $w > \Gamma$,

$$\begin{aligned} x_+ &= w^2 - \frac{w^2}{w^2 - \Gamma^2} \lambda \mp \Theta(\lambda^2) \\ x_- &= \Gamma^2 + \frac{\Gamma^2}{w^2 - \Gamma^2} \lambda \pm \Theta(\lambda^2). \end{aligned} \quad (27)$$

If $w < \Gamma$, then x_+ and x_- should be switched above. Always, $x_+ > x_- > 0$. Let $\gamma = x_-/x_+ \in (0, 1)$.

The multiples a_\pm depend on the initial conditions $m_{-1} = a_+ + a_-$ and $m_0 = a_+ x_+ + a_- x_- = \frac{\sigma}{2} m_{-1} + \frac{\sqrt{\delta}}{2} (a_+ - a_-)$. Hence $a_+ - a_- = \frac{2}{\sqrt{\delta}} (m_0 - \frac{\sigma}{2} m_{-1})$, so $\sqrt{\delta} a_\pm = \mp x_\mp m_{-1} \pm m_0$. We conclude

$$m_i = \frac{1}{\sqrt{\delta w}} \begin{pmatrix} (-x_{w,-} m_{-1} + m_0) x_{w,+}^{i+1} \\ + (x_{w,+} m_{-1} - m_0) x_{w,-}^{i+1} \end{pmatrix}, \quad (28)$$

where the w subscripts on variables from (26) indicate the coupling weight at which they are calculated.

5.3.2 First Sector $\{p_i\}$

From (28),

$$p_i = \frac{p_{-1}}{\sqrt{\delta w_1}} \begin{pmatrix} (-x_{w_1,-} + p_0/p_{-1}) x_{w_1,+}^{i+1} \\ + (x_{w_1,+} - p_0/p_{-1}) x_{w_1,-}^{i+1} \end{pmatrix}. \quad (29)$$

For $w_1 > \Gamma$, the first term in (29) is $-x_{w_1,-} + \Gamma^2 - \lambda = -\Theta(\lambda)$, while the second term is $\Theta(1)$. The first term dominates, sending p_i negative, if $\lambda = \Omega(\gamma_{w_1}^{n_1})$. By Lemmas 6 and 5, this proves the first part of Theorem 4. Also for $\lambda = \Omega(\gamma_{w_1}^{n_1})$,

$$\begin{aligned} \frac{p_{n_1}/p_{n_1-1}}{x_{w_1,+}} &= \frac{1 - \Theta(1/\lambda) \gamma_{w_1}^{n_1+1}}{1 - \Theta(1/\lambda) \gamma_{w_1}^{n_1}} \\ &\in (1 + (1 - \gamma_{w_1}) \Theta(1/\lambda) \gamma_{w_1}^{n_1}, 1 + \Theta(1/\lambda) \gamma_{w_1}^{n_1}). \end{aligned} \quad (30)$$

This follows since a fraction $\frac{1 - a\gamma^{n+1}}{1 - a\gamma^n}$ can be expanded $1 + (1 - \gamma)(a\gamma^n) + (1 - \gamma)(a\gamma^n)^2 + \dots$. For $a\gamma^n$ smaller than a constant, terms decrease and alternate.

5.3.3 Second Sector $\{q_i\}$

From (28),

$$q_i = \frac{p_{n_1-1}}{\sqrt{\delta w_2}} \begin{pmatrix} (-x_{w_2,-} + p_{n_1}/p_{n_1-1}) x_{w_2,+}^{i+1} \\ + (x_{w_2,+} - p_{n_1}/p_{n_1-1}) x_{w_2,-}^{i+1} \end{pmatrix}. \quad (31)$$

For $w_2 < \Gamma$, by (30) the first term in (31) is positive and the second term negative. Since the sum of the terms is initially positive, the first term will dominate throughout and the sequence does not change signs. Each term has magnitude $\Theta(1)$. Hence for n_2 at least some constant,

$$\frac{q_{n_2}/q_{n_2-1}}{x_{w_2,+}} \in (1 + (1 - \gamma_{w_2}) \Theta(1) \gamma_{w_2}^{n_2}, 1 + \Theta(1) \gamma_{w_2}^{n_2}). \quad (32)$$

5.3.4 Third Sector $\{r_i\}$

From (28),

$$r_i = \frac{q_{n_2-1}}{\sqrt{\delta w_1}} \begin{pmatrix} (-x_{w_1,-} + q_{n_2}/q_{n_2-1}) x_{w_1,+}^{i+1} \\ + (x_{w_1,+} - q_{n_2}/q_{n_2-1}) x_{w_1,-}^{i+1} \end{pmatrix}. \quad (33)$$

By (32) the second term in (33) is $\Theta(1)$. The first term, $q_{n_2}/q_{n_2-1} - x_{w_1,-}$, is small and of indeterminate sign. Since from (32) and (27)

$$\begin{aligned} q_{n_2}/q_{n_2-1} &< x_{w_2,+} (1 + c\gamma_{w_2}^{n_2}) \\ &= (\Gamma^2 - \frac{\Gamma^2}{\Gamma^2 - w_2^2} \lambda) (1 + c\gamma_{w_2}^{n_2}) - O(\lambda^2) \\ x_{w_1,-} &> \Gamma^2 + \frac{\Gamma^2}{w_1^2 - \Gamma^2} \lambda, \end{aligned} \quad (34)$$

we get

$$\frac{q_{n_2}}{q_{n_2-1}} - x_{w_1,-} < \Gamma^2 c\gamma_{w_2}^{n_2} - \Gamma^2 \left(\frac{1 + c\gamma_{w_2}^{n_2}}{w_2^2 - \Gamma^2} + \frac{1}{w_1^2 - \Gamma^2} \right) \lambda. \quad (35)$$

This is $\Theta(\gamma_{w_2}^{n_2}) - \Theta(\lambda)$, which is $-\Theta(\lambda)$ for $\lambda = \Omega(\gamma_{w_2}^{n_2})$. For this term to eventually dominate the second term, λ must be $\Omega(\gamma_{w_1}^{n_3})$.

Hence if $w_2 < \Gamma < w_1$, and λ is $\Omega(\gamma_{w_1}^{n_1})$, $\Omega(\gamma_{w_2}^{n_2})$ and $\Omega(\gamma_{w_1}^{n_3})$, $(A - B)(A + B)$ has two eigenvalues less than λ . When $n_1 = n_2 = n_3 = n$, this proves the second part of Theorem 4 for $b = 1$. Moreover,

$$\frac{r_{n_3}/r_{n_3-1}}{x_{w_1,+}} \in (1 + (1 - \gamma_{w_1}) \Theta(1/\lambda) \gamma_{w_1}^{n_1}, 1 + \Theta(1/\lambda) \gamma_{w_1}^{n_1}). \quad (36)$$

This bound is the same as (30) on p_{n_1}/p_{n_1-1} . We may even assume the $\Theta(1/\lambda)$ term has the same constants. Hence the argument can be repeated indefinitely, proving Theorem 4 for general b . Note that the bounds asymptotically balance for $\Gamma = \sqrt{w_1 w_2}$, when $\gamma_{w_1} \approx \gamma_{w_2} \approx w_2/w_1$. For example, if all sectors have width n and $\Gamma = \sqrt{w_1 w_2}$, then the Sturm sequence changes sign in each high-weight sector, provided $\lambda = \Omega((w_2/w_1 + \epsilon)^n)$, for any $\epsilon > 0$. Since ϵ can be made exponentially small, it can be taken out of the exponential and absorbed into the leading constant.

6. CONCLUSION

The adiabatic optimization algorithm is partly appealing because of its black box, prescriptive nature. To minimize any computable function f , we simply set up f along the diagonal of a final Hamiltonian, and starting with the ground state of some initial Hamiltonian, adiabatically interpolate between the two Hamiltonians. The adiabatic theorem – which we have rigorously justified – guarantees that this algorithm *will* find the minimum of f if run for a long enough time. The quantum wave function can sometimes tunnel through obstacles that would stymie classical search algorithms, and its tunneling ability ought to provide other optimization problems where this technique can be profitably applied.

However we have shown that despite its power, the adiabatic algorithm can still be vulnerable to the same sorts of locality traps that trip up classical algorithms. The adiabatic algorithm is no more a universal black box solution than classical simulated annealing, and needs to be designed and analyzed carefully. Moreover, these results provide insight for physics into the behavior of a simple and natural adiabatic system.

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APPENDIX

A. PROOF OF THE QUANTUM ADIABATIC THEOREM

To prove our Adiabatic Theorem, we recursively apply [2, Lemma 2.5] and then compute explicit error bounds. Set $\hbar = 1$, and $\dot{A} \equiv \frac{d}{ds}A$.

Define the “adiabatic evolution” U_A by

$$\dot{U}_A = -i\tau H_A U_A, \quad U_A(0) = I, \quad (37)$$

where

$$H_A = H + \frac{i}{\tau}[\dot{P}, P]. \quad (38)$$

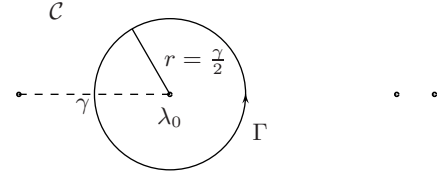


Figure 2.

Since P and \dot{P} are Hermitian, $i[\dot{P}, P]$ is Hermitian, so U_A is unitary.

LEMMA 7. U_A as defined above satisfies the “intertwining property”:

$$U_A(s)P_0 = P(s)U_A(s). \quad (39)$$

Lemma 7 says that if we start in the eigenstate corresponding to P_0 and apply U_A then we end up in the eigenstate corresponding to $P(s)$ (in this case $P_0|\psi\rangle = |\psi\rangle$, so the lemma says $P(U_A|\psi) = U_A|\psi\rangle$). We have included a proof at the end of this section for completeness, or see [2]. We wish to show that the Hamiltonian evolution U is close to the adiabatic evolution U_A for τ large.

Let $W = U_A^\dagger U$, and $Q = I - P$. Then since $QP = 0$, and by the intertwining property Eq. (39),

$$\begin{aligned} QUP_0 &= Q(U - U_A)P_0 \\ &= QU_A(W - 1)P_0 \\ &= U_A Q_0 W P_0, \end{aligned} \quad (40)$$

so we only need to bound $\|Q_0 W P_0\|$.

For fixed s , define the resolvent $R(z)$, $z \in \mathcal{C}$, by $R = (H - zI)^{-1}$. Writing $H = \sum_j \lambda_j |j\rangle\langle j|$, $R = \sum_j \frac{1}{\lambda_j - z} |j\rangle\langle j|$. Let Γ be a circle in the complex plane centered at λ_0 and with radius exactly $r = \gamma/2$, as in Fig. 2. We choose this radius to get the best upper bound for $\|R\|$ on Γ , namely $2/\gamma = 1/r$. Then by residues calculus

$$P = -\frac{1}{2\pi i} \int_{\Gamma} R(z) dz. \quad (41)$$

Also, $\dot{R} = -R\dot{H}R$. This implies, for example, that

$$\dot{P} = \frac{1}{2\pi i} \int_{\Gamma} R\dot{H}R. \quad (42)$$

We can bound this integral by its circumference $2\pi r$ times a bound on $\|R\|^2 \|\dot{H}\|$ on Γ :

$$\|\dot{P}\| \leq \frac{2\pi r}{2\pi} \frac{1}{r^2} \|\dot{H}\| = \frac{2}{\gamma} \|\dot{H}\| \leq \frac{2}{\gamma} h. \quad (43)$$

(With a result in [6] one can show $\|\dot{P}\| \leq \|\dot{H}\|/\gamma$.) For $k \geq 2$, we will also need a bound on the norm of

$$\ddot{P} = \frac{1}{2\pi i} \int_{\Gamma} -2R\dot{H}R\dot{H}R + R\ddot{H}R. \quad (44)$$

By the same argument as above, $\|\ddot{P}\| \leq \frac{2}{\gamma^2} h^2 + \frac{1}{\gamma} h$. Since $\gamma \leq 2\|H\| \leq 2h$, $\frac{h}{\gamma} \geq 1$, so $\|\ddot{P}\| \leq 3\frac{h^2}{\gamma^2}$. More generally, for $l \leq k$, we can conservatively count the number of terms in the l th derivative to get

$$\left\| \left(\frac{d}{ds} \right)^l P \right\| \leq (2l-1)!! \left(\frac{h}{\gamma/2} \right)^l, \quad (45)$$

where $(2l-1)!! \equiv \prod_{m=1}^l (2m-1)$ – a constant independent of h or τ .

The following lemma gives the key integration-by-parts step of the proof. A proof of the lemma is given at the end of this section, or see [2].

LEMMA 8 ([2]). *Given X, Y linear operators, let $\tilde{X} = \frac{1}{2\pi i} \int_{\Gamma} R X R$. Then*

$$\begin{aligned} & \int_0^s Q_0 U_A^\dagger X U_A P_0 Y \\ &= \frac{i}{\tau} Q_0 \left(U_A^\dagger \tilde{X} U_A P_0 Y \Big|_0^s - \int_0^s U_A^\dagger \tilde{X} U_A P_0 \dot{Y} \right. \\ & \quad \left. - \int_0^s U_A^\dagger (\dot{\tilde{X}} + [\dot{P}, \tilde{X}]) U_A P_0 Y \right). \end{aligned} \quad (46)$$

The two right-hand integral terms in Eq. (46) are of the form required for applying Lemma 8 again; in the first term we have $X' = \tilde{X}$, $Y' = Y$ and in the second term $X'' = \dot{\tilde{X}} + [\dot{P}, \tilde{X}]$, $Y'' = Y$. Therefore the lemma can be applied recursively. Applying the lemma k times will leave $2^k - 1$ boundary terms and 2^k integral terms.

We can estimate $\|\tilde{X}\| = O_1(\frac{1}{\gamma}\|X\|)$, where we have started using big- O_l notation to hide constants depending only possibly on the recursion step $l \leq k$. Therefore also $\|\dot{\tilde{X}}\| = O_1(\frac{1}{\gamma}\|\dot{X}\| + \frac{h}{\gamma^2}\|X\|)$, so $\|\dot{\tilde{X}} + [\dot{P}, \tilde{X}]\| = O_1(\frac{1}{\gamma}\|\dot{X}\| + \frac{h}{\gamma^2}\|X\|)$.

Assume now that $\|(\frac{d}{ds})^l X\| = O_l((h/\gamma)^l \|X\|)$, $l \leq k$. Then by the same sort of argument used for Eq. (45), also $\|(\frac{d}{ds})^l X'\| = \|(\frac{d}{ds})^l \tilde{X}\| = O_l((h/\gamma)^l \|X'\|)$. Similarly, for X'' each differentiation pulls out a factor of h/γ , so too $\|(\frac{d}{ds})^l X''\| = O_l((h/\gamma)^l \|X''\|)$. By induction, if X_m appears in the “ X ” position of Lemma 8 at recursion level $m \leq k$, then

$$\|(\frac{d}{ds})^l X_m\| = O_k((h/\gamma)^l \|X_m\|), \quad m \leq k-l. \quad (47)$$

In particular,

$$\|X'_m\| = O_1(\frac{1}{\gamma}\|X_m\|) \quad (48a)$$

$$\|X''_m\| = O_m(\frac{h}{\gamma^2}\|X_m\|). \quad (48b)$$

Assume also that $\|(\frac{d}{ds})^l Y\| = O_l((h/\gamma)^l \|Y\|)$, $l \leq k$. If Y_m appears in the “ Y ” position of Lemma 8 at recursion level m , then $Y_m = (\frac{d}{ds})^l Y$ for some $l \leq m$. Therefore

$$\|Y'_m\| = O_m(\frac{h}{\gamma}\|Y_m\|) \quad (49a)$$

$$\|Y''_m\| = O_1(\|Y_m\|). \quad (49b)$$

Hence, under these assumptions on X and Y , each time we apply Lemma 8, $\|X'\| \|Y'\|$ and $\|X''\| \|Y''\|$ pick up a factor of h/γ^2 . The boundary terms associated with these integrals, $\|X'\| \|Y'\|$ and $\|X''\| \|Y''\|$, pick up a factor of h/γ^2 also, compared to the boundary term at the previous level. Thus if $\|X\| = O_1(\frac{1}{\gamma})$, $Y = O_1(1)$ originally, then after k recursions, we’ll have boundary terms of order $O_l((h/(\tau\gamma^2))^l)$ for each $l = 1, \dots, k$, and integrals which can be bounded by $O_k(\frac{1}{\tau^k} \frac{h^{2k}}{\gamma^{2k+1}})$.

Now we can finish the proof of the k th order adiabatic theorem. Since

$$\dot{W} = -KW, \quad K = U_A^\dagger [\dot{P}, P] U_A, \quad (50)$$

$W = I - \int_0^s KW$. Also, it is easy to check that $Q_0 K = K P_0$ (and $P_0 K = K Q_0$). Hence

$$-Q_0 W P_0 = \int_0^s Q_0 K W P_0 = \int_0^s Q_0 K P_0 W P_0, \quad (51)$$

an integral of the proper form, with $X = [\dot{P}, P]$ and $Y = W$. Also, $\|X\| = O_1(h/\gamma)$, $\|Y\| = 1$. Simple calculations show $\|(\frac{d}{ds})^l X\| = O_l(h^l/\gamma^{l+1})$ and $\|(\frac{d}{ds})^l Y\| = O_l(h^l/\gamma^l)$, the necessary assumptions to apply the above error analysis. \square

For completeness, we now give the proofs of Lemmas 7 and 8.

Proof of Lemma 7: True at $s = 0$. Differentiate $U_A^\dagger P U_A$:

$$(U_A^\dagger \dot{P} U_A) = U_A^\dagger (\dot{P} + i\tau[H_A, P]) U_A. \quad (52)$$

Now, noting that H commutes with P a projector onto one of its eigenspaces,

$$\begin{aligned} i\tau[H_A, P] &= i\tau[\cancel{H}, \cancel{P}] - [[\dot{P}, P], P] \\ &= -\dot{P}P + 2P\dot{P}P - P\dot{P} \\ &= -\dot{P}. \end{aligned} \quad (53)$$

Here we used that $P^2 = P$, which implies $\dot{P} = \dot{P}P + P\dot{P}$ and also $P\dot{P}P = 0$. \square

Proof of Lemma 8: First we check that

$$QXP = -Q([H_A, \tilde{X}] - \frac{i}{\tau}[\dot{P}, \tilde{X}])P. \quad (54)$$

Indeed, $QXP = -Q[P, X]P$ and, since $[zI, R X R] = 0$,

$$\begin{aligned} [H, \tilde{X}] &= \frac{1}{2\pi i} \int_{\Gamma} [H - zI, R X R] \\ &= [X, \frac{1}{2\pi i} \int_{\Gamma} R] = [P, X]. \end{aligned} \quad (55)$$

Thus,

$$\begin{aligned} QXP &= -Q[P, X]P = -Q[H, \tilde{X}] \\ &= -Q([H_A, \tilde{X}] - \frac{i}{\tau}[\dot{P}, \tilde{X}])P, \end{aligned} \quad (56)$$

and Eq. (54) follows from $Q[[\dot{P}, P], \tilde{X}]P = Q[\dot{P}, \tilde{X}]P$.

Now

$$\begin{aligned} Q_0 U_A^\dagger X U_A P_0 &= Q_0 U_A^\dagger QXP U_A P_0 \\ &= -Q_0 U_A^\dagger ([H_A, \tilde{X}] - \frac{i}{\tau}[\dot{P}, \tilde{X}]) U_A P_0 \\ &= \frac{i}{\tau} Q_0 [(U_A^\dagger \dot{X} U_A) - U_A^\dagger (\dot{X} + [\dot{P}, \tilde{X}]) U_A] P_0, \end{aligned} \quad (57)$$

where in the last step we used Eq. (37), then integrated by parts. \square

B. DIAGONALIZE THE QUADRATIC FORM OF FERMION OPERATORS

Following the classic paper by Lieb et al [12], we’ll show how to diagonalize a Hamiltonian of the form

$$H = \sum_{ij} a_i^\dagger A_{ij} a_j + \frac{1}{2} (a_i^\dagger B_{ij} a_j^\dagger + a_i B_{ji} a_j), \quad (58)$$

where a_i 's and a_i^\dagger 's are Fermi annihilation and creation operators. Since H is Hermitian, so is A . By the anticommutation rules, B is antisymmetric. Assume A and B are real.

We'll try to write

$$H = \sum_k \Lambda_k \eta_k^\dagger \eta_k + \text{constant} , \quad (59)$$

where the η_k^\dagger 's and η_k 's are themselves Fermi operators. Note that $\eta_k^\dagger \eta_k$'s are commuting projections: $(\eta_k^\dagger \eta_k)^2 = \eta_k^\dagger (1 - \eta_k^\dagger \eta_k) \eta_k = \eta_k^\dagger \eta_k$, $\eta_k^\dagger \eta_k \eta_j^\dagger \eta_j = (-1)^4 \eta_j^\dagger \eta_j \eta_k^\dagger \eta_k$, $j \neq k$. Therefore they can be simultaneously diagonalized, and the eigenvalues of H are sums of subsets of the Λ_k , plus a constant [13]. Each elementary excitation Λ_k can be interpreted as the energy of a quasiparticle; the constant is the energy of a "vacuum."

How do we find the η_k and Λ_k ?

$$[\eta_k, H] = \sum_{j \neq k} \left(\Lambda_j (\eta_k \eta_j^\dagger \eta_j - \eta_j^\dagger \eta_j \eta_k) + \Lambda_k (\eta_k \eta_k^\dagger \eta_k - \eta_k^\dagger \eta_k^2) \right) = \Lambda_k \eta_k . \quad (60)$$

Expand the η_k 's in terms of the original Fermi operators

$$\eta_k = \sum_i g_{ki} a_i + h_{ki} a_i^\dagger \quad (61)$$

and plug (60) back into (58). From the Fermi anticommutation rules and some case-checking,

$$[a_i, H] = \sum_j A_{ij} a_j + B_{ij} a_j^\dagger, \quad [a_i^\dagger, H] = -[a_i, H]^\dagger . \quad (62)$$

Considering the coefficients of a_j and a_j^\dagger , respectively, then gives

$$\Lambda_k g_{kj} = \sum_i g_{ki} A_{ij} + h_{ki} B_{ij}, \quad \Lambda_k h_{kj} = \sum_i g_{ki} B_{ij} - h_{ki} A_{ij}, \quad (63)$$

or $\Lambda_k g_k = A g_k + B h_k$, $\Lambda_k h_k = -B g_k - A h_k$ in vector notation. Let $\phi_k^\pm = g_k \pm h_k$. Then $\Lambda_k \phi_k^\pm = (A \mp B) \phi_k^\mp$, so $\Lambda_k^2 \phi_k^\pm = (A \mp B)(A \pm B) \phi_k^\pm$. Since $(A - B)^\dagger = A + B$, the matrices $(A \mp B)(A \pm B)$ are symmetric, positive semi-definite. With a little algebra, one can show that the ϕ_k^\pm 's are orthonormal iff the η_k and η_k^\dagger 's are Fermi operators: $g_j \cdot g_k + h_j \cdot h_k = \delta_{jk}$, $g_j \cdot h_k + h_j \cdot g_k = 0$.