

Unstructured Adiabatic Quantum Optimization

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by

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CERTIFICATE

It is certified that the work contained in this thesis, titled “Unstructured Adiabatic Quantum Optimization” by Alapan Chaudhuri, has been carried out under my supervision and is not submitted elsewhere for a degree.

Date

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To a world that feels like it's splitting apart.
May we keep repairing what we can.

“Computers are more forgiving than bare-bone nature or mathematics
— both of which are infinitely more forgiving than academia.”

Abstract

[TODO]

Acknowledgement

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Adiabatic Quantum Optimization

The adiabatic version of Grover's algorithm, due to Roland and Cerf [1], finds a single marked item among $N = 2^n$ by slowly interpolating between a uniform superposition and a problem Hamiltonian that penalizes all unmarked items. The crossing between the two lowest energy levels occurs at $s = 1/2$, its position independent of the Hamiltonian's spectrum. The minimum spectral gap scales as $1/\sqrt{N}$, and a schedule that slows near the crossing achieves the optimal $O(\sqrt{N})$ runtime.

Consider a cost function encoded in an n -qubit Hamiltonian diagonal in the computational basis, with M distinct energy levels, arbitrary degeneracies, and a spectral gap that may vary with the number of qubits. The ground states encode solutions to a combinatorial optimization problem. Can the adiabatic approach still match the $\Theta(\sqrt{N})$ lower bound for unstructured search [2]? Partial answers exist: Žnidarič and Horvat [3] showed via analytical and heuristic arguments that the minimum gap scales as $\sqrt{d_0/2^n}$ for 3-SAT instances and identified the crossing position, but did not rigorously bound the runtime. Hen [4] proved a quadratic speedup for a random Hamiltonian whose energy distribution ensures a crossing position independent of the spectrum, avoiding the central difficulty.

The answer in full generality is yes, but with complications that do not arise in the single-marked-item case. The spectrum of the interpolated Hamiltonian is far richer: instead of a two-level system plus a degenerate bulk, there are M interacting energy levels in a symmetric subspace, with avoided crossings between higher excited states that obscure the gap between the two lowest. The position of the ground-state avoided crossing depends nontrivially on the degeneracy structure of the problem Hamiltonian. And the minimum gap, while still scaling as $\Theta(1/\sqrt{N})$ up to spectral factors, occurs at a position that must be known to exponential precision for the schedule to be correct.

This chapter builds the framework for analyzing adiabatic quantum optimization with general diagonal Hamiltonians. We define the problem Hamiltonian and the interpolation, identify the spectral parameters that govern the crossing, reduce the N -dimensional eigenvalue problem to M dimensions, derive the eigenvalue equation, and locate the avoided crossing with its minimum gap. The next three chapters use this framework: Chapter 6 bounds the spectral gap across the full adiabatic path, Chapter 7 derives the optimal runtime, and Chapter 8 proves that computing the crossing position is NP-hard.

5.1 The Problem

Consider an n -qubit Hamiltonian H_z that is diagonal in the computational basis:

$$H_z = \sum_{z \in \{0,1\}^n} E_z |z\rangle\langle z|, \quad (5.1.1)$$

where E_z is the energy assigned to bit-string z . Since H_z acts diagonally, it encodes a classical cost function: the energy E_z is the cost of configuration z , and the ground states are the optimal solutions. Without loss of generality, we rescale and shift so that all eigenvalues lie in $[0, 1]$.

Suppose H_z has M distinct energy levels with eigenvalues

$$0 \leq E_0 < E_1 < \dots < E_{M-1} \leq 1. \quad (5.1.2)$$

For each level k , the set of bit-strings at that energy is

$$\Omega_k = \{z \in \{0,1\}^n : H_z |z\rangle = E_k |z\rangle\}, \quad (5.1.3)$$

with degeneracy $d_k = |\Omega_k|$. The degeneracies partition the full Hilbert space: $\sum_{k=0}^{M-1} d_k = 2^n = N$. The spectral gap of the problem Hamiltonian is $\Delta = E_1 - E_0$, the energy difference between the ground state and the first excited level.

A concrete and important instance is the 2-local Ising Hamiltonian

$$H_\sigma = \sum_{\langle i,j \rangle} J_{ij} \sigma_z^i \sigma_z^j + \sum_{j=1}^n h_j \sigma_z^j, \quad (5.1.4)$$

where $J_{ij}, h_j \in \{-m, -m+1, \dots, m\}$ for some constant positive integer m . After normalization, H_σ has $M \in \text{poly}(n)$ distinct eigenvalues and a spectral gap $\Delta \geq 1/\text{poly}(n)$. Solutions to NP-hard problems such as MaxCut and QUBO encode directly in the ground states of H_σ with minimal overhead [5, 6].

For the running example, take unstructured search: $M = 2$ energy levels, a single ground state ($d_0 = 1$) with energy $E_0 = 0$, and $N - 1$ excited states ($d_1 = N - 1$) at energy $E_1 = 1$. The ground state is the “marked item.” Classical search requires $\Theta(N)$ queries; Grover’s circuit algorithm requires $\Theta(\sqrt{N})$ [7, 8].

To solve this optimization problem adiabatically, we interpolate between an initial Hamiltonian whose ground state is easy to prepare and the problem Hamiltonian whose ground state encodes the solution. The initial Hamiltonian is the rank-one projector

$$H_0 = -|\psi_0\rangle\langle\psi_0|, \quad |\psi_0\rangle = |+\rangle^{\otimes n} = \frac{1}{\sqrt{N}} \sum_{z \in \{0,1\}^n} |z\rangle. \quad (5.1.5)$$

Every computational basis state receives equal amplitude, so $|\psi_0\rangle$ introduces no bias toward any particular solution.

The adiabatic Hamiltonian is the linear interpolation

$$H(s) = -(1-s)|\psi_0\rangle\langle\psi_0| + sH_z, \quad s \in [0, 1]. \quad (5.1.6)$$

At $s = 0$, the ground state is $|\psi_0\rangle$ with energy -1 , and all other states have energy 0 . At $s = 1$, the Hamiltonian is H_z itself, and its ground states encode the solutions. The adiabatic theorem guarantees that if the schedule $s(t)$ traverses $[0, 1]$ slowly enough, the evolved state remains close to the instantaneous ground state throughout, arriving at the end in a state with high overlap with the ground space of H_z .

The choice of a rank-one projector for H_0 , rather than a more general Hamiltonian, has a structural consequence. At $s = 0$, the spectrum of $H(s)$ has a single non-degenerate eigenvalue at -1 (the ground state) and an $(N - 1)$ -fold degenerate eigenvalue at 0 . As s increases, the degeneracy splits according to the spectrum of H_z , but the ground state can only interact with one effective excited state at a time. This produces a single avoided crossing between the two lowest energy levels, in contrast to generic AQC Hamiltonians that may exhibit multiple crossings requiring different analytical techniques [9]. The single-crossing structure is what makes a complete spectral analysis tractable.

For the running example, $H(s) = -(1-s)|\psi_0\rangle\langle\psi_0| + s(I - |w\rangle\langle w|)$, where $|w\rangle$ is the marked item. Up to a global energy shift of s , this is the Roland-Cerf Hamiltonian [1]. The spectrum has $N - 2$ states at energy s (degenerate, orthogonal to both $|\psi_0\rangle$ and $|w\rangle$) and two states whose energies depend on s and undergo an avoided crossing near $s = 1/2$.

5.2 Spectral Parameters

In the Roland-Cerf setting, the crossing position ($s^* = 1/2$), its width, and the minimum gap are all determined by a single quantity: N . For a general problem Hamiltonian H_z with M energy levels and arbitrary degeneracies, no single number suffices. The relevant information is captured by a family of spectral parameters that aggregate the degeneracy structure weighted by inverse energy gaps.

Definition 5.2.1 (Spectral parameters). *For the problem Hamiltonian H_z with eigenvalues $E_0 < E_1 < \dots < E_{M-1}$ and degeneracies d_k , define*

$$A_p = \frac{1}{N} \sum_{k=1}^{M-1} \frac{d_k}{(E_k - E_0)^p}, \quad p \in \mathbb{N}. \quad (5.2.1)$$

Each excited level contributes its degeneracy d_k weighted by the inverse p -th power of its distance to the ground energy. Higher values of p emphasize levels closer to the ground state. The normalization by $N = 2^n$ makes A_p an average over the full Hilbert space.

For the running example ($M = 2$, $d_0 = 1$, $d_1 = N - 1$, $E_0 = 0$, $E_1 = 1$):

$$A_p = \frac{N-1}{N} \approx 1 \quad \text{for all } p, \quad (5.2.2)$$

since $E_1 - E_0 = 1$. The spectral parameters are trivial in this case, which is precisely why the Roland-Cerf analysis is simple.

For a general Ising Hamiltonian with $\Delta \geq 1/\text{poly}(n)$ and $M \in \text{poly}(n)$, the bound $A_1 \leq (1 - d_0/N)/\Delta$ gives $A_1 = O(\text{poly}(n))$, while $A_2 \geq 1 - d_0/N$ ensures $A_2 = \Theta(1)$ at minimum.

The first two parameters play distinct roles that will become precise in subsequent sections. The parameter A_1 determines the position of the avoided crossing: $s^* = A_1/(A_1 + 1)$. The parameter A_2 enters the minimum spectral gap: $g_{\min} = \Theta(\sqrt{d_0/(NA_2)})$. Both appear in the runtime: $T = O((\sqrt{A_2}/A_1^2\Delta^2)\sqrt{N/d_0})$.

Since every eigenvalue gap satisfies $E_k - E_0 \leq 1$ and the total excited degeneracy is $\sum_{k \geq 1} d_k = N - d_0$, we have

$$A_2 \geq \frac{1}{N} \sum_{k=1}^{M-1} d_k = 1 - \frac{d_0}{N}. \quad (5.2.3)$$

For $d_0 \ll N$ (few solutions), $A_2 \geq 1 - 1/N$ is close to 1. Also, $A_1 \leq (1 - d_0/N)/\Delta$, since $(E_k - E_0)^{-1} \leq \Delta^{-1}$ for all $k \geq 1$. Since $E_k - E_0 \geq \Delta$ for all $k \geq 1$, termwise comparison gives $A_1 \geq A_2\Delta$. Since $E_k - E_0 \leq 1$, we also have $A_1 \leq A_2$. Together: $A_2\Delta \leq A_1 \leq A_2$.

The behavior of the adiabatic Hamiltonian is well-controlled only when the avoided crossing region is narrow compared to the interval $[0, 1]$. This is ensured by a spectral condition on H_z .

Definition 5.2.2 (Spectral condition). *The problem Hamiltonian H_z satisfies the spectral condition if there exists a constant $c \ll 1$ such that*

$$\frac{1}{\Delta} \sqrt{\frac{d_0}{A_2 N}} < c. \quad (5.2.4)$$

The quantity on the left is the ratio of the crossing width parameter to the spectral gap, up to constant factors. When it is small, the two-level approximation near the crossing is accurate (the higher levels do not interfere), and the crossing window occupies a negligible fraction of $[0, 1]$. The appendix of the published paper shows that $c \approx 0.02$ suffices [10].

For any H_z with $\Delta > (1/c)\sqrt{d_0/N}$, the condition holds, using $A_2 \geq 1 - d_0/N$. For the Ising Hamiltonian with $\Delta \geq 1/\text{poly}(n)$ and d_0 not scaling with N , the left side is exponentially small in n , so the condition is easily satisfied. For the running example with $\Delta = 1$ and $d_0 = 1$, the left side is $1/\sqrt{N}$, well below any constant c for $N \geq 2$.

5.3 Symmetry Reduction

The Hilbert space of $H(s)$ has dimension $N = 2^n$, exponentially large in the number of qubits. Direct spectral analysis is intractable. But the problem Hamiltonian H_z has only M distinct energy levels, and the initial state $|\psi_0\rangle$ treats all bit-strings at the same energy identically. This permutation symmetry within each degenerate subspace reduces the eigenvalue problem from N dimensions to M .

For each energy level k , define the symmetric state

$$|k\rangle = \frac{1}{\sqrt{d_k}} \sum_{z \in \Omega_k} |z\rangle, \quad 0 \leq k \leq M-1. \quad (5.3.1)$$

These M states are orthonormal: $\langle j|k\rangle = \delta_{jk}$. They span the M -dimensional symmetric subspace

$$\mathcal{H}_S = \text{span} \{ |k\rangle : 0 \leq k \leq M-1 \}. \quad (5.3.2)$$

In this basis, the problem Hamiltonian has M non-degenerate eigenvalues:

$$H_z = \sum_{k=0}^{M-1} E_k |k\rangle \langle k| \quad \text{on } \mathcal{H}_S, \quad (5.3.3)$$

and the initial state decomposes as

$$|\psi_0\rangle = \sum_{k=0}^{M-1} \sqrt{\frac{d_k}{N}} |k\rangle. \quad (5.3.4)$$

Since $|\psi_0\rangle \in \mathcal{H}_S$ and both H_z and $|\psi_0\rangle\langle\psi_0|$ map \mathcal{H}_S to itself, the adiabatic Hamiltonian $H(s)$ leaves \mathcal{H}_S invariant. The time evolution starting from $|\psi_0\rangle$ remains in \mathcal{H}_S for all s .

The complement \mathcal{H}_S^\perp has dimension $N-M$ and is spanned by states orthogonal to $|\psi_0\rangle$ within each degenerate subspace. For each level k , order the bit-strings in Ω_k as $z_k^{(1)}, \dots, z_k^{(d_k)}$ and define the Fourier basis

$$|k^{(\ell)}\rangle = \frac{1}{\sqrt{d_k}} \sum_{\ell'=1}^{d_k} \exp \left[\frac{i 2\pi \ell \ell'}{d_k} \right] |z_k^{(\ell')}\rangle, \quad 1 \leq \ell \leq d_k - 1. \quad (5.3.5)$$

Note that $|k^{(0)}\rangle = |k\rangle$ is the symmetric state already in \mathcal{H}_S . The remaining $d_k - 1$ states for each level k form a basis for \mathcal{H}_S^\perp :

$$\mathcal{H}_S^\perp = \text{span} \left\{ |k^{(\ell)}\rangle : 0 \leq k \leq M-1, 1 \leq \ell \leq d_k - 1 \right\}. \quad (5.3.6)$$

Each $|k^{(\ell)}\rangle$ is an eigenstate of $H(s)$ with eigenvalue sE_k :

$$H(s)|k^{(\ell)}\rangle = -(1-s)|\psi_0\rangle \underbrace{\langle\psi_0|}_{=0} k^{(\ell)} + sE_k |k^{(\ell)}\rangle = sE_k |k^{(\ell)}\rangle. \quad (5.3.7)$$

The inner product vanishes because $|k^{(\ell)}\rangle$ is orthogonal to $|k\rangle = |k^{(0)}\rangle$ by construction, and $|\psi_0\rangle$ is a linear combination of the $|k\rangle$ states. These $N-M$ eigenstates are spectators: their eigenvalues sE_k are trivially known and they do not participate in the adiabatic evolution.

Henceforth, $H(s)$ denotes its restriction to the symmetric subspace \mathcal{H}_S :

$$H(s) = -(1-s)|\psi_0\rangle\langle\psi_0| + s \sum_{k=0}^{M-1} E_k |k\rangle\langle k|. \quad (5.3.8)$$

This is a rank-one perturbation of the diagonal matrix sH_z . Its eigenvalues can be characterized exactly.

Lemma 5.3.1 (Eigenvalue equation). *Let $H(s)$ be the adiabatic Hamiltonian restricted to \mathcal{H}_S as in Eq. (5.3.8). Then $\lambda(s)$ is an eigenvalue of $H(s)$ if and only if*

$$\frac{1}{1-s} = \frac{1}{N} \sum_{k=0}^{M-1} \frac{d_k}{sE_k - \lambda(s)}. \quad (5.3.9)$$

Proof. Let $|\psi\rangle = \sum_{k=0}^{M-1} \alpha_k |k\rangle$ be an eigenstate of $H(s)$ with eigenvalue λ , and set $\gamma = \langle\psi_0|\psi\rangle$. Acting with $H(s)$ on $|\psi\rangle$:

$$H(s)|\psi\rangle = s \sum_{k=0}^{M-1} E_k \alpha_k |k\rangle - (1-s)\gamma |\psi_0\rangle = \lambda \sum_{k=0}^{M-1} \alpha_k |k\rangle. \quad (5.3.10)$$

Comparing coefficients of $|k\rangle$ and using $\langle\psi_0|k\rangle = \sqrt{d_k/N}$ gives

$$\alpha_k = \frac{(1-s)\gamma \sqrt{d_k/N}}{sE_k - \lambda}. \quad (5.3.11)$$

Since $\gamma = \langle\psi_0|\psi\rangle = (1/\sqrt{N}) \sum_k \alpha_k \sqrt{d_k}$, substituting Eq. (5.3.11) yields

$$1 = \frac{1-s}{N} \sum_{k=0}^{M-1} \frac{d_k}{sE_k - \lambda}, \quad (5.3.12)$$

which is equivalent to Eq. (5.3.9). Each step is reversible: given a solution λ of Eq. (5.3.9), the coefficients in Eq. (5.3.11) define an eigenstate (after normalization), provided $\gamma \neq 0$. The case $\gamma = 0$ corresponds to $\lambda = sE_k$ for some k , which are the eigenvalues in \mathcal{H}_S^\perp already accounted for. \square

The right-hand side of Eq. (5.3.9), viewed as a function of λ , is a sum of M terms, each a decreasing function with a vertical asymptote at $\lambda = sE_k$. Between consecutive poles sE_{k-1} and sE_k , the function decreases monotonically from $+\infty$ to $-\infty$, producing exactly one root per interval. Below the lowest pole sE_0 , there is one additional root. The total count is M eigenvalues in \mathcal{H}_S , consistent with the dimension.

The two lowest eigenvalues are $\lambda_0(s) < sE_0$ (ground state) and $\lambda_1(s) \in (sE_0, sE_1)$ (first excited state). The spectral gap is $g(s) = \lambda_1(s) - \lambda_0(s) > 0$. However, the eigenvalue equation alone gives only the trivial bound

$0 < g(s) < s\Delta$, since $\lambda_0(s)$ could be arbitrarily close to sE_0 from below while $\lambda_1(s)$ could be close to sE_0 from above. Extracting tight bounds requires analyzing the eigenvalue equation in the vicinity of the crossing.

For the running example ($M = 2$), Eq. (5.3.9) becomes

$$\frac{1}{1-s} = \frac{1}{N} \cdot \frac{1}{-\lambda} + \frac{N-1}{N} \cdot \frac{1}{s-\lambda}, \quad (5.3.13)$$

where we set $E_0 = 0$ and $E_1 = 1$. Clearing denominators produces the quadratic $N\lambda^2 - N(2s-1)\lambda - s(1-s) = 0$, whose two roots give the ground and first excited energies:

$$\lambda_{\pm}(s) = \frac{2s-1}{2} \pm \frac{1}{2} \sqrt{(2s-1)^2 + \frac{4s(1-s)}{N}}. \quad (5.3.14)$$

At $s = 0$, the ground energy is $\lambda_- = -1$ and the first excited energy is $\lambda_+ = 0$, consistent with the spectrum of $H(0) = -|\psi_0\rangle\langle\psi_0|$. The gap $g(s) = \lambda_+(s) - \lambda_-(s)$ simplifies to

$$g(s) = \sqrt{(2s-1)^2 + \frac{4s(1-s)}{N}}, \quad (5.3.15)$$

which is minimized at $s = 1/2$ exactly, giving $g_{\min} = 1/\sqrt{N}$. This is the Roland-Cerf gap. The general theory of the next section reproduces this scaling as a special case.

5.4 The Avoided Crossing

The eigenvalue equation (Lemma 5.3.1) characterizes the spectrum of $H(s)$ implicitly. We now extract explicit formulas for the crossing position, its width, and the minimum gap by analyzing the equation near the ground state energy. Near the crossing, the ground and first excited states behave like a two-level system, with the higher levels acting as a perturbation controlled by the spectral condition.

The two lowest eigenvalues have the form $\lambda(s) = sE_0 + \delta(s)$, where $\delta(s)$ is a correction to the trivial energy sE_0 . Substituting into Eq. (5.3.9) [11]:

$$-\frac{d_0}{N\delta} + \frac{1}{N} \sum_{k=1}^{M-1} \frac{d_k}{s(E_k - E_0) - \delta} = \frac{1}{1-s}. \quad (5.4.1)$$

The first term has a pole at $\delta = 0$; the sum has poles at $\delta = s(E_k - E_0)$ for $k \geq 1$. When $|\delta| \ll s\Delta$ (guaranteed by the spectral condition), the sum can be expanded in powers of $\delta/(s(E_k - E_0))$:

$$\frac{1}{N} \sum_{k=1}^{M-1} \frac{d_k}{s(E_k - E_0) - \delta} = \frac{1}{s} \left(A_1 + \frac{\delta}{s} A_2 + \frac{\delta^2}{s^2} A_3 + \dots \right). \quad (5.4.2)$$

Truncating at the A_2 term and rearranging Eq. (5.4.1) gives a quadratic in δ whose two roots are the corrections $\delta_0^+(s)$ and $\delta_0^-(s)$ for the first excited and ground states, respectively:

$$\delta_0^{\pm}(s) = \frac{s(A_1 + 1)}{2A_2(1-s)} \left[(s - s^*) \pm \sqrt{(s^* - s)^2 + \frac{4A_2 d_0}{N(A_1 + 1)^2} (1-s)^2} \right], \quad (5.4.3)$$

Here $\delta_0^+(s) > 0$ corresponds to the first excited state and $\delta_0^-(s) < 0$ to the ground state: the superscript indicates the sign of the correction relative to sE_0 . The crossing position is

$$s^* = \frac{A_1}{A_1 + 1}. \quad (5.4.4)$$

The quantity s^* is the position of the avoided crossing. It is entirely determined by A_1 , and hence by the degeneracy-weighted inverse gaps of the problem Hamiltonian. For the Ising Hamiltonian with $\Delta \geq 1/\text{poly}(n)$, we have $A_1 \geq \Theta(1)$, so s^* is bounded away from both 0 and 1. In the limit $A_1 \rightarrow \infty$ (many levels near the ground state), $s^* \rightarrow 1$; when A_1 is small, s^* is closer to 0.

The crossing position marks a balance in the eigenvalue equation: $A_1/s^* = 1/(1-s^*)$, where the left side is the aggregate spectral pull of the excited levels toward sE_0 and the right side is the projector strength. At $s = s^*$, the linear coefficient in the quadratic for δ (Eq. (5.4.3)) vanishes, and the two roots δ_0^{\pm} are symmetric

about zero. The gap is determined entirely by the constant term d_0/N : the ground-state degeneracy is what opens the minimum gap.

The truncation is an approximation. The actual roots $\delta_{\pm}(s)$ of the full equation differ from $\delta_0^{\pm}(s)$ by a relative error controlled by the spectral condition. The following result, whose proof uses the intermediate value theorem on the full equation after bounding the remainder using A_3 and the spectral condition, makes this precise [10, 12].

Lemma 5.4.1 (Validity of approximation). *Let H_z satisfy the spectral condition (Definition 5.2.2) with constant $c \approx 0.02$, and define*

$$\delta_s = \frac{2}{(A_1 + 1)^2} \sqrt{\frac{d_0 A_2}{N}}. \quad (5.4.5)$$

Then for any $s \in \mathcal{I}_{s^} = [s^* - \delta_s, s^* + \delta_s]$, there exists a constant $\eta \ll 1$ such that the two lowest eigenvalues of $H(s)$ satisfy*

$$\delta_+(s) \in ((1 - \eta) \delta_0^+(s), (1 + \eta) \delta_0^+(s)), \quad (5.4.6)$$

$$\delta_-(s) \in ((1 + \eta) \delta_0^-(s), (1 - \eta) \delta_0^-(s)), \quad (5.4.7)$$

where $\delta_0^{\pm}(s)$ are given by Eq. (5.4.3).

The proof evaluates the full equation (5.4.1) at $\delta_0^{\pm}(1 \pm \eta)$ and shows, using the spectral condition to bound the truncated Taylor remainder, that the full equation changes sign between these points. The intermediate value theorem then guarantees a root in the interval. The spectral condition enters through the bound $|\delta_0^{\pm}(s)|/(s\Delta) \leq \kappa c < 1$, where κ is a constant depending on c , ensuring the geometric series in the Taylor expansion converges. The constant $c \approx 0.02$ is sufficient for $\eta \leq 0.1$. The complete calculation appears in the appendix of the published paper [10].

The spectral gap $g(s) = \delta_+(s) - \delta_-(s)$ is therefore approximated to within a factor of $1 \pm 2\eta$ by $\delta_0^+(s) - \delta_0^-(s)$, which evaluates to

$$g(s) = (1 \pm 2\eta) \cdot \frac{s(A_1 + 1)}{A_2(1 - s)} \sqrt{(s^* - s)^2 + \frac{4A_2 d_0}{N(A_1 + 1)^2} (1 - s)^2}. \quad (5.4.8)$$

At $s = s^*$, the first term under the square root vanishes, leaving only the second:

$$g_{\min} = g(s^*) \geq (1 - 2\eta) \cdot \frac{2A_1}{A_1 + 1} \sqrt{\frac{d_0}{NA_2}}. \quad (5.4.9)$$

This is the minimum spectral gap of $H(s)$.

The formulas decompose as follows. The factor $2A_1/(A_1 + 1)$ captures the position of the crossing: a crossing near the boundary ($s^* \rightarrow 0$ or $s^* \rightarrow 1$) reduces the gap. The factor $\sqrt{d_0/N}$ is the Grover-like contribution: more solutions (larger d_0) increase the gap and reduce the runtime. The factor $1/\sqrt{A_2}$ encodes the spectral structure beyond the simplest two-level case.

The crossing position s^* , the window width δ_s , and the leading-order minimum gap are connected by an exact algebraic identity. Writing $\hat{g} = \frac{2A_1}{A_1 + 1} \sqrt{\frac{d_0}{NA_2}}$ for the leading-order expression, direct substitution gives

$$\frac{s^*(A_1 + 1)^2}{A_2} \cdot \delta_s = \hat{g}, \quad (5.4.10)$$

and by Eq. (5.4.9), $g_{\min} \geq (1 - 2\eta)\hat{g}$. This relation will be used in Chapter 7 to verify the runtime calculation.

The interval $[0, 1]$ splits into three regions based on the crossing:

$$\mathcal{I}_{s^-} = [0, s^* - \delta_s], \quad \mathcal{I}_{s^*} = [s^* - \delta_s, s^* + \delta_s], \quad \mathcal{I}_{s^+} = (s^* + \delta_s, 1]. \quad (5.4.11)$$

Within the window \mathcal{I}_{s^*} , the gap is bounded both from below and above in terms of g_{\min} .

Lemma 5.4.2 (Gap within the crossing window). *Let H_z satisfy the spectral condition with constant c , and define*

$$\kappa' = \frac{(1 + 2\eta)(1 + 2c)}{(1 - 2\eta)(1 - 2c)} \sqrt{1 + (1 - 2c)^2}. \quad (5.4.12)$$

Then for any $s \in \mathcal{I}_{s^}$,*

$$g_{\min} \leq g(s) \leq \kappa' \cdot g_{\min}. \quad (5.4.13)$$

Proof. The lower bound is immediate from the definition of g_{\min} as the minimum over \mathcal{I}_{s^*} . For the upper bound, start from Eq. (5.4.8) with $|s - s^*| \leq \delta_s$:

$$g(s) \leq \frac{s(A_1 + 1)}{A_2(1-s)} \sqrt{\delta_s^2 + \frac{4A_2d_0}{N(A_1 + 1)^2}(1-s)^2}. \quad (5.4.14)$$

Factoring out $(A_1 + 1)\delta_s(1-s)$ under the square root and using $s/s^* \leq 1 + \delta_s/s^*$:

$$g(s) \leq \frac{s^*(A_1 + 1)^2}{A_2} \delta_s \cdot \frac{s}{s^*} \cdot \sqrt{\frac{1}{(1-s)^2(A_1 + 1)^2} + 1}. \quad (5.4.15)$$

The first factor equals \hat{g} by Eq. (5.4.10). The spectral condition gives $\delta_s/(1-s^*) \leq 2c$ and $\delta_s/s^* \leq 2c$. To see the first, compute

$$\frac{\delta_s}{1-s^*} = \frac{2}{1+A_1} \sqrt{\frac{d_0 A_2}{N}} = \frac{2A_2 \Delta}{1+A_1} \cdot \frac{1}{\Delta} \sqrt{\frac{d_0}{A_2 N}} \leq 2s^* c \leq 2c, \quad (5.4.16)$$

where we used $A_2 \Delta / (1 + A_1) \leq A_1 / (1 + A_1) = s^*$. The bound $\delta_s/s^* \leq 2c$ follows similarly. Substituting into the upper bound:

$$g(s) \leq (1+2\eta)\hat{g} \cdot (1+2c) \sqrt{1+(1-2c)^2} \leq \kappa' \cdot g_{\min}, \quad (5.4.17)$$

where the factor $(1+2\eta)$ comes from the upper approximation in Eq. (5.4.8), and the last step uses $\hat{g} \leq g_{\min}/(1-2\eta)$. \square

The spectral gap is therefore of order g_{\min} throughout \mathcal{I}_{s^*} and strictly larger outside this window, as the next section establishes. The avoided crossing is localized.

For the running example, the formulas specialize cleanly. With $A_1 = A_2 = (N-1)/N$:

$$s^* = \frac{(N-1)/N}{(N-1)/N + 1} = \frac{N-1}{2N-1} \approx \frac{1}{2}, \quad (5.4.18)$$

$$g_{\min} = \frac{2(N-1)/(2N-1)}{\sqrt{N \cdot (N-1)/N}} = \frac{2(N-1)}{(2N-1)\sqrt{N-1}} \approx \frac{1}{\sqrt{N}}, \quad (5.4.19)$$

$$\delta_s = \frac{2N^2}{(2N-1)^2} \sqrt{\frac{N-1}{N^2}} \approx \frac{1}{2\sqrt{N}}. \quad (5.4.20)$$

The crossing is at $s^* \approx 1/2$, the minimum gap scales as $1/\sqrt{N}$, and the window width scales as $1/\sqrt{N}$. These agree asymptotically with the exact quadratic solution in Eq. (5.3.15), confirming the general theory reproduces the known scaling. The small discrepancy between $s^* = (N-1)/(2N-1)$ and the exact minimum at $s=1/2$ is a higher-order effect of the two-level truncation, vanishing as $O(1/N)$.

5.5 Gap Structure

The previous section characterized the spectral gap within the crossing window \mathcal{I}_{s^*} : it is $\Theta(g_{\min})$ throughout. For the adiabatic algorithm, we also need the gap outside this window. The local adaptive schedule that achieves optimal runtime requires knowing how the gap grows as s moves away from s^* , so that the evolution speeds up in regions of larger gap.

The following two results, proved in Chapter 6, bound the gap in the left and right regions.

Lemma 5.5.1 (Gap to the left of the crossing). *For any $s \in \mathcal{I}_{s^-} = [0, s^* - \delta_s]$, the spectral gap of $H(s)$ satisfies*

$$g(s) \geq \frac{A_1(A_1 + 1)}{A_2}(s^* - s). \quad (5.5.1)$$

The proof, detailed in Chapter 6, uses the variational principle: an explicit ansatz $|\phi\rangle$ provides an upper bound on the ground energy $\lambda_0(s) \leq \langle \phi | H(s) | \phi \rangle$, while the eigenvalue equation gives the lower bound $\lambda_1(s) \geq sE_0$ on the first excited energy. The ansatz is

$$|\phi\rangle = \frac{1}{\sqrt{A_2 N}} \sum_{k=1}^{M-1} \frac{\sqrt{d_k}}{E_k - E_0} |k\rangle, \quad (5.5.2)$$

which concentrates amplitude on levels close to the ground energy, yielding a tight upper bound on $\lambda_0(s)$. A second route uses concavity: since $\lambda_0(s) = \min_{|\psi\rangle} \langle \psi | H(s) | \psi \rangle$ is the pointwise minimum of functions linear in s , it is concave. The tangent to a concave function lies above it, so the tangent to λ_0 at s^* gives a linear upper bound that, combined with $\lambda_1(s) \geq sE_0$, reproduces Eq. (5.5.1). Chapter 6 develops both approaches.

Lemma 5.5.2 (Gap to the right of the crossing). *Let $k = 1/4$, $a = 4k^2\Delta/3$, and*

$$s_0 = s^* - \frac{k g_{\min}(1 - s^*)}{a - k g_{\min}}. \quad (5.5.3)$$

Then for all $s \geq s^$, the spectral gap of $H(s)$ satisfies*

$$g(s) \geq \frac{\Delta}{30} \cdot \frac{s - s_0}{1 - s_0}. \quad (5.5.4)$$

This bound is linear in $s - s_0$, with a slope proportional to Δ . The proof, also in Chapter 6, uses the resolvent method: a line $\gamma(s) = sE_0 + \beta(s)$ is placed between the two lowest eigenvalues, and the Sherman-Morrison formula [13] bounds the resolvent norm $\|R_{H(s)}(\gamma)\|$, giving $g(s) \geq 2/\|R_{H(s)}(\gamma)\|$. The constants $k = 1/4$ and $a = 4k^2\Delta/3$ are tuned to make the resulting function $f(s)$ monotonically decreasing on $[s^*, 1]$, yielding the clean bound $\Delta/30$.

Both bounds exceed g_{\min} at the window boundary. At $s = s^* - \delta_s$ (left boundary), the left bound gives

$$g(s^* - \delta_s) \geq \frac{A_1(A_1 + 1)}{A_2} \cdot \delta_s = \frac{2A_1}{A_1 + 1} \sqrt{\frac{d_0}{NA_2}} = \hat{g}, \quad (5.5.5)$$

which satisfies $\hat{g} \geq g_{\min}/(1 - 2\eta)$ by Eq. (5.4.9). At $s = s^*$ (right boundary start), $\beta(s^*) \geq k g_{\min}$, so $g(s^*) \geq 2k g_{\min}/(1 + f(s^*)) = O(g_{\min})$ since $f(s^*) = \Theta(1)$. The gap profile is therefore continuous across region boundaries: it dips to g_{\min} at s^* and rises linearly on both sides.

The complete gap profile feeds directly into the runtime calculation. The optimal local adaptive schedule has $ds/dt \propto g(s)^2$: the evolution slows quadratically as the gap decreases. The total runtime is

$$T \propto \int_0^1 \frac{ds}{g(s)^2}, \quad (5.5.6)$$

split across the three regions. In the left and right regions, the linear growth $g(s) \propto |s - s^*|$ makes $1/g(s)^2 \propto 1/(s - s^*)^2$, which integrates to a logarithmic contribution. In the window, $g(s) = \Theta(g_{\min})$ is approximately constant, giving a contribution proportional to $2\delta_s/g_{\min}^2$. The window dominates:

$$\frac{\delta_s}{g_{\min}^2} \propto \frac{\sqrt{A_2}}{A_1^2 \Delta^2} \sqrt{\frac{N}{d_0}}, \quad (5.5.7)$$

yielding the runtime of Theorem 1 in the published paper [10]. For the Ising Hamiltonian with $A_1, A_2 = O(\text{poly}(n))$ and $\Delta \geq 1/\text{poly}(n)$, this gives $T = \tilde{O}(\sqrt{N/d_0})$, matching the Grover lower bound up to polylogarithmic factors. Chapter 7 carries out this calculation rigorously.

5.6 The Central Questions

The framework is now complete. The adiabatic Hamiltonian $H(s)$ interpolates between the easy initial state and the problem Hamiltonian. The symmetry reduction collapses the N -dimensional problem to M dimensions. The eigenvalue equation characterizes the spectrum implicitly, and the two-level approximation near the crossing yields explicit formulas for s^* , δ_s , and g_{\min} . The gap is $\Theta(g_{\min})$ in the crossing window and grows linearly outside it.

The first question is technical: are the gap bounds in the left and right regions tight? The variational bound for the left region and the resolvent bound for the right region have been stated but not proved. Chapter 6 develops both proofs in full, including the construction of the variational ansatz, the Sherman-Morrison resolvent calculation, and the monotonicity analysis for the function $f(s)$.

The second question is the main positive result: what is the optimal runtime? The answer, derived in Chapter 7, is

$$T = O\left(\frac{1}{\varepsilon} \cdot \frac{\sqrt{A_2}}{A_1^2 \Delta^2} \cdot \sqrt{\frac{N}{d_0}}\right), \quad (5.6.1)$$

where ε is the target error. For Ising Hamiltonians, this is $\tilde{O}(\sqrt{N/d_0})$, matching the lower bound of Farhi, Goldstone, and Gutmann [2]. Adiabatic quantum optimization achieves the Grover speedup.

The third question reveals the limitation. The local adaptive schedule requires knowing s^* to precision $O(\delta_s) = O(2^{-n/2})$, which requires knowing A_1 to comparable precision. How hard is this computation? Chapter

8 proves that approximating A_1 to additive accuracy $1/\text{poly}(n)$ is NP-hard: two queries to such an oracle suffice to solve 3-SAT. Computing A_1 exactly, or to accuracy $O(2^{-\text{poly}(n)})$, is $\#P$ -hard: polynomial interpolation extracts all degeneracies d_k from $O(\text{poly}(n))$ exact queries. There is an exponential gap between the precision needed ($O(2^{-n/2})$) and the precision at which the problem is already NP-hard ($1/\text{poly}(n)$).

The fourth question confronts this tension. In the circuit model, Grover's algorithm achieves $\tilde{O}(\sqrt{N/d_0})$ without pre-computing any spectral parameter: the oracle queries gather the needed information adaptively during execution. The adiabatic framework requires the schedule to be fixed before the evolution begins, necessitating the NP-hard pre-computation. This asymmetry is not an artifact of the analysis but a genuine difference between the two computational models. The paper [10] calls this “optimality with limitations”: the adiabatic speedup exists but is contingent on solving a hard problem first. Chapter 9 characterizes this information-runtime tradeoff precisely, proving a separation theorem for uninformed schedules, a smooth interpolation for partial information, and an adaptive measurement protocol that circumvents the classical hardness.

For the running example, the limitation vanishes: $A_1 = (N-1)/N \approx 1$ is trivially known, so $s^* \approx 1/2$ requires no hard computation. The complexity arises only for problem Hamiltonians with rich spectral structure, where the degeneracies d_k and energy gaps $E_k - E_0$ are not known in advance. The Ising Hamiltonian encoding an NP-hard problem is precisely such a case.

Chapter 6

Spectral Analysis

Chapter 5 established the crossing window \mathcal{I}_{s^*} where the spectral gap satisfies $g(s) = \Theta(g_{\min})$, and stated two bounds for the regions outside: a linear lower bound to the left ([Lemma 5.5.1](#)) and a linear lower bound to the right ([Lemma 5.5.2](#)). The complete gap profile determines the runtime of the adiabatic algorithm through the integral $\int_0^1 g(s)^{-2} ds$. This chapter proves both lemmas.

The two proofs use different techniques, reflecting different spectral structures on each side of the crossing. To the left of s^* , the ground energy $\lambda_0(s)$ sits below sE_0 while the first excited energy $\lambda_1(s)$ sits above it. The variational principle bounds how far below sE_0 the ground energy can be, yielding a linear gap bound. To the right of s^* , the eigenvalues of sH_z crowd the interval $[sE_0, sE_1]$, and the variational approach no longer applies. Instead, a resolvent identity combined with the Sherman-Morrison formula for rank-one perturbations tracks the gap through this congested region. The resulting piecewise linear profile — steep on the left, shallower on the right, flat in the window — feeds directly into the runtime calculation of Chapter 7.

6.1 Gap to the Left of the Crossing

The eigenvalue equation ([Lemma 5.3.1](#)) places the ground state energy at $\lambda_0(s) < sE_0$ and the first excited energy at $\lambda_1(s) \in (sE_0, sE_1)$. The gap $g(s) = \lambda_1(s) - \lambda_0(s)$ is therefore positive, but these bounds alone give only the trivial estimate $g(s) < s\Delta$. For the runtime integral, we need a tight lower bound that captures the linear growth of the gap as s decreases away from s^* .

The strategy is to tighten the upper bound on $\lambda_0(s)$. Two approaches give the same result. The first uses the variational principle: for any normalized state $|\phi\rangle$, the ground energy satisfies $\lambda_0(s) \leq \langle \phi | H(s) | \phi \rangle$, so a well-chosen ansatz produces a quantitative upper bound. The second uses concavity: since $\lambda_0(s) = \min_{|\psi\rangle} \langle \psi | H(s) | \psi \rangle$ is the pointwise minimum of affine functions in s , it is concave, and any tangent line lies above it. The variational approach is more direct — it produces the bound in a single calculation — so we present it here.

Lemma 6.1.1 (Gap to the left of the crossing). *For any $s \in \mathcal{I}_{s^-} = [0, s^* - \delta_s]$, the spectral gap of $H(s)$ satisfies*

$$g(s) \geq \frac{A_1(A_1 + 1)}{A_2} (s^* - s). \quad (6.1.1)$$

Proof. We upper-bound $\lambda_0(s)$ via the variational principle and lower-bound $\lambda_1(s)$ from the eigenvalue equation.

The ansatz must live in the span of $\{|k\rangle : k \geq 1\}$, orthogonal to the ground-state component $|0\rangle$, and should concentrate amplitude on levels close to E_0 where the energy expectation is lowest. The natural weighting is the inverse energy gap: levels near E_0 receive more amplitude. Requiring unit norm fixes the overall scale, giving

$$|\phi\rangle = \frac{1}{\sqrt{A_2 N}} \sum_{k=1}^{M-1} \frac{\sqrt{d_k}}{E_k - E_0} |k\rangle. \quad (6.1.2)$$

This weighting arises naturally in first-order perturbation theory: the correction to the ground state of sH_z due to the perturbation $-(1-s)|\psi_0\rangle\langle\psi_0|$ has exactly this form. Normalization is immediate:

$$\langle \phi | \phi \rangle = \frac{1}{A_2 N} \sum_{k=1}^{M-1} \frac{d_k}{(E_k - E_0)^2} = \frac{A_2}{A_2} = 1. \quad (6.1.3)$$

To compute $\langle \phi | H(s) | \phi \rangle$, decompose $H(s) = -(1-s)|\psi_0\rangle\langle\psi_0| + s(H_z - E_0) + sE_0$. Each term contributes separately.

The projector term gives

$$-(1-s)|\langle\psi_0|\phi|^2 = -(1-s)\left(\frac{1}{\sqrt{A_2N}}\sum_{k=1}^{M-1}\frac{d_k}{(E_k-E_0)\sqrt{N}}\right)^2 = -(1-s)\frac{A_1^2}{A_2}, \quad (6.1.4)$$

where $\langle\psi_0|\phi = A_1/\sqrt{A_2}$ follows from $\langle\psi_0|k = \sqrt{d_k/N}$ and the definition of A_1 .

The shifted diagonal term gives

$$s\langle\phi|(H_z - E_0)|\phi\rangle = \frac{s}{A_2N}\sum_{k=1}^{M-1}\frac{d_k}{(E_k-E_0)^2}\cdot(E_k-E_0) = \frac{s}{A_2N}\sum_{k=1}^{M-1}\frac{d_k}{E_k-E_0} = \frac{sA_1}{A_2}. \quad (6.1.5)$$

The constant term contributes $sE_0\langle\phi|\phi = sE_0$. Combining:

$$\lambda_0(s) \leq \langle\phi|H(s)|\phi\rangle = sE_0 - (1-s)\frac{A_1^2}{A_2} + s\frac{A_1}{A_2} = sE_0 + \frac{A_1}{A_2}(s(1+A_1) - A_1). \quad (6.1.6)$$

Since $s^*(1+A_1) = A_1$, we have $s(1+A_1) - A_1 = (1+A_1)(s-s^*) = (s-s^*)/(1-s^*)$, so

$$\lambda_0(s) \leq sE_0 + \frac{A_1}{A_2}\cdot\frac{s-s^*}{1-s^*}. \quad (6.1.7)$$

For $s < s^*$, the second term is negative, confirming $\lambda_0(s) < sE_0$.

For the first excited state, the eigenvalue equation (Lemma 5.3.1) confines $\lambda_1(s)$ to the interval (sE_0, sE_1) , so

$$\lambda_1(s) \geq sE_0. \quad (6.1.8)$$

The gap is therefore

$$g(s) = \lambda_1(s) - \lambda_0(s) \geq sE_0 - sE_0 - \frac{A_1}{A_2}\cdot\frac{s-s^*}{1-s^*} = \frac{A_1}{A_2}\cdot\frac{s^*-s}{1-s^*}. \quad (6.1.9)$$

Since $1/(1-s^*) = A_1 + 1$, we obtain $g(s) \geq A_1(A_1+1)(s^*-s)/A_2$. \square

At the left boundary of the crossing window, $s = s^* - \delta_s$, the bound gives

$$g(s^* - \delta_s) \geq \frac{A_1(A_1+1)}{A_2}\cdot\delta_s = \hat{g} \geq \frac{g_{\min}}{1-2\eta}, \quad (6.1.10)$$

using $A_1(A_1+1)\delta_s/A_2 = \hat{g}$ from Eq. (5.4.10) (equivalently, $A_1 = s^*(A_1+1)$) and $g_{\min} \geq (1-2\eta)\hat{g}$ from Eq. (5.4.9). The gap at the window boundary exceeds g_{\min} , confirming that the minimum gap lies within \mathcal{I}_{s^*} .

The same bound follows from concavity. The second derivative of $\lambda_0(s)$ satisfies $\ddot{\lambda}_0(s) = -2\sum_{j\geq 1}|\langle\phi_j(s)|\dot{H}|\phi_0(s)\rangle|^2/(E_j-E_0(s)) \leq 0$, where $\dot{H} = H_z + |\psi_0\rangle\langle\psi_0|$ and $|\phi_j(s)\rangle$ are the instantaneous eigenstates. The tangent to the concave function $\lambda_0(s)$ at $s = s^*$ lies above it everywhere, and its slope evaluated using Eq. (6.1.7) reproduces the same linear bound.

For the running example ($M = 2$, $d_0 = 1$, $d_1 = N - 1$, $E_0 = 0$, $E_1 = 1$), the ansatz reduces to $|\phi\rangle = |1\rangle$, and the bound becomes

$$g(s) \geq \frac{(N-1)/N \cdot (2N-1)/N}{(N-1)/N}\left(\frac{1}{2}-s\right) = \frac{2N-1}{N}\left(\frac{1}{2}-s\right) \approx 2\left(\frac{1}{2}-s\right). \quad (6.1.11)$$

The exact gap $g(s) = \sqrt{(2s-1)^2 + 4s(1-s)/N}$ at $s = 1/4$ equals $\sqrt{1/4 + 3/(4N)} \approx 1/2$, while the bound gives $(2N-1)/(4N) \approx 1/2$. The bound is tight near s^* and only becomes loose as s approaches 0, where the true gap approaches 1 while the bound continues growing. Since the runtime integral is dominated by the crossing window, this looseness far from s^* has negligible effect.

6.2 Gap to the Right of the Crossing

Bounding the spectral gap to the right of s^* is the main technical challenge of this chapter. The variational principle that worked on the left does not extend: it provides upper bounds on $\lambda_0(s)$, but what we need on the right is a lower bound on $\lambda_1(s) - \lambda_0(s)$ that captures the linear reopening of the gap. The variational principle bounds ground energies from above, not excited energies from below.

The obstacle is structural. On the left, the first excited eigenvalue $\lambda_1(s)$ is bounded below by sE_0 from the eigenvalue equation, giving a clean reference point. On the right, $\lambda_1(s)$ lies between sE_0 and sE_1 , but so do eigenvalues from the higher levels of sH_z , which undergo their own avoided crossings with the first excited state. Tracking $\lambda_1(s)$ through this congested region requires a tool that bounds the distance from a given point to the spectrum without identifying individual eigenvalues.

The resolvent provides exactly this. For a self-adjoint operator A with spectrum $\sigma(A)$ and any $\lambda \notin \sigma(A)$, the resolvent

$$R_A(\lambda) = (\lambda I - A)^{-1} \quad (6.2.1)$$

is a bounded operator whose norm equals the inverse distance from λ to the spectrum:

$$\|R_A(\lambda)\| = \frac{1}{\text{dist}(\lambda, \sigma(A))}. \quad (6.2.2)$$

This follows from the spectral theorem: in the eigenbasis of A with eigenvalues $\{\lambda_j\}$, the resolvent is diagonal with entries $1/(\lambda - \lambda_j)$, and its operator norm is the maximum absolute value $\max_j |1/(\lambda - \lambda_j)| = 1/\min_j |\lambda - \lambda_j|$. If a point γ lies between two consecutive eigenvalues λ_0 and λ_1 , then $\text{dist}(\gamma, \sigma(A)) = \min(\gamma - \lambda_0, \lambda_1 - \gamma) \leq g/2$, since the minimum of two non-negative numbers summing to g is at most $g/2$. Therefore $\|R_A(\gamma)\| = 1/\text{dist}(\gamma, \sigma(A)) \geq 2/g$, and the useful contrapositive is

$$g(s) \geq \frac{2}{\|R_{H(s)}(\gamma)\|}. \quad (6.2.3)$$

Bounding the gap from below reduces to bounding the resolvent norm from above.

The adiabatic Hamiltonian $H(s) = sH_z - (1-s)|\psi_0\rangle\langle\psi_0|$ is a rank-one perturbation of sH_z . Rank-one perturbations have a classical inversion formula. The Sherman-Morrison identity [13] states that for an invertible operator A and vectors $|u\rangle, \langle v|$,

$$(A + |u\rangle\langle v|)^{-1} = A^{-1} - \frac{A^{-1}|u\rangle\langle v|A^{-1}}{1 + \langle v|A^{-1}|u\rangle}, \quad (6.2.4)$$

provided $1 + \langle v|A^{-1}|u\rangle \neq 0$. Applying this to the resolvent of $H(s)$ decomposes it into the resolvent of sH_z (whose spectrum is known explicitly) and a correction from the rank-one term $-(1-s)|\psi_0\rangle\langle\psi_0|$. The triangle inequality then yields an upper bound on $\|R_{H(s)}(\gamma)\|$.

The strategy is: choose a line $\gamma(s)$ that lies between $\lambda_0(s)$ and $\lambda_1(s)$ for all $s \geq s^*$, apply the Sherman-Morrison decomposition, bound each piece using the spectral parameters A_1 and A_2 , and show that the resulting bound on $\|R_{H(s)}(\gamma)\|$ yields a linear lower bound on $g(s)$.

The simplest choice for $\gamma(s)$ is a line starting at sE_0 when $s = s^*$ and ending between E_0 and E_1 at $s = 1$: take $\beta(s) = a(s-s^*)/(1-s^*)$ with $a < \Delta$ and set $\gamma(s) = sE_0 + \beta(s)$. With $a = \Delta/6$, the function $f(s)$ controlling the resolvent bound can be shown to satisfy $f(s) \leq 1$ for all $s \geq s^*$, giving $g(s) \geq \beta(s) = (\Delta/6)(s-s^*)/(1-s^*)$. This bound has a problem: at the window boundary $s = s^* + \delta_s$, it gives $g(s^* + \delta_s) \geq (\Delta/6) \cdot \delta_s/(1-s^*) = (\Delta A_2)/(3A_1) \cdot g_{\min}$. Since $\Delta A_2 \leq A_1$, this is at most $g_{\min}/3$, and for Hamiltonians with $\Delta A_2 \ll A_1$, it can be polynomially smaller than g_{\min} . At $s = s^*$ itself, the bound gives $g(s^*) \geq 0$, missing the true gap entirely.

The failure has a geometric explanation. At s^* , the ground energy $\lambda_0(s^*)$ is not at s^*E_0 but rather $g_{\min}/2$ below it. The line $\gamma(s)$ passes through s^*E_0 at $s = s^*$, so it sits between the two eigenvalues but with zero margin below. The resolvent norm at a point equidistant from two eigenvalues has norm $2/g$, but at a point touching one eigenvalue, the norm diverges. The line must start with $O(g_{\min})$ separation from both eigenvalues at s^* .

The fix is to shift the line's origin from s^* to a point $s_0 < s^*$ so that $\beta(s^*) = k g_{\min}$ for a constant $k < 1$. With $\beta(s) = a(s - s_0)/(1 - s_0)$, the constraint $\beta(s^*) = k g_{\min}$ determines

$$s_0 = s^* - \frac{k g_{\min}(1 - s^*)}{a - k g_{\min}}. \quad (6.2.5)$$

The line now passes through $\gamma(s^*) = s^*E_0 + k g_{\min}$, which lies between $\lambda_0(s^*)$ and $\lambda_1(s^*)$ when k is chosen appropriately. The price is that $s_0 < s^*$ introduces additional terms in the monotonicity analysis for $f(s)$, requiring a careful choice of a .

Lemma 6.2.1 (Gap to the right of the crossing). *Let $k = 1/4$, $a = 4k^2\Delta/3 = \Delta/12$, and s_0 as in Eq. (6.2.5). Then for all $s \geq s^*$, the spectral gap of $H(s)$ satisfies*

$$g(s) \geq \frac{\Delta}{30} \cdot \frac{s - s_0}{1 - s_0}. \quad (6.2.6)$$

Proof. Set $\gamma(s) = sE_0 + \beta(s)$ with $\beta(s) = a(s - s_0)/(1 - s_0)$. We bound $\|R_{H(s)}(\gamma)\|$ from above using the Sherman-Morrison formula.

Since $H(s) = sH_z - (1 - s)|\psi_0\rangle\langle\psi_0|$, the resolvent of $H(s)$ at γ satisfies, via Eq. (6.2.4) and the triangle inequality,

$$\|R_{H(s)}(\gamma)\| \leq \|R_{sH_z}(\gamma)\| + (1 - s) \frac{\|R_{sH_z}(\gamma)|\psi_0\rangle\langle\psi_0|R_{sH_z}(\gamma)\|}{1 + (1 - s)\langle\psi_0|R_{sH_z}(\gamma)|\psi_0\rangle}. \quad (6.2.7)$$

The unperturbed resolvent $R_{sH_z}(\gamma)$ is diagonal in the $|k\rangle$ basis with entries $1/(\gamma - sE_k) = 1/(\beta - s(E_k - E_0))$ for $k \geq 1$ and $1/\beta$ for $k = 0$. The nearest eigenvalue of sH_z to γ is sE_0 , at distance β , so $\|R_{sH_z}(\gamma)\| = 1/\beta$.

We bound the numerator and denominator of the second term separately. Both require that $\beta(s) \leq s(E_k - E_0)/2$ for all $k \geq 1$, which ensures the Taylor expansion in powers of $\beta/(s(E_k - E_0))$ converges rapidly. Since $\beta(s) \leq a = \Delta/12$ and $s(E_k - E_0) \geq s^*\Delta \geq \Delta/3$ (using $s^* = A_1/(A_1 + 1) \geq 1/3$, which holds when $A_1 \geq 1/2$, i.e., $d_0 \leq N/2$), we have $\beta \leq \Delta/12 < \Delta/6 \leq s(E_k - E_0)/2$. When $d_0 > N/2$, the majority of states are ground states and random sampling finds a solution with constant probability, making the adiabatic approach unnecessary.

Numerator bound. The squared norm of $R_{sH_z}(\gamma)|\psi_0\rangle$ expands as

$$\|R_{sH_z}(\gamma)|\psi_0\rangle\|^2 = \frac{d_0}{N\beta^2} + \frac{1}{N} \sum_{k=1}^{M-1} \frac{d_k}{(s(E_k - E_0) - \beta)^2}. \quad (6.2.8)$$

Using $s(E_k - E_0) - \beta \geq s(E_k - E_0)/2$, each term in the sum is at most $4d_k/(Ns^2(E_k - E_0)^2)$, giving

$$\|R_{sH_z}(\gamma)|\psi_0\rangle\langle\psi_0|R_{sH_z}(\gamma)\| \leq \|R_{sH_z}(\gamma)|\psi_0\rangle\|^2 \leq \frac{d_0}{N\beta^2} + \frac{4A_2}{s^2}. \quad (6.2.9)$$

Denominator bound. Expanding the expectation value:

$$\begin{aligned} 1 + (1 - s)\langle\psi_0|R_{sH_z}(\gamma)|\psi_0\rangle &= 1 + \frac{(1 - s)d_0}{N\beta} - \frac{1 - s}{N} \sum_{k=1}^{M-1} \frac{d_k}{s(E_k - E_0) - \beta} \\ &= 1 + \frac{(1 - s)d_0}{N\beta} - \frac{1 - s}{s} \sum_{k=1}^{M-1} \frac{d_k}{N(E_k - E_0)} \sum_{\ell=0}^{\infty} \left(\frac{\beta}{s(E_k - E_0)} \right)^\ell. \end{aligned} \quad (6.2.10)$$

Using $\beta/(s(E_k - E_0)) \leq 1/2$ to bound the geometric series by $1 + 2\beta/(s(E_k - E_0))$:

$$1 + (1 - s)\langle\psi_0|R_{sH_z}(\gamma)|\psi_0\rangle \geq 1 + \frac{(1 - s)d_0}{N\beta} - (1 - s) \left(\frac{A_1}{s} + \frac{2A_2\beta}{s^2} \right). \quad (6.2.11)$$

Collecting terms. Substituting the bounds (6.2.9) and (6.2.11) into (6.2.7) and factoring:

$$\|R_{H(s)}(\gamma)\| \leq \frac{1}{\beta} (1 + f(s)), \quad (6.2.12)$$

where, writing $\epsilon_0 = d_0/N$,

$$f(s) = \frac{\epsilon_0 s^2(1 - s) + 4A_2\beta^2(1 - s)}{\epsilon_0 s^2(1 - s) + \beta s \frac{s - s^*}{1 - s^*} - 2A_2\beta^2(1 - s)}. \quad (6.2.13)$$

To obtain this form, multiply numerator and denominator of the second term in (6.2.7) by β , then multiply by $s^2(1 - s)$ to clear fractions. The key step is rewriting the denominator's constant-plus-linear terms. Using $A_1 = s^*/(1 - s^*)$:

$$1 - \frac{(1 - s)A_1}{s} + \frac{(1 - s)\epsilon_0}{\beta} = \frac{s - s^*}{s(1 - s^*)} + \frac{(1 - s)\epsilon_0}{\beta}, \quad (6.2.14)$$

since $1 - A_1(1 - s)/s = (s - A_1(1 - s))/s = (s - s^*(1 - s)/(1 - s^*))/s = (s(1 - s^*) - s^*(1 - s))/(s(1 - s^*)) = (s - s^*)/(s(1 - s^*))$. Multiplying through by $\beta s^2(1 - s)$ and collecting the Taylor-bounded terms into the $A_2\beta^2$ contributions gives Eq. (6.2.13).

The numerator of $f(s)$ measures the rank-one perturbation's effect on the resolvent: the ϵ_0 term comes from the $|0\rangle$ component of $|\psi_0\rangle$ (the ground-state overlap), while the A_2 term comes from the excited components. The denominator captures the spectral rigidity: the term $\beta s(s - s^*)/(1 - s^*)$ grows as γ moves away from the crossing, stabilizing the resolvent against the perturbation. Near s^* , the denominator is small (the gap is small), so $f(s^*)$ is $O(1)$. As s increases, the denominator grows and $f(s) \rightarrow 0$.

From (6.2.12) and (6.2.3), the spectral gap satisfies

$$g(s) \geq \frac{2\beta(s)}{1 + f(s)} \geq \frac{2\beta(s)}{1 + \max_{s \geq s^*} f(s)}. \quad (6.2.15)$$

If f is monotonically decreasing on $[s^*, 1]$, then $\max_{s \geq s^*} f(s) = f(s^*)$, and the bound becomes $g(s) \geq 2\beta(s)/(1 + f(s^*))$, which is linear in $s - s_0$.

Monotonicity of f . We show $f'(s) < 0$ for $s \in [s^*, 1]$. Write $f = u/v$ with

$$\begin{aligned} u &= \epsilon_0 s^2(1 - s) + 4A_2\beta^2(1 - s), \\ v &= \epsilon_0 s^2(1 - s) + \beta s \frac{s - s^*}{1 - s^*} - 2A_2\beta^2(1 - s). \end{aligned} \quad (6.2.16)$$

Then $f' = (u'v - uv')/v^2$, so the sign of f' is determined by $u'v - uv'$.

Computing u' and v' using $\beta' = a/(1 - s_0)$:

$$\begin{aligned} u' &= \frac{4aA_2\beta}{1 - s_0}(2 + s_0 - 3s) + \epsilon_0 s(2 - 3s), \\ v' &= \frac{a(3s^2 - 2s(s^* + s_0) + s^*s_0)}{(1 - s_0)(1 - s^*)} - \frac{2aA_2\beta}{1 - s_0}(2 + s_0 - 3s) + \epsilon_0 s(2 - 3s). \end{aligned} \quad (6.2.17)$$

Expanding $u'v$ and uv' and taking the difference, two terms cancel exactly: the $\epsilon_0^2 s^3(2 - 3s)(1 - s)$ term and the $8aA_2^2\beta^3(1 - s)(2 + s_0 - 3s)/(1 - s_0)$ term. The remaining expression has three terms [10]:

$$\begin{aligned} u'v - uv' &= -\frac{4aA_2\beta^2}{(1 - s_0)(1 - s^*)} \left(s^2(1 + s_0 - s^*) - 2s s_0 + s^* s_0 \right) \\ &\quad + \frac{12aA_2\epsilon_0\beta}{1 - s_0} s(1 - s)^2 s_0 \\ &\quad - \frac{\epsilon_0 s^2 a}{(1 - s_0)(1 - s^*)} \left(-s^2(s^* + s_0 - 1) + 2s s_0 s^* - s^* s_0 \right). \end{aligned} \quad (6.2.18)$$

The first and third terms are negative; the second is positive (it is the only term involving $\epsilon_0 s_0$, which arises from the shift of s_0 below s^*). We must show the first negative term dominates the positive one.

Factor out $-4aA_2\beta/(1 - s_0)$ from the sum of the first two terms:

$$-\frac{4aA_2\beta}{1 - s_0} \left(\frac{\beta}{1 - s^*} \left(s^2(1 + s_0 - s^*) - 2s s_0 + s^* s_0 \right) - 3\epsilon_0 s_0 s(1 - s)^2 \right). \quad (6.2.19)$$

The quadratic $s^2(1 + s_0 - s^*) - 2s s_0 + s^* s_0$ is a convex function of s that is minimized at some $s_m < s^*$ and is positive for $s \geq s^*$. The cubic $s(1 - s)^2$ is maximized at $s = 1/3 \leq s^*$. Therefore, on $[s^*, 1]$, the bracket in (6.2.19) is bounded below by its value at $s = s^*$:

$$\frac{a(s^* - s_0)^2}{1 - s_0} - 3\epsilon_0 s_0(1 - s^*)^2. \quad (6.2.20)$$

Using $s_0 \leq s^*$ and $s^* - s_0 = k g_{\min}(1 - s^*)/(a - k g_{\min})$, this is positive whenever

$$a < \frac{4}{3}k^2 \frac{A_1}{A_2}. \quad (6.2.21)$$

Since $\Delta A_2 \leq A_1$ (because $A_2 \leq \sum_{k \geq 1} d_k/(N(E_k - E_0)^2) \leq A_1/\Delta$), the choice $a = (4/3)k^2\Delta$ satisfies (6.2.21). With this choice, $u'v - uv' < 0$ on $[s^*, 1]$, so f is monotonically decreasing.

Evaluating $f(s^*)$. At $s = s^*$, $\beta(s^*) = k g_{\min}$. The term $\beta s(s - s^*)/(1 - s^*)$ vanishes, so

$$f(s^*) = \frac{\epsilon_0 s^{*2}(1 - s^*) + 4A_2 k^2 g_{\min}^2(1 - s^*)}{\epsilon_0 s^{*2}(1 - s^*) - 2A_2 k^2 g_{\min}^2(1 - s^*)}. \quad (6.2.22)$$

Using $g_{\min} \approx (2s^*/\sqrt{A_2})\sqrt{\epsilon_0}$ (from Eq. (5.4.9) with $\hat{g} = 2s^*\sqrt{\epsilon_0/A_2}$), we have $A_2 k^2 g_{\min}^2 \approx 4k^2 s^{*2} \epsilon_0$. Substituting:

$$f(s^*) = \frac{1 + 16k^2}{1 - 8k^2}. \quad (6.2.23)$$

For $k = 1/4$: $f(s^*) = (1 + 1)/(1 - 1/2) = 4$, so $1 + f(s^*) = 5$.

Final bound. From (6.2.15):

$$g(s) \geq \frac{2\beta(s)}{1 + f(s^*)} = \frac{2a}{1 + f(s^*)} \cdot \frac{s - s_0}{1 - s_0}. \quad (6.2.24)$$

The prefactor evaluates to

$$\frac{2a}{1 + f(s^*)} = \frac{2 \cdot (4/3)k^2 \Delta}{1 + (1 + 16k^2)/(1 - 8k^2)} = \frac{4}{3}k^2 \cdot \frac{1 - 8k^2}{1 + 4k^2} \cdot \Delta. \quad (6.2.25)$$

The function $P(k) = (4/3)k^2(1 - 8k^2)/(1 + 4k^2)$ is maximized at $k_{\text{opt}} = \frac{1}{2}\sqrt{\sqrt{3/2} - 1} \approx 0.237$, where $P(k_{\text{opt}}) = \frac{1}{3}(5 - 2\sqrt{6}) \approx 0.034$. For $k = 1/4$:

$$P(1/4) = \frac{4}{3} \cdot \frac{1}{16} \cdot \frac{1/2}{5/4} = \frac{1}{30}. \quad (6.2.26)$$

Therefore $g(s) \geq (\Delta/30)(s - s_0)/(1 - s_0)$. \square

For the running example ($M = 2$, $\Delta = 1$), the bound gives $g(s) \geq (1/30)(s - s_0)/(1 - s_0)$, where $s_0 = 1/2 - O(1/\sqrt{N})$ is close to $s^* \approx 1/2$ for large N . Near $s = 3/4$, the exact gap from Eq. (5.3.15) is $g(3/4) = \sqrt{1/4 + 3/(16N)} \approx 1/2$, while the bound gives approximately $(1/30)(1/4)/(1/2) = 1/60$. The bound is conservative by a factor of approximately 30 but correctly captures the linear growth. This constant is the price of a clean, uniform bound valid for all problem Hamiltonians satisfying the spectral condition.

6.3 The Complete Gap Profile

Combining the results of this chapter with those of Chapter 5, the spectral gap $g(s)$ is bounded below across all of $[0, 1]$.

Theorem 6.3.1 (Complete gap profile). *Let H_z satisfy the spectral condition (Definition 5.2.2). The spectral gap of $H(s) = -(1 - s)|\psi_0\rangle\langle\psi_0| + sH_z$ satisfies, for all $s \in [0, 1]$:*

$$g(s) \geq \begin{cases} \frac{A_1(A_1 + 1)}{A_2} (s^* - s), & s \in \mathcal{I}_{s^-} = [0, s^* - \delta_s], \\ g_{\min}, & s \in \mathcal{I}_{s^*} = [s^* - \delta_s, s^* + \delta_s], \\ \frac{\Delta}{30} \cdot \frac{s - s_0}{1 - s_0}, & s \in \mathcal{I}_{s^+} = (s^* + \delta_s, 1], \end{cases} \quad (6.3.1)$$

where $s_0 = s^* - k g_{\min}(1 - s^*)/(a - k g_{\min})$ with $k = 1/4$ and $a = \Delta/12$.

Proof. The three cases follow from Lemma 5.4.2 (window, proved in Chapter 5), Lemma 6.1.1 (left), and Lemma 6.2.1 (right). The right bound holds for all $s \geq s^*$ and therefore covers \mathcal{I}_{s^+} . The window bound $g(s) \geq g_{\min}$ is tighter than the right bound at s^* but weaker far from the crossing. \square

The bounds match across region boundaries. At the left boundary $s = s^* - \delta_s$:

$$\frac{A_1(A_1 + 1)}{A_2} \cdot \delta_s = \hat{g} \geq \frac{g_{\min}}{1 - 2\eta} > g_{\min}, \quad (6.3.2)$$

so the left bound exceeds the window bound. At $s = s^*$, the right bound gives $g(s^*) \geq 2\beta(s^*)/(1 + f(s^*)) = 2k g_{\min}/5 = g_{\min}/10$, which is below g_{\min} by a constant factor but still $O(g_{\min})$. The window bound provides the tighter estimate $g(s^*) = g_{\min}$.

The gap profile has a characteristic shape. It forms a broad V centered at s^* , with a narrow rounded minimum of width approximately $2\delta_s$. The left arm has slope $A_1(A_1 + 1)/A_2$, which is $O(\text{poly}(n))$ for Ising Hamiltonians. The right arm has the shallower slope $\Delta/(30(1 - s_0))$, controlled by the spectral gap Δ of the

problem Hamiltonian. The asymmetry in the bounds — steep on the left, shallow on the right — is a proof artifact: the variational bound captures the true slope closely, while the resolvent bound sacrifices tightness for uniform validity across a more complicated spectral landscape. At the endpoints, $g(0) = 1$ (the initial gap between eigenvalues -1 and 0 of H_0) and $g(1) = \Delta$ (the gap of H_z).

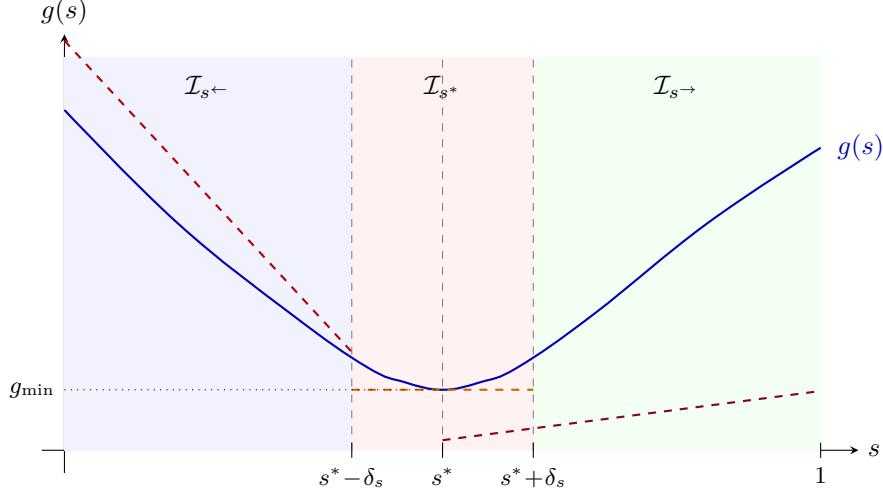


Figure 6.1: Schematic gap profile for $H(s)$. The solid curve shows the true spectral gap $g(s)$, which dips to g_{\min} at $s = s^*$ and rises on both sides. The dashed lines show the piecewise lower bounds: linear on the left (steep), constant in the window, and linear on the right (shallow). The three regions $\mathcal{I}_{s\leftarrow}$, \mathcal{I}_{s^*} , $\mathcal{I}_{s\rightarrow}$ are indicated.

Given any problem Hamiltonian H_z satisfying the spectral condition, the gap is bounded across $[0, 1]$ by the piecewise profile of [Theorem 6.3.1](#), determined up to constant factors by A_1 , A_2 , d_0 , and Δ . The minimum gap $g_{\min} = \Theta(\sqrt{d_0/(N A_2)})$ occurs at $s^* = A_1/(A_1 + 1)$ and is exponentially small in n when $d_0 = O(1)$. The crossing position depends only on A_1 , not on A_2 or d_0 . More solutions (larger d_0) widen the gap; richer spectral structure (larger A_2) narrows it. The gap reaches Δ at $s = 1$, the spectral gap of the problem Hamiltonian itself.

For the running example, the exact gap $g(s) = \sqrt{(2s-1)^2 + 4s(1-s)/N}$ and the piecewise bound from [Theorem 6.3.1](#) can be compared directly. The left bound has slope approximately 2, matching the exact slope $|g'(s^*)| = 2\sqrt{1-1/N} \approx 2$. The window bound $g_{\min} = 1/\sqrt{N}$ is exact. The right bound has slope approximately $1/15$ near s^* , weaker than the true slope by a factor of 30, but sufficient for the runtime integral since the window dominates.

The runtime integral $\int_0^1 g(s)^{-2} ds$ splits across the three regions. In the left and right regions, $g(s) \sim C|s-s^*|$ for constants C , and

$$\int_{\delta_s}^{s^*} \frac{du}{(Cu)^2} = \frac{1}{C^2} \left(\frac{1}{\delta_s} - \frac{1}{s^*} \right) \leq \frac{1}{C^2 \delta_s}, \quad (6.3.3)$$

which is $O(1/(C^2 \delta_s))$. In the window, $g(s) \geq g_{\min}$ gives $\int_{s^* - \delta_s}^{s^* + \delta_s} g(s)^{-2} ds \leq 2\delta_s/g_{\min}^2$. The window contribution $\delta_s/g_{\min}^2 = \Theta(A_2^{3/2}/A_1^2 \cdot \sqrt{N/d_0})$ dominates the outer regions, and the full integral — including the Δ -dependent right-arm contribution — yields the runtime $T = O((\sqrt{A_2}/(A_1^2 \Delta^2)) \sqrt{N/d_0})$ that Chapter 7 derives rigorously.

Chapter 7

Optimal Schedule

Chapter 8

Hardness of Optimality

Chapter 9

Information Gap

Chapter 10

Formalization

Chapter 11

Conclusion

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