ABSTRACT

Title of dissertation: SPECTRAL GRAPH THEORY WITH
                           APPLICATIONS TO QUANTUM ADIABATIC
                           OPTIMIZATION

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In this dissertation I draw a connection between quantum adiabatic optimization, spectral graph theory, heat-diffusion, and sub-stochastic processes through the operators that govern these processes and their associated spectra. In particular, we study Hamiltonians which have recently become known as "stoquastic" or, equivalently, the generators of sub-stochastic processes. The operators corresponding to these Hamiltonians are of interest in all of the settings mentioned above.

I predominantly explore the connection between the spectral gap of an operator, or the difference between the two lowest energies of that operator, and certain equilibrium behavior. In the context of adiabatic optimization, this corresponds to the likelihood of solving the optimization problem of interest. I will provide an instance of an optimization problem that is easy to solve classically, but leaves open the possibility to being difficult adiabatically.

Aside from this concrete example, the work in this dissertation is predominantly mathematical and we focus on bounding the spectral gap. Our primary tool for doing this is

spectral graph theory, which provides the most natural approach to this task by simply considering Dirichlet eigenvalues of subgraphs of host graphs. I will derive tight bounds for the gap of one-dimensional, hypercube, and general convex subgraphs. The techniques used will also adapt methods recently used by Andrews and Clutterbuck to prove the long-standing "Fundamental Gap Conjecture".

SPECTRAL GRAPH THEORY WITH APPLICATIONS TO QUANTUM ADIABATIC OPTIMIZATION

by

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Dedication

To the ignorance of youth, without which this never would have happened.

Acknowledgments

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Chapter 1:   Introduction

This dissertation focuses on the problem of bounding the difference between the two lowest eigenvalues of Schrödinger operators, or quantum Hamiltonians, which are used to represent the energy of the physical system.[1] This difference, denoted by γ throughout, is known as the "spectral gap" of the corresponding operator. Although of reasonably broad mathematical interest, our primary motivation for studying this problem arises in the context of adiabatic quantum computing. Roughly speaking, adiabatic quantum algorithms slowly vary a quantum state that is easy to prepare into one that encodes the solution to some computational problem [35]. Although adiabatic quantum computation can perform universal quantum computation [1], the technique is most naturally applied to optimization problems, our current focus. Quantum adiabatic theorems tell us precisely how slowly our variation must progress. Understanding the speed at which the adiabatic process can progress helps us to understand the power of the algorithm.

The dynamics of an adiabatic process, and of course all quantum processes, are governed by Schrödinger's equation, $i\partial_t \psi(t) = H(t)\psi(t)$. The Hermitian operator H is known as the Hamiltonian of the system, and we denote its spectrum $\lambda_0 \leq \lambda_1 \leq \lambda_2 \ldots \leq \lambda_N$. We call $\gamma(s) = \lambda_1(s) - \lambda_0(s)$ the spectral gap of $H(s)$ and let $\gamma_{\min} = \min_s \gamma(s)$. If $\gamma_{\min} > 0$ we call the Hamiltonian "gapped". Most adiabatic theorems focus on such gapped Hamiltoni-

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[1]In general, these Hermitian operators H are known as either Hamiltonians or Schrödinger operators, where the term "Schrödinger operator" is preferred in the differential equations literature, seemingly because of increased generality. Although "Hamiltonian" might imply something physical about the operator, in this dissertation we use the two terms synonymously, as we are predominantly concerned with the mathematical properties of such operators.

ans, and our goal will be to develop techniques for estimating the spectral gap given that it is non-zero.

In this chapter we introduce the basics of adiabatic quantum computation, heat diffusion, and discrete sub-stochastic processes. Certain information about all three of these processes, in each a particular form of equilibration, can be addressed through an analysis of the spectral gap of a corresponding operator. The primary goal of this chapter is to make clear the connection between these three areas of study and the question of determining the spectral gap. In Section 1.1, we will introduce the model of quantum adiabatic optimization and recall certain well-known theorems about adiabaticity. In Section 1.2, we will introduce heat diffusion, its relationship to adiabatic optimization, and estimates on the equilibration time of a heat-diffusion process. In Section 1.3, we will define a sub-stochastic process and prove estimates on their equilibration time by relating them back to heat diffusion. In Section 1.4, we introduce the Rayleigh quotient, or the energy associated with a particular state, and state some of its properties. We conclude the chapter with some general properties of the spectral gap in adiabatic optimization problems in Section 1.5.

1.1 Adiabatic Optimization

Adiabatic optimization is a strategy for quantum computing where we assume that we are given a Hamiltonian $H(T)$ with ground-state ϕ that encodes the solution to some optimization problem of interest. Our strategy is to prepare a known ground-state $u(0)$ of some other Hamiltonian $H(0)$ and slowly adjust H from $H(0)$ into $H(T)$ according to some continuous path $H(t)$. The probability of success of this strategy, then, is given by how closely our actual final state $u(T)$ resembles ϕ. In turn, this behavior is governed by the adiabatic theorem.

A proof of the adiabatic theorem is beyond the scope of this chapter, however numerous

versions exist [40, 44, 60]. Some work has been done on deriving adiabatic theorems for operators without a spectral gap [16, 17, 55], but folklore amongst most physicists remains that a spectral gap is required for adiabatic behavior. Our interest at present, therefore, is restricted to "gapped" adiabatic theorems. We recall what is perhaps the most widely used adiabatic theorem adapted from Jansen, Ruskai, and Seiler [40, Theorem 4]:

Theorem 1.1 (Adiabatic theorem). *Let $\psi(t)$ be the ground state of a Hamiltonian $H(t/\tau)$. Then, if $\phi(t)$ satisfies*

$$\begin{cases} i\frac{d\phi}{dt} = H\left(\frac{t}{\tau}\right)\phi(t) \\ \phi(0) = \psi(0) \end{cases}$$

we have that

$$\|\phi(t) - \psi(t)\| \lesssim O\left(\frac{mh_{\max}}{\tau\gamma_{\min}^2}\right)$$

where $\gamma_{\min} = \min_s \gamma(s)$, m is the number of eigenvalues of H, and

$$h_{\max} = \sup_s \max\left\{\|H(s)\|, \|\dot{H}(s)\|, \|\dddot{H}(s)\|\right\}.$$

The adiabatic theorem is the primary tool for determining the runtime of an adiabatic optimization algorithm. In particular we see that the theorem predicts convergence of a state prepared in an initial ground-state $\psi(0)$ to the final ground state $\psi(\tau)$ if $\tau \sim \gamma_{\min}^{-2}$.

The general recipe for the adiabatic optimization algorithm, then, is to create the known $\phi(0)$ and vary it by the conditions of Theorem 1.1 into $\phi(\tau)$. By choosing τ to be sufficiently large, where "large" is determined by the theorem, we can guarantee convergence in ℓ^2-norm of the $\phi(\tau)$ to the final ground-state $\psi(\tau)$. If we can construct a final Hamiltonian $H(\tau)$ such that $\psi(\tau)$ encodes the solution to a problem of interest, we claim that we have solved the problem.

1.2   Heat Diffusion

Another process which depends on the spectral gap is heat diffusion. Suppose that $H \geq 0$ is a positive, semi-definite operator with spectrum $0 \leq \lambda_0 < \lambda_1 \leq \ldots \leq \lambda_n$. The heat diffusion process for $t \in [0, T]$ with initial distribution f_0 is then given by the initial-value problem

$$\begin{cases} f(0) = f_0 \\ \frac{df}{dt} = -Hf. \end{cases} \tag{1.1}$$

If we assume that the eigenfunction of H corresponding to λ_i is u_i, then it is a well-known fact that eq. (1.1) has the general solution

$$f(t) = \sum_i C_i u_i e^{-\lambda_i t} \tag{1.2}$$

where the constants C_i are uniquely determined by

$$C_i = \frac{f(0) \cdot u_i}{u_i^2}.$$

Now, we wish to examine the rate at which f approaches something proportional to the lowest eigenfunction u_0, which we assume is everywhere nonzero. Also, without loss of generality, we assume that $C_0 > 0$, or that our initial $f(0)$ is not completely orthogonal to u_0. What we want to consider is the rate at which our arbitrary function f approaches the current ground state $u_0 e^{-\lambda_0 t}$. To do so, we look at the ratio $f/(u_0 e^{-\lambda_0 t})$. If these two states are similar, then the ratio should be close to 1. In particular, we consider componentwise ratios $g_i = u_i/(C_0 u_0)$ and rewrite eq. (1.2) as

$$f(t) = C_0 u_0 e^{-\lambda_0 t} \sum_i \frac{C_i}{C_0} g_i e^{-(\lambda_i - \lambda_0)t}. \tag{1.3}$$

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Since all g_i are bounded, we find that

$$\frac{f(t)}{C_0 u_0 e^{-\lambda_0 t}} = \sum_i \frac{C_i}{C_0} g_i e^{-(\lambda_i - \lambda_0)t}$$
$$= 1 + \sum_{i>0} \frac{C_i}{C_0} g_i e^{-(\lambda_i - \lambda_0)t}.$$

Now, we derive a bound by considering the ℓ^2-norm of the difference

$$\left\| \frac{f(t)}{C_0 u_0 e^{-\lambda_0 t}} - 1 \right\| = \left\| \sum_{i>0} \frac{C_i}{C_0} g_i e^{-(\lambda_i - \lambda_0)t} \right\|$$
$$\leq \sum_{i>0} \left\| \frac{C_i}{C_0} g_i e^{-(\lambda_i - \lambda_0)t} \right\|$$
$$\leq \sum_{i>0} \left\| \frac{C_i}{C_0} g_i \right\| e^{-\gamma t}$$
$$= C e^{-\gamma t}$$

for some absolute constant C. Above, the second inequality follows from the fact that $\lambda_1 \leq \lambda_{i \geq 1}$. Hence, we see that deviations from the ground state are bounded as a function of the spectral gap γ.

In fact, because heat diffusion is equivalent to to Schrödinger evolution by the Wick rotation[2] $i \mapsto it$, one may naturally think of the role of the gap as similar in both adiabatic optimization and heat diffusion.

1.3   Sub-stochastic Processes

Similar to heat diffusion are sub-stochastic processes. A sub-stochastic process is a Markov process for a population that trends almost surely to death [27, 29]. Although less studied than traditional Markov processes, sub-stochastic processes have broad applications from ecology and population dynamics to classical algorithms [47, 49]. To characterize a sub-stochastic process, we define a measurable state space $\mathscr{X} \cup \partial \mathscr{X}$. We consider a

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[2]or one can transform eq. (1.1) into a Schrödinger equation by this transformation

Markov process $X = (X_t : t \geq 0)$ on $\mathcal{X} \cup \partial\mathcal{X}$ and consider the family of distributions $\mathbb{P}_x$ for some initial condition $x \in \mathcal{X}$. The boundary $\partial\mathcal{X}$ is taken to be absorbing or

$$\mathbb{P}.(x_{t>t_0} \in \partial\mathcal{X} | x_{t_0} \in \partial\mathcal{X}) = 1.$$

All that this says is that we consider a random walk on a properly defined (discrete) state space, where some boundary sites are capable of "killing" walkers, or forever trapping them. In this context, our primary interest is in quasi-stationary distributions (QSDs). A QSD is a distribution ν, such that

$$\mathbb{P}_\nu(x_t \in B | x_t \notin \partial\mathcal{X}) = \nu(B)$$

for a subset $B \in \mathcal{X}$, or a distribution which is stationary when conditioned on remaining alive. The quasi-stationary distribution, then, is the distribution which if achieved by a walker, is only deviated from by the death of that walker. Hence, a walker with probability distributed by the QSD retains probability distributed by the QSD until its death.

Our interest in these processes arises mostly due to their similarity to heat diffusion. The QSD can be thought of as the ground state in heat diffusion. Even though such a state may decay in amplitude with time, the *relative* amplitudes of that state remain constant. In particular, for a finite, discrete state space, we encode a sub-stochastic process in a matrix H satisfying

1. $H_{xy} \geq 0 \ \forall \, x, y \in \mathcal{X}$ and

2. $\sum_y H_{x,y} \leq 1 \ \forall \, x \in \mathcal{X}$.

Under these restrictions, we again wish to see how rapidly an arbitrary distribution f approaches a quasi-stationary distribution. Similar to (but in reverse order from) eq. (1.1)

we write the eigenvalues of H as $1 \geq \lambda_0 > \lambda_1 \geq \lambda_2 \ldots \geq \lambda_N \geq 0$ and corresponding eigen-vectors $u_0, u_1, \ldots, u_N$. (The restriction to $\lambda_0 > \lambda_1$ corresponds to the restriction that our walk is over a connected space. For details, see [25].) In this case, we define the spectral gap $\gamma = \lambda_0 - \lambda_1$. Then, we apply the walk t times

$$H^t v = \sum_i C_i u_i \lambda_i^t$$

where we again assume that $C_0 \neq 0$. Now, exactly like Section 1.2,

$$\left\| \frac{H^t v}{C_0 u_0 \lambda_0^t} - 1 \right\| = \left\| \sum_{i>0} f_i \frac{\lambda_i^t}{\lambda_0^t} \right\|$$

where $f_i = (C_i u_i)/(C_0 u_0)$. Note that the λ_i are arranged in decreasing order so that

$$
\begin{aligned}
\left\| \frac{H^t v}{C_0 u_0 \lambda_0^t} - 1 \right\| &\leq \left\| \sum_{i>0} f_i \right\| \frac{\lambda_1^t}{\lambda_0^t} \\
&= C \frac{\lambda_1^t}{\lambda_0^t} \\
&= C \frac{(\lambda_0 - \gamma)^t}{\lambda_0^t} \\
&= C \left(1 - \frac{\gamma}{\lambda_0} \right)^t \\
&\leq C (1 - \gamma)^t \\
&\leq C e^{-\gamma t}
\end{aligned}
$$

for some absolute constant C. Above, the second inequality follows from the fact that $\lambda_0 \leq 1$ and $t > 0$. (The third inequality just follows from a standard exponential inequality, $(1 - x) \leq e^{-x}$.) Hence, we see that a sub-stochastic process approaches its quasi-stationary distribution with the same asymptotic bound in γ as a heat-diffusive process.

1.4 The Rayleigh Quotient

Important to our discussion throughout the subsequent chapters will be the Rayleigh quotient. In general, for a Hermitian operator H and some nonzero function u

$$\frac{\sum_i u_i^* H_{ij} u_j}{u^* u} \equiv \langle H \rangle_u$$

is known as a Rayleigh quotient. The Rayleigh quotient, in quantum-mechanical terms, is nothing more than the expected value of the operator H under the state u. In the present case, it is simply the energy associated with the state u for the system given by H. If H has eigenfunctions $\{u_i\}$, then its eigenvalues are given by

$$\lambda_i = \langle H \rangle_{u_i}.$$

It is easy to see, then, that the lowest eigenvalue λ_0 is given by

$$\lambda_0 = \inf_{u \neq 0} \langle H \rangle_u$$

since the Rayleigh quotient must always be greater than or equal to the lowest eigenvalue. If H is nondegenerate, or has spectrum $\lambda_0 < \lambda_1 < \dots \lambda_n$, let S_i be the space spanned by the i lowest eigenvectors. Then,

$$\lambda_i = \inf_{\substack{u \perp S_i \\ u \neq 0}} \langle H \rangle_u. \tag{1.4}$$

This particular form of the Rayleigh quotient will be the object we are most interested in what follows. By utilizing a more careful definition of S_i, we could accommodate degenerate spectra. Nonetheless, because we are never going to be interested in $i > 1$ and we will always restrict ourselves to the case that $\lambda_1 - \lambda_0 > 0$, we hereafter assume that all operators

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discussed have nondegenerate spectra without loss of generality.

1.5 Minimal gap conservation

An interesting property that one can derive about interpolated Hamiltonians (such as the standard adiabatic linear interpolation $H(t) = (1-t)H_0 + tH_1$) is that critical points in the spectrum are conserved over the course of an interpolation. This is an immediate consequence of the well-known Hellman-Feynman theorem, which will also be used in later chapters.

Theorem 1.2. *Let $H(\alpha)$ be a Hermitian operator (matrix) dependent upon a parameter α with non-degenerate eigenvalue $\lambda(\alpha)$ and associated eigenfunction $u(\lambda; \alpha)$. Then*

$$\frac{d\lambda(\alpha)}{d\alpha} = \sum_{i,j} u_i^*(\lambda; \alpha) \frac{dH(\alpha)_{ij}}{d\alpha} u_j(\lambda; \alpha) \equiv \left\langle \frac{dH(\alpha)}{d\alpha} \right\rangle_{u(\lambda; \alpha)}$$

where $u_i(\lambda; \alpha)$ is the ith component of $\mathbf{u}(\lambda; \alpha)$.

It should be noted that the theorem is typically stated for a Hermitian operator $H(\alpha)$ with eigenvalues $\lambda_0 < \lambda_1 < \cdots < \lambda_N$. Care must be taken in the application of this theorem when considering degenerate eigenvalues [59, 62] which can sometimes occur. For instance, the ring graph with constant potential has degeneracies. Nonetheless, since the cases we consider in this dissertation are non-degenerate, we can use this theorem in its above-stated form.

The Hellman-Feynman theorem will be utilized in Chapter 4 for proving a one dimensional gap theorem. However, even in the context of adiabatic optimization, it has a non-trivial, somewhat surprising consequence.

Theorem 1.3. *Let $H(s) = (1 - a(s))H_0 + a(s)H_1$ be a Hermitian operator with non-zero spectral gap $\gamma(s)$ and a monotone-increasing and once differentiable for $s \in I$. Suppose*

that $\gamma(s)$ has a stationary point s_0 internal to I. Then, the two lowest eigenfunctions u, v of $H(s_0)$ satisfy

$$\gamma(s_0) = \langle H(s) \rangle_v - \langle H(s) \rangle_u$$

for all s.

Proof. Let $\lambda_0(s) < \lambda_1(s)$ be the two lowest eigenvalues of $H(s)$ with corresponding eigenfunctions $u(s)$ and $v(s)$. With s_0 as stated above, we know that $\gamma(s_0) = \lambda_1(s_0) - \lambda_0(s_0)$. Furthermore, by Theorem 1.2, we have that

$$\frac{d\gamma}{ds} = \left\langle \frac{dH}{ds} \right\rangle_{v(s)} - \left\langle \frac{dH}{ds} \right\rangle_{u(s)}$$
$$= a'(s) \left(\langle H_1 - H_0 \rangle_{v(s)} - \langle H_1 - H_0 \rangle_{u(s)} \right).$$

We wish to evaluate the function at $s = s_0$, which because $a'(s) > 0$ yields

$$0 = \langle H_1 - H_0 \rangle_{v(s_0)} - \langle H_1 - H_0 \rangle_{u(s_0)}.$$

Now, consider $H(s)$,

$$\langle H(s) \rangle_{v(s_0)} = \langle H_0 \rangle_{v(s_0)} + a(s) \langle (H_1 - H_0) \rangle_{v(s_0)}$$
$$= \langle H_0 \rangle_{v(s_0)} + a(s) \langle (H_1 - H_0) \rangle_{u(s_0)}$$
$$= \langle H_0 \rangle_{v(s_0)} - \langle H_0 \rangle_{u(s)} + \langle H(s) \rangle_{u(s_0)}.$$

Thus, we find that,

$$\langle H(s) \rangle_{v(s_0)} - \langle H(s) \rangle_{u(s_0)} = \langle H_0 \rangle_{v(s_0)} - \langle H_0 \rangle_{u(s_0)}.$$

In other words, the quantity $\langle H(s) \rangle_{v(s_0)} - \langle H(s) \rangle_{u(s_0)}$ is independent of s. Because we know that $\gamma(s_0) = \langle H(s_0) \rangle_{v(s_0)} - \langle H(s_0) \rangle_{u(s_0)}$ and $\langle H(s) \rangle_{v(s_0)} - \langle H(s) \rangle_{u(s_0)}$ is independent of s, our proof is complete. $\square$

We have incidentally also proven the following:

Corollary 1.1. *Let H, v, u, γ be defined as in theorem 1.3. Then, if $\gamma(s)$ attains its minimum interior to I,*

$$\gamma_{\min} = \langle H(s) \rangle_{v(s_0)} - \langle H(s) \rangle_{u(s_0)}$$

is independent of s.

Chapter 2:   Spectral Graph Theory

The most natural mathematical formalism for analyzing the spectral gap of the opera-
tors governing the processes discussed in the previous chapter is spectral graph theory. In
particular, we choose the formalism of combinatorial graph Laplacians, instead of normal-
ized graph Laplacians. [1] Typically, the framework of normalized graph Laplacians is the
more powerful approach, but in our context has great limitations. Most notably, the lowest
eigenvector (ground-state) of a combinatorial Laplacian is always the uniform distribution
and, for most of the processes that we wish to consider, is a (*the*) physically-relevant distri-
bution. In the case of normalized graph Laplacians, although regular graphs have a uniform
ground-state, in general, the ground state at vertex x is distributed like $d_x^{-1/2}$ where d_x is
the degree of vertex x.

This adjusted ground-state, while mathematically advantageous, is difficult to under-
stand physically and not a useful starting point for the adiabatic algorithm. Furthermore,
there is presently no clear mapping between the spectrum of the normalized Laplacian and
the combinatorial Laplacian, other than in the case of regular graphs.[2] This requires us to
focus our attention primarily on the combinatorial Laplacian. Although not our focus, when
not too distracting, we will occasionally explore properties of the normalized Laplacian.

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[1]For a review of the distinction, see [25].

[2]Results in either setting apply equally well to both combinatorial and normalized Laplacians of k-regular
graphs, since the spectrum maps neatly from the combinatorial to normalized case by a multiplicative factor
of $1/k$.

2.1 Weighted Graph Laplacians

Our object of interest is the weighted, undirected "combinatorial" graph Laplacian associated with a graph $G = (V, E, w)$ with weight function $w : V \times V \to \mathbb{R}^+$. We will somewhat abusively refer to eigenvalues of the combinatorial Laplacian of a graph G as eigenvalues of G and denote by λ_i the i-th eigenvalue of G. We choose w to satisfy the following three constraints,

1. $w(x, y) = 0$ if $(x, y) \notin E$,

2. $w(x, y) = w(y, x)$ for all $(x, y) \in E$, and

3. $w(x, x) = \sum_{\{x,y\} \in E} w(x, y)$.

Although our analysis will apply equally well to disconnected graphs, we will always impose the further constraint that our graph be connected, or that G cannot be decomposed into union of two disjoint graphs.

The Laplacian then takes the form,

$$L(x, y) = \begin{cases} w(x, x) & \text{if } x = y \\ -w(x, y) & \text{if } x \neq y. \end{cases} \tag{2.1}$$

It is also useful to write the Laplacian as a linear operator on the space of functions $\{f : V \to \mathbb{R}\}$. In keeping with spectral graph theory convention, we write $Lf(y)$ compactly for $[Lf](y)$. It should be clear from eq. (2.1) that

$$Lf(y) = w(y, y)f(y) - \sum_{x \in V} w(y, x)f(x)$$

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and utilizing the constraints on w,

$$Lf(y) = \sum_{\{x,y\} \in E} (f(y) - f(x)) w(x,y). \tag{2.2}$$

It is instructive to reconstruct the unweighted Laplacian for G from this definition. Simply let $w(x,y) = 1$ for all $(x,y) \in E$. Then, $w(x,x) = \sum_{y \sim x} 1 = d_x$. Thus, one finds that

$$L(x,y) = \begin{cases} d_x & \text{if } x = y \\ -1 & \text{if } (x,y) \in E \\ 0 & \text{otherwise.} \end{cases}$$

Furthermore, the key property of a constant lowest eigenvector is preserved through this definition. To see this, we begin by examining the Rayleigh quotient

$$\lambda_0 = \inf_f \frac{\sum_{x,y} f_x f_y w(x,y)}{\sum_x f_x^2}$$

$$= \inf_f \frac{\sum_x f_x^2 w(x,x) + \sum_{x \neq y} f_x f_y w(x,y)}{\sum_x f_x^2}$$

$$= \inf_f \frac{\sum_x \sum_{y \sim x} f_x^2 w(x,y) + 2 \sum_{\{x,y\} \in E} f_x f_y w(x,y)}{\sum_x f_x^2}$$

$$= \inf_f \frac{2 \sum_{\{x,y\} \in E} f_x^2 w(x,y) + 2 \sum_{\{x,y\} \in E} f_x f_y w(x,y)}{\sum_x f_x^2}$$

$$= \inf_f \frac{\sum_{\{x,y\} \in E} (f_x^2 + f_y^2) w(x,y) + 2 \sum_{\{x,y\} \in E} f_x f_y w(x,y)}{\sum_x f_x^2}$$

$$= \inf_f \frac{\sum_{\{x,y\}\in E} (f_x^2 + f_y^2 - 2f_xf_y)w(x,y)}{\sum_x f_x^2}$$

$$= \inf_f \frac{\sum_{\{x,y\}\in E} (f_x - f_y)^2 w(x,y)}{\sum_x f_x^2}.$$

Above, the third equality follows from the first and third constraints on w and the fifth equality from the second constraint on w. Now, note that $w(x,y)(f_x - f_y)^2 \geq 0$ independently of the choice of x, y. This clearly implies that $\lambda_0 \geq 0$. By choosing $f_x = f_y = C$ for all $x \in V$, we see that $\lambda_0 = 0$ is achieved, and hence $f_x = f_y = C$ is an eigenvector associated with eigenvalue 0.

It is easy to see that we can achieve 0 in the numerator if and only if $f_x - f_y = 0$ whenever $w(x,y) \neq 0$. If the graph were disconnected, we could indeed choose $f_x = f_y = C_1$ for all x, y in one connected component and $f_x' = f_y' = C_2$ in the other connected component and still achieve $\lambda_0 = 0$. This, however, clearly requires $C_1 = C_2$ in the case of a connected graph. Hence, in the case of a connected graph, the ground-state is unique.

The first nontrivial eigenvalue of G is clearly given by the Rayleigh quotient,

$$\lambda_1 = \inf_{f \perp \mathbf{1}} \frac{\sum_{(x,y)\in E} (f_x - f_y)^2 w(x,y)}{\sum_x f_x^2}$$

and furthermore,

$$\lambda_i = \inf_{f \perp S_i} \frac{\sum_{(x,y)\in E} (f_x - f_y)^2 w(x,y)}{\sum_x f_x^2} \tag{2.3}$$

where S_i is the subspace spanned by the i lowest eigenvectors. The spectral gap γ of a graph G is then,

$$\gamma := \lambda_1 - \lambda_0 = \lambda_1.$$

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2.2 Dirichlet Eigenvalues

To fully utilize the graph formalism, we consider a subgraph S of a graph G. Let $V(S) \subseteq V$ be the vertices of S and $E(S) \subseteq E$ be the edges of S. We write $\partial S = \{(x,y) \in E \mid x \in V(S), y \notin V(S)\}$ and $\delta S = \{x \in V \setminus V(S) \mid (x,y) \in \partial S \text{ for some } y \in V\}$. In other words, ∂S is the set of all edges of G with only one end in S. Then, δS is the set of all vertices in $G \setminus S$ that are connected by an edge to some vertex in S.

Now, consider functions $f : S \cup \delta S \to \mathbb{R}^+$. We write

$$\lambda_i^{(D)} = \inf_{\substack{f \in D* \\ f \perp S_i^*}} \frac{\displaystyle\sum_{\{x,y\} \in E(S) \cup \partial S} (f_x - f_y)^2 w(x,y)}{\displaystyle\sum_x f_x^2} \tag{2.4}$$

where $D*$ is the space of functions $\{f : S \cup \delta S \to \mathbb{R}^+\}$ satisfying the Dirichlet condition

$$f(x \in \delta S) = 0.$$

Note that, through an appropriate choice of w, one can specify the eigenvalues of all stoquastic Hamiltonians. To see this, fix a Hamiltonian

$$H = L + W \tag{2.5}$$

where L is a combinatorial graph Laplacian and W is some diagonal matrix which can be identified with a physical potential. Because shifts $H \mapsto H + cI$ adjust the spectrum by uniformly adding the constant c, we can restrict to the case that $W \geq 0$ without loss of generality. Then, W is a linear operator satisfying $W : S \to \mathbb{R}^+$.

We choose a host graph G for S such that

1. S is the graph corresponding to L, and

2. $W(x) = \sum_{y \in \delta S} w(x,y)$.

Then, eq. (2.4) becomes

$$\lambda_i^{(D)} = \inf_{\substack{f \in D_* \\ f \perp S_i^*}} \frac{\displaystyle\sum_{\{x,y\} \in E(S) \cup \partial S} (f_x - f_y)^2 w(x,y)}{\displaystyle\sum_{x \in V(S)} f_x^2}$$

$$= \inf_{\substack{f \in D_* \\ f \perp S_i^*}} \frac{\displaystyle\sum_{\{x,y\} \in E(S)} (f_x - f_y)^2 w(x,y) + \sum_{(x,y) \in \partial S} (f_x - f_y)^2 w(x,y)}{\displaystyle\sum_{x \in V(S)} f_x^2}$$

$$= \inf_{\substack{f \in D_* \\ f \perp S_i^*}} \frac{\displaystyle\sum_{\{x,y\} \in E(S)} (f_x - f_y)^2 w(x,y) + \sum_{x \in V(S)} \sum_{y \in \delta S} (f_x - f_y)^2 w(x,y)}{\displaystyle\sum_{x \in V(S)} f_x^2}$$

$$= \inf_{\substack{f \in D_* \\ f \perp S_i^*}} \frac{\displaystyle\sum_{\{x,y\} \in E(S)} (f_x - f_y)^2 w(x,y) + \sum_{x \in V(S)} \sum_{y \in \delta S} f_x^2 w(x,y)}{\displaystyle\sum_{x \in V(S)} f_x^2}$$

$$= \inf_{\substack{f \in D_* \\ f \perp S_i^*}} \frac{\displaystyle\sum_{\{x,y\} \in E(S)} (f_x - f_y)^2 w(x,y) + \sum_{x \in V(S)} f_x^2 W(x)}{\displaystyle\sum_{x \in V(S)} f_x^2}$$

which are clearly the eigenvalues of H. Note that, above, the fourth step follows by explicitly imposing the Dirichlet condition.

One can also derive an operator equation for H. Like above, both L and W can be viewed as linear operators on $\{f : S \cup \delta S \to \mathbb{R} | f(x \in \delta S) = 0\}$, where the action of L is given by eq. (2.2) and the action of W is simply

$$W f(y) = w(y,y) f(y) = \sum_{x \in \delta S} w(y,x) f(y).$$

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Combining these facts,

$$Hf(y) = \sum_{x \in V(S) \cup \delta S} (f(y) - f(x))w(y,x). \tag{2.6}$$

2.2.1 Dirichlet gap

Because the Dirichlet eigenvalues are the eigenvalues that we are typically interested in, we look to also define a spectral gap. The obvious choice is

$$\gamma^{(D)} := \lambda_1^{(D)} - \lambda_0^{(D)}. \tag{2.7}$$

Since $\lambda_0^{(D)} > 0$ whenever the Dirichlet boundary is nonempty (see spectral interlacing), the spectral gap of the Dirichlet eigenvalues is more difficult to analyze than that of the host graph. Our goal in this section is to seek a functional definition for the spectral gap, like that of eq. (2.3). We derive a theorem similar to Proposition 1.1 of [26].

Theorem 2.1. *Suppose u is the first Dirichlet eigenfunction corresponding to eigenvalue $\lambda_0^{(D)}$ of the induced subgraph S of G. Let $\lambda_1^{(D)} > \lambda_0^{(D)}$ be the next-lowest non-trivial Dirichlet eigenvalue. Then, the spectral gap $\gamma^{(D)} = \lambda_1^{(D)} - \lambda_0^{(D)}$ is given by*

$$\gamma^{(D)} = \inf_{f \perp \mathbf{1}} \frac{\displaystyle\sum_{\{x,y\} \in E(S)} (f_x - f_y)^2 w(x,y)u_x u_y}{\displaystyle\sum_{x \in V(S)} f_x^2 u_x^2}.$$

Proof. We begin by noting that u is an eigenfunction of the appropriate operator H. Then, eq. (2.6) yields

$$\begin{aligned}
\lambda_0^{(D)} u_y &= H u_y \\
&= \sum_{x \in V(S) \cup \delta S} (u_y - u_x)w(y,x)
\end{aligned}$$

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Thus, for an arbitrary function $f : S \cup \delta S \to \mathbb{R}$,

$$\lambda_0^{(D)} u_y^2 f_y^2 = \sum_{x \in V(S) \cup \delta S} (u_y - u_x) w_{yx} f_y^2 u_y$$

$$\lambda_0^{(D)} \sum_y u_y^2 f_y^2 = \sum_{y \in V(S)} \sum_{x \in V(S) \cup \delta S} w_{yx} (u_y - u_x) f_y^2 u_y$$

$$= \sum_{\{x,y\} \in \partial S} w_{yx} (u_y - u_x)(f_y^2 u_y - f_x^2 u_x)$$

$$= \sum_{\{x,y\} \in \partial S} w_{yx} \left((f_y u_y - f_x u_x)^2 - (f_y^2 u_x u_y + f_x^2 u_x u_y - 2 f_x f_y u_x u_y) \right)$$

$$= \sum_{\{x,y\} \in \partial S} w_{yx} \left((f_y u_y - f_x u_x)^2 - (f_y - f_x)^2 u_x u_y \right).$$

Thus,

$$\frac{\sum_{\{x,y\} \in \partial S} w(y,x) (f_y u_y - f_x u_x)^2}{\sum_y u_y^2 f_y^2} = \frac{\sum_{\{x,y\} \in \partial S} (f_y - f_x)^2 u_x u_y w(x,y)}{\sum_y u_y^2 f_y^2} + \lambda_0^{(D)}. \qquad (2.8)$$

Now, examining eq. (2.4),

$$\lambda_1^{(D)} = \inf_{\substack{g \in D* \\ g \perp u}} \frac{\sum_{\{x,y\} \in E(S) \cup \partial S} (g_x - g_y)^2 w(x,y)}{\sum_x g_x^2}$$

we choose $g = fu$ and see that

$$\lambda_1^{(D)} = \inf_{\substack{f \in D* \\ f \perp u^2}} \frac{\sum_{\{x,y\} \in E(S) \cup \partial S} (f_x u_x - f_y u_y)^2 w(x,y)}{\sum_x f_x^2}.$$

$$= \inf_{\substack{f \in D* \\ f \perp u^2}} \frac{\sum_{\{x,y\} \in \partial S} w(y,x) (f_y u_y - f_x u_x)^2}{\sum_y u_y^2 f_y^2}$$

$$= \inf_{\substack{f \in D* \\ f \perp u^2}} \frac{\sum_{\{x,y\} \in \partial S} (f_y - f_x)^2 w(x,y) u_x u_y}{\sum_y u_y^2 f_y^2} + \lambda_0^{(D)}.$$

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Thus, we finally arrive at

$$\gamma^{(D)} = \inf_{\substack{f \in D* \\ f \perp u^2}} \frac{\sum_{\{x,y\} \in \partial S} (f_y - f_x)^2 w(x,y) u_x u_y}{\sum_y u_y^2 f_y^2}.$$

$\square$

2.3 Cheeger Inequalities

Isoperimetric inequalities bound the volume of a region of a graph by the surface area of that region. Roughly speaking, the ratio of surface area to volume is bounded by a constant, known as an isoperimetric constant. The simplest and perhaps most commonly used isoperimetric inequality is known as a Cheeger inequality, which relates this ratio to an isoperimetric constant known as the Cheeger constant. In the context of Markov chains, this constant is often referred to as the conductance.

The utility of Cheeger inequalities is most easily seen by first deriving the Cheeger upper bound. Our approach follows [25]. First, we define the Cheeger constant for a subset A of $V(S)$. Let $\overline{A} = V(S) \setminus A$. Then, define

$$h_S(A) = \frac{\sum_{\substack{x \in A \\ y \in \overline{A}}} w(x,y) u_x u_y}{\min(\text{vol}(A), \text{vol}(\overline{A}))}$$

where $\text{vol}(A) = \sum_{x \in A} u_x^2$.

Now, we wish to minimize different "cuts". We hence arrive at the Cheeger constant *of the subgraph S*

$$h_S = \min_A h_S(A). \tag{2.9}$$

This constant provides a simple upper bound to the spectral gap $\gamma^{(D)}$.

Theorem 2.2.

$$\gamma^{(D)} \leq 2h_S$$

Proof. Consider the *A* that actually achieves this minimum. We wish to maximize contributions from the cut itself, while minimizing contributions from either side internal to the cut. To do so, we choose a step function, orthogonal to u^2, that changes sign at the cut itself. (The sign change at the cut insures that $(f_x - f_y)^2 \geq f_x^2 + f_y^2$.)

$$f(y) = \begin{cases} \frac{1}{\text{vol}(A)} & y \in A \\ -\frac{1}{\text{vol}(\overline{A})} & y \in \overline{A} \end{cases}$$

Now, by Theorem 2.1,

$$\gamma^{(D)} \leq \frac{\sum\limits_{\{x,y\} \in E(S)} (f_x - f_y)^2 w(x,y) u_x u_y}{\sum\limits_{x \in V(S)} f_x^2 u_x^2}.$$

$$= \frac{\sum\limits_{\substack{x \in A \\ y \in \overline{A}}} (\frac{1}{\text{vol}(A)} + \frac{1}{\text{vol}(\overline{A})})^2 w(x,y) u_x u_y}{\frac{1}{\text{vol}(A)} + \frac{1}{\text{vol}(\overline{A})}}.$$

$$= \sum\limits_{\substack{x \in A \\ y \in \overline{A}}} (\frac{1}{\text{vol}(A)} + \frac{1}{\text{vol}(\overline{A})}) w(x,y) u_x u_y$$

$$\leq \frac{2}{\min(\text{vol}(A), \text{vol}(\overline{A}))} \sum\limits_{\substack{x \in A \\ y \in \overline{A}}} w(x,y) u_x u_y.$$

$$= 2h_S$$

$\square$

We now wish to derive a Cheeger lower bound. Before we start, it helps to derive a relationship similar to eq. (2.6), except for $\gamma^{(D)}$.

Lemma 2.1. *Suppose v and u be the Dirichlet eigenfunctions corresponding to eigenvalues $\lambda_1^{(D)}$ and $\lambda_0^{(D)}$. Let $f = v/u$ and $\gamma^{(D)} = \lambda_1^{(D)} - \lambda_0^{(D)}$. Then,*

$$\gamma^{(D)} f_y u_y^2 = \sum_{x \in V(S) \cup \delta S} w(y,x)\, (f_y - f_x)\, u_x u_y.$$

Proof. Let v and u represent the Dirichlet eigenfunctions corresponding to eigenvalues $\lambda_1^{(D)}$ and $\lambda_0^{(D)}$ respectively. Then, by eq. (2.6)

$$\lambda_1^{(D)} v_y = \sum_{x \in V(S) \cup \delta S} (v_y - v_x) w(y,x)$$

$$\lambda_1^{(D)} v_y u_y = \sum_{x \in V(S) \cup \delta S} (v_y - v_x) u_y w(y,x).$$

Similarly,

$$\lambda_0^{(D)} v_y u_y = \sum_{x \in V(S) \cup \delta S} (u_y - u_x) v_y w(y,x).$$

Combining these,

$$\gamma^{(D)} v_y u_y = \sum_{x \in V(S) \cup \delta S} (v_y - v_x) u_y w(y,x) - \sum_{x \in V(S) \cup \delta S} (u_y - u_x) v_y w(y,x)$$

$$= \sum_{x \in V(S) \cup \delta S} w(y,x)\, \big((v_y - v_x) u_y - (u_y - u_x) v_y\big)$$

$$= \sum_{x \in V(S) \cup \delta S} w(y,x)\, (u_x v_y - v_x u_y)\,.$$

Now, substituting $f = v/u$

$$\gamma^{(D)} f_y u_y^2 = \sum_{x \in V(S) \cup \delta S} w(y,x)\, (u_x u_y f_y - f_x u_x u_y)\,.$$

$$= \sum_{x \in V(S) \cup \delta S} w(y,x)\, (f_y - f_x)\, u_x u_y.$$

$\square$

Remark. *Note that one can also derive the above expression through variational considerations of the Theorem 2.1. This approach is used by Chung in [25]. Alternatively, one*

might also derive this expression by considering rates of heat diffusion. This method will be explored in Chapter 5.

Theorem 2.3. *Let $\lambda_0^{(D)} < \lambda_1^{(D)}$ be the two lowest Dirichlet eigenvalues of $S \cup \delta S$ with corresponding eigenvectors u, v. Then,*

$$\gamma^{(D)} \geq \frac{h_S^2}{2\left(\langle D \rangle_v - 2\lambda_0\right)}$$

where $\langle D \rangle_v = \sum_{x \in S} d_{v_x} v_x^2$.

Proof. Let $S^+ = \{x \in V(S) | v \geq 0\}$. Assume that the host graph $S \cup \delta S$ has corresponding Laplacian $L = D - A$, where $Dx = \sum_{y \sim x} w(y, x) x$ and $Ax = \sum_{y \sim x} w(y, x) y$. Without loss of generality, we assume that $\langle D \rangle_{v|_{S^+}} \leq \langle D \rangle_{v..}$ (Note that if this were not true, we could simply take $v \mapsto -v$. We begin by recalling Lemma 2.1,

$$\gamma^{(D)} f_y u_y^2 = \sum_{x \in V(S) \cup \delta S} w(y, x) \left(f_y - f_x\right) u_x u_y$$

$$\gamma^{(D)} \sum_{f_y > 0} f_y^2 u_y^2 = \sum_{f_y > 0} \sum_{x \in V(S) \cup \delta S} w(y, x) \left(f_y - f_x\right) f_y u_x u_y$$

Now, we introduce the function

$$g(y) = \begin{cases} f(y) & \text{if } f(y) > 0 \\ \\ 0 & \text{otherwise.} \end{cases}$$

Hence, we arrive at,

$$\gamma^{(D)} \sum_y g_y^2 u_y^2 \geq \sum_y \sum_{x \in V(S) \cup \delta S} w(y, x) \left(g_y - g_x\right) g_y u_x u_y.$$

We then rearrange this expression to obtain an inequality explicitly for the gap.

$$\gamma^{(D)} \geq \frac{\sum_y \sum_{x \in V(S) \cup \delta S} w(y, x) \left(g_y - g_x\right) g_y u_x u_y}{\sum_y g_y^2 u_y^2}$$

$$\geq \frac{\displaystyle\sum_{\{y,x\}\in E(S)} w(y,x)\,(g_y - g_x)^2\,u_x u_y}{\displaystyle\sum_y g_y^2 u_y^2}$$

$$= \Phi$$

Now,

$$\Phi = \frac{\displaystyle\sum_{\{y,x\}\in E(S)} w(y,x)\,(g_y - g_x)^2\,u_x u_y}{\displaystyle\sum_y g_y^2 u_y^2} \cdot \frac{\displaystyle\sum_{\{y,x\}\in E(S)} (g_y + g_x)^2\,u_x u_y w(y,x)}{\displaystyle\sum_{\{y,x\}\in E(S)} (g_y + g_x)^2\,u_y u_x w(y,x)}$$

$$\geq \frac{\left(\displaystyle\sum_{\{y,x\}\in E(S)} |g_y^2 - g_x^2|\,u_x u_y w(y,x)\right)^2}{\displaystyle\sum_y g_y^2 u_y^2 \left(\sum_{\{y,x\}\in E(S)} (g_y + g_x)^2\,u_y u_x w(y,x)\right)}$$

$$= \frac{\left(\displaystyle\sum_{\{y,x\}\in E(S)} |g_y^2 - g_x^2|\,u_x u_y w(y,x)\right)^2}{\displaystyle\sum_y g_y^2 u_y^2 \left(\sum_{\{y,x\}\in E(S)} \left(2g_y^2 + 2g_x^2 - (g_y - g_x)^2\right)\,u_y u_x w(y,x)\right)}$$

$$= \frac{\left(\displaystyle\sum_{\{y,x\}\in E(S)} |g_y^2 - g_x^2|\,u_x u_y w(y,x)\right)^2}{\displaystyle\sum_y g_y^2 u_y^2 \left(2\sum_y g_y^2 u_y \sum_x u_x w(y,x) - \sum_{\{y,x\}\in E(S)} \left((g_y - g_x)^2\right)\,u_y u_x w(y,x)\right)}$$

where the inequality follows directly from Cauchy-Schwarz. Next, for the denominator, we recall eq. (2.6),

$$\frac{\left(\displaystyle\sum_{\{y,x\}\in E(S)} |g_y^2 - g_x^2|\,u_x u_y w(y,x)\right)^2}{\displaystyle\sum_y g_y^2 u_y^2 \left(2\sum_y g_y^2 u_y \left(\sum_x w(y,x) - \lambda_0^{(D)}\right) u_y - \sum_{\{y,x\}\in E(S)} \left((g_y - g_x)^2\right)\,u_y u_x w(y,x)\right)}$$

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$$= \frac{\left(\sum\limits_{\{y,x\}\in E(S)} |g_y^2 - g_x^2| u_x u_y w(y,x) \right)^2}{\sum\limits_y g_y^2 u_y^2 \left(2\sum\limits_y g_y^2 u_y^2 \left(\sum\limits_x w(y,x) - \lambda_0^{(D)} \right) - \sum\limits_{\{y,x\}\in E(S)} (g_y - g_x)^2 u_y u_x w(y,x) \right)}$$

$$= \frac{\left(\sum\limits_{\{y,x\}\in E(S)} |g_y^2 - g_x^2| u_x u_y w(y,x) \right)^2}{\left(\sum\limits_y g_y^2 u_y^2 \right)^2 \left(2\frac{\sum\limits_y g_y^2 u_y^2 \sum\limits_x w(y,x)}{\sum\limits_y g_y^2 u_y^2} - 2\lambda_0^{(D)} - \Phi \right)}$$

$$= \frac{\left(\sum\limits_{\{y,x\}\in E(S)} |g_y^2 - g_x^2| u_x u_y w(y,x) \right)^2}{\left(\sum\limits_y g_y^2 u_y^2 \right)^2 \left(2\frac{\sum\limits_y g_y^2 u_y^2 d_y}{\sum\limits_y g_y^2 u_y^2} - 2\lambda_0^{(D)} - \Phi \right)}.$$

In order to derive a bound, we now sort the components of v supported by S^+. In particular, we order the components such that $0 < v_{x_i} \le v_{x_{i+1}}$ for all $x_i, x_{i+1} \in S^+$. We construct cuts C_i such that,

$$C_i = \{\{x_j, x_k\} \in E(S) | j \le i < k\}$$

or, in other words, we cut vertices that connect amplitudes of v less than or equal to v_i to amplitudes of v greater than v_i. Then, by noting that our ordering guarantees $|g_x^2 - g_y^2| \ge |g_{x_i}^2 - g_{x_{i+1}}^2|$ and considering our choice of cut for i, we have that

$$\Phi \ge \frac{\left(\sum\limits_i |g_{v_i}^2 - g_{v_{i+1}}^2| \sum\limits_{C_i} u_x u_y w(y,x) \right)^2}{\left(\sum\limits_y g_y^2 u_y^2 \right)^2 \left(2\frac{\sum\limits_y g_y^2 u_y^2 d_y}{\sum\limits_y g_y^2 u_y^2} - 2\lambda_0^{(D)} - \Phi \right)}$$

$$\geq \frac{\left(\sum_i |g_{v_i}^2 - g_{v_{i+1}}^2| \sum_{j \leq i} h_S u_i^2\right)^2}{\left(\sum_y g_y^2 u_y^2\right)^2 \left(2\frac{\sum_y g_y^2 u_y^2 d_y}{\sum_y g_y^2 u_y^2} - 2\lambda_0^{(D)} - \Phi\right)}$$

$$\geq \frac{h_S^2}{2\langle D \rangle_v - 2\lambda_0 - \Phi}$$

$$\geq \frac{h_S^2}{2\langle D \rangle_v - 2\lambda_0}$$

where the second inequality followed from our assumption that $\langle D \rangle_{v|_{S^+}} \leq \langle D \rangle_v$. $\qquad \square$

At this point, one might wish to note that in the context of adiabatic optimization, one can combine Theorem 2.3 with Theorem 1.3 to derive a bound explicitly in terms of the ground-state and applied directly to the gap minimum. Considerations of this sort will be considered in the next chapter.

Chapter 3:   Adiabatic optimization without local minima

3.1   Introduction

An original intuition of adiabatic quantum computation (and an earlier classical algorithm called quantum annealing [36]) is that quantum optimization algorithms can in some cases tunnel out of local minima that would trap a classical algorithm known as simulated annealing. The runtime of adiabatic algorithms for variousspecific potentials with local minima has been analyzed in [6, 7, 33, 54, 57, 58]. In this chapter we investigate the more basic question of whether quantum adiabatic algorithms always efficiently solve "trivial" optimization problems, or problems where the only local energy minimum is the global minimum. As one might intuit from Theorem 2.3, we can construct a Hamiltonian with an exponentially small "bottleneck" in the distribution, thus causing an exponentially small gap.

Specifically, we consider Hamiltonians associated with graphs, consisting of the graph Laplacian plus a potential on the vertices. (The dimension of the Hilbert space is the number of vertices in the graph. The vertices may be labeled with bit strings corresponding to basis states of a set of qubits. Physically, one can interpret the Hamiltonian as describing a single particle hopping amongst the vertices.) In Section 3.3 we construct a single-basin potential on a graph such that the eigenvalue gap between the ground state and first excited state is exponentially small as a function of the number of vertices. This corresponds to a trivial optimization problem for which classical gradient descent finds the minimal-energy

vertex in linear time.

Strictly speaking, the exponentially small eigenvalue gap in our example does not necessarily imply that an adiabatic algorithm fails to solve this problem. For this one would need to invoke a converse of the adiabatic theorem, and one would furthermore need to show that diabatic transitions between eigenstates cause algorithmic failure in a practical sense. (Indeed, an example of algorithmic success despite failure of adiabaticity is given in [50].) However, our construction serves as a counterexample to a natural and perhaps even widely assumed conjecture, namely that potentials without local minima yield polynomial eigenvalue gaps.

Our counterexample has a ground state consisting of two "lobes" with exponentially small amplitude in the region between them. In Section 3.4 we use arguments based on conductance of Markov chains to show that the eigenvalue gap shrinks at worst quadratically with the number of vertices provided the ground state wavefunction is single-peaked. (See Lemma 3.4.) Thus, the two-lobed nature of the ground state in our counterexample is an essential feature. In other words, we find that the structure of local extrema in the potential does not neatly characterize the eigenvalue gap, but the structure of the local extrema of the ground state wavefunction does.

We also specifically investigate the one-dimensional case, called the path graph. We show that for convex[1] potentials, the ground state wavefunction is single-peaked. This yields, as a consequence of proposition 3.4, an $\Omega(1/(|W|\ell^2))$ lower bound on the gap for the path of ℓ vertices and a potential of norm $|W|$. By adapting Poincaré's inequality we are able to obtain an $\Omega(1/\ell^2)$ lower bound, with no dependence on $|W|$. This lower bound is tight to within a constant factor [41], and forms a discrete analog of [52]. Previous work has shown that for symmetric potentials on the path graph that increase as one moves

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[1]Actually, our result holds under the slightly weaker condition that the potential be "single-basin". See §3.4.3.

away from the center, the eigenvalue gap is lower bounded by $\Omega(1/\ell^2)$ [15]. Our result is incomparable to that of [15] in that such potentials are not a special case of convex potentials nor vice-versa.

Much of the research on adiabatic quantum algorithms seeks to achieve exponential speedups over classical algorithms. For this purpose, one seeks to find a potential on a highly-connected graph of exponentially many vertices (often the hypercube) such that the eigenvalue gap is only polynomially small. This differs somewhat from the setting studied in the present chapter - we consider graphs of polynomially many vertices and ask whether the gap is exponentially small or polynomially small. Thus, our counterexample in which the gap is already exponentially small on a graph of only polynomially many vertices constitutes an even more extreme gap collapse than previous examples such as [5].

In this chapter, since the math is somewhat less technical, we adopt standard Dirac notation. Most of the content of this section can also be found in [42].

3.2   Preliminaries

Let G be a graph with vertices V_G and edges $E_G \subseteq V_G \times V_G$. Let $\mathscr{H}_G = \mathrm{span}\{|x\rangle \,|\, x \in V_G\}$ be a complex Hilbert space with $\langle x|y\rangle = \delta_{x,y}$. Let L_G denote the Laplacian of G acting on $\mathscr{H}$. That is,

$$L_G = \sum_{x \in V_G} d_x |x\rangle\langle x| - \sum_{(x,y) \in E_G} |x\rangle\langle y|, \tag{3.1}$$

where d_x denotes the degree of vertex x.

In this chapter, we consider the Dirichlet graph described by

$$H_{G,W} = L_G + \sum_{x \in V_G} W(x)|x\rangle\langle x|, \tag{3.2}$$

where $W : V_G \to \mathbb{R}$ can be thought of as a potential energy function.

We say that $x \in V_G$ is a local minimum of W if $W(x) \le W(y)$ for all y such that $(x,y) \in E_G$. By the Perron-Frobenius theorem, the ground state of $H_{G,W}$ can be expressed in the form

$$|\psi\rangle = \sum_{x \in V_G} \psi(x)|x\rangle \qquad (3.3)$$

with $\psi(x) > 0$ for all $x \in V_G$. We say that ψ has a local maximum at x if

$$\psi(x) \ge \psi(y) \ \forall y \text{ s.t. } (x,y) \in E_G. \qquad (3.4)$$

In Section 3.4.2 we prove a lower bound on the eigenvalue gap in the case that the ground state wavefunction is single-peaked. By this, we mean that the set of local maxima of ψ form a connected set of vertices in G. This is a weaker condition than demanding that ψ have only a single local maximum, in that we allow the peak to consist of multiple vertices on which ψ is constant.

Most adiabatic optimization algorithms proposed to date use the following formulation. The optimization problem is formalized as a search on a graph G. The edges of the graph E_G represent the allowed moves within the search space. The vertices V_G represent the possible solutions, and one seeks to minimize the cost function $W : V_G \to \mathbb{R}$. For simplicity we assume that W has a unique global minimum $x_{\min} \in V_G$. Let

$$H_{G,W}(s) = (1-s)L_G + s \sum_{x \in V_G} W(x)|x\rangle\langle x|. \qquad (3.5)$$

The computation starts in the uniform superposition over vertices of G, which is the ground state of $H_{G,W}(0)$. Then, one applies a slowly-varying Hamiltonian $H_{G,W}(t/\tau)$. According to the adiabatic theorem, if τ is taken sufficiently large, the system will track the instantaneous ground state, and at the end of the computation, one will be left with the ground state of $H(1)$, namely $|x_{\min}\rangle$. More quantitatively, the adiabatic theorem [40] shows that it suf-

fices to take $\tau = O(1/\gamma^3)$, where $\gamma = \min_{0 \leq s \leq 1} \gamma(s)$ and $\gamma(s)$ is the eigenvalue gap between the ground energy and first excited energy of $H_{G,W}(s)$. (Heuristic arguments suggest that in many cases $\tau = O(1/\gamma^2)$ suffices [48]. For careful choices of $s(t)$, which do not include the choice $s = t/\tau$ considered here, this has been shown to hold rigorously [31]. See §3.6 for more discussion of this point.)

Let

$$\hat{H}_{G,W}(s) = \frac{H_{G,W}(s)}{1-s}. \tag{3.6}$$

One sees that $\hat{H}_{G,W}(s)$ is of the form (3.2) for all $s \in [0,1)$. Furthermore, the eigenvalue gap $\gamma(s)$ is given by

$$\gamma(s) = (1-s)\hat{\gamma}(s), \tag{3.7}$$

where $\hat{\gamma}(s)$ is the eigenvalue gap of $\hat{H}_{G,W}(s)$. Thus, theorems yielding upper or lower bounds on the eigenvalue gap of Hamiltonians of the form (3.2) yield useful bounds on the eigenvalue gap of $H_{G,W}(s)$ throughout the adiabatic algorithm except when s is very close to one. The gap analysis for s very close to one can be performed by other means, as discussed in §3.6. Throughout the rest of this paper, our focus will be on bounding gaps for Hamiltonians of the form (3.2).

Some works, such as [28, 32, 34], have considered adiabatic optimization algorithms with paths other than the linear interpolation defined by (3.5). In certain cases this has been shown to improve runtime. Most of the proposed alternative paths involve non-uniform changes to the off-diagonal matrix elements. Unlike (3.5), such Hamiltonians cannot be put into the form (3.2) by rescaling. Instead, they correspond to (3.2) where the Laplacian is of a weighted graph. The analysis of such Hamiltonians thus goes beyond the scope of this paper, although techniques related to those described here may be applicable.

3.3   Small Gaps Without Local Minima

Given a connected graph G, a potential W on the vertices, and a Hamiltonian $H_{G,W}$ of the form given in (3.2), one is tempted to conjecture that if G has only polynomially many vertices and W has no local minima (other than a global minimum) then $H_{G,W}$ can't have an exponentially small gap. In this section we construct a counterexample to this conjecture. In fact, beyond lack of local minima, our counterexample satisfies the even stronger condition that the potential forms a monotonic basin leading to a unique vertex of minimal potential. That is, there is no connected region of constant potential.

Consider the following "caterpillar" graph of $6\ell - 1$ vertices, as illustrated below.
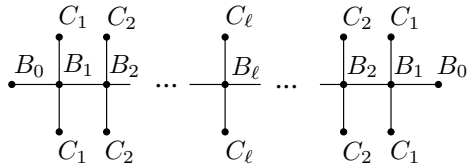
We consider a potential on the vertices with left-right and top-bottom mirror symmetries, and we correspondingly label equivalent vertices with identical labels. Our potential is as follows[2].

$$
\begin{aligned}
W(B_0) &= 0 \\
W(B_j) &= -\tfrac{1}{2} - \tfrac{j}{4l} \quad j \in \{1,\dots,\ell\} \\
W(C_1) &= \tfrac{1}{\frac{11}{12} - \frac{1}{8\ell}} - 1 \\
W(C_\ell) &= 7 \\
W(C_j) &= \tfrac{1}{\frac{2}{3} - \frac{j}{8\ell}} - 1 \quad j \in \{2,\dots,\ell-1\}
\end{aligned}
\tag{3.8}
$$

---

[2]Curious readers may wonder how this potential was arrived at. One can choose a desired ground state and potential on the B vertices, set the ground energy to zero, and solve for the wavefunction and potential on the C vertices. With some trial and error one can find choices such that the wavefunction at B_ℓ is exponentially small, yet the potential on each C vertex is greater than the potential on the B vertex to which it is connected and the ground state amplitudes are nonnegative on all vertices.

One sees that this potential is a single basin funneling to the unique minimum-potential vertex B_ℓ. (See Fig. 3.1.) The following unnormalized eigenstate has eigenvalue zero.

$$
\begin{aligned}
\psi(B_0) &= \tfrac{2}{3} \\
\psi(B_j) &= \left(\tfrac{2}{3}\right)^j && j \in \{1,\ldots,\ell\} \\
\psi(C_\ell) &= \tfrac{1}{8}\left(\tfrac{2}{3}\right)^\ell \\
\psi(C_1) &= \tfrac{2}{3}\left(\tfrac{11}{12} - \tfrac{1}{8\ell}\right) \\
\psi(C_j) &= \left(\tfrac{2}{3} - \tfrac{j}{8\ell}\right)\left(\tfrac{2}{3}\right)^j && j \in \{2,\ldots,\ell-1\}
\end{aligned}
\tag{3.9}
$$

All off-diagonal elements of the Hamiltonian $H_{G,W}$ are nonpositive. Therefore, by the Perron-Frobenius theorem, its ground state is the only eigenstate with all nonnegative amplitudes [45]. Hence, we can identify ψ as the ground state of $H_{G,W}$.

A ground state consisting of two symmetric lobes, such as ψ, implies a small eigenvalue gap because, by flipping the signs of the amplitudes in one lobe, one obtains an orthogonal state of only slightly higher energy. This energy cost, which upper-bounds the eigenvalue gap, is small due to the smallness of the amplitudes between the lobes.

More precisely, consider the wavefunction ϕ, which equals ψ for all vertices to the left of B_ℓ, equals $-\psi$ for all vertices to the right of B_ℓ, and equals zero at B_ℓ and C_ℓ. One sees that ϕ is orthogonal to ψ. Let $\eta = \langle\phi|\phi\rangle$ and let $|\widetilde{\phi}\rangle = \frac{1}{\sqrt{\eta}}|\phi\rangle$ be the normalized version of $|\phi\rangle$. The first excited state is variationally characterized as the lowest energy state orthogonal to the ground state. Therefore the energy of the first excited state is at most $\langle\widetilde{\phi}|H_{G,W}|\widetilde{\phi}\rangle$. Because the ground energy is zero we thus have

$$
\gamma \leq \langle\widetilde{\phi}|H_{G,W}|\widetilde{\phi}\rangle.
\tag{3.10}
$$

By construction, $|\phi\rangle$ satisfies the eigenvalue zero equation everywhere except at the B_ℓ
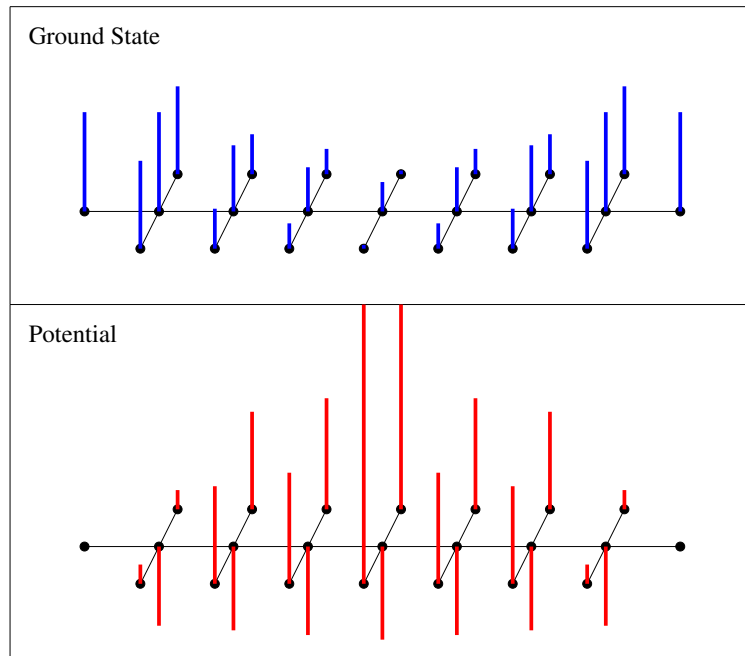
Figure 3.1: We illustrate the ground state wavefunction ψ and the potential W for $\ell = 4$. The ground state ψ consists of two lobes separated by a region of small amplitude in the center. The potential along the "spine" of the caterpillar is negative and decreasing as one approaches the central vertex B_4. The potential is positive on the "legs" of the caterpillar. Thus, the classical steepest-descent algorithm starting from any initial vertex will reach the minimum (B_4) by the shortest path. Note that the potential on the C_4 vertices is approximately ten times as large as the second largest value of the potential, and thus it is cut off by the boundaries of the figure.

vertex and the two $B_{\ell-1}$ vertices. Using this fact, one finds

$$\langle \phi | H_{G,W} | \phi \rangle = 2\psi(B_\ell)\psi(B_{\ell-1}). \tag{3.11}$$

By (3.9) one sees that $\eta > 1$. Therefore, (3.10) yields

$$\begin{align}
\gamma \quad &\leq \quad 2\eta^{-1}\psi(B_\ell)\psi(B_{\ell-1}) \tag{3.12} \\
&< \quad 2\psi(B_\ell)\psi(B_{\ell-1}) \tag{3.13} \\
&= \quad 2\left(\frac{2}{3}\right)^{2\ell-1}. \tag{3.14}
\end{align}$$

Hence, without any local minima in the potential and with only $O(\ell)$ vertices we obtain an eigenvalue gap of $O((2/3)^{2\ell})$.

3.4 Conductance-based Gap Bounds

In the preceding section, we showed that a ground state consisting of two symmetric lobes separated by a region of small amplitude implies a small eigenvalue gap. We relied on the symmetry of the lobes to construct a low-energy state orthogonal to the ground state by flipping the sign of the amplitudes on one lobe. However, it is true more generally that lobes separated by a region of small amplitude imply a small gap even if the lobes are asymmetric, provided the imbalance is not too severe. In this section we use concept of conductance to make this precise, and conversely to prove that if the ground state wavefunction is single-peaked, then the eigenvalue gap cannot be smaller than $\Omega(|V_G|^{-2})$.

3.4.1 Conductance

Motivated by applications to rapidly mixing Markov chains, sophisticated tools have been developed to bound the difference between the largest and second-largest eigenvalues of stochastic matrices. In this subsection, we recount one such tool, known as conductance.

Consider a discrete-time random walk on G defined by transition matrix P. That is, for $x, y \in V_G$, P_{xy} is the probability for a walker at x to transition to y in a given timestep. Thus, P is a row-stochastic matrix. Conductance provides upper and lower bounds on the gap between the largest and second largest eigenvalues of row-stochastic matrices in the case that the random walks they define are ergodic and reversible. Ergodicity means that the random walk converges to the same limiting distribution independent of the starting point of the walker. Reversibility means that, in the limiting distribution, the probability of traversing a given edge in one direction is equal to the probability of traversing it in the opposite direction. More formally, we recount the following definitions and facts from [56].

Definition 3.1. *The random walk defined by transition matrix P on vertex set V_G is ergodic if*

$$\lim_{s \to \infty} (P^s)_{xy} = \pi_y \quad \text{independent of } x. \tag{3.15}$$

The probability distribution π is then called the limiting distribution of the random walk.

Lemma 3.1. *The following conditions are necessary and sufficient for ergodicity of P.*

1. *P is irreducible. That is, for each $x, y \in V_G$ there is $s \in \mathbb{N}$ such that $(P^s)_{xy} > 0$.*

2. *P is aperiodic. That is, for all x, y, $\gcd\{s | (P^s)_{xy} > 0\} = 1$.*

Definition 3.2. *An ergodic random walk given by transition matrix P on vertex set V_G is*

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reversible if

$$\pi_x P_{xy} = \pi_y P_{yx} \quad \forall x, y \in V_G, \tag{3.16}$$

where π is the limiting distribution.

Definition 3.3. *Let P be the transition matrix of a reversible ergodic random walk on graph G with vertices V_G and edges E_G. Let π be the corresponding limiting distribution. Let S be any non-empty subset of V_G and let $\bar{S} = V_G/S$ be its complement. Let*

$$F_S = \sum_{\substack{(x,y) \in E_G \\ x \in S, y \in \bar{S}}} \pi_x P_{xy} \tag{3.17}$$

$$C_S = \sum_{x \in S} \pi_x \tag{3.18}$$

$$\Phi_S(P) = \frac{F_S}{\min\{C_S, C_{\bar{S}}\}} \tag{3.19}$$

$$\Phi(P) = \min_{S \subset V_G} \Phi_S(P). \tag{3.20}$$

$\Phi(P)$ *is called the conductance of P.*

The quantity F_S is called the flow of S, and the quantity P_S is called the probability of S. Note that, for reversible random walks, $F_S = F_{\bar{S}}$. By the Perron-Frobenius theorem, the largest eigenvalue of any irreducible stochastic matrix is 1 and the corresponding eigenspace is one-dimensional. Furthermore, this eigenvector can be written with all non-negative entries. Adapting theorems 2.4 and 2.6 of [56] one has the following.

Lemma 3.2. *(from [56]) Let matrix P define a reversible ergodic random walk with conductance $\Phi(P)$. Let γ denote the gap between the largest eigenvalue of P (which is 1) and the second-largest eigenvalue. Then*

$$\frac{\Phi(P)^2}{2} \leq \gamma \leq 2\Phi(P). \tag{3.21}$$

Proposition 3.2 is based on Cheeger's inequality [22] for the spectrum of Laplacians of manifolds, which was adapted to graphs by Alon and Milman [4], and extended to stochastic matrices by Sinclair [56].

3.4.2 Conductance Bound

In this subsection we use conductance to prove lower bounds on the gap of Hamiltonians of the form $H_{G,W}$ given in (3.2), culminating in a proof that the "lobed" nature of the ground state wavefunction in the counterexample from §3.3 is a necessary feature to obtain exponentially small gap. Specifically, we show that if $H_{G,W}$ has a single-peaked ground state then its eigenvalue gap has an $\Omega(|W|^{-1}|V_G|^{-2})$ lower bound, where $|V_G|$ is the number of vertices in the graph G and $|W| = \max_{x \in V_G} W(x) - \min_{x \in V_G} W(x)$.

Given a connected graph G, and a potential W on the vertices, let $H_{G,W}$ be the corresponding Hamiltonian of the form (3.2). Let γ denote the energy gap between the ground state and first excited state of $H_{G,W}$. For the purpose of bounding γ we may assume without loss of generality that the potential satisfies $W(x) < -d_G \quad \forall x \in V_G$, where d_G is the maximum degree of any vertex in G. If this is not the case, one can always subtract a sufficiently large multiple of the identity matrix to make it so without affecting γ.

Let $|\psi\rangle = \sum_{x \in V_G} \psi(x)|x\rangle$ denote the ground state of $H_{G,W}$ and E the ground energy. Let N_x be the neighbors of vertex x. That is,

$$N_x = \{y \in V_G | (x,y) \in E_G\}. \tag{3.22}$$

In this notation,

$$(d_x + W(x))\psi(x) - \sum_{y \in N_x} \psi(y) = E\psi(x). \tag{3.23}$$

For connected G,

$$\psi(x) > 0 \quad \forall x. \tag{3.24}$$

Thus we may rearrange (3.23) to obtain

$$d_x + W(x) - \sum_{y \in N_x} \psi(y)/\psi(x) = E. \tag{3.25}$$

Also, note that H has all nonpositive entries, so $E < 0$.

We next adapt a technique from [2, 3, 21] to relate the spectrum of $H_{G,W}$ to the spectrum of a random walk. Let $D = \mathrm{diag}\{\psi(x)|x \in V_G\}$. By (3.24), D is an invertible matrix with $D^{-1} = \mathrm{diag}\{\psi(x)^{-1}|x \in V_G\}$. Let

$$P = \frac{1}{E}D^{-1}H_{G,W}D. \tag{3.26}$$

By (3.25), $\sum_{y \in V_G}\langle x|P|y \rangle = 1$. That is, P is a row-stochastic matrix.

Because $E < 0$, the lowest eigenvalue of H corresponds to the highest eigenvalue of P, which is 1. Specifically, let

$$|\psi^2\rangle = \sum_{x \in V_G} \psi(x)^2|x\rangle. \tag{3.27}$$

One sees that

$$\langle \psi^2|P = \langle \psi^2|. \tag{3.28}$$

Hence the probability distribution ψ^2 is a limiting distribution of the random walk defined by P. Connectedness of the graph G suffices to ensure that condition 1 of proposition 3.1 is satisfied. The requirement that $W(x) < -d_G$ for all $x \in V_G$ ensures that condition 2 of proposition 3.1 is satisfied [56]. Thus, P is an ergodic random walk. In other words, ψ^2 is the unique limiting distribution of P and correspondingly $|\psi\rangle$ is the nondegenerate ground

state of $H_{G,W}$. By direct calculation, one finds

$$\psi(x)^2 P_{xy} = \psi(y)^2 P_{yx} = \begin{cases} -\frac{1}{E}\psi(x)\psi(y) & \text{if } (x,y) \in E_g \\ 0 & \text{otherwise.} \end{cases} \tag{3.29}$$

Thus, P is a reversible ergodic random walk. Therefore, by proposition 3.2 and equation (3.26), the energy gap γ between the ground and first-excited states of $H_{G,W}$ satisfies

$$-\frac{E}{2}\Phi^2(P) \leq \gamma \leq -2E\Phi(P). \tag{3.30}$$

One sees that the flow between $S \subset V_G$ and its complement determined by P is

$$F_S(P) = \sum_{\substack{x \in S \\ y \in \bar{S}}} \frac{\psi(x)\psi(y)}{-E} \tag{3.31}$$

and the corresponding probability is

$$C_S(P) = \sum_{x \in S} \psi(x)^2. \tag{3.32}$$

Thus, by (3.30) one obtains the following result.

Lemma 3.3. *(cf. [2, 3, 21]) Let $H_{G,W}$ be a Hamiltonian of the form (3.2) with $W(x) \leq -d_G \quad \forall x \in V_G$. Let ψ denote the ground state of $H_{G,W}$, let E denote the ground energy, and let γ denote the gap between the ground energy and the first excited energy. Then,*

$$-\frac{1}{2E}\Phi_H^2 \leq \gamma \leq 2\Phi_H \tag{3.33}$$

where

$$\Phi_H = \min_{S \subset V_G} \frac{F_S}{\min\{C_S, C_{\bar{S}}\}} \tag{3.34}$$

$$F_S = \sum_{(x,y) \in B} \psi(x)\psi(y) \tag{3.35}$$

$$B = \{(x,y) | x \in S, y \notin S, (x,y) \in E_G\} \tag{3.36}$$

$$C_S = \sum_{x \in S} \psi(x)^2 \tag{3.37}$$

$$C_{\bar{S}} = \sum_{\substack{x \in V_G \\ x \notin S}} \psi(x)^2. \tag{3.38}$$

Note that $E < 0$ and therefore the lower bound on γ given by (3.33) is nonnegative.

Examining (3.33) one sees that the gap is exponentially small if and only if the ground state has a pair of not-too-unbalanced lobes separated by a region of exponentially small amplitude. Choosing S and $\bar{S}$ to be the lobes, one sees that S and $\bar{S}$ must have reasonably well-balanced ground state probabilities for the denominator $\min\{C_S, C_{\bar{S}}\}$ to remain large, and the amplitudes along the cut separating S from $\bar{S}$ must all be small for the numerator F_S to be small. More precisely, recalling from §3.2 the definition of single-peaked, we have the following, which is the main result of this section.

Lemma 3.4. *Let G be a connected graph with vertices V_G, edges E_G, and maximum degree d_G. Let $W : V_G \to \mathbb{R}$ be a potential, and $H_{G,W}$ the corresponding Hamiltonian described in (3.2). Let ψ denote the ground state of $H_{G,W}$ and let γ denote the eigenvalue gap between the ground state and first excited state of $H_{G,W}$. If ψ is single-peaked then*

$$\gamma \geq \frac{1}{2(|W| + d_G)|V_G|^2} \tag{3.39}$$

where

$$|W| = \max_{x \in V_G} W(x) - \min_{x \in V_G} W(x). \tag{3.40}$$

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Proof. Let

$$H_{G,W}^{(-)} = H_{G,W} - (W_{\max} + d_G)\mathbb{1} \tag{3.41}$$

where $W_{\max} = \max_{x \in V_G} W(x)$. One sees that $H_{G,W}^{(-)}$ has the same ground state ψ and same gap γ as $H_{G,W}$ and that all matrix elements in $H_{G,W}^{(-)}$ are nonpositive. Hence, by proposition 3.3,

$$\gamma \geq -\frac{1}{2E^{(-)}} \left(\min_{S \subset V_G} \frac{F_S}{\min\{C_S, C_{\bar{S}}\}} \right)^2 \tag{3.42}$$

where $E^{(-)}$ is the ground energy of $H_{G,W}^{(-)}$, namely

$$E^{(-)} = E - (W_{\max} + d_G), \tag{3.43}$$

and F_S, C_S, and $C_{\bar{S}}$ are as in (3.35)-(3.38). Graph Laplacians are positive semidefinite, and therefore $E \geq W_{\min}$. Thus,

$$E^{(-)} \geq -|W| - d_G. \tag{3.44}$$

Hence, (3.42) yields

$$\gamma \geq \frac{1}{2(|W| + d_G)} \left(\min_{S \subset V_G} \frac{F_S}{\min\{C_S, C_{\bar{S}}\}} \right)^2. \tag{3.45}$$

We now consider two cases: 1) the peak of ψ spans the cut $\{S, \bar{S}\}$, and 2) the peak of ψ is contained entirely within one side of the cut.

Case 1: If the peak of ψ spans the cut then there exist $x \in S$ and $y \in \bar{S}$ such that $(x, y) \in E_G$ and $\psi(x) = \psi(y) \geq \psi(z)$ $\forall z \in V_G$. We can lower bound γ by throwing away the flows across all edges in the numerator other than (x, y). Thus,

$$\gamma \geq \frac{1}{2(|W| + d_G)} \left(\frac{\psi(x)^2}{\min\{C_S, C_{\bar{S}}\}} \right)^2. \tag{3.46}$$

Furthermore, $\min\{C_S, C_{\bar{S}}\} \leq \psi(x)^2 |V_G|$, and therefore $\gamma \geq \frac{1}{2(|W|+d)|V_G|^2}$.

Case 2: If the peak of ψ is contained within one side of the cut, we may, without loss of generality, call the side containing the peak S and the other side $\bar{S}$. Let $x_{\max}$ be the vertex in $\bar{S}$ that maximizes ψ. Because ψ is single-peaked, there must be a neighbor z of $x_{\max}$ such that $\psi(z) > \psi(x_{\max})$. Because $\psi(x_{\max})$ maximizes ψ in $\bar{S}$, z must be contained in S. We can lower bound γ by throwing away the flows across all edges in the numerator other than $(x_{\max}, z)$. Thus,

$$\gamma \geq \frac{1}{2(|W|+d_G)} \left(\frac{\psi(x_{\max})\psi(z)}{\min\{C_S, C_{\bar{S}}\}} \right)^2 \geq \frac{1}{2(|W|+d_G)} \left(\frac{\psi(x_{\max})^2}{\min\{C_S, C_{\bar{S}}\}} \right)^2. \tag{3.47}$$

Furthermore, $C_{\bar{S}} \leq \psi(x_{\max})^2 |V_G|$, and therefore $\min\{C_S, C_{\bar{S}}\} \leq \psi(x_{\max})^2 |V_G|$. Thus, in this case also, $\gamma \geq \frac{1}{2(|W|+d_G)|V_G|^2}$. $\qquad\square$

3.4.3 Conductance Bound for Path Graphs

Here we note some consequences of proposition 3.4 in the case that G is the path graph of l vertices, G_l.

$$G_l \quad = \quad \overset{1}{\bullet}\!\!-\!\!\overset{2}{\bullet}\!\!-\!\!\bullet \quad \cdots \quad -\!\!\overset{l}{\bullet}$$

Definition 3.4. *Let G be a graph with vertices V_G and edges E_G. Let $W : V_G \to \mathbb{R}$ be a potential. We say W is a single-basin potential if the set $\{x \in V_G | W(x) < E\}$ is a connected set of vertices in G for all E.*

As we now show, single-basin potentials on the path graph have single-peaked ground states and hence a large eigenvalue gap by proposition 3.4. For intuition, recall that, for a single particle in the one-dimensional continuum, the time-independent Schrödinger equation can be written as $-\frac{d^2\psi}{dx^2} = (E - W(x))\psi$. The ground state can be expressed with all real non-negative amplitudes. Hence the sign of $\frac{d^2\psi}{dx^2}$ is the same as the sign of $W(x) - E$. Thus,

the ground state of a convex potential has simple structure: inside the well, $W(x) - E < 0$ and the wavefunction is concave down, whereas outside the well $W(x) - E > 0$ and the wavefunction is concave up. The path graph case, described below, is essentially a discrete analogue to this.

Remark: The notion of a single-basin potential is well-defined on any graph. On path graphs one can also easily define the notion of a convex potential. Simply think of the l vertices as corresponding to the integers $\{1, \ldots, l\}$ and demand that the potential on the vertices be equal to some convex function on $\mathbb{R}$ evaluated at these integer points. It is not hard to show that single-basin is a slightly weaker condition than convex. That is, on the path graph, all convex potentials are single-basin, but not all single-basin potentials are convex.

For a wavefunction ψ on the vertices of G, define

$$\Delta^2 \psi(x) = -d_x \psi(x) + \sum_{y \in N_x} \psi(y), \tag{3.48}$$

where d_x is the degree of vertex x and N_x is the set vertices neighboring x. Thus,

$$L_G |\psi\rangle = -\sum_{x \in V_G} \Delta^2 \psi(x) |x\rangle. \tag{3.49}$$

Lemma 3.5. *Suppose W is a single-basin potential on graph G. Let ψ be the ground state of the corresponding Hamiltonian $H_{G,W}$, and let*

$$S[\psi] = \{x \in V_G | \Delta^2 \psi(x) < 0\}. \tag{3.50}$$

Then, $S[\psi]$ is a connected set of vertices in G.

Proof. Let E denote the ground energy of $H_{G,W}$. Thus, by (3.49),

$$\Delta^2 \psi(x) = (W(x) - E)\psi(x) \tag{3.51}$$

Recall that $\psi(x) > 0 \quad \forall x \in V_G$. Thus, $\Delta^2 \psi(x)$ has the same sign as $W(x) - E$. The connectedness of $S[\psi]$ then follows directly from the single-basin property. $\quad\square$

In special case that G is a path graph, the connectedness of $S[\psi]$ implies that ψ has only one local maximum. Thus, as a corollary of proposition 3.4, one obtains proposition 3.6. Note that on more general graphs, connectedness of $S[\psi]$ does not imply that ψ has only one local maximum.

Lemma 3.6. *Let W be a single-basin potential on the path graph G_l. Let $H_{G,W}$ be the corresponding Hamiltonian of the form (3.2). Let γ denote the gap between the ground energy and first excited energy of $H_{G,W}$. Then $\gamma \geq \frac{1}{2(|W|+2)l^2}$ where $|W| = \max_{x \in V_G} W(x) - \min_{x \in V_G} W(x)$.*

Proposition 3.6 shows that for single-basin potentials on G_l, the eigenvalue gap obeys $\gamma = \Omega(1/l^2)$. In the special case of a flat potential, it is easy to solve for the eigenvalue gap exactly, which is $O(1/l^2)$. However, the bound of proposition 3.6 is not tight due to the dependence on $|W|$. In the next section, we obtain a tighter bound by applying the Poincaré inequality.

3.5 Poincaré-based Gap Bounds

Two of the main tools for proving lower bounds on the eigenvalue gap of stochastic matrices are the Cheeger inequality and the Poincaré inequality. Conductance methods, such as those described in §3.4.1, are originally derived from the Cheeger inequality [22]. For some random walks, the Poincaré inequality yields stronger lower bounds than the

Cheeger inequality [30, 37], and for other random walks the reverse is true [53]. In §3.5.1, we recount the version of the Poincaré inequality given in [30] and apply it to Hamiltonians $H_{G,W}$ of the form (3.2). In §3.5.2 we specialize to the case of path graphs, obtaining a tighter bound than our conductance-based bound (proposition 3.6). (For a previous example in which Poincaré's inequality is used to bound the gap of a Hamiltonian see [19].)

3.5.1 The Poincaré Inequality

Let P be the transition matrix for an ergodic reversible discrete-time random walk on a graph G. Let π denote the limiting distribution and let γ denote the gap between the highest and second-highest eigenvalues of P. For any edge e in the graph G, let e_1, e_2 denote the vertices at its endpoints. Let $Q(e)$ denote the flow across edge e in the limiting distribution.

$$Q(e) = \pi_{e_1} P_{e_1, e_2} = \pi_{e_2} P_{e_2, e_1}. \tag{3.52}$$

The latter equality expresses the reversibility of the random walk. For each ordered pair (x, y) of distinct vertices in G, choose a canonical path γ_{xy} from x to y. Vertices may be repeated in a path, but no edge may be traversed more than once. Let Γ be the collection of canonical paths, one for each ordered pair of vertices. For $\gamma_{xy} \in \Gamma$, let

$$|\gamma_{xy}| = \sum_{e \in \gamma_{xy}} Q(e)^{-1} \tag{3.53}$$

where the sum is over the edges in path γ_{xy}. Let

$$\kappa(\Gamma) = \max_e \sum_{\gamma_{xy} \ni e} |\gamma_{xy}| \pi_x \pi_y. \tag{3.54}$$

The Poincaré inequality states [30]

$$\gamma \geq \frac{1}{\kappa}. \tag{3.55}$$

To obtain a tight bound on γ one must make a good choice of Γ.

Intuitively, the quantity $\frac{1}{\kappa}$, like the conductance Φ, quantifies the presence of a bottleneck across which the flow is small. As an example, consider a graph consisting of two large subgraphs connected by only a single edge e. In this case, every pair of vertices spanning the pair of subgraphs has a canonical path crossing e. Correspondingly, $\sum_{\gamma_{xy} \ni e} |\gamma_{xy}| \pi_x \pi_y$ will be large, which implies large κ. Similarly, κ will be large if there are many edges connecting the two subgraphs to each other but the flow $Q(e)$ across all such edges is small. Only in the absence of such bottlenecks does (3.55) yield a large lower bound on the gap.

As in §3.4.2, we use (3.26) to obtain a stochastic matrix P from our Hamiltonian H such that the eigenvalue gap γ of P relates to the eigenvalue gap γ_H of H according to

$$\gamma_H = -E\gamma, \tag{3.56}$$

where E is the ground energy of H. The eigenvalue gap of P can be lower-bounded using the Poincaré inequality. Specifically, by (3.26), we have the following.

$$Q(x,y) = \frac{\psi(x)\psi(y)}{-E} \tag{3.57}$$

$$\pi_x = \psi(x)^2 \tag{3.58}$$

$$\kappa = \max_e \sum_{\gamma_{xy} \ni e} \psi(x)^2 \psi(y)^2 \sum_{g \in \gamma_{xy}} \frac{-E}{\psi(g_1)\psi(g_2)}. \tag{3.59}$$

Here ψ is the ground state of H, and g_1, g_2 are the two vertices connected by edge g. By (3.56) the ground energy cancels from the final bound on γ_H. Summarizing:

$$\gamma_H \geq \frac{1}{\kappa'}, \tag{3.60}$$

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where

$$\kappa' = \max_e \sum_{\gamma_{xy} \ni e} \psi(x)^2 \psi(y)^2 \sum_{g \in \gamma_{xy}} \frac{1}{\psi(g_1)\psi(g_2)}. \tag{3.61}$$

3.5.2 Poincaré Bound for Path Graphs

For path graphs, there is only one valid choice of canonical paths Γ. Specifically, for a pair of vertices $s < f$ the canonical path is $s, s+1, \ldots, f$. For $f < s$ one takes the reverse path. Thus, (3.61) reduces to

$$\kappa' = \max_{1 \le j \le l-1} 2 \sum_{s \le j} \sum_{f > j} R(s, f) \tag{3.62}$$

where

$$R(s, f) = \psi(s)^2 \psi(f)^2 \sum_{s \le v < f} \frac{1}{\psi(v)\psi(v+1)}. \tag{3.63}$$

The factor of 2 in (3.62) arises because we sum only over the paths with $s < f$ and use the fact that $R(s, f) = R(f, s)$.

As discussed in §3.4.3, if the potential on the path graph is single-basin, then the ground state wavefunction has only one local maximum. Thus, the minimum of $\psi(v)$ along a segment $s \le v < f$ must occur at one of the endpoints. If the minimum is at s then (3.63) yields

$$R(s, f) \le \psi(s)^2 \psi(f)^2 \sum_{s \le v < f} \frac{1}{\psi(s)^2} \tag{3.64}$$

$$= (f - s)\psi(f)^2. \tag{3.65}$$

Similarly, if the minimum is at f then one has $R(s, f) \le (f - s)\psi(s)^2$.

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Let J be the value of j that achieves the maximum in (3.62). Then

$$\kappa' \leq 2 \sum_{s \leq J} \sum_{f > J} (f - s) \psi(b_{s,f})^2 \tag{3.66}$$

where $b_{s,f}$ is either s or f depending on which is smaller amongst $\psi(s)^2$ and $\psi(f)^2$. We can rewrite this sum over pairs of vertices as

$$\sum_{s \leq J} \sum_{f > J} (f - s) \psi(b_{s,f})^2 = \sum_{b=1}^{l} \sum_{a \in S_b} |a - b| \psi(b)^2, \tag{3.67}$$

where, for a given vertex b, S_b is the set of vertices on the other side of edge J such that $\psi(a)^2 \leq \psi(b)^2$. (For some b, S_b can be empty.) From (3.67) we have

$$\kappa' \leq 2 \sum_{b=1}^{l} \psi(b)^2 \sum_{a \in S_b} |a - b| \tag{3.68}$$

$$\leq 2 \sum_{b=1}^{l} \psi(b)^2 \sum_{a=1}^{l-1} a \tag{3.69}$$

$$= \sum_{b=1}^{l} \psi(b)^2 l(l-1) \tag{3.70}$$

$$\leq l(l-1). \tag{3.71}$$

The last equality follows from the fact that $\psi(b)^2$ is a probability distribution over $1, \ldots, l$. Thus, by (3.60),

$$\gamma_H \geq \frac{1}{l(l-1)}. \tag{3.72}$$

By direct calculation, one finds that the eigenvalue gap for the length l chain with no potential ($W = 0$) is $4 \sin^2 \left(\frac{\pi}{2l} \right)$. Thus, the bound (3.72) is asymptotically tight to within a factor of π^2 [41].

3.6 Application to Adiabatic Optimization Algorithms

In this section, we show that, as a corollary of proposition 3.4, adiabatic optimization algorithms in which the ground state $\psi(s)$ is single-peaked for all s, have minimum gap at least $\Omega(1/|V_G|^2)$ and therefore run in $\widetilde{O}(|V_G|^4)$ time, by an adiabatic theorem [31]. (The $\widetilde{O}$ notation indicates that we are omitting logarithmic factors.) This result cannot be used directly to find algorithmic speedups, as exhaustive search runs in $O(|V_G|)$ time. However, we believe this analysis may be useful in cases of high symmetry such as [33, 54, 57], where the eigenvalue gap on exponentially large graphs can be determined by analyzing the spectrum of polynomial-size graphs. In addition, the analysis in this section provides an illustrative example of how proposition 3.4 may be applied to the analysis of adiabatic optimization problems.

Consider an adiabatic optimization algorithm using a Hamiltonian $H_{G,W}(s)$ of the form shown in (3.5). Then

$$\hat{H}_{G,W}(s) = \frac{1}{1-s} H_{G,W}(s) \tag{3.73}$$

is of the form (3.2) addressed by proposition 3.4. $\hat{H}_{G,W}(s)$ and $H_{G,W}(s)$ have the same ground state, which we denote $\psi(s)$. Thus, if $\psi(s)$ is single-peaked for all $s \in [0,1)$ we may conclude from proposition 3.4 that

$$\hat{\gamma}(s) \geq \frac{1}{2\left(|\hat{W}(s)|+d_G\right)|V_G|^2}, \tag{3.74}$$

where $\hat{W}(s) = \frac{s}{1-s}W$ is the potential in $\hat{H}_{G,W}(s)$. Hence, one substitutes $|\hat{W}(s)| = \frac{s}{1-s}|W|$ and $\gamma(s) = (1-s)\hat{\gamma}(s)$ into (3.74), obtaining

$$\gamma(s) \geq \frac{1-s}{2\left(\frac{s}{1-s}|W|+d_G\right)|V_G|^2}. \tag{3.75}$$

One sees that this lower bound on $\gamma(s)$ becomes very small as s closely approaches 1. For the final part of the adiabatic optimization algorithm we therefore use a different method to lower-bound the eigenvalue gap. As an illustrative example, we suppose that the gap between the minimum of W and the second smallest value taken by W is one. Thus, by (3.5), $\gamma(1) = 1$. Generalization to other values of $\gamma(1)$ is straightforward and yields the same scaling with $|V_G|$ and d_G. At $s = 1 - \delta$, one has

$$H(s) = \delta L_G + (1 - \delta)W. \tag{3.76}$$

By Gershgorin's circle theorem, one sees that the operator norm of L_G is at most $2d_G$. Thus, the operator norm of δL_G is at most $2\delta d_G$. Hence, Weyl's inequalities show that the worst case is that the addition of δL_G to $(1 - \delta)W$ shifts the ground energy up by $2\delta d_G$ and shifts the first excited energy down by $2\delta d_G$. Thus, adding δL_G to $(1 - \delta)W$ at worst decreases the gap from $1 - \delta$ to $1 - \delta - 4\delta d_G$. Thus,

$$\gamma(s) \geq \frac{1}{2} - \frac{1}{8d_G} \quad \forall s \in \left[1 - \frac{1}{8d_G}, 1\right]. \tag{3.77}$$

The degree d_G is at least 2 for any connected graph of more than two vertices, so for all nontrivial cases one has

$$\gamma(s) \geq \frac{7}{16} \quad \forall s \in \left[1 - \frac{1}{8d_G}, 1\right]. \tag{3.78}$$

For the remaining values of s, (3.75) yields

$$\gamma(s) \geq \frac{\frac{1}{8d_G}}{2\left(8d_G|W| + d_G\right)|V_G|^2} \quad \forall s \in \left[0, 1 - \frac{1}{8d_G}\right]. \tag{3.79}$$

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Together, (3.78) and (3.79) yield

$$\gamma(s) = \Omega \left(\frac{1}{d_G^2 |W| |V_G|^2} \right) \quad \forall s \in [0, 1]. \tag{3.80}$$

The adiabatic theorem of [40] shows that adiabaticity will be maintained by evolving according to the linear-interpolation Hamiltonian $H_{G,W}(t/\tau)$ with runtime τ bounded by

$$\tau = O \left(\frac{\left\| \frac{dH}{ds} \right\|^2}{\gamma^3} \right). \tag{3.81}$$

By (3.5), $\left\| \frac{dH}{ds} \right\| = O(d_G + |W|)$. Thus, by (3.80) and (3.81),

$$\tau = O \left(d_G^6 |W|^3 |V_G|^6 (|W| + d_G)^2 \right). \tag{3.82}$$

As shown in [31], a tighter bound on running time can be obtained by choosing a more optimized interpolation schedule between the initial and final Hamiltonians. Specifically, one should choose the interpolation such that $H(t)$ is infinitely differentiable but is time-independent outside of $t \in [0, \tau]$. For example, let

$$H(t) = (1 - s(t/\tau))L_G + s(t/\tau)W \tag{3.83}$$

where s is the following "switching function", which is infinitely differentiable, and satisfies $s(0) = 0$, $s(1) = 1$, and $s'(x) = 0 \; \forall x \notin (0, 1)$:

$$s(x) \;\; = \;\; \int_{-\infty}^{x} g(y) dy \tag{3.84}$$

$$g(y) \;\; = \;\; \begin{cases} 0 & \text{if } y \notin [0, 1] \\ \beta \exp \left(-\frac{1}{y(1-y)} \right) & \text{if } y \in (0, 1) \end{cases}. \tag{3.85}$$

$$\tag{3.86}$$

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Here, β is the normalization constant yielding $f(1) = 1$. In this case, as shown in [31], by evolving with $H(t)$ from time zero to τ one achieves adiabaticity with runtime

$$\tau = O\left(\frac{(\log(1/\gamma))^{12}}{\gamma^2}\right).$$

(3.87)

For a Hamiltonian in which the ground state is always single-peaked, (3.87) and (3.80) yield runtime

$$\tau = \widetilde{O}(V_G^4).$$

(3.88)

Chapter 4: One dimensional fundamental gap theorem

4.1 Introduction

The Fundamental Gap Conjecture proposed a tight lower bound of $3\pi^2/D^2$ to the difference between the two lowest eigenvalues (the gap) of a Schrödinger operator $-\nabla^2 + V(x)$ with convex potential V on a compact convex domain $\Omega \subset \mathbb{R}^n$ of diameter D and subject to Dirichlet boundary conditions. Recently, Andrews and Clutterbuck proved the conjecture for all "semiconvex" potentials (which include convex potentials as a special case) in arbitrary dimensions [12]. Although the community's focus has largely centered on the continuum[12, 14, 46, 61], as early as 1990 Ashbaugh and Benguria saw the potential for extending their results to discrete Laplacians. In their work, they proved a lower bound to the gap for a particular class of discrete Laplacians with symmetric-decreasing potentials [15]. Indeed, recent interest in adiabatic quantum computing justifies their vision and motivates our interest in lifting continuum results to graph Laplacians[33, 35].

Previously to the approach below first found in [41], in the setting of quantum computation, gap bounds were derived on an as-needed basis. For instance, in an analysis of the power of adiabatic algorithms, van Dam et al. bounded eigenvalue gaps in the minimum Hamming weight problem by considering an explicit gap and then bounding the maximum error on this gap from perturbations[57]. In another instance, Reichardt considers the eigenvalue gap for an Ising system by using properties of the operator's principal submatrices[54]. (At least in the case of the path graph, Reichardt's Sturm sequences are

similar in form to our eigenvector recurrence of eq. (4.12). For an explicit examination of the link between principal submatrices and the eigenvector recurrences, see Gantmakher and Kreĭn[38].) Unlike the constructions above, this chapter develops a tight bound, general bound.

In this chapter, we consider specifically Schrödinger operators corresponding to graph Laplacians with suitably defined convex potential terms. Here, the potential is restricted to the vertices and can be seen either as a site-dependent physical potential (as in the physics literature) or as a weighted graph with loops (as in the mathematical and computer science literature). Thus, for a graph $\mathbb{G} = (V, E)$ with graph Laplacian $\mathbf{L}(\mathbb{G})$ and subjected to a potential $W(\cdot)$ we consider Schrödinger operators of the form

$$\mathbf{H}_W(\mathbb{G}) = \mathbf{L}(\mathbb{G}) + \mathbf{W} \tag{4.1}$$

where

$$[\mathbf{W}(V)]_{ij} = W(V_i)\delta_{ij}. \tag{4.2}$$

Although our problem is analogous to the Fundamental Gap Conjecture as proven in the continuum, lifting existing results to the discrete realm and maintaining tight bounds is nontrivial. Perhaps the most obvious challenge we face is the transition from well-understood boundary conditions to discrete boundary conditions and, for this reason, this chapter focuses on only the one dimensional case. In the first case, our restriction is identifiable with discrete Neumann boundary conditions and thus our result bears some resemblance to the continuum one of Payne and Weinberger [51] and indeed converges upon this result asymptotically. (For the physicist, our path graph Hamiltonian can be viewed as a 1-dimensional chain with a nearest-neighbor interaction term and a convex, site-dependent potential term. See Figure 4.1. Up to an identity term, the Laplacian of the hypercube graph of 2^N ver-

tices, $\mathbb{H}_{2^N}$, is equivalent to a sum of the Pauli σ_x operators acting on each of N qubits. In particular, transverse Ising models such as those studied in [35] can be cast as potentials on the hypercube. Here, like Reichardt[54] and van Dam et al. [57], but unlike Farhi et al.[35], we focus on the case that the potential depends only on the Hamming distance from a minimum. For the hypercube graph see Figure 4.1.)
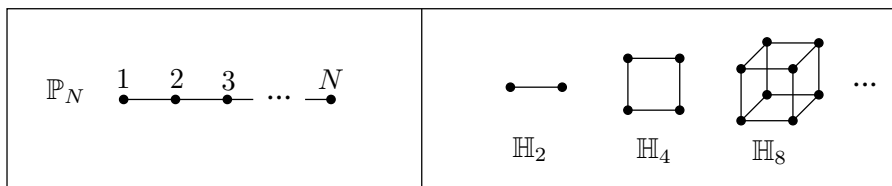
Figure 4.1: The path graph $\mathbb{P}_N$ of length N and the first three hypercube graphs $\mathbb{H}_2, \mathbb{H}_4$, and $\mathbb{H}_8$.

In particular, we show that for convex potentials on the path graph $\mathbb{P}_N$ of length N the gap Γ is bounded by the gap corresponding to the flat potential

$$\Gamma \geq 2\left(1 - \cos\left(\frac{\pi}{N}\right)\right). \tag{4.3}$$

On the hypercube graph $\mathbb{H}_{2^N}$, for convex potentials dependent only upon vertex Hamming weight, we prove a similar flat-potential lower bound given by

$$\Gamma \geq 2. \tag{4.4}$$

4.2   Preliminaries

4.2.1   The graph Laplacian and its Eigenvalues

Let $\mathbb{G} = (V, E)$ be an undirected graph with vertex set V and edge set $E \subseteq V \times V$. Then we associate with $\mathbb{G}$ a degree matrix $\mathbf{D}(\mathbb{G})$ and an adjacency matrix $\mathbf{A}(\mathbb{G})$.

We now extend our attention to a more general class of Schrödinger operators of the

form

$$\mathbf{H}_W(\mathbb{G}) \stackrel{\text{def}}{=} \mathbf{L}(\mathbb{G}) + \mathbf{W}(V) \tag{4.5}$$

where for some function $W : V \to \mathbb{R}$, $\mathbf{W}$ is the diagonal matrix defined by

$$[\mathbf{W}(V)]_{ij} \stackrel{\text{def}}{=} W(V_i)\delta_{ij}. \tag{4.6}$$

We can think of the resulting matrix as either the Dirichlet graph Laplacian for some host graph or as a Schrödinger operator (Hamiltonian) with an external potential. The eigenvalue spectrum of $\mathbf{H}_W(\mathbb{G})$ is $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{|V|}$ with associated, normalized eigenvectors $\mathbf{u}(\lambda_1), \mathbf{u}(\lambda_2), \ldots, \mathbf{u}(\lambda_{|V|})$. Suppose now that we consider the one parameter family $\mathbf{H}_W(\mathbb{G}; \alpha)$ with

$$\mathbf{H}_W(\mathbb{G}) = \mathbf{H}_W(\mathbb{G}; \alpha)\Big|_{\alpha=0}. \tag{4.7}$$

If λ_k is an eigenvalue of $\mathbf{H}_W(\mathbb{G}; \alpha)$ with no degeneracy, the Hellman-Feynman theorem governs the relationship between λ_k and α. That is,

Theorem 1.2. *Let $H(\alpha)$ be a Hermitian operator (matrix) dependent upon a parameter α with non-degenerate eigenvalue $\lambda(\alpha)$ and associated eigenfunction $u(\lambda; \alpha)$. Then*

$$\frac{d\lambda(\alpha)}{d\alpha} = \sum_{i,j} u_i^*(\lambda; \alpha) \frac{dH(\alpha)_{ij}}{d\alpha} u_j(\lambda; \alpha) \equiv \left\langle \frac{dH(\alpha)}{d\alpha} \right\rangle_{u(\lambda; \alpha)}$$

where $u_i(\lambda; \alpha)$ is the ith component of $\mathbf{u}(\lambda; \alpha)$.

Assuming that both λ_1 and λ_2 are non-degenerate eigenvalues, by Theorem 1.2 we have that

$$\frac{d\Gamma(\alpha)}{d\alpha} = \left\langle \frac{d\mathbf{H}_W(\mathbb{G}; \alpha)}{d\alpha} \right\rangle_{\mathbf{u}(\lambda_2)} - \left\langle \frac{d\mathbf{H}_W(\mathbb{G}; \alpha)}{d\alpha} \right\rangle_{\mathbf{u}(\lambda_1)} \tag{4.8}$$

where if we consider $\mathbf{H}_W(\mathbb{G}; \alpha) = \mathbf{H}_{\alpha W}(\mathbb{G})$,

$$\frac{d\Gamma(\alpha)}{d\alpha} = \langle \mathbf{W} \rangle \mathbf{u}(\lambda_2) - \langle \mathbf{W} \rangle \mathbf{u}(\lambda_1). \tag{4.9}$$

4.2.2 Eigenvectors of $\mathbf{H}_W(\mathbb{G})$

In deriving bounds for Γ we make extensive use of the recurrence relations satisfied by the eigenvectors of $\mathbf{H}_W(\mathbb{G})$. Expressing the eigenvalue equation

$$\mathbf{H}_W(\mathbb{G})\mathbf{u}(\lambda) - \lambda \mathbf{u}(\lambda) = 0 \tag{4.10}$$

componentwise, we obtain the following set of linear equations.

$$(d_i + W_i - \lambda)u_i(\lambda) = \sum_{(V_i, V_j) \in E} u_j(\lambda) \ \text{ for } V_i \in V \tag{4.11}$$

where for simplicity we let $W_i = W(V_i)$.

When $\mathbb{G}$ is the path graph, we always consider the labeling of V such that $(V_i, V_j) \in E \implies j = i \pm 1$. Then, eq. (4.11) reduces to

$$(2 + W_i - \lambda)u_i(\lambda) = u_{i-1}(\lambda) + u_{i+1}(\lambda) \ \text{ for } V_i \in V. \tag{4.12}$$

Here, to simplify the treatment, we introduce fictitious vertices $u_0(\lambda)$ and $u_{|V|+1}(\lambda)$. We correspondingly set $u_0(\lambda) = u_1(\lambda)$ and $u_{|V|+1}(\lambda) = u_{|V|}(\lambda)$ for the path graph.

For our purposes, it is often convenient to express eq. (4.12) in terms of difference equations. For this, we need the forward difference operator.

Definition 4.1 (Forward Difference Operator). *For a given sequence (u_i), we define Δ, the forward difference operator, by $\Delta u_i = u_{i+1} - u_i$. We further define Δ^2, the second difference*

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operator, by $\Delta^2 u_i = u_{i+1} - 2u_i + u_{i-1}.$

It is also useful to note that for any sequence (u_i),

$$\sum_{i=a}^{b} \Delta u_i = u_{b+1} - u_a. \tag{4.13}$$

Remark. *The reader should note that our notation yields* $\Delta(\Delta u_i) \neq \Delta^2 u_i$. *This makes* Δ^2 *a central difference operator, not a forward difference operator. This choice is convenient, since it allows us to easily keep track of indices as seen below in eq. (4.14).*

Now, applying Definition 4.1, eq. (4.12) becomes

$$\Delta^2 u_i(\lambda) = (W_i - \lambda)u_i(\lambda) \tag{4.14}$$

which, similar to the second derivative of a continuous function, is an expression of the convexity of **u** at u_i.

We now define some other useful properties of sequences, which we will apply to both sequences and vectors without restatement.

Definition 4.2 (Generalized Zero). *For a given sequence* (u_i) *we call* $u_m \in (u_i)$ *a generalized zero if* $u_m u_{m+1} < 0$ *or* $u_m = 0.$

Definition 4.3. *For a given sequence* (u_i) *we call the piecewise linear curve connecting Cartesian coordinates* (i, u_i) *the* **u***-line.*

Definition 4.4. *For a given sequence* (u_i) *we call a point at which the* **u** $-$ *line intersects zero a node and label it by its x-coordinate. From Definition 4.2 if* $u_m \in (u_i)$ *is a generalized zero, then the* **u***-line has a node at x with* $x \in [m, m+1).$

For two sequences $(u_i), (v_i)$ we will frequently need the discrete analogue of the Wronskian, the Casoratian sequence (w_i). Suppose that $\mathbf{u}(\mu; \beta), \mathbf{u}(\lambda; \alpha)$ are two sequences (vec-

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tors) with $\mu > \lambda$, satisfying eq. (4.12), and parameterized by β and α respectively. Then, we are interested in

$$w_i(\mathbf{u}(\mu;\beta),\mathbf{u}(\lambda;\alpha)) = u_{i+1}(\mu;\beta)u_i(\lambda;\alpha) - u_i(\mu;\beta)u_{i+1}(\lambda;\alpha) \qquad (4.15)$$

which, when applied to eq. (4.12) yields

$$\Delta w_{i-1}(\mathbf{u}(\mu;\beta),\mathbf{u}(\lambda;\alpha)) = \Theta_{W,i}(\mu - \lambda;\beta,\alpha)u_i(\mu;\beta)u_i(\lambda;\alpha) \qquad (4.16)$$

where

$$\Theta_{W,i}(\gamma;\beta,\alpha) \overset{\text{def}}{=} W_i(\beta) - W_i(\alpha) - \gamma. \qquad (4.17)$$

4.3   The Path Graph $\mathbb{P}_N$

For the path graph $\mathbb{P}_N$ depicted in Figure 4.1, we are interested in the case of convex potentials, for which we offer the following definition:

Definition 4.5. *Let $[\![a,b]\!] = \{a,a+1,\ldots,b-1,b\}$. Let $\mathbb{P}_N$ be the path graph with vertex set $V = \{V_i\}_{i\in[\![1,N]\!]}$ and edge set $E = \{(V_i,V_{i+1})\}_{i\in[\![1,N-1]\!]}$. Let $\mathscr{W}$ be the set of all convex functions $w : \mathbb{R} \to \mathbb{R}$. We call $W : V \to \mathbb{R}$ convex if there exists some $w \in \mathscr{W}$ such that $W(V_i) = w(i) \ \forall \ V_i \in V$.*

We similarly define the term "linear" and denote its set $\mathscr{L}$.

We begin by using variational arguments to demonstrate that the gap corresponding to each $W \in \mathscr{W}$ is bounded from below by the gap corresponding to some $L \in \mathscr{L}$. This approach is modeled on that used by Lavine in the continuum.[46] Then, we use the geometry of the eigenvectors of $\mathbf{H}_L(\mathbb{P}_N)$ to demonstrate that the gap of each linear potential L is bounded from below by the gap for a constant potential.

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4.3.1 The gap for convex potentials is lower bounded by the gap for linear potentials.

The eigenvalues of $\mathbf{H}_W(\mathbb{P}_N)$ are real and ordered $\lambda_1 < \lambda_2 < \cdots < \lambda_N$. Also, recall that we have introduced fictitious points $u_0(\lambda)$ and $u_{N+1}(\lambda)$ to satisfy the recurrence eq. (4.12). Then we have the following fact about the intersections of the $\mathbf{u}(\lambda_1)$-line and $\mathbf{u}(\lambda_2)$-line.

Lemma 4.1. *Let $0 \leq \lambda_1 < \lambda_2$ be the two lowest eigenvalues of $\mathbf{H}_W(\mathbb{P}_N)$ for convex W, and let $\mathbf{u}(\lambda_1), \mathbf{u}(\lambda_2)$ be their corresponding eigenvectors. Then, $\exists m < n \in [\![1, N]\!]$ such that $u_i^2(\lambda_2) - u_i^2(\lambda_1) \geq 0$ for all $i \in [\![1, m]\!] \cup [\![n+1, N]\!]$ and $u_i^2(\lambda_2) - u_i^2(\lambda_1) < 0$ for all $i \in [\![m+1, n]\!]$.*

Proof. The intersections of $\mathbf{u}(\lambda_1)$ and $\mathbf{u}(\lambda_2)$ can be characterized by the behavior of the quantity

$$\Delta\left(\frac{u_i(\lambda_2)}{u_i(\lambda_1)}\right) = \frac{u_{i+1}(\lambda_2)u_i(\lambda_1) - u_i(\lambda_2)u_{i+1}(\lambda_1)}{u_{i+1}(\lambda_1)u_i(\lambda_1)} \tag{4.18}$$

$$\equiv \frac{w_i(\mathbf{u}(\lambda_2), \mathbf{u}(\lambda_1))}{u_{i+1}(\lambda_1)u_i(\lambda_1)}. \tag{4.19}$$

For simplicity, let $w_i = w_i(\mathbf{u}(\lambda_2), \mathbf{u}(\lambda_1))$. Then, in eq. (4.16) we can set $\alpha = \beta = 0$, yielding

$$\Delta w_{i-1} = -\Gamma u_i(\lambda_2) u_i(\lambda_1) \tag{4.20}$$

and since $u_0(\cdot) = u_1(\cdot)$ and $u_N(\cdot) = u_{N+1}(\cdot)$, $w_0 = w_N = 0$. Thus, from eqs. (4.13) and (4.20)

we have

$$w_n = w_0 + \sum_{i=0}^{n-1} \Delta w_i \tag{4.21}$$

$$= -\Gamma \sum_{i=0}^{n-1} u_{i+1}(\lambda_2) u_{i+1}(\lambda_1) \tag{4.22}$$

$$= \Gamma \sum_{i=n}^{N-1} u_{i+1}(\lambda_2) u_{i+1}(\lambda_1). \tag{4.23}$$

Here, because $\mathbf{H}_W(\mathbb{P}_N)$ is a Jacobi matrix, we are free to choose $\mathbf{u}(\lambda_1)$ as everywhere positive and $\mathbf{u}(\lambda_2)$ as initially positive with no loss of generality. Further, it is known that $\mathbf{u}(\lambda_1)$ has no generalized zeros and $\mathbf{u}(\lambda_2)$ has exactly one, which we identify with $u_\sigma(\lambda_2)$. (See *e.g.* Gantmakher.[38]) Then, from eq. (4.22)

$$w_{n \leq \sigma} = -\Gamma \sum_{i=0}^{n-1} u_{i+1}(\lambda_2) u_{i+1}(\lambda_1) \tag{4.24}$$

$$\leq 0 \tag{4.25}$$

Similarly, from eq. (4.23)

$$w_{n > \sigma} = \Gamma \sum_{i=n}^{N-1} u_{i+1}(\lambda_2) u_{i+1}(\lambda_1) \tag{4.26}$$

$$\leq 0 \tag{4.27}$$

so that we have $w_n \leq 0 \; \forall \, n \in [\![0, N]\!]$.

Finally, by eq. (4.19) we arrive at

$$\Delta \left(\frac{u_i(\lambda_2)}{u_i(\lambda_1)} \right) \leq 0 \; \forall \, i \in [\![0, N]\!] . \tag{4.28}$$

Now, this sequence can be divided into three regions, where we will find that at least two of these regions are nonempty. Specifically, that this quantity is always decreasing guarantees

that there exists some choice of $m < n \in [\![1,N]\!]$ such that

$$
\begin{cases}
\left(\frac{u_i(\lambda_2)}{u_i(\lambda_1)}\right) > 1, & i \in [\![1,m]\!] \\[2mm]
-1 \leq \left(\frac{u_i(\lambda_2)}{u_i(\lambda_1)}\right) \leq 1, & i \in [\![m+1,n]\!] \\[2mm]
\left(\frac{u_i(\lambda_2)}{u_i(\lambda_1)}\right) < -1, & i \in [\![n+1,N]\!]
\end{cases}
\tag{4.29}
$$

and hence $(u_i^2(\lambda_2) - u_i^2(\lambda_1))_{i=1}^N$ has at most two generalized zeros. Further, that $u_i(\lambda_2), u_i(\lambda_1)$ are normalized and orthogonal eigenvectors guarantees that $(u_i^2(\lambda_2) - u_i^2(\lambda_1))_{i=1}^N$ has at least one generalized zero. Thus, our proof is complete. $\qquad\square$

Using Lemma 4.1 we now prove a discrete analogue of Lemma 3.2 from Lavine[46]:

Lemma 4.2. *Let $\mathscr{W}$ be the set of convex potentials and $\mathscr{L} \subseteq \mathscr{W}$ be the set of linear potentials. Let $\mathbf{u}(\lambda_1)$, $\mathbf{u}(\lambda_2)$ be the two lowest eigenvectors of some $\mathbf{H}_W(\mathbb{P}_N)$ satisfying eq. (4.29). Then, $\forall\, W \in \mathscr{W} \;\exists\, L \in \mathscr{L} \mid \Gamma(\mathbf{H}_W(\mathbb{P}_N)) \geq \Gamma(\mathbf{H}_L(\mathbb{P}_N))$.*

Proof. Identify with $W(V_i)$ a convex function $w : \mathbb{R} \to \mathbb{R}$ such that $w(i) = W(V_i) \;\forall\, i \in [\![1,N]\!]$. Then, we define the linear function $l_w : \mathbb{R} \to \mathbb{R}$ as

$$
l_w(i) = \frac{1}{n-m}\Big((n-i)w(m) + (i-m)w(n) \Big)
\tag{4.30}
$$

with n and m defined as in Lemma 4.1, and identify it with the corresponding $L_W \in \mathscr{L}$. Notably, $L_W(V_i) \leq W(V_i) \;\forall\, i \in [\![1,m]\!] \cup [\![n+1,N]\!]$ and $L(V_i) \geq W(V_i) \;\forall\, i \in [\![m+1,n]\!]$. Then, clearly

$$
\langle \mathbf{W} - \mathbf{L}_W \rangle_{\mathbf{u}(\lambda_2)} - \langle \mathbf{W} - \mathbf{L}_W \rangle_{\mathbf{u}(\lambda_1)} \geq 0
\tag{4.31}
$$

where equality is obtained only when $W = L_W$.

Now we consider the Schrödinger operator that satisfies

$$\mathbf{H}_W(\mathbb{P}_N; \alpha) = \mathbf{H}_{W(\alpha)}(\mathbb{P}_N) \tag{4.32}$$

and identify with $W(\alpha)$ the convex function $w(i; \alpha)$

$$w(i; 0) = w(i) \tag{4.33}$$

$$\frac{dw}{d\alpha}(i; \alpha) = l_{w(\cdot; \alpha)}(i) - w(i; \alpha). \tag{4.34}$$

Thus, by eqs. (4.8) and (4.31) we have that the gap of $\mathbf{H}_{W(\alpha)}(\mathbb{P}_N)$ decreases with α and additionally that

$$w(i; \alpha) = e^{-\alpha} w(i) + \int_0^\alpha \frac{e^{s-\alpha}}{n(s) - m(s)} \bigg((n(s) - i) w(m(s); s) + (i - m(s)) w(n(s); s) \bigg) ds. \tag{4.35}$$

Hence, as α increases, we have that $w(i; \alpha)$ gets arbitrarily close to a linear function and therefore $W(\alpha)$ gets arbitrarily close to some function in $\mathscr{L}$. $\qquad\square$

4.3.2 The gap for linear potentials is lower bounded by the gap for constant potentials.

We start with $\mathbf{u}(\lambda_2), \mathbf{u}(\lambda_1)$ as the eigenvectors of $\mathbf{H}_W(\mathbb{P}_N)$ for some $W \in \mathscr{W}$. By Lemma 4.2 we need only demonstrate that gaps associated with the class of linear potentials are lower bounded by the gaps associated with the constant potential. Because we are confined to a discrete setting, this takes a bit of work. The overall strategy is as follows: First, we restrict ourselves to a particular class of linear potentials and demonstrate that $\mathbf{u}(\lambda_1)$ is strictly decreasing. Then, we prove some facts about the ordering of the components of $\mathbf{u}(\lambda_2)$ around its node. Next, we demonstrate that for positive slopes, $\mathbf{u}(\lambda_2)$ always

has a node left of center. These facts combine to complete our proof.

We introduce the notation $[\mathbf{U}]_{ij} = (i-1)\delta_{ij}$ for the unit linear potential. Note that for any linear potential $L \in \mathscr{L}$ with slope α, the potential αU has the same gap. Thus, we restrict our study to the unit potential multiplied by some parameter α. Further, symmetry allows us to restrict ourselves to the case that $\alpha \geq 0$.

Our goal is to demonstrate that

$$\frac{d\Gamma(\alpha)}{d\alpha} > 0 \tag{4.36}$$

for all $\alpha \geq 0$.

We make use of the following lemma to reduce to the case that $u_1^2(\lambda_2) > u_1^2(\lambda_1)$:

Lemma 4.3. *Let $\alpha U \in \mathscr{L}$ where U is the unit-linear potential. Then, for $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$, if $u_1^2(\lambda_2) \leq u_1^2(\lambda_1)$, eq. (4.36) is satisfied.*

Proof. By eq. (4.8),

$$\frac{d\Gamma(\alpha)}{d\alpha} = \sum_{i=1}^{N} \left(u_i^2(\lambda_2) - u_i^2(\lambda_1) \right) (i-1) \tag{4.37}$$

$$= \sum_{i=1}^{N} \left(u_i^2(\lambda_2) - u_i^2(\lambda_1) \right) (i-c) \tag{4.38}$$

for any constant c. (Recall that the $\mathbf{u}(\lambda)$ are normalized eigenvectors.) From Lemma 4.1 we know that if $u_1^2(\lambda_2) \leq u_1^2(\lambda_1)$ then $\exists n < N$ such that $u_i^2(\lambda_2) - u_i^2(\lambda_1) > 0$ for all $i > n$. Choosing $c = n$ we get that eq. (4.38) is non-negative for each term of the sum, thus completing the proof. $\square$

Having reduced to the case that $u_1^2(\lambda_2) \geq u_1^2(\lambda_1)$, we now prove that $\mathbf{u}(\lambda_1)$ is a decreasing sequence:

Lemma 4.4. *Let $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ be defined as in Lemma 4.3. Then, $\mathbf{u}(\lambda_1)$ is a decreasing sequence. Further, for $\alpha > 0$, $\mathbf{u}(\lambda_1)$ is strictly decreasing.*

Proof. First we note that at the boundaries, $\Delta u_0(\lambda_1) = \Delta u_N(\lambda_1) = 0$. Thus we know that the boundaries are local extrema of the $\mathbf{u}(\lambda_1)$-line. Now, we note that by eq. (4.12)

$$\frac{u_2(\lambda_1)}{u_1(\lambda_1)} = (1 - \lambda_1) \leq 1 \tag{4.39}$$

where the inequality is strict for $\alpha > 0$ since this requires that $\lambda_1 > 0$. Thus, the $\mathbf{u}(\lambda_1)$-line is initially decreasing. Note that from eq. (4.14) when $\mathbf{W} = \mathbf{U}$, $\Delta^2 u_i(\lambda_1)$ has at most one sign change. Thus, the second boundary term cannot be a maximum and, therefore, both boundaries must be global extrema. We therefore have that $\mathbf{u}(\lambda_1)$ is decreasing for $\alpha \geq 0$ and strictly decreasing for $\alpha > 0$. $\qquad \square$

We now recall a theorem by Cauchy and use it to derive an upper bound for λ_2:

Theorem 4.1 (Cauchy Interlace Theorem)**.** *Let $\mathbf{A}$ be an $N \times N$ Hermitian matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$. Suppose that B is an $(N-1) \times (N-1)$ principal submatrix of $\mathbf{A}$ with eigenvalues $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_{N-1}$. Then, the eigenvalues are ordered such that $\lambda_1 \leq \mu_1 \leq \lambda_2 \leq \mu_2 \leq \ldots \leq \lambda_{N-1} \leq \mu_{N-1} \leq \lambda_N$.*

Proof. For proof, we refer the reader to Hwang. [39] $\qquad \square$

Lemma 4.5. *Suppose that an $N \times N$ Hermitian matrix $\mathbf{A}$ with $N \geq 3$ has the 3×3 principal submatrix*

$$\mathbf{B}(\delta) = \begin{pmatrix} 2 - \delta & -1 & 0 \\ -1 & 2 + \alpha & -1 \\ 0 & -1 & 2 + 2\alpha \end{pmatrix}$$

with $\delta \geq 0$. Then, if λ_2 is the second lowest eigenvalue of $\mathbf{A}$, $\lambda_2 \leq 2 + \alpha$.

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Proof. Let $\mu_1(\delta) \leq \mu_2(\delta) \leq \mu_3(\delta)$ be the eigenvalues of $\mathbf{B}(\delta)$. That $\lambda_2 \leq \mu_2(\delta)$ is obvious from repeated applications of Theorem 4.1. From, Theorem 1.2,

$$\frac{d\mu_2(\delta)}{d\delta} \leq 0 \tag{4.40}$$

and by direct calculation, $\mu_2(0) = 2 + \alpha$. Thus, $\lambda_2 \leq 2 + \alpha$. $\qquad\square$

Lemma 4.5 now combines with the following fact to give an ordering of the components of $\mathbf{u}(\lambda_2)$:

Lemma 4.6. *Let $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ be defined as in lemma 4.3 and let $\mathbf{u}(\lambda)$ be an eigenvector. Define the quantity*

$$u_{i+\varepsilon}(\lambda) \stackrel{def}{=} \varepsilon u_{i+1}(\lambda) + (1 - \varepsilon)u_i(\lambda). \tag{4.41}$$

Then, for $u_i(\lambda)$ not a generalized zero,

$$u_{i+1+\varepsilon}(\lambda) = (2 + \alpha(j_{i+\varepsilon} - 1) - \lambda) u_{i+\varepsilon} - u_{i-1+\varepsilon} \tag{4.42}$$

for some $j_{i+\varepsilon} \in [i, i+1]$.

Proof. First, note that from eq. (4.12)

$$u_{i+1+\varepsilon}(\lambda) = (2 - \lambda) u_{i+\varepsilon}(\lambda) + \alpha \left(i\varepsilon u_{i+1}(\lambda) + (i-1)(1-\varepsilon)u_i(\lambda)\right) - u_{i-1+\varepsilon}(\lambda). \tag{4.43}$$

Now, with $\text{sign}(u_{i+1}(\lambda)) = \text{sign}(u_i(\lambda))$, there exists a $j_{i+\varepsilon} \in [i, i+1]$ such that

$$i\varepsilon u_{i+1}(\lambda) + (i-1)(1-\varepsilon)u_i(\lambda) = (j_{i+\varepsilon} - 1)(\varepsilon u_{i+1}(\lambda) + (1-\varepsilon)u_i(\lambda)). \tag{4.44}$$

Thus, eq. (4.43) becomes

$$u_{i+1+\varepsilon}(\lambda) = (2 + \alpha(j_{i+\varepsilon} - 1) - \lambda)u_{i+\varepsilon}(\lambda) - u_{i-1+\varepsilon}(\lambda). \tag{4.45}$$

$\square$

Lemma 4.7 (Ordering $\mathbf{u}(\lambda_2)$). *Let $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ be defined as in Lemma 4.3. Let x represent the first node of the $\mathbf{u}(\lambda_2)$-line and let $u_m(\lambda_2)$ be the corresponding generalized zero. Suppose that $x \le (N+1)/2$. Let $u_{i+\varepsilon}(\lambda)$ be defined as in Lemma 4.6. Then,*

$$-1 \ge \begin{cases} \frac{u_{m+k+\varepsilon}(\lambda_2)}{u_{m-1-k+\varepsilon}(\lambda_2)} & \text{for } m \le x \le m + \frac{1}{2} \text{ and } k \in [\![0, m-1]\!] \\ \frac{u_{m+k+\varepsilon}(\lambda_2)}{u_{m-k+\varepsilon}(\lambda_2)} & \text{for } m + \frac{1}{2} < x \le m+1 \text{ and } k \in [\![1, m]\!]. \end{cases} \tag{4.46}$$

Proof. We proceed to prove this lemma by induction. First, consider the case that $m + 1/2 \le x < m+1$ for some $m \in [\![1, \lfloor N/2 \rfloor]\!]$. For simplicity, let $\mathbf{u}(\lambda_2) = \mathbf{u}$. Then, there exists an ε such that $(1-\varepsilon)u_m + \varepsilon u_{m+1} = 0$. So, from eq. (4.43) we can consider the base case

$$u_{m+1+\varepsilon} = \varepsilon \alpha u_{m+1} - u_{m-1+\varepsilon} \tag{4.47}$$

$$< -u_{m-1+\varepsilon}. \tag{4.48}$$

For the induction, rearrange eq. (4.42) for terms left and right of the node,

$$\frac{u_{m+k+2+\varepsilon} + u_{m+k+\varepsilon}}{u_{m+k+1+\varepsilon}} - \frac{u_{m-k-2+\varepsilon} + u_{m-k+\varepsilon}}{u_{m-k-1+\varepsilon}} = \alpha(j_{m+k+1+\varepsilon} - j_{m-k-1+\varepsilon}) > 0. \tag{4.49}$$

Now assume

$$\frac{u_{m+k+\varepsilon}}{u_{m+k+1+\varepsilon}} \le \frac{u_{m-k+\varepsilon}}{u_{m-k-1+\varepsilon}} \tag{4.50}$$

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thus, by eq. (4.49)

$$\frac{u_{m+k+2+\varepsilon}}{u_{m+k+1+\varepsilon}} \geq \frac{u_{m-k-2+\varepsilon}}{u_{m-k-1+\varepsilon}}. \tag{4.51}$$

Thus,

$$\frac{u_{m+k+2+\varepsilon}}{u_{m-k-2+\varepsilon}} \leq \frac{u_{m+k+1+\varepsilon}}{u_{m-k-1+\varepsilon}}. \tag{4.52}$$

Finally, taking $k = 0$, eq. (4.47) satisfies eq. (4.50) and

$$\frac{u_{m+k'+\varepsilon}}{u_{m-k'+\varepsilon}} \leq -1 \tag{4.53}$$

for all $k' \in [\![1, m]\!]$.

Next we consider the case that $m \leq x < m + 1/2$. In this case, by Definition 4.4 we can choose ε such that $u_{m+\varepsilon} = -u_{m-1+\varepsilon}$. Then,

$$\frac{u_{m+k+1+\varepsilon} + u_{m+k-1+\varepsilon}}{u_{m+k+\varepsilon}} - \frac{u_{m-k-2+\varepsilon} + u_{m-k+\varepsilon}}{u_{m-k-1+\varepsilon}} = \alpha(j_{m+k+\varepsilon} - j_{m-k-1+\varepsilon}) > 0. \tag{4.54}$$

This time, assume

$$\frac{u_{m+k-1+\varepsilon}}{u_{m+k+\varepsilon}} \leq \frac{u_{m-k+\varepsilon}}{u_{m-k-1+\varepsilon}} \tag{4.55}$$

then, by eq. (4.54)

$$\frac{u_{m+k+1+\varepsilon}}{u_{m+k+\varepsilon}} \geq \frac{u_{m-k-2+\varepsilon}}{u_{m-k-1+\varepsilon}}. \tag{4.56}$$

Hence,

$$\frac{u_{m+k+1+\varepsilon}}{u_{m-k-2+\varepsilon}} \leq \frac{u_{m+k+\varepsilon}}{u_{m-k-1+\varepsilon}}. \tag{4.57}$$

Again, taking $k = 0$, we have that

$$\frac{u_{m+k'+\varepsilon}}{u_{m-1-k'+\varepsilon}} \leq \frac{u_{m+\varepsilon}}{u_{m-1+\varepsilon}} \leq -1. \tag{4.58}$$

for all $k' \in [\![0, m-1]\!]$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Now, we recall a theorem due to Gantmakher and Kreĭn:[38]

Theorem 4.2. *Let* $\mathbf{u}(\mu; \alpha), \mathbf{u}(\lambda; \beta)$ *be two vectors of length N satisfying eq.* (4.12) *and with*

$$\Theta_{W,i}(\mu - \lambda; \alpha, \beta) \leq 0 \ \forall \ i \in [\![m, n]\!] \tag{4.59}$$

where $\Theta_{W,i}(\mu - \lambda; \alpha, \beta) < 0$ *for at least some* $i \in [\![m, n]\!]$. *We extend both vectors to length* $N+2$ *by including nodes at* u_0 *and* u_{N+1}. *(So long as eq.* (4.12) *is satisfied, despite previous choices of* u_0 *and* u_{N+1}, *these points are always considered nodes.) Let* $\eta \in [m-1, m), \xi \in (n, n+1]$ *be two adjacent nodes of* $\mathbf{u}(\lambda; \beta)$ *with* $m \leq n \in [\![0, N+1]\!]$. *Then there exists at least one node of* $\mathbf{u}(\mu; \alpha)$ *between* η *and* ξ.

Proof. This fact is adapted directly from Gantmakher and Kreĭn, with modifications made to allow for our parameterization. The argument is provided in detail in Appendix A for the unfamiliar reader. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

Lemma 4.8. *Let* $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ *be defined as in Lemma 4.3.* $\mathbf{u}(\lambda_2)$ *always has a node at or left of* $x = (N+1)/2$.

Proof. We only want to consider variations with respect to one parameter, so we fix $\lambda = \mu_0, \alpha = \beta_0$. Then, we note that, by eq. (4.17), $\Theta_{U,i}$ is an increasing sequence in i. Now, we assume that there exists a node of $\mathbf{u}(\mu_0)$ at $x = (N+1)/2$. Next, at $\beta = \beta_0$ and $\mu = \mu_0$, $\Theta_{U,i}$ is identically 0. Then,

$$\left. \frac{d\Theta_{U,i}}{d\beta} \right|_{\mu=\mu_0} = U_i - \left. \frac{d\mu}{d\beta} \right|_{\mu=\mu_0} = U_i - \langle \mathbf{U} \rangle_{\mathbf{u}(\mu_0)} \tag{4.60}$$

Our assumption that $\mathbf{u}(\mu_0)$ at $x = (N+1)/2$ requires that $\varepsilon = 1$ in Lemma 4.7. Then, Lemma 4.7 becomes an exact statement about the ordering of the components of $\mathbf{u}(\mu_0)$.

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Hence, $\langle \mathbf{U} \rangle_{\mathbf{u}(\mu_0)} \geq (N-1)/2$ and we have that

$$U_{\left\lfloor \frac{N+1}{2} \right\rfloor} - \langle \mathbf{U} \rangle_{\mathbf{u}(\mu_0)} \leq U_{\left\lfloor \frac{N+1}{2} \right\rfloor} - \frac{N-1}{2} \tag{4.61}$$

$$= \left(\left\lfloor \frac{N+1}{2} \right\rfloor - 1 \right) - \frac{N-1}{2} \tag{4.62}$$

$$\leq 0. \tag{4.63}$$

Further, in the same fashion

$$U_{\left\lfloor \frac{N+1}{2} - 1 \right\rfloor} - \langle \mathbf{U} \rangle_{\mathbf{u}(\mu_0)} < 0. \tag{4.64}$$

Hence, for some $\beta - \beta_0 = \xi > 0$ with ξ sufficiently close to 0, $\Theta_{U,i} \leq 0 \, \forall \, i \in [\![1, \lfloor (N+1)/2 \rfloor]\!]$ with at least some i such that $\Theta_{U,i} < 0$. Thus, at $\beta = \beta_0$ the node of $\mathbf{u}(\lambda_2)$ shifts left as β increases. Note that if $\beta = \beta_0 = 0$, symmetry forces the node of the $\mathbf{u}(\mu)$-line to occur at $x = (N+1)/2$. Thus, there is initially a node at $(N+1)/2$ and whenever there is a node at $x = (N+1)/2$ it shifts left. Hence, there is always a node at or left of $(N+1)/2$. $\qquad \square$

Remark. *In fact, with some of the facts that follow, we demonstrate that the node shifts left with increasing α. For proof, see Appendix B.*

Lemma 4.8 allows us to strengthen Lemma 4.7 through the following fact:

Lemma 4.9. *Let $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ be defined as in Lemma 4.3. Let x represent the first node of the $\mathbf{u}(\lambda_2)$-line. Then, there exists a symmetric region $S = [\![1, m]\!]$ about x such that $\mathbf{u}(\lambda_2)$ is a decreasing sequence.*

Proof. We begin by considering the first point after the node such that $\mathbf{u}(\lambda_2)$ is increasing and label it by m such that $\Delta u_m(\lambda_2) \Delta u_{m-1}(\lambda_2) < 0$. Then,

$$u_{m+1}(\lambda_2) = (2 + \alpha(m-1) - \lambda_2) u_m(\lambda_2) - u_{m-1}(\lambda_2). \tag{4.65}$$

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Now, rearranging eq. (4.65)

$$u_m(\lambda_2) = \left(2 + \left(1 - \frac{u_{m+1}(\lambda_2)}{u_m(\lambda_2)}\right) + \alpha(m-1) - \lambda_2\right) u_m(\lambda_2) - u_{m-1}(\lambda_2). \qquad (4.66)$$

Note that in eq. (4.66), because $u_m(\lambda_2) \leq u_{m+1}(\lambda_2) < 0$, we know that $1 > u_{m+1}(\lambda_2)/u_m(\lambda_2)$ and thus $(u_i(\lambda_2))_{i \in [\![1,m]\!]}$ is an eigenvector of $\mathbf{H}_W(\mathbb{P}_m)$ where

$$W_i = \alpha U_i + \delta_{im}\left(1 - \frac{u_{m+1}(\lambda_2)}{u_m(\lambda_2)}\right). \qquad (4.67)$$

By Lemma 4.8 the second eigenvector of $\mathbf{H}_{\alpha U}(\mathbb{P}_m)$ has a node left of center. Since λ_2 is greater than the second eigenvalue of $\mathbf{H}_{\alpha U}(\mathbb{P}_m)$ and we know that $\mathbf{W}$ is identical to $\mathbf{U}$ in all but the mth component, we have by Theorem 4.2 that $(u_i(\lambda_2))_{i \in [\![1,m]\!]}$ has a node left of center. Further, by our assumptions, $(u_i(\lambda_2))_{i \in [\![1,m]\!]}$ is a decreasing sequence. Therefore, there exists a symmetric region $S = [\![1,m]\!]$ about x such that $\mathbf{u}(\lambda_2)$ is strictly decreasing. $\square$

Using Lemma 4.9 we now prove a corollary to Lemma 4.7 that holds regardless of whether the node falls directly on a vertex:

Corollary 4.1. *Let $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ and x be defined as in lemma 4.7. Let $\mathbf{u}(\lambda_2)$ be a decreasing sequence. Then,*

$$-1 \geq \begin{cases} \frac{u_{m+k+1}(\lambda_2)}{u_{m-k}(\lambda_2)} \text{ for } m \leq x \leq m + \frac{1}{2}\forall k \in [\![0, m-1]\!] \\ \frac{u_{m+2+k}(\lambda_2)}{u_{m-k}(\lambda_2)} \text{ for } m + \frac{1}{2} < x \leq m + 1\forall k \in [\![1, m]\!]. \end{cases} \qquad (4.68)$$

Proof. For the first case, assume that $m + 1/2 \leq x < m + 1$ for some $m \in [\![1, \lfloor N/2 \rfloor]\!]$. Then, from Lemma 4.7 we have that

$$-1 \geq \frac{u_{m+k+\varepsilon}(\lambda_2)}{u_{m-k+\varepsilon}(\lambda_2)} \text{ for } m + \frac{1}{2} < x \leq m + 1\forall k \in [\![1, m]\!]. \qquad (4.69)$$

Then, since $\mathbf{u}(\lambda_2)$ is decreasing, $u_{m+1+k} \leq u_{m+k+\varepsilon}$ and also $u_{m-k+\varepsilon} \geq u_{m+1-k}$. Thus,

$$-1 \geq \frac{u_{m+k+\varepsilon}(\lambda_2)}{u_{m-k+\varepsilon}(\lambda_2)} \geq \frac{u_{m+1+k}(\lambda_2)}{u_{m+1-k}(\lambda_2)}. \tag{4.70}$$

Similarly, for the case that $m \leq x < m+1/2$, we have that

$$-1 \geq \frac{u_{m+k+\varepsilon}(\lambda_2)}{u_{m-1-k+\varepsilon}(\lambda_2)} \quad \text{for } m \leq x \leq m + \frac{1}{2} \forall k \in [\![1, m-1]\!]. \tag{4.71}$$

In this case, we have that $u_{m-1-k+\varepsilon} \geq u_{m-k}$. So that finally,

$$-1 \geq \frac{u_{m+k+\varepsilon}(\lambda_2)}{u_{m-1-k+\varepsilon}(\lambda_2)} \geq \frac{u_{m+1+k}(\lambda_2)}{u_{m-k}(\lambda_2)}. \tag{4.72}$$

$\square$

Theorem 4.3. *For* $\mathbb{P}_N$,

$$\Gamma_{W \in \mathscr{W}} \geq 2\left(1 - \cos\left(\frac{\pi}{N}\right)\right). \tag{4.73}$$

Proof. From Theorem 1.2 we know that so long as $\langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_2)} - \langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_1)} > 0$, the gap is increasing.

Consider a set of indices S_m symmetric about m, the index corresponding to the first generalized zero $u_m(\lambda_2)$ of $\mathbf{u}(\lambda_2)$. Now, define $\mathbf{v}(\lambda_i) = (u(\lambda_i))_{i \in S_m}$. From Lemmas 4.4 and 4.7 we know that

$$\langle \mathbf{U} \rangle_{\mathbf{v}(\lambda_2)} \geq \langle \mathbf{U} \rangle_{\mathbf{v}(\lambda_1)}. \tag{4.74}$$

where we restrict $\mathbf{U}$ to the same number of terms as $\mathbf{v}(\lambda_2)$. By Lemma 4.8 we know that the node of the $\mathbf{u}(\lambda_2)$-line must occur at or before the midpoint of $\mathbf{u}(\lambda_2)$. Thus, S_m can be taken as $S_m = [\![1, 2m+1]\!]$. By Lemma 4.3 we restrict ourselves to the case that $u_1^2(\lambda_2) > u_1^2(\lambda_1)$. With this restriction, Lemmas 4.4 and 4.7 insist that $u_k^2(\lambda_2) > u_k^2(\lambda_1) \ \forall k \in [\![1, N]\!]/S_m$. It is

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then obvious that

$$\langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_2)} \geq \langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_1)} \tag{4.75}$$

for $\alpha \geq 0$. Thus, we know that Γ is at a minimum for $\alpha = 0$. Now, at $\alpha = 0$ we find that $\lambda_1 = 0$ and thus $\Gamma = \lambda_2$. Hence,

$$\Gamma_{W \in \mathscr{W}} \geq 2 \left(1 - \cos \left(\frac{\pi}{N} \right) \right). \tag{4.76}$$

$\square$

4.4 The Hypercube Graph

In this section we find a tight lower bound for the gap for Hamming-symmetric convex potentials on the N-dimensional hypercube graph $\mathbb{H}_{2^N} = (V, E)$. To define $\mathbb{H}_{2^N}$, we identify with each vertex $V_i \in V$ a unique vector $\mathbf{b}_i \in \{0,1\}^N$. Then, we choose $E = \{(V_i, V_j) \mid |\mathbf{v}_i - \mathbf{v}_j| = 1\}$, where $|\cdot|$ here denotes the 1-norm. (In the language of computer science, $\mathbf{b}_i, \mathbf{b}_j$ are bit-strings and $|\mathbf{b}_i - \mathbf{b}_j|$ is their Hamming distance.) As in (4.5) the Schrödinger operator includes a potential term $\mathbf{W}$. Thus, an eigenvector $u(\lambda)$ of eigenvalue λ satisfies

$$(N + W_i - \lambda)u_i(\lambda) = \sum_{(V_i, V_j) \in E} u_j(\lambda) \text{ for } V_i \in V. \tag{4.77}$$

Here we restrict our attention to the case that the potential depends only on Hamming distance from the vertex of minimum potential. We can label this minimum by the all zeros string, and therefore $W_i = W_{|b_i|}$. In this case, the set of Hamming-symmetric vectors are an invariant subspace of the Schrödinger operator.

Remark. *In the language of quantum-mechanics, this is the space spanned by the $N+1$ state vectors that are uniform superpositions over bit-strings of a given Hamming weight.*

By Schrödinger's equation, no time-evolution induced by a (possibly time-dependent) Hamming symmetric Hamiltonian will ever drive transitions out of this subspace. For many cases, it is only the gap within this subspace that is of interest.

Below, we will bound the gap within the Hamming-symmetric subspace. Here, the (normalized) uniform superpositions over bit-strings of each Hamming weight form an orthonormal basis for this subspace. Given a state-vector $\mathbf{u}(\lambda)$, let $v_m(\lambda)$ denote the inner product of $\mathbf{u}(\lambda)$ with the Hamming-weight-m basis vector. That is,

$$v_m(\lambda) = \frac{1}{\sqrt{\binom{N}{m}}} \sum_{|b_i|=m} u_i(\lambda). \tag{4.78}$$

Because $\mathbf{u}(\lambda)$ lies within the symmetric subspace, this corresponds to rewriting the vector in a different basis. For arbitrary vectors in the full Hilbert space, this would be a projection onto the symmetric subspace.

Then, with a bit of work, eq. (4.77) becomes

$$(N + W_m - \lambda)v_m(\lambda) = h(m-1)v_{m-1}(\lambda) + h(m)v_{m+1}(\lambda) \tag{4.79}$$

where

$$h(m) = \sqrt{(m+1)(N-m)}. \tag{4.80}$$

Now, we know that eq. (4.79) is the recurrence relation satisfied by some Jacobi matrix $\mathbf{J}$ with eigenvalue $\lambda \in (\lambda_i)_{i=1}^{N}$. In keeping with our typical ordering, we choose $\lambda_1 < \lambda_2 < \cdots < \lambda_N$. Further, since we know that we can shift the diagonal by any $c\mathbb{1}, c \in \mathbb{R}$ without altering the gap, we instead consider $\mathbf{J} \to \mathbf{J} - N\mathbb{1}$ which satisfies the recurrence relation

$$(W_m - \lambda)v_m(\lambda) = h(m-1)v_{m-1}(\lambda) + h(m)v_{m+1}(\lambda) \tag{4.81}$$

without any loss of generality.

Remark. *The reader should note that unlike Section 4.3, $v_0(\lambda)$ is not a boundary term, but $v_{N+1}(\lambda)$ is. This inconsistency is an artifact of labeling vertices by their Hamming weights as there are vertices with Hamming weight 0, but none with Hamming weight $N+1$. The boundary terms will be defined where appropriate.*

Now, we define the transformation,

$$v'_m(\lambda) \stackrel{\text{def}}{=} f(m)v_m(\lambda) \tag{4.82}$$

where $f(m)$ is given by

$$f(m) \stackrel{\text{def}}{=} \begin{cases} f_0 \prod_{\substack{j \in \text{Odd} \\ 0 < j < m}} \frac{h(j-1)}{h(j)} & \text{if } m \text{ is even} \\[2em] f_1 \prod_{\substack{j \in \text{Even} \\ 0 \le j < m}} \frac{h(j-1)}{h(j)} & \text{if } m \text{ is odd} \end{cases} \tag{4.83}$$

and we choose,

$$\frac{f_1}{f_0} = \frac{\sqrt{N}\,\Gamma(N)}{2^{N-1}(\Gamma(\frac{N+1}{2}))^2} \tag{4.84}$$

where the Γ above represents the gamma function, not the gap.

With this transformation, we have from eqs. (4.81) and (4.82)

$$v'_{m-1}(\lambda) - 2v'_m(\lambda) + v'_{m+1}(\lambda) = \frac{f(m)}{h(m)}f(m+1)(W_m - q_m - \lambda)v'_m(\lambda) \tag{4.85}$$

where

$$q_m \stackrel{\text{def}}{=} \frac{2h(m)f(m+1)}{f(m)}. \tag{4.86}$$

Here, our choice of q_m (alternatively our choice of f_1/f_0) maintains symmetry and consistency across various choices of N.

Now we consider the Casoratian sequence corresponding to eq. (4.16).

$$w_i(\mathbf{v}'(\lambda_2), \mathbf{v}'(\lambda_1)) = v'_{i+1}(\lambda_2)v'_i(\lambda_1) - v'_{i+1}(\lambda_1)v'_i(\lambda_2) \tag{4.87}$$

For consistency, we choose $v'_{-1}(\cdot) = v'_{N+1}(\cdot) = 0$ and we get that $w_{-1} = w_{N+1} = 0$. Then, from eq. (4.85), similarly to eq. (4.20), we have that

$$\Delta w_{k-1} = -\Gamma \frac{f(k)}{h(k)f(k+1)} v'_k(\lambda_2)v'_k(\lambda_1). \tag{4.88}$$

We note that since $\mathbf{v}(\cdot)$ are the eigenvectors of a Jacobi matrix, $\mathbf{v}(\lambda_1)$ has no generalized zeros and $\mathbf{v}(\lambda_2)$ has precisely one generalized zero. Then, since $f(m) > 0 \; \forall m \in [\![0,N]\!]$ we know that $\mathbf{v}'(\lambda_1)$ has no zeros and $\mathbf{v}'(\lambda_2)$ has precisely one. Thus, labeling the generalized zero of $\mathbf{v}'(\lambda_2)$ by n, we have that

$$
\begin{align}
w_{m \leq n} &= \sum_{k=-1}^{m-1} \Delta w_i \tag{4.89}\\
&= -\Gamma \sum_{k=-1}^{k-1} \frac{f(k)}{h(k)f(k+1)} v'_k(\lambda_2)v'_k(\lambda_1) \tag{4.90}\\
&< 0 \tag{4.91}
\end{align}
$$

and similarly

$$
\begin{align}
w_{m > n} &= -\sum_{k=m}^{N} \Delta w_i \tag{4.92}\\
&= \Gamma \sum_{k=m}^{N} \frac{f(k)}{h(k)f(k+1)} v'_k(\lambda_2)v'_k(\lambda_1) \tag{4.93}\\
&< 0 \tag{4.94}
\end{align}
$$

so that $w_i < 0 \; \forall \, i \in [\![0,N]\!]$. As we have already seen in eq. (4.29), this guarantees that

$\left(v_i'^2(\lambda_2) - v_i'^2(\lambda_1) \right)_{i=0}^{N}$ has at most two generalized zeros. Now, because we have that

$$v_i'^2(\lambda_2) - v_i'^2(\lambda_1) = f(k)^2 \left(v_i^2(\lambda_2) - v_i^2(\lambda_1) \right) \tag{4.95}$$

$v_i'^2(\lambda_2) - v_i'^2(\lambda_1)$ has the same sign as $v_i^2(\lambda_2) - v_i^2(\lambda_1)$ and thus, $\left(v_i^2(\lambda_2) - v_i^2(\lambda_1) \right)_{i=0}^{N}$ has at most two generalized zeros. That $\mathbf{v}(\lambda_2)$ is orthogonal to $\mathbf{v}(\lambda_1)$ guarantees that it has at least one generalized zero.

At this point, we have satisfied the necessary conditions to apply an obvious analogue of Lemma 4.2:

Lemma 4.10. *Let $\mathscr{W}$ be the set of convex potentials and $\mathscr{L} \subseteq \mathscr{W}$ be the set of linear potentials. Let $\mathbf{u}(\lambda_1)$, $\mathbf{u}(\lambda_2)$ satisfying eq. (4.29) be real-valued eigenvectors corresponding to the two lowest eigenvalues of some matrix $\mathbf{H}_W(\mathbb{P}_N) + \mathbf{M}$ with real eigenvalues, where $\mathbf{M}$ is an arbitrary $N \times N$ matrix independent of W. Then, $\forall W \in \mathscr{W} \; \exists L \in \mathscr{L} \mid \Gamma(\mathbf{H}_W + \mathbf{M}) \geq \Gamma(\mathbf{H}_L + \mathbf{M})$.*

Proof. We note that because Lemma 4.2 depends only upon the variational term $\mathbf{W}(\alpha)$, when some matrix some matrix $\mathbf{H}_W(\mathbb{P}_N) + \mathbf{M}$ satisfies eq. (4.29), the proof is identical to that of Lemma 4.2. Therefore, this proof is omitted. $\qquad \square$

The reduced Hamming-symmetric matrix corresponding to eq. (4.79) is equivalent to $\mathbf{H}_W(\mathbb{P}_{N+1}) + \mathbf{M}$ for some choice of $\mathbf{M}$. Thus, by Lemma 4.10 it has a lower bound for a linear, Hamming-symmetric potential. Now, for such a linear potential we can consider $\alpha L_i = \alpha(i - N/2)$. Here, the eigenvalues are exactly solvable and given by

$$\lambda_k = k\sqrt{4 + \alpha^2} \quad \forall k \in \{-N/2, -(N-1)/2, \ldots, (N-1)/2, N/2\}. \tag{4.96}$$

Then,

$$\Gamma_{\alpha L \in \mathscr{L}} = \sqrt{4 + \alpha^2} \qquad (4.97)$$

which is clearly minimized for $\alpha = 0$. Thus, for convex, Hamming-symmetric potentials on the hypercube

$$\Gamma \geq 2 \qquad (4.98)$$

within the Hamming-symmetric subspace.

Chapter 5: Modulus of continuity oscillation estimates

5.1   Introduction

This chapter studies the spectral structure of combinatorial graph Laplacians by adapting recent advances in the spectral theory of Schrödinger operators on $\mathbb{R}^n$. To proceed, we introduce a technique based largely on the work of Ben Andrews, Julie Clutterbuck, and collaborators [8–13]. Additionally, we attempt an approach similar to [12] to bounding the spectral gap. In graph theory, the current setting, these Hamiltonians correspond to Laplacians of subgraphs of weighted graphs with Dirichlet boundary, as discussed in Sections 2.2 and 5.4 and elaborated on in [25]. Much of this chapter is taken verbatim from [43].

That the lowest eigenvalue of H is no longer 0 and the corresponding eigenvector is nonuniform makes determining the spectral gap of H a more challenging problem than that of a simple graph Laplacian. In this chapter, we reduce such a bound to an estimate involving the log-concavity of the lowest eigenvector u_0 of H.

Our approach follows [12], where the authors proved the Fundamental Gap Conjecture. In particular, we study the behavior of oscillations in functions defined on the graph $V(S)$. In [12], the authors studied the time-extended behavior of these oscillation terms when introduced into the heat equation, since such terms cannot decay any slower than $Ce^{-\lambda_1(L)t}$ for some constant C. These oscillation terms are characterized by a modulus of continuity, a construct which typically tracks how uniformly continuous a function is, but we can think of as quantifying the size of oscillations separated by a particular distance. More

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specifically, for a function $f : V(S) \longrightarrow \mathbb{R}$ we say that it has modulus of continuity η if

$$|f(y) - f(x)| \leq \eta(d(y,x)) \text{ for all } y, x \in V(S)$$

where $d(y,x)$ is the shortest path length between vertices $y, x \in V(S)$. We will further formalize this modulus in Section 5.3.1.

By sacrificing some tightness, one can apply modulus of continuity estimates without utilizing the heat equation at all. Instead one can derive bounds in terms of the ℓ^2-norm of the modulus. Nonetheless, our intuition stems from the heat equation and we expect that the heat equation will prove useful in subsequent work, so we derive our results from this perspective.

In Section 5.3.1, we prove the primary result of this paper:

Theorem 5.1. *Let L be the combinatorial Laplacian for a strongly convex subgraph $S \subseteq G$ of an invariant homogeneous graph G. Then,*

$$\lambda_1(L) \geq 2 \left(1 - \cos \left(\frac{\pi}{D+1} \right) \right)$$

where D is the diameter of S.

This theorem gives a nice lower bound to the spectral gap of combinatorial Laplacians in terms of the diameter of the corresponding graph. Although there is a long history of results comparing eigenvalues to diameters, this particular bound relates $\lambda_1(L)$ to the first eigenvalue of the path graph of $D+1$ vertices. This bound is also tight, since it is always achieved for $S \subset G$ such that S is the path graph with D edges. As a corollary to Theorem 5.1, this bounds the eigenvalues of the normalized laplacian $\mathscr{L}$ of S. Thus, this provides a tight bound comparable to that of [23], where the author derives a lower bound of $1/(8kD^2)$ for the Neumann eigenvalues of S where k is the degree of S.

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In Section 5.3.3, the proof strategy of Theorem 5.1 is adapted to the case of the hyper-cube graph. In particular, we recover the following, well-known bound:

Theorem 5.2. *Let L be the combinatorial Laplacian for a hypercube graph. Then, $\lambda_1(L) \geq 2$.*

Since one can directly calculate that $\lambda_1(L) = 2$ independently of D, this result is tight and demonstrates the power of modulus of continuity estimates adapted to spectral graph theory. In physical contexts, this estimate may also prove useful. We begin to explore such physical cases in Section 5.4, where we consider matrices of the form $H = L + W$ where W is any diagonal matrix and L is a combinatorial Laplacian. For simplicity, we restrict W to be positive-semidefinite, but since the spectral gap of H is unaltered by an addition of a constant multiple of the identity matrix, our results apply equally well to all diagonal W. In particular, we derive the following bound on the spectral gap $\gamma(H) = \lambda_1(H) - \lambda_0(H)$:

Theorem 5.3. *Let (u_0, λ) and $(u_1, \lambda + \gamma)$ be the two lowest eigenvector-eigenvalue pairs of $H = L + W$ where L is a combinatorial Laplacian of a strongly convex subgraph of an invariant homogeneous graph and W is a diagonal positive-semidefinite matrix. Let the componentwise ratio $f = u_1 / u_0$ have modulus of continuity η and $g = \log(u_0)$. Then,*

$$\gamma \geq 2C_{u_0} \left(1 - \cos\left(\frac{\pi}{D+1} \right) \right)$$

where D is the diameter of S,

$$C_{u_0} = \inf_{(y,x) \in \xi} \frac{\displaystyle\sum_{a \in \mathscr{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum_{a \in \mathscr{K}} \Delta_a f(x) e^{g(ax) - g(x)}}{\displaystyle\sum_{a \in \mathscr{K}} \Delta_a f(y) - \sum_{a \in \mathscr{K}} \Delta_a f(x)},$$

and

$$\xi = \left\{ (y,x) \in V(S) \mid \eta\left(|y^{-1}x| \right) = f(y) - f(x) \right\}.$$

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Above, $\Delta_a f(x) = f(ax) - f(x)$ for $x \in V(S)$. This result reduces the task of bounding $\gamma(H)$ to determining an appropriate constant C_{u_0} and is motivated similarly to the approach taken in [12], where the authors prove the longstanding fundamental gap conjecture.

Extending results of the fundamental gap literature to discrete Laplacians was first considered by Ashbaugh and Benguria in Ashbaugh1990, where the authors proved a fundamental gap-type theorem for the case of symmetric, single-well potentials on a one-dimensional Dirichlet Laplacian. More recently, in [41] we proved another fundamental gap-type theorem for the case of convex potentials on one-dimensional combinatorial Laplacians and Hamming-symmetric convex potentials on hypercube combinatorial Laplacians by following the method of Lavine1994a. In the context of hypercube combinatorial Laplacians L, we find in Section 5.4:

Theorem 5.4. *Let (u_0, λ) and $(u_1, \lambda + \gamma)$ be the two lowest eigenvector-eigenvalue pairs of $H = L + W$ where L is the combinatorial Laplacian of a Hypercube graph G and W is some diagonal positive-semidefinite matrix. Let the componentwise ratio $f = u_1/u_0$ have modulus of continuity η. Let $g = \log(u_0)$. Then, $\gamma \geq 2C_{u_0}$ with*

$$
C_{u_0} = \frac{\displaystyle\sum_{a \in \mathcal{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)}}{\displaystyle\sum_{a \in \mathcal{K}} \Delta_a f(y) - \sum_{a \in \mathcal{K}} \Delta_a f(x)}
$$

for $y, x \in V(G)$ such that $f(y) - f(x) = \eta(2)$.

Here, C_{u_0} is restricted to admit y, x only if they are separated by at most a path of length 2. Hence, Theorem 5.4 presents a much more local property than Theorem 5.3.

We also make use of a modulus of concavity ω of $\log(u_0)$ where u_0 is the ground-state of the operator H. By *modulus of concavity*, we mean that for each pair of $y, x \in V(S)$ and

some generator $a \in \mathcal{H}$ falling along a shortest path connecting y to x,

$$\Delta_a \log(u_0(y)) + \Delta_{a^{-1}} \log(u_0(x)) \geq \omega(d(y,x)) \text{ for all } x, y \in V(S).$$

We apply the results of Section 5.4 to the case of path graphs with log-concave ground states to obtain the following bound:

Theorem 5.5. *Suppose $H = L + W$ with ground state u_0, where L is the combinatorial Laplacian for some path graph S with diameter D and $W : V(S) \longrightarrow \mathbb{R}_{\geq 0}$. Then,*

$$\gamma(H) \geq 4 \left(2\cosh(\overline{\omega}) - 1\right) \left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right)$$
$$\geq 4 \left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right)$$

for $\log(u_0)$ having non-negative modulus of concavity ω and $\overline{\omega} = \inf_s \omega(s)$.

We can actually apply a closer analysis in deriving Theorem 5.5, assuming that we know a bound on the gradient of the modulus of concavity ω:

Theorem 5.6. *Suppose $H = L + W$ with ground state u_0, where L is the combinatorial Laplacian for some path graph S with diameter D and $W : V(S) \longrightarrow \mathbb{R}_{\geq 0}$. Then,*

$$\gamma(H) \geq 4 \left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right) + 2\inf_s \left(\Delta^- \cosh(\omega(s))\right)$$

for $\log(u_0)$ with non-negative modulus of concavity ω where $\omega(D + 1) = 0$ and $\overline{\omega} = \inf_s \omega(s)$. Above,

$$\Delta^- \cosh(\omega(s)) = \cosh(\omega(s)) - \cosh(\omega(s+1)).$$

This equation is particularly useful if we choose the modulus of concavity of ω to be

convex. Such a restriction is always possible without altering our analysis, because we are concerned with finite graphs, but these considerations will be discussed in future work. Under such restrictions, Theorem 5.6 provides the bound

$$\gamma(H) \geq 4\left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right) + 2\left(\cosh(\overline{\omega}) - 1\right) \tag{5.1}$$

with $\overline{\omega}$ defined as in Theorem 5.5. It is easy to see that Theorem 5.6 is indeed an improvement over Theorem 5.5.

5.2 Preliminaries

In this paper we restrict our attention to spectra of invariant, homogeneous graphs and their strongly convex subgraphs. We introduce some algebraic tools for discussing such graphs in Section 5.2.1. In Section 5.2.2, we introduce the *combinatorial Laplacian* and properties of its spectra.

5.2.1 Invariant homogeneous graphs

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. We call G *homogeneous* if there exists a group $\mathcal{H}$ acting on G such that for $\{u, v\} \in E(G)$, $\{au, av\} \in E(G) \ \forall \, a \in \mathcal{H}$ and $\forall u', v' \in V(G) \ \exists \, a_0 \in \mathcal{H}$ such that $a_0 u' = v'$. We call the set $\mathcal{K} \subset \mathcal{H}$ the edge generating set if $a \in \mathcal{K} \iff \{v, av\} \in E(G) \ \forall \, v \in V(G)$.

We restrict to the case that G is undirected; hence, if $\{v, av\} \in E(G)$ we also have that $\{av, v\} \in E(G)$. This restriction is equivalent to requiring that $a \in \mathcal{K} \iff a^{-1} \in \mathcal{K}$.[1] To simplify our problem further, we reduce our class of graphs by insisting that these graphs be *invariant* homogeneous graphs, or that $a\mathcal{K}a^{-1} = \mathcal{K} \ \forall \, a \in \mathcal{K}$.

---

[1]Note that if $v = av$ and $g(av) = v$, then $g = a^{-1}$.

We also need a notion of distance in the graph. Typically, we use $d(x,y)$, the length of the shortest path connecting vertex x to vertex y. In our setting, it helps to formalize this in group-theoretic terms. Because we are considering invariant homogeneous graphs, we can take $d(x,y) = |w|$, where $|\cdot|$ represents the *word metric* over $\mathscr{K}$ and $|w|$ is the length of the shortest word w written in terms of elements of $\mathscr{K}$ such that $wx = y$.

Lemma 5.1. *Let G be an invariant homogeneous graph with generating set $\mathscr{K}$. Then, for $x,y \in V(G)$ and $a \in \mathscr{K}$, $d(ax,ay) = d(x,y)$.*

Proof. This follows immediately from the equivalence of the shortest path and the word metric. Begin by writing $wx = y$. Then, for some $a \in \mathscr{K}$, $awa^{-1}(ax) = ay$. By invariance, $|awa^{-1}| = |w|$ and we have that $d(ax,ay) = d(x,y)$. □

Because Lemma 5.1 demonstrates the proper equivalence between the word-metric measured in generators of $\mathscr{K}$ and the distance between vertices y,x, we will write $|y^{-1}x|$ to represent $d(y,x)$.

Now, let S be an induced subgraph of G. We label the boundary of S by $\delta S = \{v \in V(G) \setminus V(S) | v \sim u \in S\}$. S is said to be *strongly convex* if it satisfies the following two (equivalent) properties:

1. For all pairs of vertices $y,x \in S$, the shortest path connecting y to x is also in S.

2. For all $a,b \in \mathscr{K}$, $x \in \delta S$, if $ax \in S$ and $bx \in S$ then $b^{-1}a \in \mathscr{K}$.[23]

Lemma 5.2. *Let $S \subseteq G$ be a strongly convex induced subgraph of an invariant homogeneous graph G. If $x,ax,y \in S$ and $d(ax,y) = d(x,y) + 1$, then $ay \in S$.*

Proof. Suppose that $x,y \in S$ and $d(ax,y) = d(x,y) + 1$. By Lemma 5.1, we know that $d(ax,ay) = d(x,y)$ and thus there exists a shortest path traversing $ax \to ay \to y$. Hence, $ay \in S$. □

5.2.2 Graph Laplacians

The focus of this paper is the *combinatorial Laplacian L* of a graph S which for all $x, y \in S$ is given by

$$L(x,y) = \begin{cases} d_x & \text{if } x = y \\ -1 & \text{if } x \sim y \\ 0 & \text{otherwise} \end{cases} \tag{5.2}$$

where d_x is the degree of vertex x. L can also be identified with an operator on the space of functions $u : V(S) \longrightarrow \mathbb{R}$ satisfying

$$Lu(x) = \sum_{y \sim x} (u(x) - u(y)). \tag{5.3}$$

The reader should note that the operator L in eq. (5.3) should be understood to apply to u before u is evaluated at the vertex x. In the case that S is an induced subgraph of a homogeneous graph G with edge generating set $\mathcal{K}$, we can equivalently write

$$Lu(x) = \sum_{a \in \mathcal{K}_x} (u(x) - u(ax)) \tag{5.4}$$

where $\mathcal{K}_x = \{a \in \mathcal{K} \mid ax \notin \delta S\}$. Here $\mathcal{K}_x$ is simply the set that generates all vertices in S adjacent to some particular vertex $x \in V(S)$.

The operator L corresponding to a connected graph has eigenvalues $\lambda_0(L) < \lambda_1(L) \leq \ldots \leq \lambda_{|V(G)|-1}(L)$ and corresponding eigenvectors $u_0(L), u_1(L), \ldots, u_{|V(G)|-1}(L)$ with $\lambda_0(L) = 0$ and

$$\lambda_1(L) = \inf_{u \perp \mathbf{1}} \frac{\sum_{x \sim y} (u(x) - u(y))^2}{\sum_{x} u^2(x)} \tag{5.5}$$

where $\mathbf{1}$ is the constant function. u attaining the infimum in eq. (5.5) is called a *combina-*

torial harmonic eigenfunction of S and can be identified with an eigenvector of L. If (u, λ) is an eigenvector-eigenvalue pair of L, then u satisfies

$$-\lambda u(x) = \sum_{y \sim x} (u(y) - u(x)).$$ (5.6)

Although eq. (5.6) is the standard definition of an eigenvector and can be obtained by inspecting eq. (5.3), the expression can also be derived through through variational techniques on eq. (5.5)[25].

5.3   Main Results

5.3.1   Strongly convex subgraphs of invariant homogeneous graphs

Heat kernel techniques are one of the more powerful approaches to proving eigenvalue bounds [25]. In this section, we adapt the approach of [9] to combinatorial Laplacians. This technique has the advantage of often being easier to handle than known techniques, such as those of [18, 23–26], while often retaining (and potentially sharpening) these bounds. In particular, the results of this section are comparable to those of [23].

For a graph G with diameter D, we begin by considering solutions to the initial value problem

$$\begin{cases} \frac{d(s,t)\phi}{dt} = -L\phi(s,t) \\ \phi(s,0) = \phi_0(s). \end{cases}$$ (5.7)

Clearly, if we let $\phi_0 = u$ for an eigenvector-eigenvalue pair (u, λ) of L, we have that $\phi(s,t) = u(s)e^{-\lambda t}$ solves eq. (5.7). Our strategy, then, is to consider the decay rate of oscillations in u. Since $\lambda_0(L) = 0$, the slowest such oscillations decay is proportional to $e^{-\lambda_1 t}$. Thus, if we bound the decay rate of these oscillations, we implicitly bound on the spectral gap. To characterize the magnitude of oscillations, we introduce the modulus of continuity for a

function defined on a graph.

For a function $f : V(G) \times \mathbb{R}^+ \longrightarrow \mathbb{R}$, we call $\eta : [-D, D] \times \mathbb{R}^+ \longrightarrow \mathbb{R}$ its *modulus of continuity* if

$$
\eta(s,t) = \begin{cases} \sup_{y,x \in V(G)} \left\{ f(y,t) - f(x,t) \mid |y^{-1}x| \leq s \right\} & s > 0 \\ 0 & s = 0 \\ -\sup_{y,x \in V(G)} \left\{ f(y,t) - f(x,t) \mid |y^{-1}x| \leq -s \right\} & s < 0 \end{cases} \tag{5.8}
$$

Although traditionally we would define the modulus only over non-negative s, defining it as an anti-symmetric function about the origin is advantageous for the analysis that follows. Importantly, our choice of η is monotonic and sub-additive, which further simplifies many of the arguments that follow. In future settings, however, it may be worth utilizing alternatively restricted moduli, such as concave moduli. Since we are interested in finite graphs, there always exists a concave function that both lies above and touches η. In fact the analysis that follows applies to these moduli equally well, but would require more detail than is necessary in the current context.

To prove Theorem 5.1, we need the following fact.

Lemma 5.3. *Suppose $S \subseteq G$ is a finite strongly convex subgraph in an invariant homogeneous graph G with edge generating set $\mathcal{K}$. Let $u : V(S) \longrightarrow \mathbb{R}$ have modulus of continuity η. Then, for $y, x, ay \in V(S)$ either $ax \in V(S)$ or $|u(ay) - u(x)| \leq \eta\left(|y^{-1}x|\right)$.*

Proof. To prove this, simply note that from Lemma 5.2 we know that either $ax \in V(S)$ or $|y^{-1}(ax)| \leq |y^{-1}x|$. Thus, $ax \in V(S)$ or $u(ay) - u(x) \leq \eta(|y^{-1}x|)$. □

Lemma 5.4. *Suppose $S \subseteq G$ is a finite strongly convex subgraph in an invariant homogeneous graph G with edge generating set $\mathcal{K}$. Let $u : V(S) \longrightarrow \mathbb{R}$ have modulus of continuity η. Then, for $y, x \in V(S)$ achieving the supremum in $\eta(|y^{-1}x|)$ with $u(y) \geq u(x)$*

1. *if* $ay \in V(S)$ *and* $ax \notin V(S)$, *then* $u(ay) - u(y) \le 0$ *and*

2. *if* $ax \in V(S)$ *and* $ay \notin V(S)$, *then* $u(ax) - u(x) \ge 0$.

Proof. To prove item 1, assume that $ax \notin V(S)$ and write

$$
\begin{aligned}
u(ay) - u(y) &= u(ay) - u(y) + u(x) - u(x) \\
&= u(ay) - u(x) - \eta(|y^{-1}x|) \\
&\le \eta(|y^{-1}x|) - \eta(|y^{-1}x|) \\
&= 0
\end{aligned}
$$

where the inequality follows from Lemma 5.3. Item 2 is similar to item 1 and proof is omitted. $\square$

Lemma 5.5. *Suppose S is a finite strongly convex subgraph in an invariant homogeneous graph G with edge generating set $\mathcal{K}$. Let $u : V(S) \longrightarrow \mathbb{R}$ have modulus of continuity η. Then, for $y, x \in V(S)$ achieving the supremum in $\eta(|y^{-1}x|)$ with $u(y) \ge u(x)$*

$$
-Lu(y) + Lu(x) \le \sum_{a \in \mathcal{Y}} (u(ay) - u(y)) - \sum_{a \in \mathcal{X}} (u(ax) - u(x))
$$

for any $\mathcal{Y} \subseteq \mathcal{K}_y$ and $\mathcal{X} \subseteq \mathcal{K}_x$ satisfying $\mathcal{Y} \cap (\mathcal{K}_y \cap \mathcal{K}_x) = \mathcal{X} \cap (\mathcal{K}_y \cap \mathcal{K}_x)$.

Proof. From eq. (5.4) we have,

$$
\begin{aligned}
-Lu(y) + Lu(x) &= \sum_{a \in \mathcal{K}_y} (u(ay) - u(y)) - \sum_{a \in \mathcal{K}_x} (u(ax) - u(x)) \\
&= \sum_{a \in \mathcal{K}_y \cap \mathcal{K}_x} (u(ay) - u(y)) - \sum_{a \in \mathcal{K}_y \cap \mathcal{K}_x} (u(ax) - u(x)) \\
&\quad + \sum_{a \in \mathcal{K}_y \setminus \mathcal{K}_x} (u(ay) - u(y)) - \sum_{\mathcal{K}_x \setminus \mathcal{K}_y} (u(ax) - u(x)).
\end{aligned} \tag{5.9}
$$

Now, since $\mathcal{K}_y \setminus \mathcal{K}_x$ is the set of all $a \in \mathcal{K}$ such that $ay \in V(S)$ and $ax \notin V(S)$ and

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similarly for $\mathcal{K}_x \setminus \mathcal{K}_y$, from Lemma 5.4 we know that

$$\sum_{a \in \mathcal{K}_y \setminus \mathcal{K}_x} (u(ay) - u(y)) \leq \sum_{a \in \mathcal{J}_y} (u(ay) - u(y)) \tag{5.10}$$

$$- \sum_{a \in \mathcal{K}_x \setminus \mathcal{K}_y} (u(ax) - u(x)) \leq - \sum_{a \in \mathcal{J}_x} (u(ax) - u(x)) \tag{5.11}$$

for any $\mathcal{J}_y \subseteq \mathcal{K}_y \setminus \mathcal{K}_x$ and $\mathcal{J}_x \subseteq \mathcal{K}_x \setminus \mathcal{K}_y$. Now, noting that $u(y) - u(x) = \eta(|y^{-1}x|)$, Lemma 5.1 implies that $u(ay) - u(ax) \leq u(y) - u(x)$ for any $a \in \mathcal{K}_y \cap \mathcal{K}_x$. Thus,

$$\begin{aligned} \sum_{a \in \mathcal{K}_y \cap \mathcal{K}_x} (u(ay) - u(y)) &- \sum_{a \in \mathcal{K}_y \cap \mathcal{K}_x} (u(ax) - u(x)) \\ &\leq \sum_{a \in \mathcal{J}} (u(ay) - u(y)) - \sum_{a \in \mathcal{J}} (u(ax) - u(x)) \end{aligned} \tag{5.12}$$

for any $\mathcal{J} \subseteq \mathcal{K}_y \cap \mathcal{K}_x$. Combining eqs. (5.9) to (5.12) completes the proof. $\qquad\square$

Lemma 5.6. *Suppose S is a finite strongly convex subgraph with even (odd) diameter D of an invariant homogeneous graph G with edge generating set $\mathcal{K}$ and $|\mathcal{K}| = k$. If $u : V(S) \times \mathbb{R}^+ \longrightarrow \mathbb{R}$ is a solution of eq. (5.7), then the modulus of continuity η of u satisfies for positive even (odd) s,*

$$\frac{d\eta(s,t)}{dt} \leq -L_P \eta(s,t) \tag{5.13}$$

where L_P is the combinatorial Laplacian of the path graph P with $V(P) = \{s \mid s \in [\![-D,D]\!]$ and s even (odd)$\}$ and $E(P) = \{\{s, s+2\} \mid s \in [\![-D, D-2]\!]$ and s even (odd)$\}$.

Proof. Choose y, x to achieve the supremum in eq. (5.8) with $u(y) \geq u(x)$. Say that $s = |y^{-1}x| \in \mathbb{E}$ where $\mathbb{E}$ is the appropriate choice of the set of all evens or all odds. Then, we have that

$$\left. \frac{d\eta(s,t)}{dt} \right|_{t=t_0} = \left. \left(\frac{du(y,t)}{dt} - \frac{du(x,t)}{dt} \right) \right|_{t=t_0} = -Lu(y,t_0) + Lu(x,t_0) \tag{5.14}$$

where, to avoid excessive notation, we have adopted the convention $u(y) = u(y, t_0)$. Now, fix $a_0, a_1 \in \mathcal{K}$ such that $a_0 y$ and $a_1 x$ lie along a shortest path connecting y to x. By our

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choice, we know that $a_0 y \in S$ and $a_1 x \in S$. Now, we have a few cases and in each we will apply Lemma 5.5 with various choices of $\mathcal{Y}, \mathcal{X}$. (In the cases that follow, we adopt the convention that $\eta(D+2) = \eta(D+1) = \eta(D)$.)

Case 1, $a_0 x \in S$ and $a_1 y \in S$: In this case, we choose $\mathcal{Y} = \mathcal{X} = \{a_0, a_1\}$. Hence, Lemma 5.5 and eq. (5.14) yield

$$
\begin{aligned}
\frac{d\eta(s,t)}{dt} &\leq u(a_0 y) + u(a_1 y) - 2u(y) - u(a_0 x) - u(a_1 x) + 2u(x) \\
&= (u(a_0 y) - u(a_1 x)) + (u(a_1 y) - u(a_0 x)) - 2(u(y) - u(x)) \\
&\leq \eta(s-2) + \eta(s+2) - 2\eta(s) \\
&= -L_P \eta(s)
\end{aligned}
$$

where the final inequality follows from eq. (5.8).

Case 2, $a_0 x \notin S$ and $a_1 y \in S$: In this case, we choose $\mathcal{Y} = \{a_0, a_1\}$ and $\mathcal{X} = \{a_1\}$. Hence, Lemma 5.5 and eq. (5.14) yield

$$
\begin{aligned}
\frac{d\eta(s)}{dt} &\leq u(a_0 y) + u(a_1 y) - 2u(y) - u(a_1 x) + u(x) \\
&= (u(a_0 y) - u(a_1 x)) + (u(a_1 y) - u(x)) - 2(u(y) - u(x)) \\
&\leq \eta(s-2) + \eta(s+1) - 2\eta(s) \\
&\leq \eta(s-2) + \eta(s+2) - 2\eta(s) \\
&= -L_P \eta(s)
\end{aligned}
$$

where the inequalities follow from eq. (5.8).

Case 3, $a_0 x \in S$ and $a_1 y \notin S$: This is similar to Case 2 and proof is omitted.

Case 4, $a_0 x \notin S$ and $a_1 y \notin S$: In this case, we choose $\mathscr{Y} = \{a_0\}$ and $\mathscr{X} = \{a_1\}$. Hence, Lemma 5.5 and eq. (5.14) yield

$$\frac{d\eta(s)}{dt} \leq u(a_0 y) - u(y) - u(a_1 x) + u(x)$$

$$= (u(a_0 y) - u(a_1 x)) - (u(y) - u(x))$$

$$\leq \eta(s-2) - \eta(s)$$

$$\leq \eta(s-2) + \eta(s+2) - 2\eta(s)$$

$$= -L_P \eta(s)$$

where the inequalities follow from eq. (5.8).

Thus, in all cases,

$$\frac{d\eta(s)}{dt} \leq -L_P \eta(s)$$

provided $s \geq 0$. $\qquad\square$

Theorem 5.1. *Let L be the combinatorial Laplacian for a strongly convex subgraph $S \subseteq G$ of an invariant homogeneous graph G. Then,*

$$\lambda_1(L) \geq 2\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right)$$

where D is the diameter of S.

Proof. Let $\lambda_1 = \lambda_1(L)$. Suppose u_1 is a solution to eq. (5.7) and (u_1, λ_1) is the first eigenvector-eigenvalue pair of L. Let η be the modulus of continuity for u_1. For simplicity, we restrict our attention to $\eta(s)$ such that $s \in \mathbb{E}$ in accordance with Lemma 5.6. In other words, we treat η as a vector with entries indexed by $s \in \mathbb{E}$. Then, Lemma 5.6 yields

$$\frac{d\eta(s)}{dt} \leq -L_P \eta(s) \ \text{ for } s \geq 0.$$

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Noting that η as defined in Lemma 5.6 is an odd function, we immediately see that

$$\frac{d\eta(s)}{dt} \geq -L_P\eta(s) \text{ for } s < 0$$

so that we have

$$\eta^\top \frac{d\eta}{dt} \leq -\eta^\top L_P\eta.$$

Then,

$$\frac{1}{2}\frac{d|\eta|^2}{dt} \leq -\eta^\top L_P\eta$$
$$\leq -\mu|\eta|^2$$

where $\mu = 2\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right)$ is the smallest non-trivial eigenvalue of L_P. Hence, we have that

$$|\eta(s)| \leq Ce^{-\mu t}$$

for $s \in [\![-D,D]\!]$ and some constant C chosen independently of t. Then, there exist $y, x \in V(S)$ such that,

$$|u_1(y,0) - u_1(x,0)|e^{-\lambda_1 t} = \eta(s,t)$$
$$\leq Ce^{-\mu t}$$
$$|u_1(y,0) - u_1(x,0)| \leq Ce^{(\lambda_1 - \mu)t}.$$

Note that $u_1(y,0) - u_1(x,0)$ is nonzero, so that if $\lambda_1 - \mu < 0$ we arrive at a contradiction by taking $t \to \infty$. Hence, $\lambda_1 \geq \mu$. $\qquad\square$

We can alternatively prove Theorem 5.1 without using the heat equation:

Proof. Let $\lambda_1 = \lambda_1(L)$. Suppose that (u_1, λ_1) is the first eigenvector-eigenvalue pair of

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L. Let u_1 have modulus of continuity η, and let vertices x and y achieve the supremum defining $\eta(s)$ in eq. (5.8). Then

$$-Lu_1(y) + Lu_1(x) = \lambda_1 \eta(s).$$

As shown in the proof of Lemma 5.6,

$$-Lu_1(y) + Lu_1(x) \leq -L_P \eta(s).$$

Hence,

$$-\lambda_1 \eta(s) \leq -L_P \eta(s).$$

Now, since $\eta(s) > 0$ for all $s > 0$, we have that for $s > 0$,

$$-\lambda_1 \eta^2(s) \leq -\eta(s) L_P \eta(s).$$

Recalling that η is odd, this yields

$$-\lambda_1 |\eta|^2 \leq -\eta^\top L_P \eta$$
$$\leq -\mu |\eta|^2$$

where $\mu = 2\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right)$ is the smallest non-trivial eigenvalue of L_P. Thus, since $|\eta|^2$ is nonzero, $\lambda_1 \geq \mu$ and we have proven Theorem 5.1. $\qquad\square$

One should note that the two proofs of Theorem 5.1 are essentially the same, as the lower bound on the decay-rate of the heat equation can be deduced from the ℓ^2-norm of the modulus. Regardless, while the first method can be adapted to any non-constant function u_1, the latter cannot. Also, the reader familiar with normalized Laplacians should note that

as a consequence of Theorem 5.1, we obtain a lower bound of $\frac{2}{k}\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right)$ on the spectral gap of the normalized Laplacian for convex subgraphs of homogeneous graphs, where k is the degree of the graph. Thus, we can compare this result to those of [23, 25].

5.3.2 Example 1: Path graphs

Consider any path graph and note that it is a convex subgraph of some homogeneous graph. Then, Theorem 5.1 implies that the first eigenvalue

$$\lambda_1(L) \geq 2\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right).$$

This bound is tight, since the eigenvalues of the path graph are actually given by

$$\lambda_j(L) = 2\left(1 - \cos\left(\frac{j\pi}{D+1}\right)\right).$$

5.3.3 Example 2: Hypercube graphs

Theorem 5.2. *Let L be the combinatorial Laplacian for a hypercube graph. Then, $\lambda_1(L) \geq 2$.*

Proof. For the hypercube, we can choose $\mathcal{K}$ such that it is both abelian and every element $a \in \mathcal{K}$ is self-inverse. We again consider a solution u to eq. (5.14) with modulus of continuity η. Then, η either satisfies $\eta(2) > \eta(1)$ or $\eta(2) = \eta(1)$. Let y, x be the vertices that achieve the supremum in $\eta(2)$ with $u(y) \geq u(x)$.

Case 1, $|y^{-1}x| = 2$: Note that in this case we can write $y = b'bx$ for some $b, b' \in \mathcal{K}$ and that $y \neq x$ implies $b \neq b'$. Then, Equation (5.14) with $s = 2$ becomes

$$\frac{d\eta(2)}{dt} = \sum_{a \in \mathcal{K}} (u(ay) - u(y)) - \sum_{a \in \mathcal{K}} (u(ax) - u(x))$$

$$\leq (u(by) - u(bx)) + (u(b'y) - u(b'x) - 2\eta(2))$$

$$= (u(b'y) - u(bx)) + (u(by) - u(b'x)) - 2\eta(2)$$

$$= -2\eta(2).$$

Above, the first inequality follows from Lemma 5.5 with $\mathcal{Y} = \mathcal{X} = \{b, b'\}$.

Case 2, $|y^{-1}x| = 1$: Equation (5.14) with $s = 1$ becomes

$$\frac{d\eta(1)}{dt} = \sum_a (u(ay) - u(y)) - \sum_a (u(ax) - u(x))$$

$$\leq (u(by) - u(bx)) + (u(b'y) - u(b'x) - 2\eta(1))$$

$$= (u(b'y) - u(b'x)) + (u(x) - u(y)) - 2\eta(1)$$

$$\leq -2\eta(1)$$

where the first inequality follows from Lemma 5.5 with $\mathcal{X} = \mathcal{Y} = \{b, b'\}$ with b satisfying $x = by$ and $bx = y$. The second inequality follows from the definition of η. Thus, in either case we have that

$$\frac{d\eta(2)}{dt} \leq -2\eta(2). \tag{5.15}$$

Now, by either method of Theorem 5.1, $\lambda_1(L) \geq 2$ and our bound is tight. □

It is both remarkable and (perhaps) expected that the particular connectivity of the hypercube allows us to consider only points separated by a path of length 2 while still obtaining a tight bound. The modulus of continuity approach suggests that in many cases of

physical interest the spectral gap is a highly local property. This result may be exploitable in the context of quantum Ising models, where it can reduce our problem to that of estimating the log-concavity of the ground-state wavefunction (the lowest eigenvector).

5.4 Dirichlet Eigenvalues and Ising-type Hamiltonians

Now we consider the more general problem of bounding the gap of the matrix $H = L + W$, where L is the combinatorial Laplacian for some subgraph S of a homogeneous graph and W is a positive-semidefinite matrix. In the physics literature these are known as "stoquastic Hamiltonians" and have the same spectrum as the Dirichlet eigenvalues of S for an appropriate choice of host graph. The key results of Section 5.4.1 should be seen as Lemma 5.7 and Corollary 5.1.

The constant C_{u_0} introduced in Theorem 5.3 and Theorem 5.4 requires further exploration before it provides useful bounds. However, we believe that in the case that u_0 is log-concave, for some suitably-defined notion of log-concavity, $C_{u_0} \geq 1$. Section 5.4.2 applies the techniques of Section 5.4.1 to derive a bound on the spectral gap of H in the one-dimensional case. Theorem 5.5 and Theorem 5.6 should be viewed as a slightly weakened (but still strong) analogue of Theorem 5.3, demonstrating the utility of the methods of section 5.4.1 and the promise of an alternative expression for Theorem 5.5 and Theorem 5.6 entirely in terms of (a measure of) the log-concavity of u_0 and the diameter of S.

5.4.1 Induced subgraphs of weighted homogeneous graphs and Hamiltonians with potentials

In this section, we consider an induced subgraph S of a graph G with vertex set $V(S) \subseteq V(G)$ and nonempty vertex boundary δS. We let $S' = \{\{x, y\} \in E(G) \mid x \in V(S) \text{ or } y \in V(S)\}$. In other words, S' is the set of all edges with at least one end in S. Then, we define

the lowest (combinatorial) Dirichlet eigenvalue of the induced subgraph S as

$$\lambda_0^{(D)} = \inf_{u \in D^*} \frac{\sum\limits_{\{x,y\} \in S'} (u(x) - u(y))^2}{\sum\limits_{y \in V(S)} u^2(y)} \qquad (5.16)$$

where D^* is simply the set of all nonzero functions satisfying the Dirichlet condition

$$u(x) = 0 \text{ for } x \in \delta S.$$

The function $u_0 : V(S) \cup \delta S \to \mathbb{R}$ achieving the infimum in eq. (5.16) is called a Dirichlet eigenfunction and in accordance with the physics literature, we refer to u_0 as a ground-state. In the interior of S, u_0 is nonzero and has constant sign, so is taken to be completely positive. Hence, there exists a function $g : V(S) \cup \delta S \longrightarrow \mathbb{R}$ satisfying

$$u_0(y) = \begin{cases} e^{g(y)} & y \in V(S) \\ 0 & y \in \delta S. \end{cases} \qquad (5.17)$$

Above, g, the log of the ground-state, will prove a more natural consideration in much of what follows. In general, any function $u_0 : V(S) \cup \delta S \to \mathbb{R}$ such that $u_0 > 0$ interior to S is compatible with such a choice of g. To specify a function consistent with eq. (5.17) for some $u_0 > 0$, we will often write $g = \log(u_0)$.

Higher Dirichlet eigenvalues can be defined generally by

$$\lambda_i^{(D)} = \inf_{\substack{u \perp C_i \\ u \in D^*}} \frac{\sum\limits_{\{x,y\} \in S'} (u(x) - u(y))^2}{\sum\limits_{y \in V(S)} u^2(y)}$$

where C_i is the subspace spanned by the i lowest nonzero Dirichlet eigenfunctions.[2] Imposing the Dirichlet condition explicitly, we can write

$$\lambda_i^{(D)} = \inf_{u \perp C_i} \frac{\sum\limits_{x \sim y \in S} (u(x) - u(y))^2 + \sum\limits_{y \in V(S)} W(y)u^2(y)}{\sum\limits_{y \in V(S)} u^2(y)} \tag{5.18}$$

where $W(y) = |\{\{x, y\} \in S' \mid x \in \delta S\}|$. Thus, we identify $\lambda_i^{(D)}$ with the eigenvalues of the matrix $L + W$ where L is the combinatorial Laplacian of S and W is some diagonal matrix with non-negative integer-valued entries.

For the remainder of this section, we adopt a somewhat more general construction. We let $H = L + W$ where W is any positive-semidefinite diagonal matrix. Equivalently, $W : V(G) \longrightarrow \mathbb{R}_{\geq 0}$. (Since we are ultimately concerned with spectral gaps, we could equivalently discuss W as any diagonal matrix by simply shifting $W \mapsto cI + W$ for any c without impacting the spectral gap.) Despite relaxing the combinatorial constraints on W, the eigenvalues of H are still given by eq. (5.18).[3] H defined this way corresponds to a subset of so-called "stoquastic Hamiltonians" which have been of recent interest in quantum theory [20].[4] Since solutions of eq. (5.18) are simply the eigenvalues of H, for the remainder of this section we write $\lambda_i = \lambda_i^{(D)}$.

To bound the spectral gap $\gamma(H)$, we once again wish to consider solutions to the heat equation

$$\begin{cases} \frac{d\phi(s,t)}{dt} = -H\phi(s,t) \\ \phi(s,0) = \phi_0(s). \end{cases} \tag{5.19}$$

---

[2]Note that $\lambda_i^{(D)}$ differ from those of the corresponding normalized Laplacian only by a factor of k, the degree of G.

[3]These are also the Dirichlet eigenvalues for the weighted combinatorial Laplacian with $W(u) = \sum\limits_{\{v,u\} \in \partial S} w(v,u)$ and unit weight on the edges internal to S.

[4]One important stoquastic Hamiltonian would be the transverse-field Ising model with a non-negative field.

In general, we proceed by consider the componentwise ratio of two solutions u_0 and u_1 to eq. (5.19), where we choose $u_0 > 0$ in the interior of S. This situation is rather similar to that considered in Section 5.3.1, but we require a relationship like eq. (5.4) to proceed. To this end, we propose the following:

Lemma 5.7. *Let S with combinatorial Laplacian L be a convex induced subgraph of some invariant homogeneous graph. Let $u_0(x,t), u_1(x,t)$ be solutions to eq. (5.19) with $u_0(x,0) = u_0(x)$ and $u_1(x,0) = u_1(x)$ and satisfying the Dirichlet condition on δS. Suppose $u_0(x) > 0$ for all $x \in V(S)$. If*

$$f(x,t) = \frac{u_1(x,t)}{u_0(x,t)} \text{ for } x \in V(S).$$

and

$$\Delta_a f(x,t) = \begin{cases} f(ax,t) - f(x,t) & ax \in V(s) \\ 0 & ax \in \delta S. \end{cases}$$

Then,

$$\frac{df}{dt} = \sum_{a \in \mathcal{H}} \Delta_a f(x,t) e^{g(ax) - g(x)}$$

for $g = log(u)$ defined consistently with eq. (5.17).

Proof. For simplicity, we write $f = f(t)$ and similarly for $u_0(t), u_1(t)$. Then,

$$\frac{df(x)}{dt} = \frac{1}{u_0(x)} \frac{du_1(x)}{dt} - \frac{u_1(x)}{u_0^2(x)} \frac{du_0(x)}{dt}.$$

If $u_1(x) = 0$, the second term is 0 and the remainder of the proof becomes trivial. Hence, we assume that $u_1(x) \neq 0$. Now, we recall that $H = L + W$ where W is diagonal and apply eq. (5.19) to get

$$\begin{aligned} \frac{df(x)}{dt} &= f(x) \left(\frac{1}{u_1(x)} \frac{du_1(x)}{dt} - \frac{1}{u_0(x)} \frac{du_0(x)}{dt} \right) \\ &= f(x) \left(-\frac{1}{u_1(x)} Hu_1(x) + \frac{1}{u_0(x)} Hu_0(x) \right) \end{aligned}$$

$$= f(x) \left(-\frac{1}{u_1(x)} L u_1(x) + \frac{1}{u_0(x)} L u_0(x) - \frac{1}{u_1(x)} W u_1(x) + \frac{1}{u_0(x)} W u_0(x) \right)$$

$$= f(x) \left(-\frac{1}{u_1(x)} L u_1(x) + \frac{1}{u_0(x)} L u_0(x) - W(x) + W(x) \right)$$

$$= f(x) \left(\frac{1}{u_1(x)} \sum_{a \in \mathcal{K}} (u_1(ax) - u_1(x)) - \frac{1}{u_0(x)} \sum_{a \in \mathcal{K}} (u_0(ax) - u_0(x)) \right)$$

$$= f(x) \left(\sum_{a \in \mathcal{K}} \left(\frac{u_1(ax)}{u_1(x)} - 1 \right) - \sum_{a \in \mathcal{K}} \left(\frac{u_0(ax)}{u_0(x)} - 1 \right) \right)$$

$$= f(x) \sum_{a \in \mathcal{K}} \left(\frac{u_1(ax)}{u_1(x)} - \frac{u_0(ax)}{u_0(x)} \right)$$

$$= f(x) \sum_{\substack{a \in \mathcal{K} \\ ax \in V(S)}} \left(\frac{f(ax)}{f(x)} - 1 \right) \frac{u_0(ax)}{u_0(x)}$$

$$= \sum_{\substack{a \in \mathcal{K} \\ ax \in V(S)}} (f(ax) - f(x)) \frac{u_0(ax)}{u_0(x)}$$

$$= \sum_{a \in \mathcal{K}} \Delta_a f(x) \frac{u_0(ax)}{u_0(x)}$$

$$= \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)}.$$

$\square$

Corollary 5.1. *Let* $(u_0, \lambda_0), (u_1, \lambda_0 + \gamma)$ *be the first and second eigenvector-eigenvalue pair of* $H = L + W$ *where L is a combinatorial Laplacian and W is a diagonal positive-semidefinite matrix. Then, if* $u_0(t), u_1(t)$ *are solutions to eq. (5.19) with* $u_0(0) = u_0$ *and* $u_1(0) = u_1$, *we have that*

$$-\gamma f(x) = \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax,t) - g(x,t)}.$$

for g defined consistently with eq. (5.17).

Proof. This follows from Lemma 5.7 by simply noting that $f(x,t) = \frac{u_1(x)}{u_0(x)} e^{-\gamma t}$. $\square$

Note that the operator acting on f and satisfying the relationships of Lemma 5.7 and Corollary 5.1 has a constant eigenfunction with eigenvalue 0. Thus, the analysis of Section 5.3.1 carries over identically, provided that we can appropriately bound $-\gamma f(x)$. Because of this, Lemma 5.7 and Corollary 5.1 are sufficient to prove Theorem 5.3.

Theorem 5.3. *Let (u_0, λ) and $(u_1, \lambda + \gamma)$ be the two lowest eigenvector-eigenvalue pairs of $H = L + W$ where L is a combinatorial Laplacian of a strongly convex subgraph of an invariant homogeneous graph and W is a diagonal positive-semidefinite matrix. Let the componentwise ratio $f = u_1/u_0$ have modulus of continuity η and $g = \log(u_0)$. Then,*

$$\gamma \geq 2C_{u_0}\left(1 - \cos\left(\frac{\pi}{D+1}\right)\right)$$

where D is the diameter of S,

$$C_{u_0} = \inf_{(y,x)\in\xi} \frac{\displaystyle\sum_{a\in\mathcal{K}}\Delta_a f(y)e^{g(ay)-g(y)} - \sum_{a\in\mathcal{K}}\Delta_a f(x)e^{g(ax)-g(x)}}{\displaystyle\sum_{a\in\mathcal{K}}\Delta_a f(y) - \sum_{a\in\mathcal{K}}\Delta_a f(x)},$$

and

$$\xi = \left\{(y,x) \in V(S) \mid \eta\left(|y^{-1}x|\right) = f(y) - f(x)\right\}.$$

Proof. First, let η be the modulus of f. Then, note that by Lemma 5.5, for all $(y,x) \in \xi$

$$\sum_{a\in\mathcal{K}}\Delta_a f(y) - \sum_{a\in\mathcal{K}}\Delta_a f(x) < 0$$

for appropriate choice of $\mathscr{Y}, \mathscr{X}$. Additionally, by the method of Lemma 5.6

$$\sum_{a\in\mathcal{K}}\Delta_a f(y) - \sum_{a\in\mathcal{K}}\Delta_a f(x) \leq -L_P\eta\left(|y^{-1}x|\right)$$

with L_P defined as in Theorem 5.1.

Further, Corollary 5.1 requires that

$$\sum_{a \in \mathcal{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)} < 0.$$

Thus,

$$C_{u_0} = \inf_{\{y,x\} \in \xi} \frac{\sum_{a \in \mathcal{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)}}{\sum_{a \in \mathcal{K}} \Delta_a f(y) - \sum_{a \in \mathcal{K}} \Delta_a f(x)} > 0$$

Now, we apply Lemma 5.7 and obtain

$$\begin{aligned}
\frac{d\eta(s)}{dt} &= \sum_{a \in \mathcal{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)} \\
&\leq C_{u_0} \left(\sum_{a \in \mathcal{K}} \Delta_a f(y) - \sum_{a \in \mathcal{K}} \Delta_a f(x) \right) \\
&\leq -C_{u_0} L_P \eta(|y^{-1}x|).
\end{aligned}$$

Hence, by the exact same argument as Theorem 5.1, we have that $\gamma \geq C_{u_0} \mu$. Thus,

$$\gamma \geq 2C_{u_0} \left(1 - \cos\left(\frac{\pi}{D+1} \right) \right).$$

$\square$

Theorem 5.4. *Let (u_0, λ) and $(u_1, \lambda + \gamma)$ be the two lowest eigenvector-eigenvalue pairs of $H = L + W$ where L is the combinatorial Laplacian of a Hypercube graph G and W is some diagonal positive-semidefinite matrix. Let the componentwise ratio $f = u_1 / u_0$ have*

modulus of continuity η. Let $g = \log(u_0)$. Then, $\gamma \geq 2C_{u_0}$ with

$$C_{u_0} = \frac{\sum\limits_{a \in \mathcal{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum\limits_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)}}{\sum\limits_{a \in \mathcal{K}} \Delta_a f(y) - \sum\limits_{a \in \mathcal{K}} \Delta_a f(x)}$$

for $y, x \in V(G)$ such that $f(y) - f(x) = \eta(2)$.

Proof of Theorem 5.4 is omitted, since it exactly follows the approach to Theorem 5.3.

5.4.2   Example 3: Log-concave ground states

In this section we apply the techniques above to prove a gap bound in the case that $H = L + W$ has a log-concave ground state u_0 for L corresponding to a one-dimensional graph S. In particular, by log-concavity we mean that $g : V(S) \cup \delta S \longrightarrow \mathbb{R}$ defined consistently with eq. (5.17) satisfies

$$\sum_{a \in \mathcal{K}} (g(ay) - g(y)) \leq 0 \text{ for all } y \in V(S). \tag{5.20}$$

In more general settings, this is not a satisfactory notion of concavity, since the analogue of a saddle-point might also satisfy this definition. However, for the one-dimensional case considered in this section, it is appropriate. In the future, we will likely define a much stronger notion of concavity that acts as a better analogue to the continuous definition while still being useful in our setting. Regardless, note that concavity as defined by eq. (5.20) can be trivially satisfied by g at any vertex connected to the boundary δS. To see this, simply note our freedom in g in eq. (5.17) and choose $g(ay) \to -\infty$ for any $ay \in \delta S$.

In the case of the path graph S, we choose our edge generating set $\mathcal{K} = \{b, b^{-1}\}$ and log-concavity implies that $g(bx) - 2g(x) + g(b^{-1}x) \leq 0$ for all $x \in V(S)$.

We also introduce in this section a modulus of concavity for g. This modulus allows us

to prove tighter bounds than the simple assumption of log-concavity itself. For a graph S with diameter D, we call $\omega : [0, D] \longrightarrow \mathbb{R}$ the modulus of concavity of a function g defined on $V(S)$ if

$$\omega(s) = \inf_{|y^{-1}x|=s} \left\{ \frac{\Delta_{a^{-1}}g(y) + \Delta_a g(x)}{2} \;\middle|\; |y^{-1}a^2 x| \le |y^{-1}x| \right\}. \tag{5.21}$$

Basically, the modulus of concavity tells us exactly how strongly concave g is over a particular path separation s. Its utility lies in the expectation that as the ground-state becomes more contracted, the spectral gap should increase.

Lemma 5.8. *Suppose S is a path graph of diameter D and $f : V(S) \times \mathbb{R} \longrightarrow \mathbb{R}$ and γ are defined as in Corollary 5.1. Let η be the modulus of continuity of f. Then, for $s \ge 1$, η satisfies*

$$-\gamma \eta(s) \le -2L_P \eta(s) - 4(\cosh(\omega(s)) - 1)\nabla\eta(s)$$

where ω is the modulus of concavity of the ground state of S, L_P is the combinatorial Laplacian operator for the path graph P with $V(P) = [\![-D, D]\!]$ and $E(P) = \{\{s, s+1\}\}_{s \in [\![-D, D-1]\!]}$, and ∇ is the operator defined by

$$\nabla\eta(s) = \eta(s) - \eta(s-1).$$

Proof. First, we let f and g be defined as in Lemma 5.7 with f having modulus of continuity η. For simplicity, let $f(\cdot) = f(\cdot, t)$. Then, for y, x achieving $\eta(s)$ with $f(y, t) > f(x, t)$, we have that

$$-\gamma(f(y) - f(x)) = \sum_{a \in \mathcal{K}} \Delta_a f(y) e^{g(ay) - g(y)} - \sum_{a \in \mathcal{K}} \Delta_a f(x) e^{g(ax) - g(x)}.$$

Suppose that $b^{-1}y$ and bx lie along a shortest path connecting y to x. We begin by

considering the interior terms

$$\Psi_i \equiv \Delta_{b^{-1}} f(y) e^{g(b^{-1}y) - g(y)} - \Delta_b f(x) e^{g(bx) - g(x)}.$$

In particular,

$$\begin{aligned} \Delta_{b^{-1}} f(y) &= f(b^{-1}y) - f(y) \\ &= f(b^{-1}y) - f(y) + f(x) - f(x) \\ &= f(b^{-1}y) - f(x) - \eta(s) \\ &\leq \eta(s-1) - \eta(s). \end{aligned}$$

In similar fashion, we also have that $-\Delta_b f(x) \leq (\eta(s-1) - \eta(s))$. Hence,

$$\begin{aligned} \Psi_i &\leq (\eta(s-1) - \eta(s)) \left(e^{\Delta_b^{-1} g(y)} + e^{\Delta_b g(x)} \right) \\ &= (\eta(s-1) - \eta(s)) \exp\left(\frac{\Delta_{b^{-1}} g(y) + \Delta_b g(x)}{2} \right) \left(e^p + e^{-p} \right) \end{aligned}$$

where $p = \frac{\Delta_{b^{-1}} g(y) - \Delta_b g(x)}{2}$. Then,

$$\begin{aligned} \Psi_i &\leq 2\cosh(p) \left(\eta(s-1) - \eta(s) \right) \exp\left(\frac{\Delta_{b^{-1}} g(y) + \Delta_b g(x)}{2} \right) \\ &\leq 2\cosh(p) \left(\eta(s-1) - \eta(s) \right) e^{\omega(s)}. \end{aligned}$$

where the final inequality comes from the definition of ω and the fact that $\eta(s-1) \leq \eta(s)$. The outer terms follow a similar procedure, where $\Delta_b f(y) \leq \eta(s+1) - \eta(s)$ and

$-\Delta_{b-1}f(x) \leq \eta(s+1) - \eta(s)$. For these, we have that

$$\Psi_o \equiv \Delta_b f(y) e^{\Delta_b g(y)} - \Delta_{b-1} f(x) e^{\Delta_{b-1} g(x)}$$

$$\leq (\eta(s+1) - \eta(s)) \left(e^{\Delta_b g(y)} + e^{\Delta_{b-1} g(x)} \right)$$

$$\leq (\eta(s+1) - \eta(s)) \left(e^{-\Delta_{b-1} g(y)} + e^{-\Delta_b g(x)} \right)$$

$$= 2\cosh(p) \left(\eta(s+1) - \eta(s) \right) \exp\left(\frac{-\Delta_{b-1} g(y) - \Delta_b g(x)}{2} \right)$$

$$\leq 2\cosh(p) \left(\eta(s+1) - \eta(s) \right) e^{-\omega(s)}.$$

Above, the second inequality follows from log-concavity and the final inequality follows from the definition of ω.

Combining Ψ_i and Ψ_o we have that,

$$-\gamma(f(y) - f(x)) = \Psi_i + \Psi_o$$

$$\leq 2\cosh(p) \left((\eta(s-1) - \eta(s)) e^{\omega(s)} + 2(\eta(s+1) - \eta(s)) e^{-\omega(s)} \right)$$

$$\leq 2\cosh(p) \left(-L_P \eta(s) + R \right)$$

where

$$R \equiv (\eta(s-1) - \eta(s)) (e^{\omega(s)} - 1) + (\eta(s+1) - \eta(s)) (e^{-\omega(s)} - 1).$$

Above, because log-concavity requires that $\omega(s) \geq 0$ and η is monotonic, both terms in R

are independently non-positive. Thus,

$$R = (\eta(s-1) - \eta(s))(e^{\omega(s)} - 1) + (\eta(s+1) - \eta(s))(e^{-\omega(s)} - 1)$$

$$= 2(\eta(s-1) - \eta(s))(\cosh(\omega(s)) - 1) + (\eta(s+1) - \eta(s-1))(e^{-\omega(s)} - 1)$$

$$\leq 2(\eta(s-1) - \eta(s))(\cosh(\omega(s)) - 1)$$

and we arrive at

$$-\gamma\eta(s) \leq 2\cosh(p)(-L_P\eta(s) - 2(\cosh(\omega(s)) - 1)\nabla\eta(s)).$$

Since the above inequality is trivially satisfied (and hence the proposition proven) if $-L_P\eta(s) - 2(\cosh(\omega(s)) - 1)\nabla\eta(s) \geq 0$, we note that $\cosh(p) \geq 1$ and then

$$-\gamma\eta(s) \leq -2L_P\eta(s) - 4(\cosh(\omega(s)) - 1)\nabla\eta(s).$$

$\square$

We now use Lemma 5.8 to perform various estimates on the spectral gap $\gamma(H)$. For our first estimate:

Theorem 5.5. *Suppose $H = L + W$ with ground state u_0, where L is the combinatorial Laplacian for some path graph S with diameter D and $W : V(S) \longrightarrow \mathbb{R}_{\geq 0}$. Then,*

$$\gamma(H) \geq 4(2\cosh(\overline{\omega}) - 1)\left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right)$$

$$\geq 4\left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right)$$

for $\log(u_0)$ having non-negative modulus of concavity ω and $\overline{\omega} = \inf_s \omega(s)$.

Proof. We begin with Lemma 5.8,

$$-\gamma\eta(s) \leq -2L_P\eta(s) - 4\cosh(\omega(s))-1))\nabla\eta(s)$$

$$= -2L_P\eta(s) - 4(\cosh(\omega(s))-1)(\eta(s)-\eta(s-1))$$

$$\leq -2L_P\eta(s) - 4(\cosh(\omega(s))-1)(2\eta(s)-\eta(s+1)-\eta(s-1))$$

$$= -2L_P\eta(s) - 4(\cosh(\omega(s))-1)L_P\eta(s)$$

$$= -2L_P\eta(s)(2\cosh(\omega(s))-1))$$

where L_P is defined as in Lemma 5.8 and the only inequality comes from adding a multiple of the non-negative term $\eta(s+1) - \eta(s)$. Hence, by the same analysis as Theorem 5.1,

$$\gamma(H) \geq 4\inf_s(2\cosh(\omega(s))-1)\left(1-\cos\left(\frac{\pi}{2D+1}\right)\right).$$

$\square$

Although this proof follows immediately from Lemma 5.8, taking $\omega \to 0$ and comparing to Theorem 5.1 reveals that it is not tight. For one, the methods of Lemma 5.8 are loose when $\omega(s) \sim 0$. This case is, of course, better handled by an approximation using the techniques of Section 5.3.1. Nonetheless, we can still improve upon the estimate of Theorem 5.5 in the case that the gradient of ω is bounded.

Theorem 5.6. *Suppose $H = L + W$ with ground state u_0, where L is the combinatorial Laplacian for some path graph S with diameter D and $W : V(S) \longrightarrow \mathbb{R}_{\geq 0}$. Then,*

$$\gamma(H) \geq 4\left(1-\cos\left(\frac{\pi}{2D+1}\right)\right) + 2\inf_s\left(\Delta^-\cosh(\omega(s))\right)$$

for $\log(u_0)$ with non-negative modulus of concavity ω where $\omega(D+1) = 0$ and $\overline{\omega} =$

$\inf_s \omega(s)$. *Above,*

$$\Delta^- \cosh(\omega(s)) = \cosh(\omega(s)) - \cosh(\omega(s+1)).$$

Proof. We once again begin with the result of Lemma 5.8

$$-\gamma\eta(s) \le -2L_P\eta(s) - 4(\cosh(\omega(s)) - 1)\nabla\eta(s),$$

and look to estimate the contribution of the term associated with the operator ∇. To do so, we consider the expected value of the associated term under η. Now, let $\omega(D+1) = 0$ and then, if $\nabla'\eta(s) = \cosh(\omega(s)) - 1)\nabla\eta(s)$,

$$
\begin{aligned}
\eta^\top \nabla' \eta &= \sum_{s=1}^{D} \eta(s)\left(\eta(s) - \eta(s-1)\right)\left(\cosh(\omega(s)) - 1\right) \\
&\ge \sum_{s=1}^{D} \frac{\eta(s) + \eta(s-1)}{2}\left(\eta(s) - \eta(s-1)\right)\left(\cosh(\omega(s)) - 1\right) \\
&= \frac{1}{2}\sum_{s=1}^{D}\left(\eta^2(s) - \eta^2(s-1)\right)\left(\cosh(\omega(s)) - 1\right)
\end{aligned}
$$

where the inequality follows from the monotonicity of η. Then,

$$
\begin{aligned}
2\eta^\top \nabla' \eta &= \sum_{s=1}^{D} \eta^2(s)(\cosh(\omega(s)) - 1) - \sum_{s=1}^{D} \eta^2(s-1)(\cosh(\omega(s)) - 1) \\
&= \sum_{s=1}^{D} \eta^2(s)(\cosh(\omega(s)) - 1) - \sum_{s=1}^{D-1} \eta^2(s)(\cosh(\omega(s+1)) - 1) \\
&= \sum_{s=1}^{D-1} \eta^2(s)(\cosh(\omega(s)) - \cosh(\omega(s+1))) + \eta^2(D)\left(\cosh(\omega(D)) - 1\right) \\
&= \sum_{s=1}^{D} \eta^2(s)\Delta^- \cosh(\omega(s)) \\
&\ge \inf_s \left(\Delta^- \cosh(\omega(s))\right) \sum_{s=1}^{D} \eta^2(s).
\end{aligned}
$$

Hence,

$$\frac{2\eta^\top \nabla' \eta}{|\eta|^2} \geq \inf_s \Delta^- \cosh\left(\omega(s)\right).$$

Thus, our estimate from Theorem 5.5 can be improved to

$$\gamma(H) \geq 4\left(1 - \cos\left(\frac{\pi}{2D+1}\right)\right) + 2\inf_s\left(\Delta^- \cosh(\omega(s))\right).$$

$\square$

Chapter 6:   Conclusions and open problems

The examples analyzed here and in [7, 33, 54, 57, 58] show that quantum adiabatic algorithms can succeed in finding the minimum in polynomial time in cases where classical local search fails to do so, and can fail in cases where classical local search succeeds. For both classical local search and adiabatic optimization, local minima of the potential that one is seeking to minimize play an important role in determining runtime. However, as the present work shows, these local minima do not tell the whole story. In particular, absence of local minima does not imply large eigenvalue gap.

In addition, we note that there remains much to be learned regarding the performance of adiabatic optimization algorithms relative to classical computation in the general case that one is not comparing only to classical local search. In particular, the ease of modulus of continuity methods indicate that heat diffusion processes are a good foil for adiabatic quantum computing, and we are currently exploring algorithms of this nature.

Probably the most significant results of this dissertation are those of Chapter 5. In general, modulus of continuity methods seem readily adaptable to both spectral graph theory and quantum theory. In particular, the results of Section 5.3.1 demonstrate that these estimates are quite strong for at least a certain class of graphs. The results of Section 5.4 are not immediately applicable in physical contexts, however Section 5.4.2 demonstrates ways in which they might be applied. These results can be strengthened by learning more about the relationship between the ratio u_1/u_0 and u_0 itself. Additionally, although a weak restriction, log-concavity may be an overly strong characterization of u_0 for practical pur-

poses and one may prefer to derive results entirely in terms of the modulus of concavity of $\log(u_0)$. Further, bounds on the modulus of concavity of $\log(u_0)$ should be reducible to bounds on the modulus of concavity of the potential term W' as seen in [12]. This comparison theorem is saved for future work, but since the potential term W' is typically provided in both physical and quantum-computational contexts, in common settings this modulus of concavity should be explicitly calculable.

There remains a great deal of work to be done on estimating runtimes for Adiabatic, sub-stochastic, and diffusive processes as well as classical algorithms for simulating them. The similarities between these different phenomena, mainly that they all approach their ground-states in time that scales with the spectral gap, is suggestive that they share asymptotic regimes and may indeed correspond in the adiabatic limit.

Appendix A: A sufficient condition for some node of $\mathbf{u}(\mu)$ to separate adjacent nodes of $\mathbf{u}(\lambda)$

In this section we give proof of Theorem 4.2. The following proof is adapted directly from Gantmakher and Kreĭn[38], however we consider vectors $\mathbf{u}(\lambda)$ and $\mathbf{u}(\mu)$ which need not be eigenvectors of the same matrix. Rather, we require only that these vectors satisfy eq. (4.12).

Theorem 4.2. *Let $\mathbf{u}(\mu;\alpha),\mathbf{u}(\lambda;\beta)$ be two vectors of length N satisfying eq. (4.12) and with*

$$\Theta_{W,i}(\mu - \lambda;\alpha,\beta) \leq 0 \ \forall\, i \in [\![m,n]\!] \tag{4.59}$$

where $\Theta_{W,i}(\mu - \lambda;\alpha,\beta) < 0$ for at least some $i \in [\![m,n]\!]$. We extend both vectors to length $N+2$ by including nodes at u_0 and u_{N+1}. (So long as eq. (4.12) is satisfied, despite previous choices of u_0 and u_{N+1}, these points are always considered nodes.) Let $\eta \in [m-1,m), \xi \in (n,n+1]$ be two adjacent nodes of $\mathbf{u}(\lambda;\beta)$ with $m \leq n \in [\![0,N+1]\!]$. Then there exists at least one node of $\mathbf{u}(\mu;\alpha)$ between η and ξ.

Proof. First, we consider the extension of vectors $\mathbf{u}(\mu;\alpha),\mathbf{u}(\lambda;\beta)$. From eq. (4.12) we take $W_1 \mapsto W_1 + 1$ and, for $\mathbf{u}(\lambda;\beta)$ get

$$(1 + W_1 - \lambda)u_1(\lambda) = u_2(\lambda) + u_0(\lambda) \tag{A.1}$$

and similarly for $\mathbf{u}(\mu;\alpha)$. Here, to maintain consistency between eqs. (4.12) and (A.1) we

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require that in eq. (A.1) $u_0 = 0$. Thus, u_0 is a node of **u**. We similarly treat u_{N+1} as a node. Further, since we have shifted W_1, W_N by constants, eq. (4.17) is unaltered. Hence, eq. (4.16) is unchanged and we can proceed with the proof.

Let $\eta \in [m-1, m)$ and $\xi \in (n, n+1]$ be successive nodes of $\mathbf{u}(\lambda; \beta)$ with $\eta < \xi$. Without loss of generality, we assume that $u_i(\lambda; \beta) > 0 \ \forall \ i \in [\![m, n]\!]$. Then,

$$\begin{cases} (m-\eta)u_{m-1}(\lambda; \beta) + (\eta - m + 1)u_m(\lambda; \beta) &= 0 \\ (n+1-\xi)u_n(\lambda; \beta) + (\xi - n)u_{n+1}(\lambda; \beta) &= 0 \end{cases} \tag{A.2}$$

Now, again without loss of generality, we assume that $u_i(\mu; \alpha) > 0 \ \forall \ i \in [\![m, n]\!]$. Hence, if $\mathbf{u}(\mu; \alpha)$ also has no nodes in (m, n), we get that

$$\begin{cases} (m-\eta)u_{m-1}(\mu; \alpha) + (\eta - m + 1)u_m(\mu; \alpha) &\geq 0 \\ (n+1-\xi)u_n(\mu; \alpha) + (\xi - n)u_{n+1}(\mu; \alpha) &\geq 0 \end{cases} \tag{A.3}$$

Combining eqs. (A.2) and (A.3) yields the inequalities

$$w_{m-1}(\mathbf{u}(\mu; \beta), \mathbf{u}(\lambda; \alpha)) \leq 0 \tag{A.4}$$

$$w_n(\mathbf{u}(\mu; \beta), \mathbf{u}(\lambda; \alpha)) \geq 0 \tag{A.5}$$

Recall from eq. (4.16) that

$$\Delta w_{i-1}(\mathbf{u}(\mu; \beta), \mathbf{u}(\lambda; \alpha)) = \Theta_{W,i}(\mu - \lambda; \beta, \alpha)u_i(\mu; \beta)u_i(\lambda; \alpha) \tag{A.6}$$

where by summing both sides,

$$w_n(\mathbf{u}(\mu; \beta), \mathbf{u}(\lambda; \alpha)) - w_{m-1}(\mathbf{u}(\mu; \beta), \mathbf{u}(\lambda; \alpha)) = \sum_{i=m}^{n} \Theta_{W,i}(\mu - \lambda; \beta, \alpha)u_i(\mu; \beta)u_i(\lambda; \alpha) \tag{A.7}$$

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Thus, by eqs. (A.4) and (A.5) we have that the left-hand side of eq. (A.7) is non-negative. Then, by our choice of $u_i(\lambda;\alpha), u_i(\mu;\beta) > 0 \,\forall\, i \in [\![m,n]\!]$, we see that if $\Theta_{W,i}(\mu - \lambda;\beta,\alpha) \leq 0 \,\forall\, i \in [\![m,n]\!]$ with at least some $i \in [\![m,n]\!]$ such that $\Theta_{W,i}(\mu - \lambda;\beta,\alpha) < 0$ we arrive at a contradiction. $\qquad\square$

Appendix B: For $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$, the node of $\mathbf{u}(\lambda_2)$ shifts left with increasing α.

Theorem B.1. *Let $\mathbf{H}_{\alpha U}(\mathbb{P}_N)$ be defined as in Lemma 4.8. Then, the node of $\mathbf{u}(\lambda_2)$ shifts left with increasing α.*

Proof. The proof proceeds in analogy to Lemma 4.8. First, note that by Corollary 4.1,

$$\langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_2)} \geq m - 1 \tag{B.1}$$

where m corresponds to the generalized zero of $\mathbf{u}(\lambda_2)$. Then, like eq. (4.61)

$$U_m - \langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_2)} = (m-1) - \langle \mathbf{U} \rangle_{\mathbf{u}(\lambda_2)} \leq 0. \tag{B.2}$$

Note that because $\mathbf{u}(\lambda_2)$ has at least one positive and one negative term, the inequality is strict when $m = 1$. If $m > 1$,

$$U_{m-1} - \langle \check{\ }_2 \rangle_{\mathbf{u}(\lambda_2)} < 0. \tag{B.3}$$

Thus, by eq. (4.60)

$$\frac{d\Theta_{U,i}}{d\beta} < 0 \quad \forall i \in [\![1, m]\!]. \tag{B.4}$$

Hence, by the same logic as Lemma 4.8, Theorem 4.2 applies and the node always shifts left with increasing α. $\qquad\square$

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