Quantum adiabatic optimization without heuristics

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Abstract

Quantum adiabatic optimization (QAO) is performed using a time-dependent Hamiltonian $H(s)$ with spectral gap $\gamma(s)$. Assuming the existence of an oracle $\Gamma$ such that $\gamma(s) = \Theta(\Gamma(s))$, we provide an algorithm that reliably performs QAO in time $O(\gamma^{-1}_{\text{min}} \log(\gamma^{-1}_{\text{min}}))$ with $O(\log(\gamma^{-1}_{\text{min}}))$ oracle queries, where $\gamma_{\text{min}} = \min_s \gamma(s)$. Our strategy is not heuristic and does not require guessing time parameters or annealing paths. Rather, our algorithm naturally produces an annealing path such that $dH/ds \approx \gamma(s)$ and chooses its own runtime $T$ to be as close as possible to optimal while promising convergence to the ground state.

We then demonstrate the feasibility of this approach in practice by explicitly constructing a gap oracle $\Gamma$ for the problem of finding a vertex $m = \arg\min_u W(u)$ of the cost function $W : V \rightarrow [0, 1]$, restricting ourselves to computational basis measurements and driving Hamiltonian $H(0) = I - V^{-1} \sum_{u,v \in V} |u \rangle \langle v|$, with $V = |V|$. Requiring only that $W$ have a constant lower bound on its spectral gap and upper bound $\kappa$ on its spectral ratio, our QAO algorithm returns $m$ using $\Gamma$ with probability $(1 - \epsilon)(1 - e^{-1/\epsilon})$ in time $O(\epsilon^{-1} [\sqrt{V} + (\kappa - 1)^{2/3} V^{2/3}])$. This achieves a quantum advantage for all $\kappa$, and when $\kappa \approx 1$, recovers Grover scaling up to logarithmic factors. We implement the algorithm as a subroutine in an optimization procedure that produces $m$ with exponentially small failure probability and expected runtime $O(\epsilon^{-1} [\sqrt{V} + (\kappa - 1)^{2/3} V^{2/3}])$, even when $\kappa$ is not known beforehand.

1 Introduction

Although adiabatic quantum computation (AQC) using general Hamiltonians is capable of universal quantum computation, near-term devices aiming to perform AQC typically focus on specific classes of Hamiltonians that are known to be implementable. In particular, some devices implement stoquastic Hamiltonians and are used predominantly for solving optimization problems. Indeed, a large-scale quantum annealer—that is, an adiabatic quantum computer operating at non-negligible temperature—has been constructed [15]. Nonetheless, whether a quantum advantage is obtainable with such a device is hotly debated [2, 5, 11].

One of the primary challenges in creating quantum adiabatic optimization (QAO) algorithms is understanding the nature of the spectral gap, which imposes, via the quantum adiabatic theorem, the schedule required for adiabatic evolution. A successful adiabatic computation using a Hamiltonian requires a runtime
that scales inversely with a power of its spectral gap. Unfortunately, obtaining useful analytic bounds on the gap is generally infeasible, and even if the size of the minimal gap were known, determining where the gap is small may be necessary to make QAO more efficient than classical algorithms [17]. One strategy for avoiding this issue would be to search for adiabatic schedules that work for most, but not all, possible problems [20], but the standard approach to optimizing an annealing schedule requires a detailed analysis of the entire Hamiltonian [1]. Current suggestions for adaptive control of adiabatic evolution depend on minimizing an associated Lagrangian; however, this may require knowledge of the cost function (up to permutation) and an approximation for the spectral gap of the Hamiltonian [3, 16, 22, 18]. Alternative methods either abandon the adiabatic procedure altogether [19, 18] or modify the Hamiltonian [8, 21]. These methods may not work for large classes of problems, or rely on solving equations that may be unknown for an arbitrary cost function.

In this paper, we present a general algorithm for adiabatic state preparation, which we then apply to QAO. We show that given a Hamiltonian \( H(s) \) (for \( s \in [0, 1] \)) with spectral gap \( \gamma(s) \), an adiabatic optimization algorithm can be completed in time \( \tilde{O}(\gamma^{-1}_{\min}) \) with \( \mathcal{O}(\log(\gamma^{-1}_{\min})) \) queries to the oracle under relatively weak constraints. Here, \( \gamma_{\min} \equiv \min_{s \in [0, 1]} \gamma(s) \) denotes the minimum gap. Discretization methods similar to those we will utilize already exist, but their utility depends upon the choice of discretization points. In order to make a good choice, one needs to determine an appropriate adiabatic schedule in advance and may require additional machinery beyond knowledge of the initial Hamiltonian \( H(0) \) and final Hamiltonian \( H(1) \) [4, 6]. In contrast, our algorithm discovers a near-optimal path dynamically.

In the first part of the paper, we assume access to a gap oracle \( \Gamma \) for which \( \gamma(s) = \Theta(\Gamma) \). If we assume that \( I_k \equiv \{ s \in [0, 1] \mid \Gamma(s) < \max_s \|H(s)\|^2 \} \) has measure \( \mu(I_k) \leq C2^{-k} \) for all nonnegative integers \( k \), where \( C \) is a constant independent of the problem size, and if each \( I_k \) is the union of at most \( \mathcal{O}(1) \) disjoint intervals, then for a Hamiltonian with \( \max_s \|H(s)\| = \mathcal{O}(1) \) our approach requires \( \mathcal{O}(\max_s \log(1/\Gamma(s))) \) queries to the oracle and \( \mathcal{O}(\max_s 1/\Gamma(s) \log(1/\Gamma(s))) \) time to prepare the final adiabatic state. (The idea behind this constraint is that the total amount of time \( H(s) \) has a gap less than \( \gamma \) should be proportional to \( \gamma \) itself. (We actually use a stronger constraint in the main text and relax to our looser condition in Appendix A.) The runtime of our algorithm then matches the best cases achievable by the approach of, say, [4] without randomized unitaries, a need to guess at discretization points, or substantial knowledge of the cost function.

This approach obviates the need for an analytic bound on the spectral gap by creating an algorithm that learns the gap. The weighted Cheeger constant \( h \) [7, 13] serves this purpose, and sometimes may be efficiently computable. In the case of stoquastic Hamiltonians of the form \( H(s) = (1-s)L + sW \), where \( L \) is the combinatorial Laplacian for a graph with \( V \) vertices and maximum degree \( d \) and \( W \) is a real diagonal matrix,

\[
2h(s) \geq \gamma(s) \geq \sqrt{h(s)^2 + d^2 - d},
\]

where \( h(s) \) is the weighted Cheeger constant of \( H(s) \) [13]. When \( d \) does not depend on \( V \), this scales with \( h \) provided \( h \gtrsim d \). On the other hand, if \( d \) is allowed to scale with \( V \), the bound can be quadratically loose. Thus, to create an oracle for the gap, one wants to build driving Hamiltonians \( L \) such that \( H \) tracks the lower bound of \( \gamma(H) \) with high probability. Additionally, as we will show in Section 5, it appears possible to obtain tight Cheeger inequalities once \( C \) is fixed and our actual performance may depend upon our ability to do so. Indeed, our approach might instruct us as to what models are useful for near-term optimizers and how to perform optimization within those models.

In the second part of the paper, we explicitly construct a gap oracle \( \Gamma \) for the model in which the driving Hamiltonian \( H(0) \) is the Laplacian \( L \) of a complete graph, and the final Hamiltonian \( H(1) \) is an unknown diagonal \( W \). We show that with only knowledge of \( H(0) \) and no knowledge of \( H(1) \), with bounded probability we can construct the Hamiltonian \( H(s) \) and return the ground state of \( H(1) \) with runtime \( \tilde{O}(\sqrt{\nu} + (\kappa - 1)V^{2/3}) \), where \( \kappa \) is the ratio of the largest to second-smallest eigenvalue of \( H(1) \). Modulo logarithmic terms, our adiabatic algorithm scales optimally when presented with a problem similar to Grover search despite the algorithm being unaware that this was the case, and we achieve a quantum advantage over classical search in every setting.

The inherent technical difficulty above arises in problems more general than Grover search, which suffer from two inherent difficulties. First, in our picture where \( \|L\| = V \), the Grover problem utilizes a matrix \( W = \text{diag}(0, V, V, \ldots, V) \) where \( V \) is the number of vertices of the complete graph \( L \). Relaxing this constraint
to only, say, $W = \epsilon \text{diag}(0, V, V, \ldots, V)$ shifts the location of the gap minimum as can be seen in Fig. 1. In order to apply Grover-type analytic results to such a situation would require us to first learn $\epsilon$ itself. The yet more general problem we attack introduces a new issue also illustrated in Fig. 1: not only is the location of the minimal gap unknown, but the continuous profile of the gap is unknown. Thus, we need an algorithm that can, in real time, determine the size of $\gamma(s)$. In the most general case where the spectral ratio of $W$ is a constant independent of problem size $\kappa \geq 1$, the ratio of its largest to second-smallest eigenvalues, we obtain $\mathcal{O}(\sqrt{V} + (\kappa - 1)^{2/3}V^{2/3})$ scaling. It remains unclear whether the scaling with $\kappa$ can be improved in this setting.

Part I

The general algorithm

2 The Bashful Adiabatic Algorithm

The basic algorithm analyzed in this paper was first sketched in [13]. Because we do not have an analytic expression for the spectral gap, we cannot solve a differential equation to obtain an evolution strategy like that of [17]. Instead, we set “checkpoints” $s_i$ where we estimate the gap $\gamma_i$. We then use the estimates $\gamma_i$ and $\gamma_{i+1}$ to determine the rate of evolution for the interval $(s_i, s_{i+1})$. Given such a profile $\{(s_i, \gamma_i)\}$, it is straightforward to develop an algorithm for adiabatic state preparation. Formally this is presented as Algorithm 1 below, the analysis of which is covered in Section 3.1.

Algorithm 1 Adiabatic state preparation

Require: A time-dependent Hamiltonian $H(s)$ linear in $s \in [0, 1]$, $\lambda_{\text{max}}$ such that $\lambda_{\text{max}} \geq \|H(s)\|$, an array $\vec{\gamma}$, a parameter $\epsilon$, a universal constant $c_0 \in (0, 1)$.

1: function GENERATESTATE($\vec{\gamma}, \delta s, \epsilon$) \hspace{1cm} $\triangleright$ Adiabatically generate a state according to Theorem 2
2: $(s_f, \gamma_f) = \text{LAST}(\vec{\gamma})$ \hspace{1cm} $\triangleright$ Get last element of $\vec{\gamma}$
3: if $\delta s \neq 0$ then
4: $s_f \leftarrow \min(s_f + \delta s, 1)$
5: $\gamma_f \leftarrow \gamma_f - 4\delta s \lambda_{\text{max}}$
6: Append $(s_f, \gamma_f)$ to $\vec{\gamma}$ \hspace{1cm} $\triangleright$ Saturate Proposition 3
7: $\tilde{P} \leftarrow |\phi(0)\rangle \langle \phi(0)|$
8: $(s_0, \gamma_0) \leftarrow \text{NEXT}(\vec{\gamma})$ \hspace{1cm} $\triangleright$ Prepare the ground state of $H(0)$
9: while $(s_1, \gamma_1) \leftarrow \text{NEXT}(\vec{\gamma})$ do
10: $\gamma_{\text{min}} \leftarrow \frac{1}{2}(\gamma_0 + \gamma_1 - 4\lambda_{\text{max}}(s_1 - s_0))$ \hspace{1cm} $\triangleright$ Apply Proposition 3 to both endpoints
11: $H(\sigma) \leftarrow \frac{1}{\lambda_{\text{max}}} [(1 - \sigma)H(s_0) + \sigma H(s_1)]$ \hspace{1cm} $\triangleright$ Version of $H$ with norm $\mathcal{O}(1)$
12: $T \leftarrow \left(c_0 + \frac{7c_0^2}{\epsilon \gamma_{\text{min}}} \right)$ \hspace{1cm} $\triangleright$ Set time using Corollary 1
13: $\tilde{P} \leftarrow U\tilde{P}U^\dagger$ using Eq. (1) with $H(s) \leftrightarrow H(\sigma)$ and time $T$
14: $(s_0, \gamma_0) \leftarrow (s_1, \gamma_1)$
15: return $\Psi$

The idea behind the bashful adiabatic algorithm is to generate each subsequent checkpoint using information derived from its predecessors and Algorithm 1. At a high level we may treat the routine which bounds the spectral gap as an oracle, which allows us to state BAA as Algorithm 2, and analyze the number of oracle calls BAA requires in Section 3.3. The schedule ultimately produced by BAA is similar to those proposed in [4], however the primary purpose of BAA is to determine this schedule such that we know to have near-optimal scaling in the spectral gap.
The existence of the weighted Cheeger constant $h$ and the fact that it depends only on information contained in the ground-state distribution means that, at least in some circumstances, one can indeed create an oracle like that required by Algorithm 2.

3 Analysis of BAA

3.1 Modifying the Adiabatic Theorem

According to the quantum adiabatic theorem, a quantum system initially in the (non-degenerate) ground state of a time-dependent Hamiltonian will remain close to its instantaneous ground state if the Hamiltonian changes sufficiently slowly. Most quantitative versions of the theorem appear in a form similar to that of Theorem 1 below. Given a total evolution time $T$, we define a scaled time parameter $s \equiv t/T$, and consider the unitary $\hat{U}(t)$ that evolves the system governed by Hamiltonian $H(t/T)$. The Schrödinger equation reads

$$\frac{i}{\hbar} \frac{d\hat{U}(t)}{dt} = H(t/T)\hat{U}(t), \quad \hat{U}(0) = I,$$

or, equivalently,

$$\frac{i}{\hbar} \frac{dU(s)}{ds} = TH(s)U(s), \quad U(0) = I,$$

with $U(s) = \hat{U}(t)$. In [12], the authors provide quantitative bounds on the deviation of an adiabatically prepared state from the instantaneous ground-state in terms of $T$. We restate the result as Theorem 1, restricting to Hamiltonians with non-degenerate ground states.

**Theorem 1** ([12, Theorem 3]). *Suppose that $H(s)$ is a self-adjoint operator on an $N$-dimensional Hilbert space, with eigenvalues $\lambda_0(s) < \lambda_1(s) \leq \ldots \leq \lambda_{N-1}(s)$. For all $s \in [0, 1]$, let $P(s)$ denote the projector onto the ground state of $H(s)$, so that $H(s)P(s) = \lambda_0(s)P(s)$, and define $\tilde{P}(s) \equiv U(s)P(0)U(s)^\dagger$, where $U$ satisfies Eq. (1). Then*

$$\left\| \tilde{P}(s) - P(s) \right\| \leq A(s),$$

*where*

$$A(s) \leq \frac{1}{T} \left[ \frac{\| \dot{H}(0) \|}{\gamma(0)^2} + \frac{\| \dot{H}(s) \|}{\gamma(s)^2} + \int_0^s ds' \left( \frac{\| \ddot{H}(s') \|}{\gamma(s')^3} + \frac{\| \dddot{H}(s') \|}{\gamma(s')^4} \right) \right]$$

*with $\gamma(s) \equiv \lambda_1(s) - \lambda_0(s)$ and*

$$\tilde{H}(a) = \frac{dH(s)}{ds} \bigg|_{s=a}, \quad \dot{H}(a) = \frac{d^2H(s)}{ds^2} \bigg|_{s=a},$$
A simple restriction of Theorem 1 yields the following.

**Proposition 1.** Suppose all quantities are defined as in Theorem 1. If \( \|\dot{H}(s)\| \leq c_0 \gamma(s)/2 \) and \( \|\ddot{H}(s)\| \leq c_1 \gamma(s) \) for all \( s \in [0, 1] \), then

\[
A(s) \leq \frac{1}{T} \left( \frac{c_0 + 7c_0^2/4 + c_1}{\min_{s \in [0, 1]} \gamma(s)} \right).
\]

In other words, if both the first and the second derivative of \( H(s) \) are upper-bounded in terms of the spectral gap \( \gamma(s) \), and \( c_0, c_1 = O(1) \) are constants independent of \( \gamma_{\text{min}} \), then the adiabatic theorem guarantees that scaling \( T \sim \gamma^{-1}_{\text{min}} \) can arbitrarily reduce \( A \). Although Proposition 1 is not satisfied for constants \( c_0, c_1 \) by most time-dependent Hamiltonians, we can perform a computationally equivalent process by chaining together a sequence of interpolating Hamiltonians.

**Theorem 2.** For a given self-adjoint operator \( H(s) \) on a finite-dimensional space, define an associated operator \( H_L(s) \) piecewise linear in \( s \) as

\[
H_L(s) = \begin{cases} 
T_0/s_1 H(0), & s = 0 \\
\frac{1}{s_{i+1} - s_i} \left( 1 - \frac{s - s_i}{s_{i+1} - s_i} \right) H(s_i) + \frac{s - s_i}{s_{i+1} - s_i} H(s_{i+1}) \right) I(s_i, s_{i+1})(s), & s \in (0, 1]
\end{cases}
\]

for \( 0 = s_0 < s_1 < \cdots < s_q = 1 \) and \( T_0, T_1, \ldots, T_{q-1} > 0 \). For all \( s \in [0, 1] \), let \( P_L(s) \) denote the projector onto the ground state of \( H_L(s) \), and define \( \tilde{P}_L(s) \equiv U_L(s)P_L(0)U_L(s)^\dagger \), where \( U_L \) is the unitary satisfying

\[
\frac{dU_L(s)}{ds} = H_L(s)U_L(s), \quad U_L(0) = I.
\]

Then

\[
\left\| \tilde{P}_L(s_j) - P_L(s_j) \right\| \leq \sum_{i=0}^{j-1} A_i
\]

for all \( j \), where \( A_i \) is any upper bound that results from applying Theorem 1 to the Hamiltonian \( (1-s)H(s_i) + sH(s_{i+1}) \) over the interval \( s \in [0, 1] \) with total evolution time \( T_i \).

**Proof.** For \( s \in (s_i, s_{i+1}] \), \( U_L \) can be written as

\[
U_L(s) = U_i(s)U_{i-1}(s_i) \cdots U_0(s_1)
\]

where for each \( i = 0, 1, \ldots, q - 1 \), \( U_i \) satisfies

\[
\frac{dU_i(s)}{ds} = \frac{T_i}{s_{i+1} - s_i} \left[ \left( 1 - \frac{s - s_i}{s_{i+1} - s_i} \right) H(s_i) + \frac{s - s_i}{s_{i+1} - s_i} H(s_{i+1}) \right] U_i(s), \quad U_i(s_i) = I
\]

(3)

Making a change of variables

\[
\sigma_i = \frac{s - s_i}{s_{i+1} - s_i}
\]

and defining

\[
H_i(\sigma_i) = (1 - \sigma_i)H(s_i) + \sigma_i H(s_{i+1})
\]

for \( \sigma_i \in [0, 1] \), we see that Eq. (3) is equivalent to

\[
\frac{dU_i(s)}{d\sigma_i} = T_i H_i(\sigma_i)U_i(s), \quad U_i(\sigma_i = 0) = I,
\]

(4)
so Theorem 1 applies to each \( H_i \) over the interval \( \sigma_i \in [0, 1] \) (i.e., \( s \in [s_i, s_{i+1}] \)), with \( T \rightarrow T_i \) and projector \( P_L(s_i) \) onto the ground state at \( \sigma_i = 0 \). We prove Eq. (2) by induction. The base case holds since \( P_L(0) = P_L(0) \). Assume Eq. (2) is true for some integer \( j \geq 1 \). Then,

\[
\| \bar{P}_L(s_{j+1}) - P_L(s_{j+1}) \| = \| U_L(s_{j+1}) P_L(0) U_L(s_{j+1})^\dagger - P_L(s_{j+1}) \|
\]

\[
= \| U_L(s_{j+1}) U_L(s_{j+1})^\dagger U_L(s_{j+1}) - P_L(s_{j+1}) \|
\]

\[
= \| U_L(s_{j+1}) P_L(s_{j+1}) U_L(s_{j+1})^\dagger - P_L(s_{j+1}) \|
\]

\[
\leq \sum_{i=0}^{j-1} A_i + A_j
\]

\[
= \sum_{i=0}^{j} A_i,
\]

where the second inequality follows from applying the inductive hypothesis to the first term and Theorem 1 to the second. Eq. (2) is thus true for all \( j \).

Corollary 1. Suppose that \( H(s) \) is linear in \( s \). Let all quantities be defined as in Theorem 2, and let \( \gamma_{i, \min} \equiv \inf_{s \in [s_i, s_{i+1}]} \gamma(s) \), where \( \gamma(s) \) denotes the spectral gap of \( H(s) \). If for all \( i \),

\[
s_{i+1} - s_i \leq \frac{c_0 \gamma_{i, \min}}{2\|H\|}, \quad T_i \geq \frac{q(c_0 + 7c_0^2/4)}{c\gamma_{i, \min}}
\]

for some \( c_0 > 0 \) and constant \( \epsilon > 0 \), then

\[
\| \bar{P}_L(1) - P_L(1) \| \leq \epsilon.
\]

Proof. By Theorem 2,

\[
\| \bar{P}_L(1) - P_L(1) \| = \| \bar{P}_L(s_q) - P_L(s_q) \| \leq \sum_{i=0}^{q-1} A_i.
\]

Since

\[
\| dH_i(\sigma_i) \| = \| H(s_{i+1}) - H(s_i) \| = \| (s_{i+1} - s_i) \dot{H} \| \leq \frac{c_0 \gamma_i}{2}
\]

by our assumption on the step sizes \( s_{i+1} - s_i \) and \( \| d^2 H_i(\sigma_i) / d\sigma^2 \| = 0 \), Proposition 1 applies to each \( A_i \) independently, giving

\[
\sum_{i=0}^{q-1} A_i \leq \sum_{i=0}^{q-1} \frac{1}{T_i} \left( \frac{c_0 + 7c_0^2/4}{\gamma_i} \right) \leq \sum_{i=0}^{q-1} \frac{\epsilon}{q} = \epsilon,
\]

where the second inequality follows from our assumption on the bound on each \( T_i \).

Typically, a weaker form of Theorem 1 is used, with

\[
A(s) \leq \frac{1}{T} \left[ \frac{2}{\min_{s \in [0, 1]} \gamma(s)} \frac{\| \dot{H}(s') \|}{2} + \int_0^1 ds' \left( \frac{7}{\gamma(s')^3} \frac{\| \dot{H}(s') \|^2}{2} + \frac{\| \ddot{H}(s') \|}{\gamma(s')^2} \right) \right] \equiv A,
\]

(4)
for all \( s \in [0, 1] \). If \( H(s) \) is linear in \( s \), the upper bound simplifies to

\[
A = \frac{1}{T} \left[ \frac{2 \norm{\dot{H}}}{(\min_{s \in [0, 1]} \gamma(s))^2} \sum_{i=0}^{k-1} \delta s_i \norm{\frac{dH_i(s_i)}{ds}} + 7 \int_{0}^{s_{i+1}} ds \frac{\norm{\frac{dH_i(s_i)}{ds}}^2}{\gamma(s)^3} \right].
\]

(5)

Since each \( H_i(s) \) considered in Theorem 2 is linear in \( s \), we see that we can take the upper bounds \( A_i \) in Theorem 2 to be

\[
A_i = \frac{1}{T_i} \left[ \frac{2 \norm{\dot{H}_i}}{(\min_{s \in [0, 1]} \gamma_i(s))^2} \norm{\frac{dH_i(s_i)}{ds}} + 7 \int_{0}^{s_{i+1}} ds \frac{\norm{\frac{dH_i(s_i)}{ds}}^2}{\gamma_i(s)^3} \right],
\]

where \( \gamma_i(s) = \gamma(s(s_{i+1} - s_i) + s_i) \) is the spectral gap of \( H_i(s) \).

The following theorem demonstrates that if we take a prescribed linear evolution over a time \( T \) and divide it into a sequence of \( k \) linear evolutions, each taking time \( T_i \geq T \) for \( i \in [k-1] \), the total divergence from the ground state does not scale with \( k \). One can actually show that the divergence decreases, but doing so requires working directly with the proof of Theorem 1, which is beyond the scope of this paper.

**Theorem 3.** Suppose that \( H(s) \) is linear in \( s \), and let all quantities be defined as in Theorems 1 and 2. If \( T_i \geq T \) for all \( i = 0, 1, \ldots, k \), then

\[
\sum_i A_i \leq A,
\]

with \( A \) and \( A_i \) as defined in Eqs. (5) and (6).

**Proof.** Since \( H(s) \) is linear in \( s \), \( \norm{\bar{P}(1) - P(1)} \leq A \), where \( A \) is defined as in Eq. (5), and letting \( \delta s_i \equiv s_{i+1} - s_i \), we have

\[
\norm{\frac{dH_i(s_i)}{ds}} = \delta s_i \norm{\frac{dH(s)}{ds}}
\]

for all \( i = 0, 1, \ldots, k-1 \), where \( \norm{\frac{dH(s)}{ds}} \) is constant. Then, Eq. (5) can be written

\[
A = \frac{1}{T} \left[ \frac{2 \norm{\dot{H}}}{(\min_{s \in [0, 1]} \gamma(s))^2} \sum_{i=0}^{k-1} \delta s_i \norm{\frac{dH(s)}{ds}} + 7 \sum_{i=0}^{k-1} \int_{s_i}^{s_{i+1}} ds \frac{\norm{\frac{dH(s)}{ds}}^2}{\gamma(s)^3} \right]
\]

\[
= \frac{1}{T} \left[ \frac{2 \norm{\dot{H}_i}}{(\min_{s \in [0, 1]} \gamma_i(s))^2} \norm{\frac{dH_i(s_i)}{ds}} + 7 \int_{s_i}^{s_{i+1}} ds \frac{\norm{\frac{dH_i(s_i)}{ds}}^2}{\gamma_i(s)^3} \right]
\]

\[
\geq \frac{1}{T_i} \left[ \frac{2 \norm{\dot{H}_i}}{(\min_{s \in [0, 1]} \gamma_i(s))^2} \norm{\frac{dH_i(s_i)}{ds}} + 7 \int_{0}^{1} ds \frac{\norm{\frac{dH_i(s_i)}{ds}}^2}{\gamma_i(s)^3} \right].
\]

Now, since \( T_i \geq T \) for all \( i \), we have

\[
A \geq \sum_{i=0}^{k-1} \frac{1}{T_i} \left[ \frac{2 \norm{\dot{H}_i}}{(\min_{s \in [0, 1]} \gamma_i(s))^2} \norm{\frac{dH_i(s_i)}{ds}} + 7 \int_{0}^{1} ds \frac{\norm{\frac{dH_i(s_i)}{ds}}^2}{\gamma_i(s)^3} \right] = \sum_i A_i.
\]
3.2 Perturbation bounds

Since the divergence from the ground state is additive in Theorem 2, we would like each $A_j$ of Theorem 2 to satisfy Proposition 1 with $c_0, c_1 = O(1)$. Thus, we need to determine an appropriate set $\{s_i\}_i$ such that Proposition 1 applied to each interval $[s_i, s_{i+1}]$ obeys these constraints. Weyl’s inequalities allow us to bound the change in the spectral gap relative to the step size $s_{i+1} - s_i$.

**Proposition 2.** Suppose that $H(s)$ is linear in $s$ and let $\gamma(s)$ denote the spectral gap of $H(s)$. Then, for $\delta s > 0$,

$$|\gamma(s + \delta s) - \gamma(s)| \leq 2\delta s \|\dot{H}\|.$$  

*Proof.* Since $H(s)$ is linear is $s$, $H(s + \delta s) = H(s) + \delta s \dot{H}$. It follows from a straightforward application of Weyl’s inequality to the eigenvalues of $H(s + \delta s)$ that

$$\gamma(s) - 2\delta s \|\dot{H}\| \leq \gamma(s + \delta s) \leq \gamma(s) + 2\delta s \|\dot{H}\|.$$  

□

To control the algorithm, we will want to choose the largest $\delta s$ in Proposition 2 for which the change $|\gamma(s + \delta s) - \gamma(s)|$ is small relative to $\gamma(s)$. The following proposition gives us an upper bound on a suitable $\delta s$.

**Proposition 3.** Suppose that $H(s)$ is linear in $s$ and let $\gamma(s)$ denote the spectral gap of $H(s)$. If $0 < \delta s \leq c_0 \gamma(s)/2 \|\dot{H}\|$ for some $c_0 > 0$, then

$$|\gamma(s + \delta s) - \gamma(s)| \leq c_0 \gamma(s).$$

*Proof.* This follows immediately from Proposition 2. □

3.3 Number of queries

The following proposition guarantees that if we have access to an oracle that estimates the gap and this oracle admits a suitably convex modulus, then Algorithm 2 requires $O(\log(1/\min_{s} \gamma(s)))$ queries to the oracle. That is, we determine that the query complexity in GETGAP is logarithmic provided only that the minimum gap is well-behaved.

Our modulus simply implies that the width in $s$ of the minimum gap should be at worst proportional to the size of the minimum gap. In fact, this is a fairly weak constraint that we would expect this to be true for most Hamiltonians. Nonetheless, this can potentially be difficult to prove. For Hamiltonians with many local minima, we can use lower bounds from a series of envelopes like that below or show that the gap always obeys the modulus of the global minimum.

**Theorem 4.** Let all quantities be defined as in Algorithm 2, and let $\Gamma(s) = \text{GETGAP}(s, 0, \cdot)$ with oracle $\Gamma$ and constant $c_0 \in (0, 1)$. If there exist constants $\alpha, \beta \in (0, 1]$ such that

$$\Gamma(s) \geq \alpha \lambda_{\max}|s - s_{\min}| + \beta \Gamma(s_{\min}),$$

for some $s_{\min} \in [0, 1]$, then Algorithm 2 requires at most

$$2 \left\lfloor \frac{\log \left(1 + \frac{\alpha \lambda_{\max}}{2 \beta \Gamma(s_{\min})}\right)}{\log \left(1 + \frac{c_0 \alpha}{4}\right)} \right\rfloor$$

queries to GETGAP.

---

1Theorem 11 in Appendix A is more general than Theorem 4 and makes this intuition more precise, however is not always as tight. Nonetheless, because it is more generally applicable and retains the same scaling behavior, Theorem 11 may be of more interest to the casual reader.
Proof. In Algorithm 2, we query $\Gamma$ at points $\{s_i\}$ given by the recurrence relation

$$s_{i+1} = s_i + \frac{c_0 \Gamma(s_i)}{4\lambda_{\text{max}}}.$$  

First, consider the case that $s < s_{\text{min}}$. Letting $\tau_i = s_{\text{min}} - s_i$, it follows from our assumption on the $\Gamma(s)$ that

$$\tau_{i+1} = \tau_i - \frac{c_0 \Gamma(s_i)}{4\lambda_{\text{max}}} \leq \left(1 - \frac{c_0 \alpha}{4}\right) \tau_i - \frac{c_0 \beta \Gamma(s_{\text{min}})}{4\lambda_{\text{max}}}. \tag{7}$$

Imposing the boundary condition $\tau_0 = s_{\text{min}} - s_0 = s_{\text{min}},$

$$\tau_i \leq \left(1 - \frac{c_0 \alpha}{4}\right)^i \left(s_{\text{min}} + \frac{\beta \Gamma(s_{\text{min}})}{\alpha \lambda_{\text{max}}} \right) - \frac{\beta \Gamma(s_{\text{min}})}{\alpha \lambda_{\text{max}}}$$

Thus, for

$$i = \left\lceil \frac{- \log (1 + \frac{\alpha \lambda_{\text{max}}}{\beta \Gamma(s_{\text{min}})})}{\log (1 - \frac{c_0 \alpha}{4})} \right\rceil$$

we are guaranteed that $\tau_i \leq 0$ and hence $s_i \geq s_{\text{min}}$.

Now, let $j$ correspond to the first $i$ such that $s_i \geq s_{\text{min}}$. Letting $s'_i = s_{j+i} - s_{\text{min}}$,

$$s'_{i+1} = s'_i + \frac{c_0 \Gamma(s'_i)}{4\lambda_{\text{max}}} \geq \left(1 + \frac{c_0 \alpha}{4}\right) s'_i + \frac{c_0 \beta \Gamma(s_{\text{min}})}{4\lambda_{\text{max}}}.$$  

Imposing the boundary condition $\tau'_0 \geq 0$,

$$\tau' \geq \left(1 + \frac{c_0 \alpha}{4}\right)^i \frac{\beta \Gamma(s_{\text{min}})}{\alpha \lambda_{\text{max}}} - 1$$

so for

$$i = \left\lceil \frac{\log (1 + \frac{\alpha \lambda_{\text{max}}}{\beta \Gamma(s_{\text{min}})})}{\log (1 + \frac{c_0 \alpha}{4})} \right\rceil$$

we are guaranteed that $\tau'_i \geq 1$ and hence $s'_i \geq 1$.

Combining both regions, we find that the algorithm terminates after at most

$$2 \left\lceil \frac{\log (1 + \frac{\alpha \lambda_{\text{max}}}{\beta \Gamma(s_{\text{min}})})}{\log (1 + \frac{c_0 \alpha}{4})} \right\rceil$$

queries to $\Gamma$. \qed

For simplicity in the following, we define

$$Q(x, y) \equiv 2 \left\lceil \frac{\log (1 + x)}{\log (1 + y)} \right\rceil. \tag{8}$$

**Corollary 2.** Let $\gamma_{\text{min}} \equiv \min_{s} H(s)$. Under the assumptions of Theorem 4, if $\alpha, \beta \in (0, 1]$ and $\epsilon > 0$ are constants independent of $\gamma_{\text{min}}$ and $(1 + \epsilon) \Gamma(s_{\text{min}}) \leq \gamma_{\text{min}}$, then Algorithm 2 completes after at most

$$Q \left(\frac{(1 + \epsilon) \alpha \lambda_{\text{max}}}{\beta \gamma_{\text{min}}}, \frac{c_0 \alpha}{4}\right) = \Theta \left(\log \left(\frac{\lambda_{\text{max}}}{\gamma_{\text{min}}}ight) \right)$$

queries to $\text{GetGap}$.

The final theorem of this section demonstrates that Algorithm 2 will successfully produce a state within $O(\epsilon)$ of the ground state of $H(1)$ provided it satisfies the constraints above. Recall that the final step of Algorithm 2 is a call to Algorithm 1 ($\text{GenerateState}$) which adiabatically prepares the final state of $H(1)$.  

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Theorem 5. Under the conditions of Corollary 2, if \( \gamma(s) = \Omega(\Gamma(s)) \), then \( \text{GenerateState}(\vec{\gamma}, 0, \epsilon/dim(\vec{\gamma})) \) takes time \( O\left(\frac{\lambda_{\max}}{\epsilon \gamma_{\min}} \log^2 \left(\frac{\lambda_{\max}}{\gamma_{\min}}\right)\right) \). Furthermore, if \( P(1) \) is the projector onto the ground state of \( H(1) \), then Algorithm 2 produces a state corresponding to projector \( \tilde{P}(1) \) such that
\[
\|\tilde{P}(1) - P(1)\| = O(\epsilon).
\]

Proof. By Proposition 3, each step of Algorithm 2 produces checkpoints \( \vec{\gamma} = ((s_i, \gamma_i)) \) such that \( \gamma(s \in [s_i, s_{i+1}]) = \Theta(\gamma_i) \). Furthermore, Corollary 2 guarantees that \( \dim(\vec{\gamma}) = O(\log(\lambda_{\max}^{-1}) \gamma_{\min}) \). Thus, each iteration of the main loop of Algorithm 1 Step 9 takes at most time \( T_i = O\left(\frac{\lambda_{\max}}{\epsilon \gamma_{\min}} \log(\lambda_{\max}^{-1}) \gamma_{\min}\right) \). Since we require \( O\left(\log(\lambda_{\max}^{-1}) \gamma_{\min}\right) \) iterations, the total time for \( \text{GenerateState}(\vec{\gamma}, 0) \) is \( O\left(\frac{\lambda_{\max}}{\gamma_{\min}} \log^2(\lambda_{\max}^{-1}) \gamma_{\min}\right) \).

By Corollary 1, this guarantees that we produce a state for which \( \|\tilde{P}(1) - P(1)\| \leq \epsilon \).

\[ \square \]

Part II

BAA on the complete graph

We will now apply Algorithm 2 to a toy model where the initial Hamiltonian \( H(0) \equiv L \) is the combinatorial Laplacian of the complete graph on \( V \) vertices and the final Hamiltonian \( H(1) \equiv \text{diag}(W) \), where \( W : V \rightarrow [0, V] \) is a cost function with a constant upper bound on its spectral ratio and \( \min_u W(u) = 0 \). Fig. 1 shows how difficult performing adiabatic optimization in this simple scenario can be. Even if \( W \) is proportional to the Grover cost function, i.e., \( W = (0, C, C, \ldots, C) \), we cannot easily apply the strategy of [17]. The position of the minimum gap shifts dramatically for even small changes to \( C \), so without first learning \( C \) we cannot solve the relevant differential equation. As can be seen by [17], nearly optimal strategies may require knowing the location of the minimal gap to within exponentially small error. As a further complication, Fig. 1 shows that a general purpose strategy that attempts to use the same schedule for all cost functions seems untenable, as arbitrary optimization problems do not fit the profile of Grover search.

Let \( W \) be a diagonal matrix with eigenvalues \( W_{u_0} < W_{u_1} \leq \ldots \leq W_{u_{V-1}} \). Unlike in the approach of [17] for adiabatic Grover search, we will not be given the promise that \( W \) has at most two unique eigenvalues. Instead, we require the following weaker promises:

1. \( W_{u_0} = 0 \),
2. a lower bound on the spectral gap \( \gamma(W) = W_{u_1} \),
3. an upper bound on the spectral ratio \( \kappa(W) = W_{u_{V-1}}/W_{u_1} \), and
4. \( \|W\| \leq V \).

Assumptions 2 and 3 merely facilitate our analysis, guaranteeing that the gap of \( W \) does not decrease with \( V \) and that the spectral ratio does not increase with \( V \). That is, since we work with the combinatorial Laplacian where \( \lambda_{\max} = V \), we require that \( W : V \rightarrow [0, V] \), or \( W \) is merely a rescaled version of \( \frac{W}{\lambda_{\max}} : V \rightarrow [0, 1] \). Analyzing other situations would be interesting and presumably require only modest, but unnecessarily technical adaptations of the theorems that follow. Restrictions on the distribution of \( W \) can also yield better scaling, such as in the case that \( W \) is proportional to the Grover cost function; however, we focus on the most general case here.

Assumption 1 is the only assumption of which the reader should be suspicious. It can actually be relaxed slightly to \( 0 \leq W_{u_0} < \epsilon V^{2/3} \). On the scale of the problem, this ends up being an exponentially small distinction, so we will proceed with Assumption 1 and leave generalizations to the interested reader. Combined with Assumption 2, this also guarantees that \( W \) has a unique minimum.

\[ ^2 \text{For an algorithm that achieves better scaling in these instances, see Algorithm 4.} \]
\[ H = (1 - s)L + sW \]

Figure 1: Comparison of the spectral gaps of a few Grover-type problems to a random optimization problem. Here, \( W \) represents the random optimization problem, whereas \( W(G) \) represents the Grover cost function. Note that although \( W \) is initially close to \( 0.50W(G) \), it rapidly diverges and is not well approximated by any Grover-type problem. We have used \( V = 2^{12} \) vertices (or 12 qubits).

In contrast to the first three assumptions, Assumption 4 is quite arbitrary and just simplifies our presentation, since it imposes the constraint that \( \|W\| \leq \|L\| = V \). An alternative presentation might use the fact that \( \|W\| = \kappa(W)\gamma(W) \) and a similar analysis would follow, however the theorems become a bit more cumbersome. In particular, as long as \( \gamma(W)/\|W\| \) is larger than some constant, the relaxation of Assumption 4 is trivial and left to the reader.

In Section 4, we propose an oracle (Algorithm 3) to take the place of \textsc{GetGap} in Algorithm 2 and discuss its behavior. The remainder of this section will be dedicated to analyzing the behavior of Algorithm 2 using Algorithm 3 as \textsc{GetGap}.

As we will see in Section 5, an efficient oracle will require us to derive a tighter Cheeger inequality particular to the complete graph. This and other useful facts arising from the spectral theory of the complete graph will be explored in Section 5. In Section 6, we will show how to apply these tools to build our oracle. Finally, in Section 6.5 we will analyze the full runtime of Algorithm 2 using the oracle of Algorithm 3.

## 4 Explicit construction of a gap oracle

In this section, we present a function \textsc{GetGap} to be used in Algorithm 2 when \( H(0) = L \), the combinatorial Laplacian of the complete graph on \( V \) vertices. After some balancing of parameters, each query to our oracle \textsc{GetGap} requires at most time \( O(V^{2/3}) \), where the actual time depends upon the ratio of the largest to second smallest eigenvalues of \( H(1) \). Thus, we seek only similar scaling from Algorithm 2.

The algorithm consists of three major parts. Prior to the gap minimum when the ground state has small amplitude on all vertices, we use a classical root-finding method to determine the appropriate Cheeger constant of \( H \). While nearing the minimum \( s_{\text{min}} \), we hit a region where \( s < s_{\text{min}} \) and the root-finding algorithm is no longer an efficient method for determining the Cheeger constant to desired precision. At this
Algorithm 3: Complete graph oracle

Require: A failure probability \( p \), the number of vertices \( V \), the cost function \( W \), a lower bound \( \chi V \leq W_{u_1} \), an upper bound \( \kappa \geq W_{u_1}/W_{u_1} \), a universal constant \( c_0 \in (0, 1) \)

1: Global \( W \leftarrow \emptyset \) \( \triangleright \) Initialize \( W \) to be empty
2: Global \( S_{\min} \leftarrow 0 \)
3: Global \( x_{\min} \leftarrow \max \left\{ \frac{1}{\kappa^3} (\kappa - 1)(V - 1)^{2/3}, 2(1 + c_0)\sqrt{V} \right\} \)
4: Global \( n \leftarrow \max \left\{ \left[ \frac{1 + c_0}{1 - c_0} \right]^2 5(V - 1)^2(\kappa - 1)^2 \ln \left( \frac{2}{p} \right), 1 \right\} \) \( \triangleright \) Choose \( n \) by Theorem 8
5: function GETGAP\( (s, \delta s, \gamma) \)
   6: if \( S_{\min} > 0 \) then return FinishSchedule\( (s, \delta s, \gamma) \)
   7: \( x_0 \leftarrow (1 + c_0) \left( \frac{2}{1 - s} + 1 \right) \) \( \triangleright \) Extract \( x_0 \) from previous gap bound
   8: if \( s = 0 \) then \( x_0 \leftarrow V \)
   9: \( x_0 \leftarrow \text{FINDROOT}(s, \delta s, x_0) \)
10: if \( x_0 = 0 \) then return FinishSchedule\( (s, \delta s, \gamma) \)
11: return \( (1 - s - \delta s) \left( \frac{x_0}{1 + c_0} - 1 \right) \) \( \triangleright \) Lower bound the gap using Theorems 6 and 8
12: function \( \tilde{\Theta}(s, x) \)
   13: while \( |W| < n \) do \( \triangleright \) Populate \( W \)
   14: \( w \leftarrow 0 \)
   15: while \( w = 0 \) do \( w \leftarrow \langle v \rvert W \rangle \) for a random vertex \( v \in V \)
   16: Append \( w \) to \( W \)
   17: return \( \frac{V - 1}{n} \sum_i \left( \frac{s}{1 - s} W_i + x \right)^{-1} + \frac{1}{x} - 1 \)
18: function FINDROOT\( (s, \delta s, x_0) \)
   19: if \( \tilde{\Theta}(s + \delta s, x_{\min}) < 0 \) or \( x_0 \leq x_{\min} \) then
   20: \( S_{\min} \leftarrow s + \frac{4(1 - s) x_{\min}}{(1 - c_0)^2 \chi V} \) \( \triangleright \) Upper bound \( s_{\min} \) using Corollaries 3 and 4
   21: \( \text{return } 0 \)
   22: \( I \leftarrow \left[ \frac{(1 - c_0)^2}{1 + c_0} x_0, \frac{(1 + c_0)^2}{1 - c_0} x_0 \right] \) \( \triangleright \) Interval from Proposition 13
   23: return \( x \in I \) such that \( \tilde{\Theta}(s + \delta s, x) \approx 0 \). \( \triangleright \) Root of Eq. (20)
24: function FinishSchedule\( (s, \delta s, \gamma) \)
   25: if \( s \leq S_{\min} \) then
   26: \( \gamma \leftarrow \max \left\{ (1 - c_0) \gamma, (1 - s - \delta s) \sqrt{V - 1}/\kappa^4 \right\} \) \( \triangleright \) Bound by Propositions 2 and 8
   27: \( \text{return } \gamma \)
   28: \( \gamma \leftarrow \frac{\chi (V - 2)}{4 \kappa^3} (s + \delta s - S_{\min}) + \frac{V - 2}{2 \kappa^4 \sqrt{V - 1}} (1 - S_{\min}) \) \( \triangleright \) Use linear lower bound from Theorem 7
   29: \( \text{return } \gamma \)
point, we use an analytic lower bound on the gap and bound the parameter $s_{\text{min}}$ determined in the first half of the algorithm until we are guaranteed that $s > s_{\text{min}}$. Finally, we use a linear envelope to complete the schedule.

5 Spectral graph theory

Consider a Hamiltonian $H = L + W$ where $L$ is the combinatorial graph Laplacian of the unweighted complete graph on $V$ vertices and $W$ is any matrix diagonal in the basis of vertices, with diagonal entries $W_u \equiv W_{uu}$. Such a Hamiltonian is stoquastic, and has non-negative eigenvalues and real eigenvectors. Let $\lambda_0 < \lambda_1 \leq \ldots \leq \lambda_{V-1}$ be the eigenvalues of $H$ with corresponding normalized eigenvectors $\phi_0, \phi_1, \ldots, \phi_{V-1}$, and let $\gamma \equiv \lambda_1 - \lambda_0$ denote the spectral gap of $H$. (It follows from the Perron-Frobenius theorem that $\lambda_0 < \lambda_1$ and that we can always choose the ground state $\phi_0$ to have strictly positive components.) By definition, the eigenvectors satisfy the equations

$$(V + W_u - \lambda_i)\phi_i(u) = \sum_v \phi_i(v),$$

for all vertices $u$, where $\phi_i(u)$ denotes the component of $\phi_i$ corresponding to $u$ and the summation is over the set $V$ of all vertices in the graph. For a subset $S \subseteq V$, we define the ratio

$$g_S \equiv \frac{\sum_{u \in S, v \not\in S} \phi_0(u)\phi_0(v)}{\sum_{u \in S} \phi_0(u)^2}. \tag{10}$$

Then, the Cheeger ratio corresponding to $S$ is given by (see [7])

$$h_S = \max\{g_S, g_{V \setminus S}\}. \tag{11}$$

and the (weighted) Cheeger constant of the Hamiltonian $H$ is

$$h = \min_{S \subseteq V} h_S. \tag{12}$$

It was shown in [13] that a general stoquastic Hamiltonian $H = L + W$, where the Laplacian $L$ need not be that of the complete graph, obeys the inequality

$$2h \geq \gamma \geq \sqrt{h^2 + d^2} - d \tag{13}$$

where $d$ is an upper bound on the degree of the graph corresponding to $L$. (For the complete graph, $d = V - 1$.)

For $h \sim V$, this inequality gives us relatively tight control over the spectral gap of $H$, but if $h$ is small, the inequality can be quadratically loose. This problem is potentially unique to graphs of exponentially large degree. If, on the other hand, $d$ is upper bounded by a constant independent of the problem size, then Eq. (13) implies that $\gamma(H) \sim h$.

In our case, $d = V - 1$ and, although potentially possible to obtain, we cannot prove scaling better than $O((V/\gamma_{\text{min}})^2) = O(V)$ out of Algorithm 2 using the tools of Section 3.1. Thus, we wish to derive a Cheeger inequality specific to the complete graph. A Cheeger inequality for a particular graph makes no sense classically, where the Cheeger constant maps each graph to a number. In particular, classical Cheeger inequalities need to be flexible enough to apply to any graph. In our setting, however, all Cheeger ratios are functions of the cost function $W$ and the graph itself is treated as a known parameter, so we can use information about graph of interest and derive Cheeger inequalities special to that graph. These inequalities, by virtue of the fact that they have been tailored to a particular graph, can be much tighter than those that are expected to work on all graphs.

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5.1 Cheeger inequalities for the complete graph

The following fact about the second smallest eigenvector of $H$ will allow us to derive a tighter Cheeger inequality in the special case of a complete graph.

**Proposition 4.** Suppose that $W$ has a unique smallest eigenvalue. Then, there exists a unique $u$ such that $\phi_1(u)\phi_1(v) < 0$ for all $v \neq u$.

**Proof.** We index the vertices as $u_0, u_1, \ldots, u_{V-1}$ such that $W_{u_0} < W_{u_1} \leq \ldots \leq W_{u_{V-1}}$. Using the Rayleigh quotient,

$$
\lambda_1 = \inf_{f \perp \phi_0} \frac{(f, Hf)}{(f, f)} = \inf_{f \perp \phi_0} \frac{\sum_{m} (f(m) - f(v))^2 + \sum_{u} f^2(u)W_{u}}{\sum_{u} f^2(u)}.
$$

Taking $f(u_0) = -\phi_0(u_1)$, $f(u_1) = \phi_0(u_0)$, and $f(u) = 0$ for all $u \neq u_0, u_1$ demonstrates that $\lambda_1 \leq V + W_{u_1}$ with equality only if $W_{u_0} = W_{u_1}$. Since $W_{u_0} < W_{u_1}$ by assumption, the inequality is strict. It then follows from Eq. (9) that $\sum_v \phi_1(v) \neq 0$ and that $\phi_1(u_k)\sum_v \phi_1(v) > 0$ for all $k \geq 1$. This in turn implies that $\phi_1(u_0)\sum_v \phi_1(v) < 0$; otherwise, all of the components of $\phi_1$ would have the same sign, contradicting $\phi_1 \perp \phi_0$ (recall that we can choose $\phi_0 > 0$ by the Perron-Frobenius theorem). Therefore, $\phi_1(u_0)\phi_1(v) < 0$ for all $v \neq u_0$.

Hereafter, we label $m \equiv u_0$, since this will correspond to the “marked” state that our algorithm aims to find.

**Theorem 6.** Suppose that $W$ has a unique smallest eigenvalue. Letting $W_m < W_{u_1} \leq \ldots \leq W_{u_{V-1}}$ denote the eigenvalues of $W$, if $W_m = 0$ and $W_{u_{V-1}}/W_{u_1} \leq \kappa$, then

$$
\gamma \geq \max \left\{ g_{\{m\}}, \frac{h_{\{m\}}}{\kappa^3} \right\}.
$$

**Proof.** As shown in the proof of Proposition 4, $\phi_1(m)\phi_1(v) < 0$ for all $v \neq m$. By Eq. (9),

$$(V + W_m - \lambda_1)\phi_0(m)\phi_1(m) = \sum_v \phi_0(v)\phi_1(m)$$

$$(V + W_m - \lambda_1)\phi_1(m)\phi_0(m) = \sum_v \phi_1(v)\phi_0(m),$$

whence

$$
\gamma \phi_0(m)\phi_1(m) = \sum_v (\phi_0(v)\phi_1(m) - \phi_0(m)\phi_1(v)).
$$

Letting $f(u) \equiv \phi_1(u)/\phi_0(u)$ for all $u$, we have

$$
\gamma \phi_0(m)^2 = \frac{1}{f(m)} \sum_{v \neq m} \phi_0(v)\phi_0(m)(f(m) - f(v)) = \phi_0(m) \sum_{v \neq m} \phi_0(v) \left(1 - \frac{f(v)}{f(m)}\right).
$$

By Eq. (10), $g_{\{m\}} = \sum_{v \neq m} \phi_0(v)/\phi_0(m)$, and, noting that $f(v)/f(m) < 0$ for all $v \neq m$ by Proposition 4, we have

$$
\gamma \phi_0(m)^2 \geq \phi_0(m) \sum_{v \neq m} \phi_0(v) = \phi_0(m)^2 g_{\{m\}},
$$

so $\gamma \geq g_{\{m\}}$.

Since the above lower bound becomes loose for large $\phi_0(m)$, we consider the case where $\phi_0(m) \geq 1/\sqrt{2}$, so that $\phi_0(m)^2 > 1 - \phi_0(m)^2$ and hence $h_{\{m\}} = \phi_0(m) \sum_{v \neq m} \phi_0(v)/(1 - \phi_0(m)^2)$ by Eq. (11). Observing from Eq. (9) that $\min_{u \neq m} \phi_0(u) = \phi_0(u_{V-1})$ and that $\lambda_0 < V$, we see that for any $v \neq m$,

$$
\frac{\min_{u \neq m} \phi_0(u)}{\phi_0(v)} \geq \phi_0(u_{V-1})/\phi_0(v) = \frac{V + W_v - \lambda_0}{V + W_{u_{V-1}} - \lambda_0} \geq \frac{V + W_{u_1} - \lambda_0}{V + W_{u_{V-1}} - \lambda_0} \geq \frac{W_{u_1}}{W_{u_{V-1}}} \geq \frac{1}{\kappa},
$$

(14)
which also implies that \( \phi_0(u)/\phi_0(v) \geq 1/\kappa \) for any \( u, v \neq m \). Thus,

\[
\gamma \phi_0(m)^2 \geq \phi_0(m) \min_{u \neq m} \phi_0(u) \sum_{v \neq m} \left( 1 - \frac{f(v)}{f(m)} \right)
\]

\[
\geq \phi_0(m) \left( \frac{1}{V-1} \sum_{u \neq m} \frac{1}{\kappa} \phi_0(u) \right) \left( V - 1 + \frac{1}{|f(m)|} \sum_{v \neq m} |f(v)| \right)
\]

\[
= \frac{1}{\kappa} \left( \phi_0(m) \sum_{u \neq m} \phi_0(u) \right) \left( 1 + \frac{1}{|f(m)|} \sum_{v \neq m} |\phi_1(v)| \right)
\]

\[
= \frac{1}{\kappa} \left( \phi_0(m) \sum_{u \neq m} \phi_0(u) \right) \left( 1 + \frac{1}{|f(m)|} \sum_{v \neq m} |\phi_1(v)| \phi_0(v) \right)
\]

\[
\geq \frac{1}{\kappa} \left( \phi_0(m) (1 - \phi_0(m)^2) \right) \left( 1 + \frac{1}{|f(m)|} \sum_{v \neq m} |\phi_1(v)| \phi_0(v) \right)
\]

\[
\geq \frac{1}{\kappa} \left( \phi_0(m) (1 - \phi_0(m)^2) \right) \left( 1 + \frac{\phi_0(m) |\phi_1(m)| \phi_0(m)}{|\phi_1(m)| \kappa^2 (1 - \phi_0(m)^2)} \right)
\]

\[
= \frac{1}{\kappa} \left( \phi_0(m) (1 - \phi_0(m)^2) + \frac{\phi_0(m)^2}{\kappa^2} \right),
\]

so

\[
\gamma \geq \frac{1}{\kappa} \left( \frac{1 - \phi_0(m)^2}{\phi_0(m)^2} + \frac{1}{\kappa^2} \right) \geq \frac{h(m)}{\kappa^3}.
\]

Since the Cheeger ratio \( h_S \) of any subset \( S \subseteq V \) upper bounds the Cheeger constant \( h \), the upper bound in Eq. (13) implies the following.

**Corollary 3.** Under the conditions of Theorem 6,

\[
2h(m) \geq \gamma \geq \frac{h(m)}{\kappa^3}.
\]

Corollary 3 demonstrates that the Cheeger ratio \( h(m) \), corresponding to the cut that isolates the marked state \( m \), determines the gap to within a constant factor whenever \( \kappa \) is a constant independent of \( V \).

For ease of presentation in what follows, we will write \( \phi \equiv \phi_0 \) for the ground state of \( H \). Noting that

\[
g(m) = \frac{\|\phi\|_1 - \phi(m)}{\phi(m)} = \frac{\|\phi\|_1}{\phi(m)} - 1,
\]

it will be convenient to introduce the notation

\[
X = \frac{\|\phi\|_1}{\phi(m)} = g(m) + 1,
\]

where \( m \) is the vertex corresponding to the smallest eigenvalue of \( W \).

We now prove a couple of useful facts about \( X \).

**Proposition 5.** Suppose that \( W_m = 0 \) is the unique smallest eigenvalue of \( W \). Then,

1. \( X = V - \lambda_0 \) and
2. \( \sum_u (X + W_u)^{-1} = 1 \).
Proof. Since \( W_m = 0 \), Eq. (9) gives
\[
(V - \lambda_0)\phi(m) = \|\phi\|_1,
\]
so
\[
V - \lambda_0 = \frac{\|\phi\|_1}{\phi(m)} = X,
\]
which establishes Fact 1.

Then,
\[
\|\phi\|_1 = \sum_u \phi(u) = \sum_u \frac{\|\phi\|_1}{V - \lambda_0 + W_u} = \|\phi\|_1 \sum_u (X + W_u)^{-1},
\]
and Fact 2 follows upon dividing both sides by \( \|\phi\|_1 \).

Using the above results, we can obtain a perturbative bound for \( g_{(m)} \). For \( s \in [0, 1) \), consider the Hamiltonian
\[
H(s) = (1 - s)L + sW = (1 - s)\left(L + \frac{s}{1 - s}W\right) \equiv (1 - s)G(s)
\]
and let \( g_S(s), h_S(s), \) and \( h(s) \) denote the quantities defined in Eqs. (10) to (12) corresponding to \( G(s) \). It is clear that the results we have proven for \( H = L + W \) extend directly to \( G(s) \).

**Proposition 6.** Suppose that \( W_m = 0 \) is the unique smallest eigenvalue of \( W \) and that \( \|W\| \leq V \). If \( 0 \leq \delta s \leq \frac{c_0}{4V}g_{(m)}(s)(1 - s) \) for some \( c_0 \in (0, 1) \), then
\[
|g_{(m)}(s + \delta s) - g_{(m)}(s)| \leq c_0 g_{(m)}(s).
\]

**Proof.** For any matrix \( M \), let \( \lambda_0(M) \) denote the smallest eigenvalue of \( M \). By Proposition 5,
\[
|g_{(m)}(s + \delta s) - g_{(m)}(s)| = |[V - \lambda_0(G(s + \delta s)) - (V - \lambda_0(G(s)))]|
= \left| \lambda_0 \left( \frac{H(s + \delta s)}{1 - (s + \delta s)} \right) - \lambda_0 \left( \frac{H(s)}{1 - s} \right) \right|
= \left| \frac{1}{1 - s - \delta s} \lambda_0(H(s + \delta s)) - \left( 1 - \frac{\delta s}{1 - s} \right) \lambda_0(H(s)) \right|
\leq \frac{1}{1 - s - \delta s} \left| \lambda_0(H(s + \delta s)) - \lambda_0(H(s)) \right| + \delta s \lambda_0(G(s))
\leq \frac{\delta s}{1 - s - \delta s}(2V + (V - g_{(m)} - 1))
\leq \frac{3Vc_0g_{(m)}(s)}{4V - c_0g_{(m)}(s)}
\leq \frac{3Vc_0g_{(m)}(s)}{4V - c_0V}
= \frac{3c_0g_{(m)}(s)}{4 - c_0}
\leq c_0 g_{(m)}(s),
\]
We arrive at the second inequality by applying Weyl’s inequality to \( H(s + \delta s) = H(s) + \delta s(-L + W) \), giving
\[
|\lambda_0(H(s + \delta s)) - \lambda_0(H(s))| \leq \delta s\| -L + W\| \leq \delta s(2V)
\]
since \( \|W\| \leq V \) by assumption. The third inequality follows from our assumption that \( \delta s/(1 - s) \leq c_0 g_{(m)}(s)/4V \), and the fourth inequality from the fact that \( 0 \leq g_{(m)} = V - \lambda_0 - 1 \leq V \), by Proposition 5. 

\( \square \)
5.2 Bounds on \( h_{\{m\}} \)

In order to apply the result of Corollary 3 in our algorithm, we require analytic bounds on the Cheeger ratio \( h_{\{m\}} \) corresponding to the marked vertex.

**Proposition 7.** Under the conditions of Theorem 6,

\[
\sqrt{V-1} \geq \sum_{u \neq m} \phi(u) \geq \frac{1}{\kappa} \sqrt{V-1} \sqrt{1 - \phi(m)^2}.
\]

**Proof.** The upper bound follows from Holder’s inequality:

\[
\sum_{u \neq m} \phi(u) \geq \frac{\sum_{u \neq m} \phi(u)}{\sqrt{\sum_{u \neq m} \phi(u)^2}} \leq \sqrt{V-1} \sqrt{1 - \phi(m)^2}.
\]

For the lower bound, we note that \( \min_{v \neq m} \phi(v) \) is achieved by \( u_{V-1} \) and that, by Eq. (14), \( \min_{v \neq m} \phi(v)^2 \geq \phi(u)^2 / \kappa^2 \) for all \( u \neq m \). Hence,

\[
\sum_{u \neq m} \phi(u) \geq \sqrt{V-1} \sum_{u \neq m} \min_{v \neq m} \phi(v)^2 \geq \sqrt{V-1} \sqrt{\sum_{u \neq m} \frac{1}{\kappa^2} \phi(u)^2} = \frac{1}{\kappa} \sqrt{V-1} \sqrt{1 - \phi(m)^2}.
\]

\[\square\]

Although \( h_{\{m\}} = g_{\{m\}} \) whenever \( \phi(m)^2 \leq 1/2 \), when \( \phi(m)^2 > 1/2 \) we would still like to express \( h_{\{m\}} \) analytically in terms of the amplitude \( \phi(m) \). We exploit the fact that \( h_{\{m\}} = g_{\{m\}} \max \left\{ 1, \frac{\phi(m)^2}{1 - \phi(m)^2} \right\} \) to obtain the following analytic bound on \( h_{\{m\}} \) for any \( \phi(m) \).

**Proposition 8.** Under the conditions of Theorem 6, if \( \phi(m) \in (0, 1) \), then

\[
\sqrt{V-1} \Phi(m) \geq h_{\{m\}} \geq \frac{1}{\kappa} \sqrt{V-1} \Phi(m)
\]

where

\[
\Phi(m) \equiv \max \left\{ \frac{\phi(m)}{\sqrt{1 - \phi(m)^2}}, \frac{\sqrt{1 - \phi(m)^2}}{\phi(m)} \right\} \geq 1.
\]

**Proof.** By definition,

\[
h_{\{m\}} = \frac{\sum_{u \neq m} \phi(u)}{\phi_m} \max \left\{ 1, \frac{\phi(m)^2}{1 - \phi(m)^2} \right\} = \sum_{u \neq m} \phi(u) \frac{\Phi(m)}{\sqrt{1 - \phi(m)^2}}.
\]

The result follows immediately from Proposition 7. \[\square\]

6 Analysis of Algorithm 3

We analyze the runtime of BAA with the oracle constructed in Algorithm 3 as follows. First, we assume that we can query the appropriate Cheeger ratios and show that they obey Theorem 4. Then, we determine the additional runtime incurred by abandoning queries to the Cheeger ratio when such queries become inefficient.

As in Section 5.1, we consider \( H(s) = (1-s)L + sW \equiv (1-s)G(s) \) and the corresponding quantities \( g_S(s), h_S(s), \) and \( h(s) \). While the results of that section apply directly to \( G(s) = L + sW/(1-s) \), it is useful to note from Equations (10) to (12) that \( g_S(s), h_S(s), \) and \( h(s) \) are functions only of the ground state and are therefore the same for both \( H(s) \) and \( G(s) \). We also define \( s_{\min} \) to be the point at which \( \phi(m) = 1/\sqrt{2} \), so that \( g_{\{m\}}(s_{\min}) = g_{\{m\}}(s_{\min}) \). Since \( \phi(m) = 1/\sqrt{V} \) at \( s = 0 \), \( \phi(m) = 1 \) at \( s = 1 \), and Proposition 16 shows that \( \phi(m) \) is strictly increasing over \( s \in [0, 1] \), this point is unique.
Proposition 9. Suppose that \( W_m = 0 \) is the unique smallest eigenvalue of \( W \), \( W_{u_1} \) is the second smallest eigenvalue of \( W \), and \( \|W\| \leq V \). Then,

\[
s_{\min} \leq \left[ \frac{1}{2} \left( 1 - \frac{1}{V - 1} \right), 1 - \frac{W_{u_1}}{5V} \right].
\]

Proof. We begin with the lower bound. For any matrix \( M \), let \( \lambda_0(M) \) denote the smallest eigenvalue of \( M \). Let \( W^{(G)} \) be the diagonal matrix with \( W_m^{(G)} = 0 \) and \( W_u^{(G)} = V \) for all \( u \neq m \). Using Proposition 5 and noting that \( W - W^{(G)} \) is negative semidefinite,

\[
g_{\{m\}}(s) = V - \lambda_0(G(s)) - 1
\]

\[
= V - \lambda_0 \left( L + \frac{s}{1 - s} W \right) - 1
\]

\[
\geq V - \lambda_0 \left( L + \frac{s}{1 - s} W^{(G)} \right) - 1
\]

\[
= V - \frac{1}{1 - s} \lambda_0 \left( (1 - s)L + sW^{(G)} \right) - 1
\]

\[
= V - \frac{1}{1 - s} V \left[ 1 - \sqrt{1 - \frac{4}{V} \left( 1 - s \right)} \right] - 1
\]

\[
= V \left\{ 1 - \frac{1}{2(1 - s)} \left[ 1 - \sqrt{1 - \frac{4}{V} \left( 1 - s \right)} \right] \right\} - 1
\]

\[
> \sqrt{V - 1}
\]

when \( s < \frac{1}{2} \left( 1 - \frac{1}{\sqrt{V - 1}} \right) \). On the other hand, at \( s = s_{\min} \), \( \Phi(m) = 1 \) and hence \( g_{\{m\}} = h_{\{m\}} \leq \sqrt{V - 1} \) by Proposition 8.

For the upper bound, let \( \gamma(s) \) be the spectral gap of \( H(s) \). Note that \( \gamma(1) = W_{u_1} \), and by Proposition 2 and our assumption that \( \|W\| \leq V \),

\[
|W_{u_1} - \gamma(s)| = |\gamma(1) - \gamma(s)|
\]

\[
\leq 4(1 - s)V,
\]

so if \( (1 - s) < \frac{1}{4\sqrt{V - 1}} |W_{u_1} - 2(1 - s)\sqrt{V - 1}| \), we would have

\[
|W_{u_1} - \gamma(s)| < W_{u_1} - 2(1 - s)\sqrt{V - 1},
\]

whence \( \gamma(s) > 2(1 - s)\sqrt{V - 1} \). Then, applying Corollary 3 to the spectral gap of \( G(s) \) implies that \( h_{\{m\}} > \sqrt{V - 1} \). On the other hand, \( h_{\{m\}} \leq \sqrt{V - 1} \) at \( s = s_{\min} \) by Proposition 8, so we must have

\[
(1 - s_{\min}) \geq \frac{1}{4\sqrt{V - 1}} |W_{u_1} - 2(1 - s_{\min})\sqrt{V - 1}|,
\]

or

\[
s_{\min} \leq 1 - \frac{W_{u_1}}{4V + 2\sqrt{V - 1}} \leq 1 - \frac{W_{u_1}}{5V}.
\]

\[
\]

6.1 The convex envelope

Theorem 7. Let \( \gamma(s) \) denote the spectral gap of \( H(s) = (1 - s)L + sW \). Suppose that \( W \) has a unique smallest eigenvalue and that \( \|W\| \leq V \). Letting \( W_m < W_{u_1} \leq \ldots W_{u_{v-1}} \) denote the eigenvalues of \( W \), if \( W_m = 0 \), \( W_{u_{v-1}}/W_{u_1} \leq \kappa \), and \( W_{u_1} \geq \chi V \) for some constant \( \chi \geq 2\sqrt{V - 1}/V \), then for all \( s \in [0,) \),

\[
2\kappa^4 \Gamma(s) \geq \gamma(s) \geq \Gamma(s),
\]

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with

\[
\Gamma(s) = \begin{cases} 
(1-s)h_{\{m\}} & s < s_{\text{min}} \\
(1-s)\sqrt{\frac{V-1}{\kappa^4}} \left( \frac{\phi(m)}{\sqrt{1 - \phi(m)^2}} \right) & s \geq s_{\text{min}}.
\end{cases}
\]  

(17)

Moreover,

\[
\Gamma(s) \geq \frac{\chi}{4\kappa^4} (V-2)|s-s_{\text{min}}| + \frac{1}{2} \left( \frac{V-2}{V-1} \right) \Gamma(s_{\text{min}}).
\]

Proof. Since \(\phi(m)\) is strictly increasing (as show by Proposition 16 in the Appendix), \(\phi(m) < 1/\sqrt{2}\) for \(s < s_{\text{min}}\) and \(\phi(m) \geq 1/\sqrt{2}\) for \(s \geq s_{\text{min}}\). Hence, by Theorem 6 and Eq. (13), the spectral gap \(\gamma(G(s))\) of \(G(s) = H(s)/(1-s)\) is bounded as \(2h_{\{m\}}(s) \geq \gamma(G(s)) \geq h_{\{m\}}(s)\) for \(s < s_{\text{min}}\) and as \(2h_{\{m\}}(s) \geq \gamma(G(s)) \geq h_{\{m\}}(s)/\kappa^3\) for \(s \geq s_{\text{min}}\). Since \(h_{\{m\}}(s)\) is invariant under rescaling \(H(s)\) by an overall factor while \(\gamma(s) = (1-s)\gamma(G(s))\), it follows that when \(s < s_{\text{min}}\), \(2(1-s)h_{\{m\}}(s) \geq \gamma(s) \geq (1-s)h_{\{m\}}(s)\) or, in terms of \(\Gamma(s)\),

\[2\Gamma(s) \geq \gamma(s) \geq \Gamma(s).
\]

Similarly, when \(s > s_{\text{min}}\), \(2(1-s)h_{\{m\}}(s) \geq \gamma(s) \geq (1-s)h_{\{m\}}(s)/\kappa^3\), and applying the bounds on \(h_{\{m\}}\) given by Proposition 8, we have

\[2\kappa^4\Gamma(s) \geq \gamma(s) \geq \Gamma(s).
\]

Thus, for all \(s \in [0,1]\), \(2\kappa^4\Gamma(s) \geq \gamma(s) \geq \Gamma(s)\).

To derive the lower bound on \(\Gamma(s)\), we consider the two regions separately.

Case 1 \([s < s_{\text{min}}]\)

In this region, \(h_{\{m\}}(s) = g_{\{m\}}(s)\) and \(\Gamma(s) = (1-s)g_{\{m\}}(s)\). Using Proposition 5 and the Hellmann-Feynmann theorem,

\[
\frac{dg_{\{m\}}(s)}{ds} = \frac{d}{ds}(V - \lambda_0(G(s)) - 1)
\]

\[= -\langle \phi, \frac{d}{ds}(L + \frac{s}{1-s} W) \rangle \phi
\]

\[= -\frac{1}{(1-s)^2} \langle \phi, W \phi \rangle
\]

\[= -\frac{1}{(1-s)^2} \sum_u \phi(u)^2 W_{uu}
\]

\[\leq -\frac{1}{(1-s)^2} (1 - \phi(m)^2) W_{uu}
\]

\[\leq -\frac{W_{uu}}{2(1-s)^2},
\]

where the first inequality follows from the assumption that \(W_m = 0\) and \(W_u \geq W_{uu}\) for all \(u \neq m\), and the second from the fact that \(\phi(m)^2 < 1/2\) in this region. Integrating both sides over \([s, s_{\text{min}}]\) for some \(s < s_{\text{min}}\), we find

\[g_{\{m\}}(s) - g_{\{m\}}(s_{\text{min}}) \geq \frac{W_{uu}}{2} \left( \frac{1}{1-s_{\text{min}}} - \frac{1}{1-s} \right) .
\]

Thus

\[
\Gamma(s) = (1-s)g_{\{m\}}(s)
\]

\[\geq (1-s_{\text{min}})g_{\{m\}}(s)
\]

\[\geq \frac{W_{uu}}{2} \frac{s_{\text{min}} - s}{1-s} + (1-s_{\text{min}})g_{\{m\}}(s_{\text{min}})
\]

\[\geq \frac{\chi V}{2} |s - s_{\text{min}}| + \lim_{s \to s_{\text{min}}} \Gamma(s)
\]

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where the last line follows from the assumption that $W_{u_1} \geq \chi V$.

**Case 2** \([s \geq s_{\text{min}}]\)

In this region, $\Gamma$ is given by

\[
\Gamma(s) = (1 - s) \frac{\sqrt{V - 1}}{\kappa^4} \frac{\phi(m)}{\sqrt{1 - \phi(m)^2}}
\]

\[
= (1 - s) \frac{\sqrt{V - 1}}{\kappa^4} \frac{1}{\sqrt{X(s)^2 \sum_{u \neq m} \left(X(s) + \frac{s}{1 - s} W_u\right)^{-2}}}
\]

\[
\geq \frac{\sqrt{V - 1}}{\kappa^4} \frac{s}{X(s) \sqrt{\sum_{u \neq m} W_u^{-2}}},
\]

where we used the fact that

\[
\frac{1 - \phi(m)^2}{\phi(m)^2} = \frac{1}{\phi(m)^2} \sum_{u \neq m} \left(\frac{\|\phi\|_1}{V - \lambda_0(G(s)) + \frac{s}{1 - s} W_u}\right)^2 = X(s)^2 \sum_{u \neq m} \left(X(s) + \frac{s}{1 - s} W_u\right)^{-2}
\]

by Eq. (9) and Proposition 5, writing $X(x) \equiv g_{\{m\}}(s) + 1$. Hence, we define

\[
\bar{\Gamma}(s) = \frac{\sqrt{V - 1}}{\kappa^4} \frac{s}{X(s) \sqrt{\sum_{u \neq m} W_u^{-2}}}
\]

as the lower bound on $\Gamma(s)$, and consider the derivative

\[
\frac{d}{ds} \left(\frac{s}{X(s)}\right) = \frac{1}{X(s)} - \frac{s}{X(s)^2} \frac{dX(s)}{ds}
\]

\[
\geq - \frac{s}{X(s)^2} \frac{dX(s)}{ds}
\]

\[
= \frac{s}{X(s)^2} \frac{1}{(1 - s)^2} (\phi|W|\phi)
\]

\[
\geq \frac{s}{X(s)^2} \frac{1}{(1 - s)^2} (1 - \phi(m)^2) W_{u_1}
\]

\[
= \frac{s W_{u_1}}{X(s)^2 (1 - s)^2} \left[\frac{\phi(m)^2 X(s)^2}{(1 - s)} \sum_{u \neq m} \left(X(s) + \frac{s}{1 - s} W_u\right)^{-2}\right]
\]

\[
\geq \frac{s W_{u_1}}{2(1 - s)^2} \frac{1}{\sum_{u \neq m} \left(W_u + \frac{s}{1 - s} W_u\right)^{-2}}
\]

\[
= \frac{s W_{u_1}}{2(1 - s)^2} \sum_{u \neq m} \left(\frac{1}{1 - s} W_u\right)^{-2}
\]

\[
\geq \frac{s W_{u_1}}{2} \sum_{u \neq m} \left(\frac{1}{W_{u_{\text{min}}}}\right)^2
\]

\[
= \frac{s (V - 1)}{2 \kappa V}.
\]
To obtain the third inequality, we used the fact that \( g(m)(s) \) is monotonically decreasing in \( s \) over \( s \in [0, 1] \), as is clear from Eq. (18) and the assumption that \( W \) is positive semidefinite, and that \( g(m)(s_{\min}) = h(m)(s_{\min}) \leq \sqrt{\frac{3}{2} \cdot 1} \) by Proposition 8. Consequently, for all \( u \neq m \)

\[
X(s) = \frac{g(m)(s) + 1 \leq g(m)(s_{\min}) + 1 \leq \sqrt{W - 1} + 1 \leq 2\sqrt{W - 1} \leq \chi V \leq W_{u_1} \leq W_u. \quad (19)
\]

The fifth inequality follows from the assumption that \( W_{u_{V-1}} \leq \kappa W_{u_1} \) and \( W_{u_{V-1}} \leq V \). Using this to bound \( d\Gamma(s)/ds \) and integrating both sides of the resultant expression over \( [s_{\min}, s] \) for some \( s \geq s_{\min} \) gives

\[
\bar{\Gamma}(s) - \Gamma(s_{\min}) \geq \frac{(V - 1)^{3/2}}{2\kappa^5 V} \left( \sum_{u \neq m} W_u^{-2} \right)^{1/2} (s^2 - s_{\min}^2)
\]

\[
\geq \frac{(V - 1)^{3/2}}{4\kappa^5 V} \left( \sum_{u \neq m} W_u^{-2} \right)^{1/2} (s + s_{\min}) |s - s_{\min}|
\]

\[
\geq \frac{V - 1}{4\kappa^5 V} W_{u_1} (2s_{\min}) |s - s_{\min}|
\]

\[
\geq \frac{V - 1}{4\kappa^5 V} (\chi V) \left( 1 - \frac{1}{V - 1} \right) |s - s_{\min}|
\]

\[
= \frac{(V - 2)}{4\kappa^5 V} |s - s_{\min}|
\]

where the second line follows from the fact that \( \sum_{u \neq m} W_u^{-2} \leq \sum_{u \neq m} W_{u_1}^{-2} = (V - 1)/W_{u_1}^{-2} \) and the fourth line follows from the assumption that \( W_{u_1} \geq \chi V \) as well as Proposition 9. Then, since

\[
\sum_{u \neq m} W_u^{-2} = \frac{1}{(1 - s)^2} \sum_{u \neq m} \left( W_u + \frac{s}{1 - s} W_u \right)^{-2} \leq \frac{1}{(1 - s)^2} \sum_{u \neq m} \left( X(s) + \frac{s}{1 - s} W_u \right)^{-2},
\]

by Eq. (19), we have \( \bar{\Gamma}(s) \geq s\Gamma(s) \). Therefore,

\[
\Gamma(s) \geq \bar{\Gamma}(s) \geq \frac{(V - 2)}{4\kappa^5 V} |s - s_{\min}| \bar{\Gamma}(s_{\min}) + \frac{1}{2} \left( \frac{V - 2}{V - 1} \right) \Gamma(s_{\min}),
\]

using Proposition 9 in the last inequality.

Since in Case 1, \( \Gamma(s) \geq \frac{\chi V}{2} |s - s_{\min}| + \lim_{s \to s_{\min}} \Gamma(s) \), and \( \lim_{s \to s_{\min}} \Gamma(s) \geq \Gamma(s_{\min}) \) by Proposition 8, we have that

\[
\Gamma(s) \geq \frac{\chi (V - 2)}{4\kappa^5 V} |s - s_{\min}| + \frac{1}{2} \left( \frac{V - 2}{V - 1} \right) \Gamma(s_{\min}),
\]

in either case. \( \square \)

Applying Theorem 4 with \( \lambda_{\max} = V \), \( \alpha = \chi (V - 2)/(4\kappa^5 V) \), and \( \beta = (V - 2)/2(V - 1) \), the total number of steps under a schedule that always follows the oracle of Theorem 7 would be given by

\[
Q \left( \frac{\alpha \lambda_{\max}}{\beta \Gamma(s_{\min})}, \frac{c_0 \alpha}{4} \right) = Q \left( \frac{\chi V}{2\kappa(1 - s_{\min})}, \frac{c_0 \chi (V - 2)}{16\kappa^3 V} \right) \leq Q \left( \frac{5V - 1}{2\kappa}, \frac{c_0 \chi (V - 2)}{16\kappa^3 V} \right),
\]

where the inequality follows from the upper bound from Proposition 9 and the assumption that \( W_{u_1} \geq \chi V \).

Step 20 of Algorithm 3 requires that we approximate \( s_{\min} \). A sufficient bound follows from the proof of Theorem 7.
Corollary 4. Under the conditions of Theorem 7, if $$\gamma(s) < \bar{\gamma}$$ for some constant $$\bar{\gamma}$$ and $$s < s_{\text{min}}$$, then

$$s_{\text{min}} \leq s + \frac{2\bar{\gamma}}{\chi V}.$$ 

Proof. This is an immediate consequence of Case 1 in the proof of Theorem 7.

6.2 The $$\Theta$$ function

In this subsection, we consider $$H = L + W$$, where $$W$$ has eigenvalues $$0 = W_m < W_u \leq \ldots \leq W_{u,V-1} \leq V$$, and determine $$X \equiv g_{\{m\}} + 1$$ up to some relative error. Recall that determining $$X$$ up to relative error will be sufficient to provide a bound on the spectral gap of $$H$$. According to Proposition 5, for any such $$W$$, $$X$$ is the zero of the function

$$\Theta(x) = \sum_u (W_u + x)^{-1} - 1.$$ 

defined on $$x \in \mathbb{R}^+$$. If we have access to $$\Theta$$, then the monotonicity of the function in the variable $$x$$ implies that the bisection method can rapidly find $$X$$ to arbitrary error. Although $$\Theta(x)$$ is simple enough to write down, determining $$\Theta(x)$$ fully would require knowledge of $$W_u$$ for every vertex $$u$$. Hence, Algorithm 3 approximates $$X$$ by finding the zero $$\tilde{X}$$ of the function

$$\tilde{\Theta}(x) = \frac{V - 1}{n} \sum_{i=0}^{n-1} (W_{y_i} + x)^{-1} + \frac{1}{x} - 1,$$ 

(20)

where $$y_0, y_1, \ldots, y_{n-1}$$ are i.i.d. random variables with $$y_i \sim \text{Uniform}(V \setminus \{m\})$$. Algorithm 3 takes $$\tilde{\Theta}(s,x)$$ as equivalent to $$\tilde{\Theta}(x)$$ with $$W \mapsto \frac{s}{1-s}W$$, which merely restricts the above expressions to a particular one-parameter family. Since we only seek to understand $$X$$ as a function of $$W$$, we suppress the $$s$$-dependence in this section.

First, we determine how close $$\tilde{\Theta}$$ must be to $$\Theta$$ for $$\tilde{X}$$ to be a good estimate of $$X$$.

Proposition 10. For any $$x > 0$$,

$$|x - X| \leq (W_{u,V-1} + x)|\Theta(x)|.$$ 

Proof. Noting that $$\Theta(X) = 0$$ implies $$\sum_u (W_u + X)^{-1} = 1$$, we have

$$\begin{align*}
(W_{u,V-1} + x) |\Theta(x)| &= (W_{u,V-1} + x) \left| \sum_u \frac{1}{W_u + x} - 1 \right| \\
&= (W_{u,V-1} + x) \left| \sum_u \left( \frac{1}{W_u + x} - \frac{1}{W_u + X} \right) \right| \\
&= |x - X| \sum_u \frac{W_{u,V-1} + x}{(W_u + x)(W_u + X)} \\
&\geq |x - X| \sum_u \frac{1}{W_u + X} \\
&= |x - X|.
\end{align*}$$

In particular, if $$\tilde{\Theta}$$ is such that $$|\Theta(\tilde{X})| \leq \epsilon X/(W_{u,V-1} + \tilde{X})$$ for some $$\epsilon > 0$$, then $$|X - \tilde{X}| \leq \epsilon X$$.

Next, we bound $$|\delta(x)|$$ in terms of the number $$n$$ of samples drawn from $$V \setminus \{m\}$$. The following proposition implies that when $$x \approx \tilde{X}$$, we are within the bounds required by Proposition 10.
Proposition 11. If $\kappa \equiv W_{uv^{-1}}/W_u > 1$ and $n = \left(\frac{(V - 1)^2(\kappa - 1)^2}{2X^2\epsilon_0^2} \ln \left(\frac{2}{p}\right)\right)$ for some $\epsilon_0 > 0$ and $p \in (0, 1]$, then with probability at least $1 - p$,
\[
\left|\Theta(x) - \tilde{\Theta}(x)\right| \leq \frac{\epsilon_0 X}{W_{uv^{-1}} + x}
\]
for all $x > 0$.

Proof. First, we note that
\[
\sum_u \frac{1}{W_u + x} = \frac{1}{x} + \sum_{u \neq m} \frac{1}{W_u + x} = \frac{1}{x} + E \left(\frac{V - 1}{W_{yi} + x}\right).
\]
for any $i$. Hence, using Hoeffding’s inequality,
\[
\Pr \left(\left|\Theta(x) - \tilde{\Theta}(x)\right| \geq t\right) = \Pr \left(\sum_u \frac{1}{W_u + x} - \frac{1}{n} \sum_{i=0}^{n-1} \frac{V - 1}{W_{yi} + x} - \frac{1}{x} \geq t\right)
= \Pr \left(\left|E \left(\frac{1}{n} \sum_{i=0}^{n-1} \frac{V - 1}{W_{yi} + x}\right) - \frac{1}{n} \sum_{i=0}^{n-1} \frac{V - 1}{W_{yi} + x} \right| \geq t\right)
\leq 2 \exp \left[-2n t^2 \left(\max_{u \neq m} \frac{V - 1}{W_u + x} - \min_{u \neq m} \frac{V - 1}{W_u + x}\right)^2\right]
= 2 \exp \left[-\frac{2nt^2}{(V - 1)^2} \left(\frac{(W_{uv^{-1}} + x)(W_{uv^{-1}} + x)}{W_{uv^{-1}} - W_u}\right)^2\right]
\]
for $t \geq 0$. Taking $t = \epsilon_0 X/(W_{uv^{-1}} + x)$, we have
\[
\Pr \left(\left|\Theta(x) - \tilde{\Theta}(x)\right| \geq \frac{\epsilon_0 X}{W_{uv^{-1}} + x}\right) \leq 2 \exp \left[-\frac{2n\epsilon_0^2 X^2}{(V - 1)^2} \left(\frac{W_{u1} + x}{W_{uv^{-1}} - W_u}\right)^2\right]
= 2 \exp \left[-\frac{2n\epsilon_0^2 X^2}{(V - 1)^2(n - 1)^2} \left(1 + \frac{x}{W_u}\right)^2\right]
\leq 2 \exp \left[-\frac{2n\epsilon_0^2 X^2}{(V - 1)^2(n - 1)^2}\right].
\]
Thus, taking $n = [(V - 1)^2(\kappa - 1)^2 \ln(2/p)/(2\epsilon_0^2 X^2)]$ yields the desired result. \hfill \Box

The observant reader may worry that while Proposition 11 yields the bound required by Proposition 10 when $x = \tilde{X}$, the bound may be insufficiently tight when $x$ is far from $\tilde{X}$. Nonetheless, the function $\tilde{X}$ is monotone decreasing and $\lim_{x \to 0^+} \Theta(x) > 0$ and $\lim_{x \to \infty} \tilde{\Theta}(x) < 0$. Thus, the bisection method, which we discuss in the following subsection, can be used to determine its zero to arbitrary accuracy.

### 6.3 The FindRoot function

In this subsection, we use $X(s)$ to denote the zero of the function
\[
\Theta(s, x) = \sum_u \left(\frac{s}{1 - s} W_u + x\right)^{-1} - 1,
\]
defined on $x \in \mathbb{R}^+$ for a given $s \in [0, 1)$, so that $X(s) \equiv g_m(s) + 1$ corresponds to $H(s) = (1 - s)L + sW$. Similarly, we write $\tilde{X}(s)$ for the zero of $\tilde{\Theta}(s, x)$, which is defined as in Eq. (20) but with $W \mapsto \frac{s}{1 - s} W$. We note
that if we take the number of samples prescribed by Proposition 11, then $|\Theta(s,x) - \bar{\Theta}(s,x)| \leq \frac{c_0 X}{\log_2 \min(W_{\alpha_{W-1}} + 1)}$ with probability $1 - p$ for any $s$. Since the vertices are sampled once at the start of the algorithm, $\bar{\Theta}$ is constructed using the same $\{W_{\alpha_{W}}\}$ at every step; consequently, with probability $1 - p$, $\bar{\Theta}$ is a good approximation of $\Theta$ all $s$ such that $X(s) \geq x_{\min}$, or whenever $\Theta$ gets called. Hence, in this section we assume that $\bar{\Theta}$ is a good approximation of $\Theta$ and do not reference the probability of success.

The \textsc{FindRoot} function in Algorithm 3 approximates $X(s + \delta s)$ as $x_0(s + \delta s)$, using $\bar{\Theta}(s,x)$ and an estimate $x_0(s)$ of $X(s)$ from the previous step. Proposition 12 determines the number of iterations of the bisection method required to determine $X(s + \delta s)$ to within some relative error, when we know that $X(s + \delta s)$ lies within a certain interval. Proposition 13 demonstrates how to constrain the interval $I$ using $X(s)$. Finally, Theorem 8 integrates all of these results and guarantees $|X(s) - x_0(s)| \leq c_0 X(s)$ whenever $X(s) \geq (1 - c_0)x_{\min}$.

$\bar{\Theta}(s,x)$ is defined such that it is monotone decreasing over $x \in \mathbb{R}^+$ and, thus, has at most one positive root for any fixed $s$. Furthermore, $\lim_{x \to 0^+} \bar{\Theta}(s,x) > 0$ and $\bar{\Theta}(s,V + \epsilon) < 0$ for any $\epsilon > 0$. Thus, the bisection method is a natural way to determine this root.

**Proposition 12.** Suppose that for a given $s$, $\tilde{\Theta}$ has a unique zero $\tilde{X}(s + \delta s)$ in the interval $[ax_0(s), bx_0(s)]$ for some $0 < a < b$. Then, the bisection method returns an $x_0(s + \delta s)$ such that $|x_0(s + \delta s) - \tilde{X}(s + \delta s)| \leq \epsilon_1 \tilde{X}(s + \delta s)$ using $|\log_2[(b/a - 1)/\epsilon_1]|$ evaluations of $\tilde{\Theta}$.

**Proof.** Since $\tilde{\Theta}$ is monotone and has precisely one zero in the interval $[ax_0(s), bx_0(s)]$, we can apply the bisection method, which returns an estimate $x_0(s + \delta s)$ such that $|x_0(s + \delta s) - X(s + \delta s)| \leq x_0(s)(b - a)/2^k$ after $k$ steps, each of which evaluates $\Theta$ once. Thus, if

$$2^k \geq \frac{x_0(s)(b - a)}{\epsilon_1 X(s + \delta s)},$$

the method finds an $x_0(s + \delta s)$ for which $|x_0(s + \delta s) - \tilde{X}(s + \delta s)| \leq \epsilon_1 \tilde{X}(s + \delta s)$. Since $\tilde{X}(s + \delta s) = ax_0(s)$, it follows that $k = [\log_2((b/a - 1)/\epsilon_1)]$ calls to $\tilde{\Theta}$ suffice.

Proposition 12 requires a particular interval such that $\tilde{X}(s + \delta s)$ is in $[ax_0(s), bx_0(s)]$ for all $s$ such that $x_0(s) \geq x_{\min}$. We provide explicit bounds on $a$ and $b$ in the following proposition.

**Proposition 13.** If $|x_0(s) - X(s)| \leq c_0 X(s)$, $0 \leq \delta s \leq \frac{c_0}{4V} \left( \frac{x_0(s)}{1 + c_0} - 1 \right)(1 - s)$, and $|\tilde{X}(s + \delta s) - X(s + \delta s)| \leq \epsilon_0 X(s + \delta s)$, for some $c_0, \epsilon_0, \in (0,1)$, then

$$\tilde{X}(s + \delta s) \in \left[1 - \epsilon_0, \frac{1 - c_0}{1 + c_0} x_0(s), (1 + \epsilon_0) \frac{1 + c_0}{1 - c_0} x_0(s)\right].$$

**Proof.** Since $|x_0(s) - X(s)| \leq c_0 X(s)$ implies that $X(s) \geq x_0(s)/(1 + c_0)$, the assumption on $\delta s$ ensures that $\delta s \leq c_0 X(s) - 1) (1 - s) / 4V = c_0 \theta_{(m)}(s)(1 - s) / 4V$. Hence, $|X(s + \delta s) - X(s)| \leq c_0 X(s)$ by Proposition 6. It follows that

$$\tilde{X}(s + \delta s) \geq (1 - \epsilon_0) X(s + \delta s) \geq (1 - \epsilon_0) (1 - c_0) X(s) \geq (1 - \epsilon_0) (1 - c_0) x_0(s) / \frac{1 + c_0}{1 - c_0} x_0(s)$$

and similarly,

$$\tilde{X}(s + \delta s) \leq (1 + \epsilon_0) X(s + \delta s) \leq (1 + \epsilon_0) (1 + c_0) X(s) \leq (1 + \epsilon_0) (1 + c_0) x_0(s) / \frac{1 - c_0}{1 + c_0} x_0(s).$$
Theorem 8. Suppose that $\kappa \equiv W_{u^2}/W_{u_1} > 1$. If for a given $s \in [0, 1)$,

1. $|x_0(s) - X(s)| \leq c_0 X(s)$ for some $c_0 \in (0, 1)$,
2. $|\tilde{X}(s) - X(s)| \leq \frac{9c_0}{10}X(s)$,
3. $\tilde{X}(s), x_0(s) > x_{\min}$ for some constant $x_{\min}$,
4. $0 \leq \delta s \leq \frac{c_0}{4V} \left( \frac{x_0(s)}{1 + c_0} - 1 \right) (1 - s)$, and
5. for all $x$,

$$\left| \Theta(s + \delta s, x) - \tilde{\Theta}(s + \delta s, x) \right| \leq \frac{9c_0}{10} \left( \frac{1 - c_0}{1 + c_0} \right) s \frac{x_{\min}}{1 - s} W_{u^2 - 1} + x$$

(21)

then FINDROOT($s, \delta s, x_0(s)$) returns an $x_0(s + \delta s)$ such that $|x_0(s + \delta s) - X(s + \delta s)| \leq c_0 X(s + \delta s)$ using at most

$$\left\lceil \left( \frac{1 + c_0}{1 - c_0} \right)^2 \frac{5(V - 1)^2(\kappa - 1)^2}{8x_{\min}^2c_0^2} \ln \left( \frac{2}{p} \right) \right\rceil \left\lceil \log_2 \left[ \frac{19}{c_0} \left( \frac{1 + c_0}{1 - c_0} \right)^3 \right] \right\rceil$$

steps, where $1 - p$ lower bounds the probability that $\tilde{\Theta}$ satisfies Eq. (21).

Proof. Assumptions 1 and 4 imply that $|X(s + \delta s) - X(s)| \leq c_0 X(s)$ by Proposition 6. Combining this with Assumptions 2 and 3, we have

$$X(s + \delta s) \geq (1 - c_0)X(s) \geq (1 - c_0)\tilde{X}(s) \geq \frac{1 - c_0}{1 + 9c_0/10} x_{\min}.$$

Hence, by Proposition 11, constructing a $\tilde{\Theta}$ obeying Eq. (21) with success probability $1 - p$ requires

$$n = \left\lceil \left( \frac{1 + c_0}{1 - c_0} \right)^2 \frac{50(V - 1)^2(\kappa - 1)^2}{8x_{\min}^2c_0^2} \ln \left( \frac{2}{p} \right) \right\rceil$$

(22)

samples of $\mathcal{V}$. Taking $x = \tilde{X}$ in Eq. (21) and Proposition 10 implies that the zero $\tilde{X}(s + \delta)$ of $\tilde{\Theta}$ satisfies

$$\left| \tilde{X}(s + \delta s) - X(s + \delta s) \right| \leq \frac{9c_0}{10} \left( \frac{1 - c_0}{1 + c_0} \right) x_{\min} \leq \frac{9c_0}{10} X(s + \delta s).$$

It then follows from Proposition 13 with $c_0 = 9c_0/10$ that $\tilde{X}(s + \delta s) \in [ax_0(s), bx_0(s)]$, where $a = (1 - 9c_0/10)/(1 - c_0)/(1 + c_0) \geq (1 - c_0)^2/(1 + c_0)$ and $b = (1 + 9c_0/10)/(1 + c_0)/(1 - c_0) \geq (1 + c_0)^2/(1 - c_0)$. Because of Assumption 3, FINDROOT proceeds to find the zero of $\tilde{\Theta}$. Using the above interval in Proposition 12 and setting $c_1 = c_0/(10 + 9c_0) > c_0/19$, we see that applying

$$k = \left\lceil \log_2 \left\{ \frac{19}{c_0} \left[ \frac{1 + c_0}{1 - c_0} \right]^2 - 1 \right\} \right\rceil$$

iterations of the bisection method returns an $x_0(s + \delta s)$ such that

$$\left| x_0(s + \delta s) - \tilde{X}(s + \delta s) \right| \leq \frac{c_0}{10 + 9c_0} \tilde{X}(s + \delta s).$$

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Each iteration evaluates \( \Theta(s + \delta s, x) \) once, and each evaluation can take as many operations as are required to construct \( \Theta \), which is determined by the number of samples, \( n \). Therefore, noting that \( \epsilon_0 + \epsilon_1 + \epsilon_0 \epsilon_1 = \epsilon_0 \), an estimate \( x_0(s + \delta s) \) satisfying

\[
| x_0(s + \delta s) - X(s + \delta s) | \leq | x_0(s + \delta s) - \bar{X}(s + \delta s) | + \bar{X}(s + \delta s) - X(s + \delta s) \\
\leq \epsilon_1 \bar{X}(s + \delta s) + x_0 X(s + \delta s) \\
\leq (\epsilon_0 + \epsilon_1 + \epsilon_0 \epsilon_1) X(s + \delta s) \\
= x_0 X(s + \delta s)
\]

can be obtained using at most \( kn \) steps. \( \square \)

Since \( H(0) = L \) is independent of \( W \), we know that \( X(0) = V \) and Line 8 of Algorithm 3 sets \( x_0(0) = X(0) \). Thus, the conditions of Theorem 8 are satisfied for the base case \( s = 0 \). By induction, if the result of the theorem holds at some \( s \), then Assumptions 1, 2, and 5 are automatically satisfied at the next step \( s + \delta s \) by choosing the step size \( \delta s \) as in Assumption 4 and taking \( n \) at least as large as that in Eq. (22). Consequently, the result of Theorem 8 holds for all steps until \( s \) is such that Assumption 3 is not true, at which point the if statement of FindRoot is executed, FindRoot returns 0, and GetGap proceeds to call the FinishSchedule function discussed in the next subsection.

The if statement of FindRoot also finds an upper bound \( S_{\text{min}} \) on \( s_{\text{min}} \) (defined as in Theorem 7), which will be useful for estimating the gap in FinishSchedule. To see why the value assigned to \( S_{\text{min}} \) in Line 20 of Algorithm 3 indeed upper bounds \( s_{\text{min}} \), suppose that \( s \) is the first point for which Assumption 3 does not hold, so that FindRoot is not used to estimate \( \bar{X}(s + \delta s) \) and instead executes Lines 20 and 21. If \( s \leq s_{\text{min}} \), then \( h_{\{m\}} = g_{\{m\}} \) (by definition of \( s_{\text{min}} \)) and by Corollary 3,

\[
\gamma(s) = (1 - s) \gamma(G(s)) \leq (1 - 2s) g_{\{m\}}(s) = 2(1 - s)(X(s) - 1) \leq 2(1 - s)X(s)
\]

Substituting this upper bound on \( \gamma(s) \) into Corollary 4, it follows that

\[
S_{\text{min}} \leq s + \frac{4(1 - s)X(s)}{\chi V}.
\]

We know from Theorem 8 that the previous call to FindRoot returned an \( x_0(s) \) such that \( | x_0(s) - X(s) | \leq \epsilon_0 X(s) \). Line 20 is executed either when \( x(s) \leq x_{\text{min}} \), in which case

\[
X(s) \leq \frac{x_0(s)}{1 - \epsilon_0} \leq \frac{x_{\text{min}}}{1 - \epsilon_0},
\]

or because \( \bar{X}(s + \delta s) < x_{\text{min}} \). Suppose that the latter condition is satisfied but the former is not, i.e., that \( \bar{X}(s + \delta s) < x_{\text{min}} \) but \( x(s) > x_{\text{min}} \). In this case, note that we would have

\[
X(s + \delta s) \geq (1 - \epsilon_0) X(s) \geq \frac{1 - \epsilon_0}{1 + \epsilon_0} x(s) \geq \frac{1 - \epsilon_0}{1 + \epsilon_0} x_{\text{min}},
\]

which means that having chosen \( n \) according to Eq. (22), \( | \bar{X}(s + \delta s) - X(s + \delta s) | \leq \epsilon_0 X(s + \delta s) \), whence

\[
X(s) \leq \frac{X(s + \delta s)}{1 - \epsilon_0} \leq \frac{\bar{X}(s + \delta s)}{(1 - \epsilon_0)^2} \leq \frac{x_{\text{min}}}{(1 - \epsilon_0)^2}.
\]

Therefore, in either case, Corollary 4 guarantees that

\[
S_{\text{min}} \leq s + \frac{4(1 - s) x_{\text{min}}}{(1 - \epsilon_0)^2 \chi V},
\]

and FindRoot sets \( S_{\text{min}} \) accordingly. If, on the other hand, \( s > S_{\text{min}} \), the above inequality is trivially true, and so \( S_{\text{min}} \) is a valid upper bound in either scenario.
Finally, it is important to note that since $\hat{\Theta}$ is constructed using the same set of vertex samples at every step throughout a given run of BAA, the probability of failure $p$ from Proposition 11 is not compounded at each step. After setting $n$ and randomly choosing $n$ vertex samples at the very first call BAA makes to FINDROOT, the resultant $\hat{\Theta}$ either approximates $\Theta$ for all subsequent $s$ at which its root is used to approximate $X$, or never does. Thus, the entire procedure evolving from $s = 0$ to $s = 1$ succeeds with probability at least $1 - p$.

### 6.4 The FinishSchedule function

The FinishSchedule function exploits the the lower bound of Theorem 7 when GetGap is called for an $s$ for which $\Theta$ cannot be used to reliably return an estimate of the gap $\gamma(s)$. Its behavior is simple: first, it underestimates the gap and returns its absolute lower bound, and then, once we know that we have definitely passed the minimum gap, it follows the linear envelope of Theorem 7 until $s = 1$. One could use computational basis measurements to avoid following the linear envelope and instead estimate the proposition determines the number of extra queries to GetGap introduced by this modified behavior.

**Proposition 14.** With all quantities as in Algorithm 3, if $x_{\text{min}} \leq \chi V$, then Algorithm 2 requires at most

$$O\left(\frac{\kappa^4 x_{\text{min}}}{\chi \sqrt{V}} + Q\left(\frac{5\sqrt{V - 1}}{2\kappa} - \frac{c_0 \chi (V - 2)}{16\kappa^4 V}\right)\right)$$

calls to FinishSchedule.

**Proof.** BAA (Algorithm 2) estimates the gap $\gamma(s)$ at a sequence of discrete points $s$, determining the step size $\delta s$ between each point in Line 6. Let $s_0 < s_1 < \ldots s_k$ denote the sequence of points at which GetGap calls FinishSchedule. Observe from Algorithm 3 that this implies that $s_0$ is the only point at which Line 20 is executed, so $S_{\text{min}}$ is set to

$$S_{\text{min}} = s_0 + \frac{4(1 - s_0)x_{\text{min}}}{(1 - c_0)^2 \chi V}$$

and remains fixed throughout the remainder of BAA. Also note that FinishSchedule is called at $s_0$ and at every subsequent step of BAA, which means that $s_0, s_1, \ldots, s_k$ are consecutive points in the sequence sampled by BAA. Therefore, it follows that $s_{i+1} = s_i + c_0 \gamma(s_i)/4V$ (unless $s_i + c_0 \gamma(s_i)/4V \leq 1$, in which case the algorithm simply sets $s_{i+1} = 1$), where $\gamma(s_i)$ is the estimate returned by GetGap in the previous step and with $\lambda_{\max} \rightarrow V$ since $\|H(0)\| = \|L\| = V$ and $\|H(1)\| = \|W\| \leq V$.

First, we consider the points $s_i \in S_{\text{min}}$, and define $f$ such that $s_{f-1} \leq S_{\text{min}}$ but $s_f > S_{\text{min}}$. We can see from Algorithm 3 that $f$ is the number of points for which the if statement of FinishSchedule is executed, and Line 26 implies that for $i = 0, 1, \ldots, f - 1$,

$$s_{i+1} \geq s_i + \frac{\sqrt{V - 1}}{4\kappa^4 V}(1 - s_i).$$

Solving the recurrence, we have

$$s_i \geq 1 - (1 - s_0)\left(1 - \frac{\sqrt{V - 1}}{4\kappa^4 V}\right)^i.$$

Thus, taking

$$g \equiv \left\lfloor \log \frac{1 - (1 - c_0)^2 \chi V}{\log \left(1 - \frac{\sqrt{V - 1}}{4\kappa^4 V}\right)} \right\rfloor,$$
we see that

\[ 1 - (1 - s_0)^g = \frac{4(1 - s_0)x_{\text{min}}}{(1 - c_0)^2 \chi V} = S_{\text{min}}, \]

and so \( g \) is an upper bound on \( f \). Since

\[
\begin{align*}
g &\leq \left( \frac{4x_{\text{min}}}{(1 - c_0)^2 \chi V} \right) \left[ 1 - \frac{4x_{\text{min}}}{(1 - c_0)^2 \chi V} \right]^{-1/2} \left( \frac{\sqrt{V - 1}}{4\kappa^{4V}} \right)^{-1} \\
&\leq \left( \frac{16}{(1 - c_0)^2 \chi \sqrt{V - 1}} \right) + O \left( \frac{\kappa^4 x_{\text{min}}^2}{\chi^2 V^{3/2}} \right) \\
&= O \left( \frac{\kappa^4 x_{\text{min}}^2}{\chi \sqrt{V}} \right),
\end{align*}
\]

it follows that Line 27 of \textsc{FinishSchedule} is reached for at most \( O \left( \frac{\kappa^4 x_{\text{min}}}{\chi \sqrt{V}} \right) \) calls to Algorithm 3.

For the remaining steps \( s_f, s_{f+1}, \ldots, s_k \) > \( S_{\text{min}} \), for which \textsc{FinishSchedule} skips to Line 28, note that \( s_k > S_{\text{min}} \) implies that \( s_k > s_{\text{min}} \) since \( S_{\text{min}} \) is an upper bound on \( s_{\text{min}} \). Hence, Theorem 7 shows that the estimate returned by Line 28 of Algorithm 3 at each remaining step is indeed a lower bound of the form required by Theorem 4, from which it follows that Line 28 is reached for at most \( Q = O \left( \frac{5\sqrt{V - 1}}{2\kappa}, \frac{\chi(V - 2)}{16\kappa^3 V} \right) \) calls to Algorithm 3. Therefore, \textsc{FinishSchedule} is executed \( O \left( \frac{\kappa^4 x_{\text{min}}}{\chi \sqrt{V}} + Q \right) \) times.

### 6.5 Full runtime

Finally, we consolidate all of the results from this section and determine the full runtime of Algorithm 2 were it to use the gap oracle constructed in Algorithm 3.

**Theorem 9.** For \( s \in [0, 1] \), let \( P(s) \) denote the projector onto the ground state of \( H(s) = (1 - s)L + sW \), and suppose that \( \chi \) and \( \kappa \geq \frac{W_{\text{max}} - 1}{W_{\text{min}}} \) are constants independent of \( V \). If Algorithm 2 uses Algorithm 3 as the gap oracle, then for any \( \epsilon > 0 \), it returns a state \( \tilde{P}(1) \) such that

\[
\left\| \tilde{P}(s) - P(s) \right\| \leq O \left( \epsilon \right)
\]

with probability at least \( 1 - e^{-1/\epsilon} \) in time

\[
O \left( \frac{1}{\epsilon} \log^2(\sqrt{V}) \left[ \sqrt{V} + (\kappa - 1)^2 V^{2/3} \right] \right).
\]

**Proof.** We see from Lines 4 and 15 of Algorithm 3 that constructing a function \( \tilde{\Theta} \) that well approximates \( \Theta \) (in the sense of Proposition 11) requires \( n = O \left( 1 + V^2(\kappa - 1)^2 x_{\text{min}}^2 \ln(1/p) \right) \) samples, conditioned on the vertex \( m \) never being sampled. Whenever \( m \) is sampled, Line 15 resamples until a different vertex is chosen. The probability of sampling \( m \) is \( 1/V \) (assuming a uniform distribution over the vertices), so the probability that, for an integer \( k \geq 0 \), Line 15 loops more than \( k \) times when it is reached is \( V^{-k} \). Since Line 15 is reached \( n \) times, the probability that every repetition of Line 15 requires more than \( k \) operations is \( V^{-kn} \). Therefore, the probability that populating \( \mathcal{V} \) in Line 13 requires no more than \( kn \) steps and that the resultant \( \tilde{\Theta} \) is a good approximation for \( \Theta \) is at least \( (1 - V^{-kn})(1 - p) \geq 1 - p - V^{-kn} \). Since \( V^{-kn} \) is doubly exponentially small, we can choose the upper bound on the failure probability to be a constant. Note from Line 13 that the global parameter \( \mathcal{V} \) is populated only once in a given run of Algorithm 2. Once \( \mathcal{V} \) is fixed, each call to \( \tilde{\Theta} \) simply executes Line 17 and returns.

\textsc{GetGap} uses \textsc{FindRoot} at each step, starting from \( s = 0 \), until the \textbf{if} statement of \textsc{FindRoot} is executed. It is clear from Line 19 that at every point \( s \) for which the \textbf{if} statement is not satisfied, it must be the case that \( x_0(s) > x_{\text{min}} \), which implies that \( X(s) \geq x_0(s)/(1 + c_0) \geq x_{\text{min}}/(1 + c_0) \). Since
$x_{\min} \geq 2(1 + c_{0})\sqrt{V}$ by Line 3 whereas $X(s) \leq \sqrt{V - 1} + 1 \leq 2\sqrt{V}$ at $s = s_{\min}$ by Proposition 7, it follows that $s < s_{\min}$ for every point $s$ at which the root-finding procedure of FindRoot is executed, with the possible exception of the very last point. Thus, the gap estimate returned by Line 11 of GetGap at these points is $\Theta(\Gamma(s))$, where $\Gamma(s)$ is defined in Theorem 7. Theorems 4 and 7 then imply that the number of calls Algorithm 2 makes to FindRoot is

$$O(Q) = O \left( Q \left( \frac{5\sqrt{V - 1}}{2\kappa}, \frac{c_{0}\chi(V - 2)}{16\kappa^{5}V} \right) \right) = O \left( \log \left( \sqrt{V} \right) \right).$$

Combining this with the number of steps required for each call to FindRoot given by Theorem 8, it follows that $O(1 + V^{2}\log(\sqrt{V})(\kappa - 1)^{2}x_{\min}^{-2}\ln(1/p))$ operations are performed before GetGap starts using FinishSchedule instead of FindRoot to estimate the gap. Proposition 14 shows that FinishSchedule is called $O(x_{\min}/\sqrt{V} + \log(\sqrt{V}))$ times, and we see from Algorithm 3 that each call performs a single elementary computation. Adding this to the steps required by FindRoot, the runtime due to Algorithm 2 calling GetGap is

$$O \left( \frac{V^{2}\log(\sqrt{V})(\kappa - 1)^{2}}{x_{\min}^{2}} \log \left( \frac{1}{p} \right) + \frac{x_{\min}}{\sqrt{V}} + \log \left( \sqrt{V} \right) \right).$$

After completing the main loop of Algorithm 2, the adiabatic state at $s = 1$ is prepared using GenerateState($\gamma, 0, \epsilon/Q$). Since Algorithm 2 calls GetGap $O(x_{\min}/\sqrt{V} + Q)$ times, $|\gamma| = O(x_{\min}/\sqrt{V} + Q)$ and there are $|\gamma|$ iterations of the main loop of Algorithm 1. For each iteration, taking $T_{i} = O(\epsilon^{-1}Q\lambda_{\max}/\gamma_{i}) = O(\epsilon^{-1}\sqrt{V}\log(\sqrt{V}))$ produces a state $\|\tilde{P}(s) - P(s)\| \leq O(\epsilon)$ by Proposition 1, Corollary 1, and Theorem 3. Multiplying this by the total number of iterations yields a runtime of

$$O \left( \frac{1}{\epsilon} \log(\sqrt{V})(x_{\min} + \sqrt{V}Q) \right) = O \left( \frac{1}{\epsilon}x_{\min}\log^{2}(\sqrt{V}) \right),$$

where we note from Line 3 that $x_{\min} \geq \sqrt{V}$.

Thus, since calls to GetGap and GenerateState are additive, the total time of the algorithm is $O(\epsilon^{-1}x_{\min}\log^{2}(\sqrt{V}) + (\kappa - 1)^{2}V^{2}\log(\sqrt{V})x_{\min}^{-2}\ln(1/p))$. Letting $p = \Omega(\epsilon^{-1}/\epsilon)$ yields a total runtime of

$$O \left( \frac{\log^{2}(\sqrt{V})}{\epsilon} \left[ x_{\min} + (\kappa - 1)^{2}V^{2}/x_{\min}^{2} \right] \right).$$

Noting that when $x_{\min} = \sqrt{V}$, the definition of $x_{\min}$ in Algorithm 3 gives

$$x_{\min} \geq (\kappa - 1)^{2/3}(V - 1)^{2/3},$$
$$x_{3}^{V} \geq (\kappa - 1)^{2}(V - 1)^{2},$$
$$x_{\min} \geq (\kappa - 1)^{2}(V - 1)^{2}/x_{\min}^{2}.$$  

Thus, since $\Omega(\sqrt{V}) = x_{\min} = O\left(1 + (\kappa - 1)^{2/3}V^{2/3}\right)$, we have a total runtime of

$$O \left( \frac{\log^{2}(\sqrt{V})}{\epsilon} \left[ x_{\min} + (\kappa - 1)^{2}V^{2}/x_{\min}^{2} \right] \right) = O \left( \frac{\log^{2}(\sqrt{V})}{\epsilon} \left( \sqrt{V} + (\kappa - 1)^{2/3}V^{2/3} \right) \right).$$
6.6 Optimization

We now present an optimization algorithm, Algorithm 4, that optimizes the runtime of Algorithm 2 using multiple copies of the gap oracle \( \text{GetGap} \) of Algorithm 3 when the spectral ratio \( \kappa \) of the cost function \( W \) is unknown. It proceeds by guessing that \( \kappa \approx 1 \) and increases \( \kappa \) until we are guaranteed that \( \kappa \) upper bounds the spectral ratio of \( W \).

**Algorithm 4 Optimize**

**Require:** \( \lambda_{\text{max}} \geq \|H\| \), the spectral gap \( \gamma(0) \) of \( H(0) \), a lower bound \( \gamma(1) \) on the spectral gap of \( H(1) \), an oracle \( \text{GetGap}_\kappa \) that depends upon the parameter \( \kappa \), a constant \( p \in (0, 1) \) independent of \( V \)

1: function Optimize\((W)\)

2: \[ \delta \leftarrow \frac{3}{2} \log_{\sqrt{V}} \left( \frac{3}{2} \right) \] \( \triangleright \) Step size by Theorem 10

3: Choose \( N \leftarrow \log \left( \frac{pV^{-1/6}}{(1-e^{-1})^2} \right) \)

4: for \( i \in \left\lfloor \frac{T}{\delta} \right\rfloor \) do

5: \[ \kappa \leftarrow 1 + \frac{V^i \delta - \frac{1}{4}}{1 - \frac{1}{4}e^{-1}} \] \( \triangleright \) Guess \( \kappa(W) \leq \kappa \)

6: \( \Psi \leftarrow [\text{BAA}(\text{GetGap}_\kappa)]_{i=0}^N \) \( \triangleright \) Collect the results of BAA

7: \( \Psi \leftarrow \text{Measure}(\Psi) \) \( \triangleright \) Measure in the computational basis

8: if \( W_b = 0 \) for any \( b \in \Psi \) then return \( |b\rangle\langle b| \)

9: \[ \kappa \leftarrow \lambda_{\text{max}} / \gamma(1) \] \( \triangleright \) Assume worst case \( \kappa \)

10: return \( \text{BAA}(\text{GetGap}_\kappa) \) \( \triangleright \) Run BAA with worst case \( \kappa \)

The following theorem shows that we can perform Algorithm 4 and achieve the runtime bound of Theorem 9 for \( \kappa \approx \kappa(W) \), with only logarithmic asymptotic overhead.

**Theorem 10.** For \( \kappa = \frac{W_{\text{max}}}{{V_{\text{max}}}^{-1}} \leq \frac{\lambda_{\text{max}}}{\gamma(1)} \), Algorithm 4 has an expected runtime of

\[
\mathcal{O} \left( \frac{\log^3(\sqrt{V})}{\epsilon \log(1/\epsilon)} \left( \sqrt{V} + (\kappa - 1)^{2/3} V^{1/3} \right) \right)
\]

and returns \( |m\rangle\langle m| \) with probability greater than \( 1 - pV^{-1/6} \).

**Proof.** Assume that \( \kappa = 1 + V^{-x} \) and \( \kappa_j = 1 + V^{j\delta - \frac{1}{4}} \). Then, there exists a first \( j \) such that \( x_j = \frac{1}{4} - j\delta \leq x \leq \frac{1}{4} - (j - 1)\delta \)

\[
|\kappa_j - \kappa| = \left| V^{j\delta - \frac{1}{4}} - V^{-x} \right|
\]

\[
= V^{-x} \left| V^{x + j\delta - \frac{1}{4}} - 1 \right|
\]

\[
= V^{\delta - x} \left| V^{x + (j-1)\delta - \frac{1}{4}} - V^{-\delta} \right|
\]

\[
\leq (\kappa - 1)V^{\delta}.\]

Taking \( \delta = \frac{3}{2} \log_{\sqrt{V}} \left( \frac{3}{2} \right) \), we have that for this \( j \),

\[
\kappa_j - \kappa = (\kappa - 1) \left( \frac{3}{2} \right)^{3/2}.
\]

Thus, for some choice of \( j \), we have that \( \kappa_j \geq \kappa \) and \( \kappa_j - 1 = \Theta(\kappa - 1) \). Thus, assuming that Algorithm 4
has not returned prior to \( j \), we wish to evaluate

\[
\sum_{i=0}^{j} (\kappa_i - 1)^{2} V^{j} = \sum_{i=0}^{j} V^{2(j-1/4 + \delta)}
\]

\[
= \sqrt{V} \sum_{i=0}^{j} V^{2(j-1/4 + \delta)}
\]

\[
= \sqrt{V} \frac{V^{2(j+1) - 1}}{V^{2(j-1/4 + \delta)} - 1}
\]

\[
\leq 2\sqrt{V} V^{2(j-1/4 + \delta)}
\]

\[
= 2V^{\frac{1}{2}} (j^{\delta} - \frac{1}{4})
\]

\[
= 2V^{\frac{1}{2}} (\kappa_j - 1)^{\frac{1}{2}}
\]

\[
\leq 2(\kappa - 1)^{\frac{1}{2}} V^{2(1 + V^{2\delta})}
\]

\[
= \frac{27}{4} (\kappa - 1)^{\frac{1}{2}} V^{2}.\]

Thus, we can reach the end of the \( j \)th iteration of Algorithm 4 Step 4 in total time

\[
O \left( N \frac{\log^{2}(\sqrt{V})}{\epsilon} \left( \sqrt{V} + (\kappa - 1)^{2/3} V^{2/3} \right) \right).
\]

On the \( j \)th iteration, we are guaranteed to satisfy the conditions of Theorem 9 and thus we produce \( N \) states such that \( \bar{P} = |m\rangle\langle m| + O(\epsilon) \), each with probability at least \( 1 - e^{-1/\epsilon} \). After measuring each in the computational basis \( N \) times, we do not return \( |m\rangle\langle m| \) with probability at most

\[
p^{N} \equiv \left( 1 - \left( (1 - \epsilon)(1 - e^{-1/\epsilon}) \right) \right)^{N}
\]

\[
\leq \left( (1 + e^{-1})\epsilon \right)^{N}.
\]

Now, let \( f \) be the the greatest value of \( i \) reached by Algorithm 4 Step 4. Let \( N T_{i} \) be the total time taken
through the end of the $i^{th}$ iteration of Algorithm 4 Step 4. Then,

$$E[T_j] = \sum_i T_i \Pr (f = i)$$

$$\leq T_j + N \sum_{i > j} \Pr (f = i) \mathcal{O} \left( \frac{V^{\frac{1}{2}} (1 + \frac{1}{2}i)}{\epsilon} \log^2 (\sqrt{V}) \right)$$

$$\leq T_j + N \sum_{i > j} \mathcal{O} \left( \frac{V^{\frac{1}{2}} (1 + \frac{1}{2}i)}{\epsilon} \log^2 (\sqrt{V}) \right) \left( (1 + e^{-1})e^{\log_{(1 + e^{-1})}(pV^{-1/6})} \right)$$

$$= T_j + N \sum_{i > j} \mathcal{O} \left( \frac{V^{\frac{1}{2}} (1 + \frac{1}{2}i)}{\epsilon} \log^2 (\sqrt{V}) \right) \left( \frac{p}{V^{1/6}} \right)$$

$$= T_j + \mathcal{O} \left( N \frac{\sqrt{V}}{\epsilon} \log^2 (\sqrt{V}) \right)$$

$$= \mathcal{O} \left( N \frac{\log^2 (\sqrt{V})}{\epsilon} \left( \sqrt{V} + (\kappa - 1)^{2/3} V^{2/3} \right) \right) + \mathcal{O} \left( N \frac{\sqrt{V}}{\epsilon} \log^2 (\sqrt{V}) \right)$$

$$= \mathcal{O} \left( \frac{\log^3 (\sqrt{V})}{\epsilon \log (1/\epsilon)} \left( \sqrt{V} + (\kappa - 1)^{2/3} V^{2/3} \right) \right).$$



7 Discussion and future work

7.1 Improving the Cheeger inequality

The bound derived in Theorem 6 is almost certainly loose by a factor of approximately $\kappa^2$, however a tighter version of this theorem remains elusive. Since improving the inequality provides no asymptotic advantage, we did not attempt to achieve a nearly optimal inequality in the present work. Nonetheless, tight inequalities are always of mathematical interest and deriving them is well-motivated, especially if one were to look to apply this algorithm in practice.

The most likely approach to successfully achieving an inequality that scales like

$$2h_{\{m\}} \geq \gamma \gtrsim \frac{h_{\{m\}}}{\kappa}$$

would be to consider the ratios of the components of $\phi_1$. That is, if $W_m < W_{u_1} \leq \ldots W_{u_{V-1}}$, we cannot get a useful bound on

$$\frac{\phi_1(u_{V-1})}{\phi_1(u_1)} = \frac{V + W_{u_1} - \lambda_1}{V + W_{u_{V-1}} - \lambda_1}$$

as the numerator can tend towards 0 for large enough $W$. Nonetheless, if we consider $\kappa_i = \frac{W_{u_{V-1}}}{W_{u_i}}$

$$\frac{\phi_1(u_{V-1})}{\phi_1(u_{j>1})} = \frac{V + W_{u_j} - \lambda_1}{V + W_{u_{V-1}} - \lambda_1} \geq \frac{\kappa_j - 1}{\kappa_1 - 1}.$$
7.2 Shaving off extra factors of $\kappa$

Note that we reach a state such that $\phi(m)^2 \geq 1/2$ before our Cheeger inequality becomes weak. Thus, if we are only looking to perform optimization and factors of $\kappa^3$ look ominous, we could stop our algorithm short and incur no factors of $\kappa$ other than insofar as they improve Proposition 11. That is, we could prepare a state such that $||m⟩ − |\phi⟩|| \leq \frac{1}{2} + \mathcal{O}(\epsilon)$. By repeating this procedure $\log_2(1/\epsilon)$ times, we would then be able to return $|m⟩$ with probability $1 - \mathcal{O}(\epsilon)$. Everything else would remain unchanged.

7.3 Multiple marked states

We should consider the case that there is more than one state $M = \{m_i\}_{i=0}^{k-1}$ such that $W_{m_i} = 0$. For this, Theorem 6 would need to be modified to handle the degeneracy, which could be done by first projecting into the subspace that identifies all marked states as a single state.

Since in the restricted subspace, if we let $\psi_i(M) = \sum_{m \in M} \phi_i(m)$ and $\psi_i(v) = \phi_i(v)$, for any eigenvector $\phi$ corresponding to eigenvalue $\lambda$, we have

$$(V + W_u - \lambda)\phi(u) = \sum_{v \neq u} (\phi(v) - \phi(u))$$

we have that

$$(V - \lambda)\psi(M) = \sum_{m \in M} \sum_{v \in M} (\phi(v) - \phi(m))$$

$$= \sum_{m \in M} \sum_{v \notin M} (\phi(v) - \phi(m)) + \sum_{m \in M} \sum_{v \in M} (\phi(v) - \phi(m))$$

$$= \sum_{v \notin M} (k\phi(v) - \psi(M)).$$

Then,

$$(\lambda_k - \lambda_0)\psi_0(M)\psi_k(M) = k \sum_{v \notin M} (\phi_0(v)\psi_k(M) - \phi_k(v)\psi_0(M)).$$

Comparing this to Theorem 6, one could clearly derive an appropriate Cheeger inequality that applies to the relevant subspace, where we are interested in the spectral gap $\lambda_k - \lambda_0$. One would need to take care, however, since above $\psi_0(M)^2 \neq \sum_{m \in M} \phi_0(m)^2$. Thus, the improvement would not be the simple factor of $k$ that we see above. The tighter bound would ultimately result from the reduced number of vertices under consideration in the equivalent of Proposition 8, using the fact that we would now be considering the point $s_{\text{min}}$ as the point at which $\sum_{m \in M} \phi(m)^2 = \frac{1}{2}$.

One could then simply proceed by calling Algorithm 2 assuming that there are $V/2^i$ marked states for $i = 0, 1, 2, \ldots, V - 1$ until some state $u$ such that $W_u = 0$ is returned. A similar approach was used by two of the authors in [14] in a completely different context, but the same technique should apply here and achieve optimal scaling. However, combining this with Algorithm 4 would require carefully balancing parameters. It is less clear whether the fixed point methods of [10] would work with BAA, though their adaptation would certainly be interesting and the claim that similar methods work in [4] suggests they might be promising.

7.4 Designing Optimization Hardware

Our results suggest that, for near-term quantum hardware, one should look to create driving Hamiltonians $L$ such that the Cheeger constant is easy to evaluate for arbitrary cost functions. Algorithm 3 demonstrates that at least under some circumstances and for particular graphs, this should indeed be possible. The numerator in the Cheeger constant itself is a measurement of the energy of some cut operator

$$C_S = \frac{1}{2} \sum_{i \in S} \sum_{j \notin S} (|i⟩⟨j| + |j⟩⟨i|).$$

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That is,
\[ g_S = \frac{\langle \phi | C_S | \phi \rangle}{\sum_{u \in S} \phi(u)^2} \]
and
\[ h_S = \max_{S' \in \{S, S\}} \frac{\langle \phi | C_{S'} | \phi \rangle}{\sum_{u \in S} \phi(u)^2}. \]

If we prepare \(|\phi\rangle\) to high enough accuracy, then we should expect that both the numerator and denominator can be measured. That is, the denominator is just the probability that \(\phi\) measured in the computational basis will be found in \(S\) and the numerator is the energy of the particular cut which, at least in our complete graph case, can be measured in the \(X\)-basis. Importantly, these bases remain fixed throughout the interpolation and so we need no knowledge of instantaneous eigenbases to determine each \(g_S\). Furthermore, for many graphs, we can probably find an appropriate set of cuts \(\{C_S\}\) such that each \(S\) is of different size and we are able to permute \(W\) to measure sets corresponding to different elements of the cost function. Thus, with only a fixed number of physical cuts, we can create a much larger number of computational cuts. The idea is sketched in Algorithm 5.

**Algorithm 5** General oracle

**Require:** A set of cuts \(S\), the cost function \(W\), a number \(N\), a known lower bound on the gap \(\gamma_{\min}\)

1. **function** GET\text{GAP}(\(s, \delta s, \gamma, c_0\))
2. **if** \(h\) is efficient to compute **then** \(h \leftarrow (1 + c_0)\gamma\) \(\triangleright\) Upper bound next \(h\)
3. **for** \(S \subset S\) **do**
4. \(P_S \leftarrow \sum_{i \in S} |i\rangle\langle i|\)
5. \(P_i \leftarrow [\text{GENERATE\text{STATE}}(s, \delta s, \gamma, c_0)]_{i=0}^{2N-1} \) \(\triangleright\) Generate some projectors at \(s + \delta s\)
6. \(E_{CS} \leftarrow \frac{1}{N} \sum_{i=0}^{N-1} \text{tr} (C_S P_i) \) \(\triangleright\) Measure the energy of the cut
7. \(p_S \leftarrow \frac{1}{N} \sum_{i=0}^{2N-1} \text{tr} (P_S P_i)\) \(\triangleright\) Measure the probability of being in the cut
8. \(h \leftarrow \min \left( h, \frac{E_{CS}}{\min(p_S, 1-p_S)} \right) \)
9. **return** \(h/2\) \(\triangleright\) Return a lower bound on the gap to within a constant factor
10. **return** \(\gamma_{\min}\) \(\triangleright\) Return a known lower bound on the gap

In fact, this oracle is the reason BAA is named such; after sampling a state \(\delta s\) away from what we presently know how to prepare, the oracle requires that we start our adiabatic procedure over entirely. Hence, we creep along slowly, only ever advancing by \(\delta s\) in a given step.

For general graphs, using adiabatic processes as subroutines may not just be useful, but is probably necessary for steering our adiabatic evolution. If we satisfy something like Theorem 11, then we are guaranteed that we need to repeat the adiabatic procedure at most \(O(\log(1/\gamma_{\min}))\) times and, thus, the need for restarts should not be concerning.

### 7.5 Improving the oracle

Although sufficient, Algorithm 3 can be greatly improved, especially after reaching the point labeled \(s_{\min}\). One method for doing so would be to sample \(\phi(m)^2\) by letting Algorithm 3 Call Algorithm 1 like discussed above, performing computational basis measurements on the result, and then exploiting Proposition 7. Proposition 7 also guarantees that \(\phi(m)^2 > \epsilon\) for some constant \(\epsilon < 1/2\) even when \(s < s_{\min}\). Thus, in some places, one might also be able to improve the provided bounds by multiple factors of \(\kappa\), by switching to a computational basis measurement procedure prior to \(s = s_{\min}\). In the present context, none of these changes would achieve better asymptotic scaling and therefore is not pursued. Nonetheless, for practical applications, optimizing constants and appropriately balancing some of the procedures presented might be necessary.
7.6 Removing the restriction $W_m = 0$

Although the existence of this condition allows us to solve the decision problem of whether $0 \in W$, it is not sufficient to arbitrarily optimize a set. For this, we may need to introduce cut operators like those discussed in Section 7.4 or improve the classical parts of our oracle. Presently, if we think of $W : V \rightarrow [0, 1]$, our algorithm is actually flexible enough to find $m$, provided that we know that a $\tilde{W}$ such that $|\tilde{W} - W_m| \leq \epsilon V^{-1/3}$. Of course, this is exponentially small on the scale of the problem and we would prefer to generalize beyond the current oracle for full optimization. Whether this can be done while remaining restricted to computational basis measurements is presently unclear.

7.7 The role of other paths

Interpolated Hamiltonians of the form

$$H_i(s) = (1-s)H(0) + s(1-s)\tilde{H}_i + sH(1)$$

where $\tilde{H}_0 = 0$ and $\tilde{H}_i$ is some arbitrary time-independent Hamiltonian are often used in the hope that $\gamma_{\min}(H_0) \leq \gamma_{\min}(H_i)$, speeding up adiabatic processes. However, numerical results suggest that doing so usually also increases the width of the corresponding gap minimum. In the language of Theorem 11, if $I_k = \{s : \gamma(H_i(s)) \leq \frac{\|H_i\|}{K} \}$ and $\mu(I_k) \leq C2^{-k}$, then we know that performing BAA on $H_0$ requires at most $O(C \log_2 \left( \frac{\|H_i\|}{\gamma_{\min}(H_0)} \right))$ queries to GETGAP. Now, if we replace this Hamiltonian with $H(s)$, but at the cost that $\mu(I_k^{(i)}) \geq \frac{\gamma_{\min}(H_i)}{\gamma_{\min}(H_0)} \mu(I_k^{(0)})$, we know that whatever performance we gain by being able to vary our Hamiltonian faster, we lose to the number of discretization points (in this case, the number of queries).

This is not to say that when the conjecture above holds true, intermediate Hamiltonians will not serve a purpose, they still might. However, the role of $H_i \neq H_0$ seems to be that these intermediate Hamiltonians may make queries to GETGAP easier. That is, if we are to consider $H_i \neq H_0$, we should probably look to determine the class $H_i$ such that we can guarantee rapid returns from GETGAP. It is possible that such an intermediate interpolation would even enhance the abilities of our oracle Algorithm 3. Additionally, using Algorithm 3, we might be able to use these intermediate Hamiltonians only when we know that queries are becoming more challenging, as is the case for $h \sim \sqrt{V}$ in Algorithm 3.

7.8 The width of the minimum gap

We believe that the mathematical project of studying the width of the minimum gap in an interpolated Hamiltonian (or the measures $\mu(I_k)$), especially in the context of the discussion of Section 7.7, would be quite interesting. Of course, this would be a question of pure analysis, but nonetheless well-motivated by BAA and Theorem 11. Understanding this relationship would, in principle, be a key component of designing optimized schedules and also determining whether algorithmically easier and faster paths exist. Furthermore, such a bound would have complexity-theoretic implications. That is, if for interpolated Hamiltonians the width of the minimal gap can indeed always be bounded as in Theorem 11, then we would know that for any driving Hamiltonian, either determining the gap is always hard for hard problems or there would be a tradeoff in the difficulty of determining the gap and the size of the gap. Otherwise, Algorithm 2 solves hard problems with bounded probability.

To the knowledge of the authors, no appropriate, general inequalities yet exist.

7.9 Classical algorithms

There is no reason that GETGAP must correspond to Algorithm 3 or, for that matter, that the driving Hamiltonian should be restricted to one considered in this paper. It seems reasonable that one might use BAA as a tool for solving classical computation problems. Indeed, the authors of [4] suggest as much

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3 Just assume that $W_m = 0$, apply Algorithm 2, and if you get 0 at the end of the day respond “yes”. 35
for their strategy. Since we know that simulated quantum annealing can potentially be faster than, say, simulated annealing, simulated quantum annealing using BAA might be faster still [9]. Furthermore, BAA may be able to expedite other Monte Carlo methods for studying phase transitions of Hamiltonian systems or be a useful component in other classical randomized approximation schemes, by automatically focusing on relevant regions of parameter space.

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A Queries under weaker constraints

In this section we prove a more general version of the query argument of Theorem 4.

**Theorem 11.** Let all quantities be defined as in Algorithm 2, and let \( \Gamma(s) = \text{GetGap}(s, 0, \cdot) \). Define \( I_k \equiv \{ s \in [0, 1] \mid \Gamma(s) \leq \lambda_{\max}/2^k \} \). If \( \mu(I_k) \leq C/2^k \) for all nonnegative integers \( k \), where \( C \) is a constant independent of the problem size, and each \( I_k \) can be written as the union of at most \( R \) disjoint intervals, then Algorithm 2 requires at most \( \mathcal{O}((C/c_0 + R) \log (\lambda_{\max}/\Gamma_{\min})) \) queries to GetGap, where \( \Gamma_{\min} \equiv \min_{s \in [0, 1]} \Gamma(s) \).

**Proof.** Let \( 0 = s_0 < s_1 < \cdots < s_{q-1} = 1 \) be the sequence of points sampled by Algorithm 2. At \( s = s_i \), Algorithm 2 chooses the size of the subsequent step so that

\[
  s_{i+1} = s_i + \frac{c_0 \Gamma(s_i)}{4 \lambda_{\max}},
\]

(unless \( c_0 \Gamma(s_i)/4 \lambda_{\max} < 1 - s_i \), in which case it simply sets \( s_{i+1} = 1 \) and makes the final step in the evolution). Now, let \( I_k \setminus I_{k+1} = \bigcup J_j \) where the \( J_j \) are disjoint intervals. Note that because both \( I_k \) and \( I_{k+1} \) can be written as the union of at most \( R \) disjoint intervals, \( I_k \setminus I_{k+1} \) can be written as the union of at most \( 2R \) disjoint intervals. Define the set \( S_k = \{ s_i \mid s_i \in I_k \setminus I_{k+1} \} \). Then, whenever \( s_i \in S_k \), we have \( s_{i+1} - s_i = c_0 \Gamma(s_i)/4 \lambda_{\max} > c_0/(4 \cdot 2^{k+1}) \), and we bound

\[
  \mu(J_j) \geq \sum_{[s_i, s_{i+1}] \subseteq J_j} (s_{i+1} - s_i) \\
  = \sum_{s_i \in J_j \cap S_k} (s_{i+1} - s_i) \\
  \geq \frac{c_0}{4 \cdot 2^{k+1}} (|S_k \cap J_j| - 1).
\]

or \( |S_k \cap J_j| \leq 2^{k+3} \mu(J_j)/c_0 + 1 \), where we used the fact that for a given interval \( J_j \), there exists at most one \( s_i \in J_j \) such that \( s_{i+1} \notin J_j \). Hence,

\[
  |S_k| = \sum_j |S_k \cap J_j| \\
  \leq \sum_j \left( \frac{2^{k+3} \mu(J_j)}{c_0} + 1 \right)
\]

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\[
\leq 8^{2k} \mu \left( \frac{I_k}{c_0} \right) + 2R \\
\leq \frac{8C}{c_0} + 2R
\]  

(23)

for any \(k\). Since the \(S_k\) are disjoint and \(S_k = \emptyset\) for \(k > \lceil \log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}) \rceil\), it follows that

\[
q + 1 = \sum_{k=0}^{\infty} |S_k| = \sum_{k=0}^{\lceil \log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}) \rceil} |S_k| \\
\leq \sum_{k=0}^{\lceil \log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}) \rceil} \left( \frac{8C}{c_0} + 2R \right) \\
= \left( \left\lceil \log_2 \left( \frac{\lambda_{\text{max}}}{\Gamma_{\text{min}}} \right) \right\rceil + 1 \right) \left( \frac{8C}{c_0} + 2R \right).
\]

Thus, Algorithm 2 requires \(O((C/c_0 + R) \log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}))\) queries to GET\textsc{Gap}.

\textbf{Theorem 12.} Under the conditions of Theorem 11, if \(R = O(1)\), then \textsc{GenerateState}(\vec{\gamma}, 0, \epsilon/\dim(\vec{\gamma}))\) takes time \(O(\epsilon^{-1} \lambda_{\text{max}} \log(\lambda_{\text{max}}/\Gamma_{\text{min}}))\). Furthermore, if \(P(1)\) is the projector onto the ground state of \(H(1)\), then Algorithm 2 produces a state corresponding to projector \(\tilde{P}(1)\) such that

\[
\| \tilde{P}(1) - P(1) \| = O(\epsilon).
\]

\textbf{Proof.} Note that \(\dim(\vec{\gamma}) = \sum_k |S_k| \leq (8C/c_0 + 2R) (\log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}) + 1)\) by Eq. (23). Then, by Algorithms 1 and 2,

\[
T_i = \frac{c_0 + 7c_0^2/4}{\epsilon \min_{s \in \mathcal{S}_i} \Gamma(s)} \lambda_{\text{max}}
\]

Then,

\[
\sum_i T_i = \frac{c_0 + 7c_0^2/4}{\epsilon} \sum_i \lambda_{\text{max}} \min_{s \in \mathcal{S}_i} \Gamma(s)
\]

\leq \frac{c_0 + 7c_0^2/4}{(1 - c_0) \epsilon} \sum_i \lambda_{\text{max}} \Gamma(s_i)
\]

\leq 2C \frac{c_0 + 7c_0^2/4}{(1 - c_0) \epsilon} \sum_{i \in S_k} 2^{k+1}
\]

\leq 2C \frac{c_0 + 7c_0^2/4}{(1 - c_0) \epsilon} \sum_{k=0}^{\infty} |S_k| 2^{k+1}
\]

\leq 2C \frac{c_0 + 7c_0^2/4}{(1 - c_0) \epsilon} \sum_{k=0}^{\lceil \log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}) \rceil} |S_k| 2^{k+1}
\]

\leq 2C \frac{c_0 + 7c_0^2/4}{(1 - c_0) \epsilon} \left( \frac{8C}{c_0} + 2R \right) \sum_{k=0}^{\lceil \log_2(\lambda_{\text{max}}/\Gamma_{\text{min}}) \rceil} 2^{k+1}
\]

\leq 4C \frac{c_0 + 7c_0^2/4}{(1 - c_0) \epsilon} \left( \frac{8C}{c_0} + 2R \right) \frac{\lambda_{\text{max}}}{\Gamma_{\text{min}}}
\]

\[
= O \left( \frac{\lambda_{\text{max}}}{\epsilon \Gamma_{\text{min}}} \right).
\]

\[
\Box
\]
Proposition 15. With all quantities as in Algorithm 3, if \( x_{\min} < \chi V \), Algorithm 2 requires at most
\[
O \left( \frac{x_{\min}}{\Gamma_{\min}} \log_2 \left( \frac{\lambda_{\max}}{\Gamma_{\min}} \right) \right)
\]
calls to FinishSchedule.

Proof. Let \( I_k' = \{ s > s_{\min} \mid s \in I_k \} \). Now, by Algorithm 3, \( \mu(S_{\min}) = (1 + c_0)(1 - s_{\min}) \frac{2x_{\min}}{\chi(V - 1)} \). Then,

\[
\mu(I_k') = \mu(S_{\min}) + \mu(I_k' \setminus S_{\min})
= (1 + c_0)(1 - s_{\min}) \frac{2x_{\min}}{\chi(V - 1)} + \mu(I_k' \setminus S_{\min}).
\]

Now, to bound \( \mu(I_k' \setminus S_{\min}) \) we can apply Theorem 7. Consider \( |s - s_{\min}| \) such that \( \Gamma(s) \leq V^{-k} \). Then,

\[
V^{-k} \geq \frac{(V - 2)\chi}{4\kappa^5} |s - s_{\min}|
\]

\[
\frac{4\kappa^5}{(V - 2)\chi} V^{-k} \geq |s - s_{\min}|
\]

\[
= \mu(I_k' \setminus S_{\min})
\]

Thus, \( \frac{8s_{\min}}{(V - 2)\chi} V^{-k} \geq \mu(I_k' \setminus S_{\min}) \). Combining these results,

\[
\mu(I_k') \leq (1 + c_0)(1 - s_0) \frac{2x_{\min}}{\chi(V - 1)} + \frac{4\kappa^5}{(V - 2)\chi} V^{-2k}
\]

\[
= \left( (1 + c_0)(1 - s_0) \frac{2x_{\min}}{\chi(V - 1)} + \frac{4\kappa^5}{(V - 2)\chi} \right) 2^{-k}.
\]

Thus, for \( \mu(I_k') \leq C 2^{-k} \) for all \( k \), the smallest \( C \) we can choose is

\[
C = \left( (1 + c_0)(1 - s_0) \frac{2x_{\min}}{\chi(V - 1)} + \frac{4\kappa^5}{(V - 2)\chi} \right)
\]

which is largest for the largest possible \( k \). Since \( k \leq \lfloor \log_2 (V/\Gamma_{\min}) \rfloor \), we have that for any \( V > 2 \) we can choose

\[
C = \left( (1 + c_0)(1 - s_0) \frac{2x_{\min}}{\chi(V - 1)} \left( \frac{V}{\Gamma_{\min}} \right) + \frac{4\kappa^5}{(V - 2)\chi} \right)
\]

\[
\leq 3 \left( (1 + c_0)(1 - s_0) \frac{2x_{\min}}{\chi \Gamma_{\min}} + \frac{4\kappa^5}{\chi} \right)
\]

\[
= O \left( \frac{x_{\min}}{\Gamma_{\min}} \log_2 \left( \frac{\lambda_{\max}}{\Gamma_{\min}} \right) \right)
\]

and satisfy Theorem 11. Thus, by Theorem 11 we require at most \( O \left( \frac{x_{\min}}{\Gamma_{\min}} \log_2 \left( \frac{\lambda_{\max}}{\Gamma_{\min}} \right) \right) \) queries to GetGap.

\[ \square \]

B Monotonicity of \( \phi(m) \)

Proposition 16. Let \( \lambda(s) \) and \( \phi > 0 \) denote the ground-state eigenvalue and normalised eigenvector of \( G(s) = L + \frac{s}{1 - s} W \) for \( s \in [0, 1) \), where \( L \) is the combinatorial graph Laplacian of the complete graph on \( V \) vertices and \( W \) is a diagonal matrix. If \( W_m = 0 \) is the unique smallest eigenvalue of \( W \), then \( d\phi(m)/ds > 0 \), where \( \phi(m) \) is the component of \( \phi \) corresponding to the vertex \( m \).
Proof. By Eq. (9),
\[
\frac{\phi(m)}{\phi(u)} = \frac{V + W_u(s) - \lambda(s)}{V - \lambda(s)} = 1 + \frac{W_u(s)}{V - \lambda(s)}
\]
for any \( u \neq m \), where \( W_u(s) \equiv sW_u/(1 - s) \). Taking the derivative,
\[
\frac{d}{ds} \left( \frac{\phi(m)}{\phi(u)} \right) = \frac{1}{V - \lambda(s)} \left( \frac{dW_u(s)}{ds} + \frac{W_u(s)}{V - \lambda(s)} \frac{d\lambda(s)}{ds} \right)
\]
\[
= \frac{1}{V - \lambda(s)} \left[ \frac{d}{ds} \left( \frac{s}{1 - s} W_u \right) + \frac{W_u(s)}{V - \lambda(s)} \langle \phi | \frac{d}{ds} \left( L + \frac{s}{1 - s} W \right) | \phi \rangle \right]
\]
\[
= \frac{1}{V - \lambda(s)} \frac{1}{(1 - s)^2} \left[ W_u + \frac{W_u(s)}{V - \lambda(s)} \frac{1}{(1 - s)^2} \langle \phi | W | \phi \rangle \right].
\]
\( \lambda(s) \leq \langle m | \left( L + \frac{s}{1 - s} W \right) | m \rangle = \langle m | L | m \rangle = V - 1 \), and \( W_u \neq m > 0 \) by assumption, so \( W_u(s), \langle \phi | W | \phi \rangle > 0 \). Thus,
\[
\frac{d}{ds} \left( \frac{\phi(m)}{\phi(u)} \right) > 0 \text{ for all } u \neq m.
\]
This together with the fact that \( \phi > 0 \) implies that
\[
\frac{d\phi(m)^2}{ds} > \frac{d\phi(u)^2}{ds}
\]
for all \( u \neq m \). Then, using the normalization condition \( 1 = \sum_u \phi(u)^2 \), we have
\[
0 = \sum_u \frac{d\phi(u)^2}{ds} \leq \sum_u \frac{d\phi(m)^2}{ds} = V \frac{d\phi(m)^2}{ds}
\]
or \( d\phi(m)^2/ds > 0 \).

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