

Improved bounds for eigenpath traversal

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We present a bound on the length of the path defined by the ground states of a continuous family of Hamiltonians in terms of the spectral gap Δ . We use this bound to obtain a significant improvement over the cost of recently proposed methods for quantum adiabatic state transformations and eigenpath traversal. In particular, we prove that a method based on evolution randomization, which is a simple extension of adiabatic quantum computation, has an average cost of order $1/\Delta^2$, and a method based on fixed-point search has a maximum cost of order $1/\Delta^{3/2}$. Additionally, if the Hamiltonians satisfy a frustration-free property, such costs can be further improved to order $1/\Delta^{3/2}$ and $1/\Delta$, respectively. Our methods offer an important advantage over adiabatic quantum computation when the gap is small, where the cost is of order $1/\Delta^3$.

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I. INTRODUCTION

Numerous problems in quantum information, physics, and optimization can be solved by preparing the low energy or other eigenstate of a Hamiltonian (cf. Refs. [1–10]). On a quantum system (e.g., an analog quantum computer), such an eigenstate can be prepared by smoothly changing the interaction parameters of the controlled Hamiltonians under which the system evolves. That is the idea of adiabatic quantum computation (AQC), which relies on the adiabatic theorem [11,12] to assert that, at any time, the evolved state is sufficiently close to an eigenstate of the system that is continuously related to the final one.

The importance of AQC for quantum speedups was demonstrated in several examples (cf. Refs. [7,13–15]). In particular, AQC is equivalent to the standard circuit model of quantum computing, implying that some quantum speedups obtained in one model may be carried to the other using methods that map quantum circuits to Hamiltonians and vice versa [16–24]. In AQC, we assume access to Hamiltonians $H(s)$, $0 \leq s \leq 1$, that have nondegenerate and continuously related eigenstates $|\psi(s)\rangle$. The goal is to prepare $|\psi(1)\rangle$ from $|\psi(0)\rangle$, up to some small approximation error ε , by increasing s from 0 to 1 with a suitable time schedule. The cost of the algorithm in AQC is determined by the total evolution time, T . This time depends on properties of the Hamiltonians used in the evolution, such as their rate of change or spectral gaps. In particular, a commonly used and rigorous quantum adiabatic approximation provides an upper bound to the cost given by (cf. Refs. [25,26])

$$T_{\text{AQC}} = \kappa \max_s \left[\frac{\|\dot{H}\|}{\varepsilon \Delta^2}, \frac{\|\dot{H}\|^2}{\varepsilon \Delta^3} \right]. \quad (1)$$

That is, increasing s according to, for example, $s(t) = t/T_{\text{AQC}}$ suffices to prepare the final eigenstate from the initial one within error ε . (The cost will be $T = T_{\text{AQC}}$ for such a schedule.) κ is a constant and Δ is the spectral gap of H , that is, the smallest (absolute) difference between the eigenvalue of $|\psi(s)\rangle$ and any other eigenvalue. Unless stated otherwise, all quantities, states, and operators depend on s , and all derivatives are with respect to s , e.g., $\dot{X} = \partial X/\partial s$ and $\ddot{X} = \partial^2 X/\partial s^2$. For an operator or matrix X and state $|\phi\rangle$ on a d -dimensional complex Hilbert space, $\|X\|$ denotes the spectral norm and $\|\phi\|$ denotes the Euclidean norm. We remark that the bound in Eq. (1) is actually tight in the sense that there exist examples (e.g., Rabi oscillations; cf. Refs. [27,28]) for which the total cost of the adiabatic evolution is also lower bounded by a quantity of order $\|\dot{H}\|^2/\Delta^3$, and $\|\dot{H}\|^2/\Delta^3 > \|\ddot{H}\|/\Delta^2$ in such examples.

A drawback with rigorous quantum adiabatic approximations is that the dependence of T_{AQC} on the gap is rather poor, especially when $\Delta \ll 1$. Also, the bound given by Eq. (1) could imply a large overestimate of the actual cost needed to prepare the final eigenstate in some cases. For these reasons, other methods for traversing the eigenstate path, which differ from AQC but may have a better cost dependence on the gap, were recently proposed [29–31]. One such method [30] is based on evolution randomization to implement a version of the quantum Zeno effect and simulate projective measurements of $|\psi(s)\rangle$. The main and only difference between this “randomization method” (RM) and AQC is that, rather than choosing the schedule $s(t) = t/T_{\text{AQC}}$ for the evolution, $s(t)$ is randomly chosen according to a probability distribution that depends on the gap and the approximation error. Another method [31] also traverses the eigenstate path by making projective measurements of $|\psi(s)\rangle$, but each measurement is implemented using the so-called phase estimation algorithm [32] and Grover’s fixed-point search technique [33]. The method in Ref. [31] requires knowing the eigenvalue of $|\psi(s)\rangle$, but this can be *learned* as the path is traversed.

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The (average) cost T , or total time of evolution under the $H(s)$, of the previous methods for eigenpath traversal depends not only on the spectral gap but also on the eigenstate path length L . This is simply the length defined in complex Hilbert space, $L = \int_0^1 ds \|\dot{\psi}\|$. For error $\varepsilon < 1$, the cost is upper bounded by

$$T_{\text{EPT}} = \kappa' \frac{L^c \ln(L/\varepsilon)}{\varepsilon \min_s \Delta}, \quad (2)$$

with $c = 1, 2$ depending on the method and κ' a constant. Having an explicit dependence in the path length is important for those cases in which L can be bounded independently of the gap. This observation was used in Ref. [7] to prove a quantum speedup of the well-known simulated annealing method used for optimization [34] (Sec. IV B). For many hard optimization problems, Δ decreases exponentially in the problem size while L increases only polynomially. Then, $T_{\text{AQC}} \gg T_{\text{EPT}}$ for these cases, and the methods in Refs. [29–31] can be used to prepare the final eigenstate with lower cost than the adiabatic method.

We remark that the upper bound of Eq. (2) can be achieved only for a uniform parametrization, under which the eigenstate satisfies $\|\dot{\psi}\| = L$, independently of s . This is a strong requirement that will not be satisfied in general. We then considered an upper bound $L^* \geq L$, which can be easily computed from known properties of the Hamiltonians, and used such a bound to obtain the corresponding T_{EPT} in Refs. [30,31] (i.e., by replacing $L \rightarrow L^*$). When $\|\dot{H}\|$ and Δ are known, a commonly used path length bound is

$$L^* = \max_s \frac{\|\dot{H}\|}{\Delta}. \quad (3)$$

Such a bound follows easily from the eigenvalue equation, which can be used to obtain $\|\dot{\psi}\| \leq \|\dot{H}\|/\Delta$ [35]. Equations (2) and (3) give an upper bound for the cost of the eigenpath traversal method as

$$T_{\text{EPT}} = \kappa' \max_s \frac{\|\dot{H}\|^c}{\varepsilon \Delta^{c+1}} \ln[\|\dot{H}\|/(\varepsilon \Delta)]. \quad (4)$$

$c = 2$ for the RM and T_{EPT} can be larger than T_{AQC} when the parametrization is different from the uniform one. Thus, the advantage of the RM over the adiabatic method is unclear in this case from the above upper bounds: both T_{AQC} and T_{EPT} depend on $1/\Delta^3$.

A main goal of this paper is to obtain better bounds for the cost of the methods of Refs. [29–31] in terms of the spectral gap, the error, $\|\dot{H}\|$ and $\|\ddot{H}\|$, giving special emphasis to the RM described in Ref. [30]. Such quantities, or their bounds, are assumed to be known. The reason why we focus more on the RM than other methods for eigenpath traversal is due to its simple connection with AQC. The other methods not only require evolving with the Hamiltonian, but also require implementing other operations such as those for the quantum Fourier transform in the phase estimation algorithm. Nevertheless, some of our results can also be used to improve the cost of those other methods as well.

Our paper is organized as follows. In Sec. II we present an improved bound on the path length where, ignoring other quantities, L^* is of order $1/\sqrt{\Delta}$ if $|\psi\rangle$ is the ground state of H . We study this bound for general Hamiltonian paths and focus also on those Hamiltonians that are *frustration free*,

due to their importance in condensed matter theory [8,36], optimization [37], and quantum information [38–40]. Then, in Sec. III, we use the improved bound to obtain an average cost for the RM of order $1/\Delta^2$, which is much smaller than T_{AQC} when $\Delta \ll 1$. In Sec. III B we improve the analysis of Ref. [30] about the cost scaling with the error and show that the logarithmic factor present in Eqs. (2) and (4) for the RM is unnecessary. In Sec. IV we apply our results to two important problems in quantum computation, namely, the preparation of projected entangled pair states [41] (i.e., generalized matrix product states or PEPS) and the quantum simulation of classical annealing processes [7,34]. We use the results for frustration-free Hamiltonians and show that the RM has an average cost of order $1/\Delta^{3/2}$ for the preparation of PEPS, while the method based on fixed-point search has cost of order $1/\Delta$ (up to a logarithmic correction). We conclude in Sec. V

II. THE PATH LENGTH

The path length of a continuous and differentiable family of unit states $\{|\psi(s)\rangle\}$, $0 \leq s \leq 1$, is

$$L = \int_0^1 ds \|\dot{\psi}\|.$$

The global phase of $|\psi\rangle$ is set so that $\langle \psi | \dot{\psi} \rangle = 0$. $|\psi\rangle$ is a nondegenerate eigenstate of H , and, without loss of generality, we assume that the eigenvalue is 0. Then, $|\dot{\psi}\rangle = -H^{-1} \dot{H} |\psi\rangle$, where H^{-1} has only support in the subspace orthogonal to $|\psi\rangle$. An upper bound of $\max_s (\|\dot{H}\|/\Delta)$ on L simply follows. Such a bound is commonly used when deriving adiabatic approximations.

Remarkably, if the state path is two times differentiable and $|\psi\rangle$ is the ground state of H (i.e., the eigenstate with lowest eigenvalue), a tighter bound on L in terms of the gap can be obtained. According to the Cauchy-Schwarz inequality,

$$L^2 \leq \int_0^1 ds \|\dot{\psi}\|^2. \quad (5)$$

By differentiation of $H|\psi\rangle = 0$, in Appendix A we obtain

$$\|\dot{\psi}\|^2 \leq \frac{1}{2\Delta} \langle \psi | \ddot{H} | \psi \rangle; \quad (6)$$

see Eq. (A2). Equations (5) and (6) yield

$$L^2 \leq \int_0^1 ds \frac{1}{2\Delta} \langle \psi | \ddot{H} | \psi \rangle.$$

If the lowest eigenvalue is $E \neq 0$, then

$$L \leq L^* = \left(\int_0^1 ds \frac{1}{2\Delta} \langle \psi | \ddot{H} - \ddot{E} | \psi \rangle \right)^{1/2}. \quad (7)$$

Equation (7) is our main result; its applications to eigenpath traversal will be discussed below.

A. General interpolations

In general, because $\langle \psi | \ddot{H} - \dot{E} | \psi \rangle \geq 0$, the right-hand side of Eq. (7) can be bounded so that

$$\begin{aligned} L^* &\leq \max_s \sqrt{\frac{\|\ddot{H}\| - [\dot{E}(1) - \dot{E}(0)]}{2\Delta}} \\ &\leq \max_s \sqrt{\frac{\|\ddot{H}\| + 2\|\dot{H}\|}{2\Delta}}. \end{aligned}$$

For eigenpath traversal, quantities such as $\|\dot{H}\|$ and $\|\ddot{H}\|$ are usually bounded by a polynomial on the problem size, while the spectral gap Δ can be exponentially small for hard instances.

B. Linear interpolations

A commonly used Hamiltonian path is given by the linear interpolation of two Hamiltonians, that is, $H = (1-s)H_0 + sH_f$. Here H_0 and H_f are the initial and final Hamiltonians, respectively. In this case,

$$L^* \leq \max_s \sqrt{\frac{\dot{E}(1) - \dot{E}(0)}{2\Delta}} \leq \max_s \sqrt{\frac{\|\dot{H}\|}{\Delta}}.$$

C. Frustration-free Hamiltonians

A Hamiltonian $H = \sum_k \Pi_k$ is said to be frustration-free if any ground state $|\psi\rangle$ of H is also a ground state of every Π_k . Typically, Π_k corresponds to local operators, and we can assume that $H|\psi\rangle = \Pi_k|\psi\rangle = 0$ for all k , and $\Pi_k \geq 0$.

For frustration-free Hamiltonians, the *local* bound on the rate of change of the state in Eq. (6) applies directly because $E = 0$, and then

$$L^* \leq \max_s \sqrt{\frac{\|\ddot{H}\|}{2\Delta}}. \quad (8)$$

III. IMPROVED BOUNDS FOR THE RANDOMIZATION METHOD

The ‘‘randomization method’’ (RM) described in Ref. [30] uses phase randomization to traverse the eigenpath. The basic idea of the RM is simple: For a Hamiltonian path $\{H(s)\}$, we choose a discretization $0 < s_1 < s_2 < \dots < s_q = 1$ that depends on the final-state preparation error. At the j th step of the RM, we evolve with the constant Hamiltonian $H(s_j)$ for random time t_j , which is drawn according to a specific distribution that depends on $\Delta(s_j)$, the gap at that step, and the error. A common example is to sample t_j from a normal distribution of zero mean and width (standard deviation) of order $1/\Delta(s_j)$. Evolution randomization will induce phase cancellation and a reduction of the *coherences* between $|\psi(s_j)\rangle$ and any other state orthogonal to it (see Secs. III A and III B). In other words, evolution randomization simulates a measurement of $|\psi(s_j)\rangle$. Then, due to a version of the quantum Zeno effect, a sequence of measurements of $|\psi(s_1)\rangle, |\psi(s_2)\rangle, \dots$ will allow the preparation of $|\psi(s_q)\rangle$, with arbitrarily high probability for

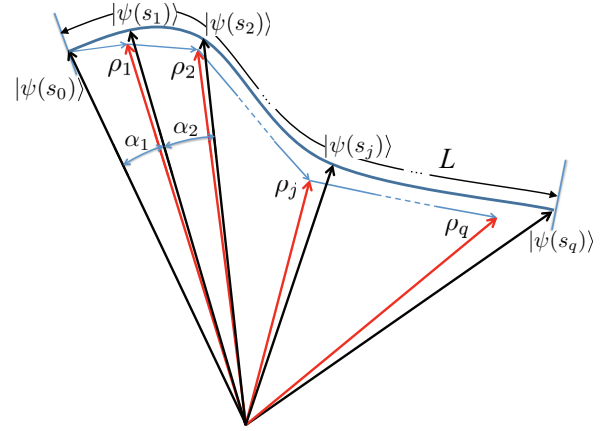


FIG. 1. (Color online) Basic steps of the RM and state representation. At the j th step, the RM prepares the mixed state ρ_j (represented by a red arrow) that has large probability of being in $|\psi(s_j)\rangle$ (represented by a black arrow) after measurement. The preparation of ρ_j is done by evolving ρ_{j-1} with the Hamiltonian $H(s_j)$ for random time. The number of steps q is obtained so that the final error probability is bounded by some given $\varepsilon > 0$.

a proper choice of s_1, s_2, \dots, s_q . The basic steps of the RM are depicted in Fig. 1; more details are in Secs. III A and III B.

The average cost of the RM is the number of steps q times the average (absolute) evolution time per randomization step; the latter is proportional to the inverse spectral gap [30]. For a uniform parametrization under which $\|\dot{\psi}\| = L$ for all s , and for error ε , we obtain $q \propto L^2/\varepsilon$, resulting in an optimal average cost of order $L^2/(\varepsilon\Delta)$. An additional logarithmic factor, coming from Eq. (4), was needed for the cost analysis of Ref. [30] if the random times are nonnegative (or nonpositive).

Nevertheless, the given parametrization is not uniform in general. In this case, the RM is guaranteed to succeed only if $q = (L^*)^2$, where L^* is an upper bound on L that can be determined from some known properties of H . As discussed, a standard choice for L^* is the one in Eq. (3), which results in an overall cost of order $1/\Delta^3$ if we disregard other quantities: the number of points in the discretization is $q \propto \max_s(1/\Delta^2)$. The goal of this section is to show that the upper bound obtained in Sec. II can be used to obtain a better discretization for the RM than that of Ref. [30], resulting in an overall, improved average cost of order $\max_s(1/\Delta^2)$. We also show how to avoid the logarithmic correction in the cost by performing a more detailed analysis of errors due to randomization, when the random times are nonnegative (or nonpositive).

A. Parametrization errors

In this section we analyze the errors due to the discretization, which assumes perfect measurements of the $|\psi(s)\rangle$ in the RM. Errors from imperfect measurements due to evolution randomization are analyzed in Sec. III B. We let $0 < s_1 < s_2 < \dots < s_q = 1$ determine any discretization of the interval $[0, 1]$, where q will be obtained below. Assuming perfect measurements of the $|\psi(s_j)\rangle$ and using the union bound, the final error or quantum *infidelity* $(1 - F)$ in the preparation of

$|\psi(s_q)\rangle$ can be bounded from above as

$$1 - F = 1 - \prod_{j=1}^q \cos^2(\alpha_j) \leq \sum_{j=1}^q \sin^2(\alpha_j),$$

where the ‘‘angles’’ α_j are determined from $\cos \alpha_j = |\langle \psi(s_{j-1}) | \psi(s_j) \rangle|$; see Fig. 1. Without loss of generality, we can assume $\sin \alpha_j \geq 0$.

In Appendix B, we show

$$\sin^2(\alpha_j) \leq (s_j - s_{j-1}) \int_{s_{j-1}}^{s_j} ds \|\dot{\psi}\|^2, \quad (9)$$

for a differentiable path. If we choose a discretization so that $s_j = j \delta s$, the choice $\delta s \leq \varepsilon / \int_0^1 ds \|\partial_s \psi(s)\|^2$ suffices to guarantee a final infidelity bounded by ε ; that is,

$$\sum_{j=1}^q \sin^2(\alpha_j) \leq \varepsilon. \quad (10)$$

We can then use the main result of Sec. II and Eq. (9) to show

$$\delta s = \frac{\varepsilon}{(L^*)^2}.$$

This bound assumes that $|\psi\rangle$ is the ground state of H . The number of points in the discretization is then

$$q = \frac{1}{\delta s} = \frac{\int_0^1 ds \langle \psi | \ddot{H} - \ddot{E} | \psi \rangle / (2\Delta)}{\varepsilon}, \quad (11)$$

which is of order $\max_s(1/\Delta)$ if we ignore other quantities. It follows that the overall, average cost of the RM is of order $\max_s(1/\Delta^2)$, implying a better gap dependence than the one obtained in Ref. [30]. In the following section we show how the measurements can be simulated and approximated by evolution randomization.

B. Imperfect measurements

A perfect, projective measurement of $|\psi\rangle$ is one that transforms all coherences between $|\psi\rangle$ and its orthogonal complement to 0. That is, if ρ denotes the density matrix after the perfect measurement, then $\langle \psi | \rho | \psi^\perp \rangle = 0$ for all states $|\psi^\perp\rangle$ satisfying $\langle \psi | \psi^\perp \rangle = 0$. In the RM of Ref. [30], we showed that a perfect measurement can only be simulated if the random evolution time t is drawn according to a distribution in which $t \in (-\infty, \infty)$. If t can be only nonnegative (or nonpositive), the coherences are reduced only by a multiplicative factor $\varepsilon' > 0$; that is, the simulated measurement is imperfect or *weak*. To achieve overall error of order ε in the preparation of the final eigenstate due to imperfect measurements, in Ref. [30] we chose $\varepsilon' = \varepsilon/q$, which easily follows from an union-like bound for a sequence of quantum operations. This introduces an additional cost to the RM given by a multiplicative factor of order $\ln(q/\varepsilon)$ [Eq. (2)], which can be large if $q \gg 1$. Nevertheless, we now present an improved error analysis of the RM than that of Ref. [30] and show that if the imperfect measurements are such that ε' is a constant independent of ε , an overall error of order ε can still be achieved. This results in an improved cost for the RM: the $\ln(q/\varepsilon)$ overhead is unnecessary.

To demonstrate the improved scaling, it is convenient to define ρ_j as the state, or density matrix, at the j th step of the RM ($j = 0, 1, \dots, q$); that is, the state after the randomized evolution with $H(s_j)$. Without loss of generality, we write

$$\rho_j = \text{Pr}(j) |\psi(s_j)\rangle \langle \psi(s_j)| + [1 - \text{Pr}(j)] \rho_j^\perp + |\xi_j\rangle \langle \psi(s_j)| + |\psi(s_j)\rangle \langle \xi_j|,$$

where $\text{Pr}(j) = \langle \psi(s_j) | \rho_j | \psi(s_j) \rangle$ is the probability of $|\psi(s_j)\rangle$ in ρ_j (i.e., the fidelity). ρ_j^\perp is a density matrix with support orthogonal to $|\psi(s_j)\rangle$ so that $\rho_j^\perp |\psi(s_j)\rangle = 0$. The (unnormalized) state $|\xi_j\rangle$ is also orthogonal to $|\psi(s_j)\rangle$ and denotes the *coherences* between $|\psi(s_j)\rangle$ and its orthogonal complement. The norm of $|\xi_j\rangle$ denotes a coherence factor:

$$c_j = \|\xi_j\|.$$

The main goal of the RM is to simulate measurements by keeping c_j sufficiently small via phase or evolution randomization.

At the $j + 1$ -th step, we evolve with $H(s_{j+1})$ for a random time drawn from some distribution $f(t)$. Then,

$$\rho_{j+1} = \int dt e^{-iH(s_{j+1})t} \rho_j e^{iH(s_{j+1})t}. \quad (12)$$

Since evolving with $H(s_{j+1})$ leaves the eigenstate $|\psi(s_{j+1})\rangle$ invariant (up to a global phase), we have

$$\begin{aligned} \text{Pr}(j+1) &= \langle \psi(s_{j+1}) | \rho_{j+1} | \psi(s_{j+1}) \rangle \\ &= \langle \psi(s_{j+1}) | \rho_j | \psi(s_{j+1}) \rangle, \end{aligned}$$

with $|\psi(s_{j+1})\rangle = \cos \alpha_{j+1} |\psi(s_j)\rangle + \sin \alpha_{j+1} |\psi^\perp(s_j)\rangle$. Then,

$$\text{Pr}(j+1) \geq \cos^2 \alpha_{j+1} \text{Pr}(j) - 2 \sin \alpha_{j+1} c_j. \quad (13)$$

Here we assumed the worst case scenario for which $\langle \xi_j | \psi(s_{j+1}) \rangle = -c_j \sin \alpha_{j+1}$ and used $\cos \alpha_{j+1} \leq 1$. In Appendix C, Eq. (C3), we show that if Eq. (10) is satisfied,

$$c_j \leq \frac{1}{1 - \varepsilon'} (\varepsilon' \sin \alpha_j + \varepsilon'^2 \sin \alpha_{j-1} + \dots + \varepsilon'^j \sin \alpha_1). \quad (14)$$

The factor $\varepsilon' < 1$ denotes the reduction in coherence due to evolution randomization per step. That is, a random evolution under $H(s_{j+1})$ applied to ρ_j transforms and reduces the coherences $|\psi(s_{j+1})\rangle \langle \psi(s_{j+1}^\perp)|$ to

$$\int dt f(t) e^{-iH(s_{j+1})t} |\psi(s_{j+1})\rangle \langle \psi(s_{j+1}^\perp)| e^{iH(s_{j+1})t},$$

where $|\psi(s_{j+1}^\perp)\rangle$ is a normalized state orthogonal to $|\psi(s_{j+1})\rangle$. Then, we can assume

$$\varepsilon' = \left\| \int dt f(t) e^{i\Delta t} \right\|, \quad (15)$$

where $\Delta \leq \Delta(s_{j+1})$.

The RM starts with $|\psi(s_0)\rangle$, so initially $\text{Pr}(0) = 1$ and $c_0 = 0$. By iteration of Eq. (13) we obtain

$$\text{Pr}(q) \geq \prod_{j=1}^q \cos^2(\alpha_j) - 2 \sum_{j=1}^q \sin \alpha_j c_{j-1}. \quad (16)$$

The first term on the right-hand side of Eq. (16) corresponds to the case where all projective measurements are implemented perfectly, i.e., when $c_j = 0$ for all j . A lower bound to such term is given by $1 - \sum_{j=1}^q \sin^2(\alpha_j) \geq 1 - \varepsilon$, as described in Sec. III A. Using Eq. (14), the second term on the right-hand side of Eq. (16) can be upper bounded by

$$\frac{2}{1 - \varepsilon} \sum_{j=1}^q \sin \alpha_j (\varepsilon' \sin \alpha_{j-1} + \varepsilon'^2 \sin \alpha_{j-2} + \dots), \quad (17)$$

and using the Cauchy-Schwarz inequality,

$$\sum_{j=1}^q \sin \alpha_j \sin \alpha_{j-k} \leq \sum_{j=1}^q \sin^2(\alpha_j) \leq \varepsilon.$$

Then, the fidelity of the RM or probability of success in the preparation of $|\psi(s_q)\rangle$ is

$$\Pr(q) \geq 1 - \varepsilon - \frac{2\varepsilon\varepsilon'}{(1 - \varepsilon)(1 - \varepsilon')}, \quad (18)$$

which follows from summing the geometric series in ε' in Eq. (17).

C. Total cost

For constant error or infidelity of order $\varepsilon < 1$, it suffices to choose a constant ε' in Eq. (18). For example, a common choice for the time distribution is a normal distribution $f(t)$ with standard deviation of order $1/\Delta$. Since the Fourier transform of $f(t)$ is a normal distribution with standard deviation of order Δ , Eq. (15) implies a constant upper bound for ε' . Then, the average cost per step of the RM is also of order $1/\Delta$. Multiplying this by q , the total number of steps in Eq. (11), provides an upper bound to the total average cost of the RM given by

$$\frac{(L^*)^2}{\varepsilon\Delta} \leq \kappa' \max_s \frac{\|\ddot{H}\| + 2\|\dot{H}\|}{\varepsilon 2\Delta^2(s)}, \quad (19)$$

for general interpolations (Sec. II A). $\kappa' \approx \sqrt{2/\pi}$ is also constant [30]. Such an upper bound can be further improved for different Hamiltonians or interpolations as described in Secs. II B and II C. Our result in Eq. (19) significantly improves upon the result in Ref. [30], for which the average cost in terms of the gap only was of order $\max_s [\ln(1/\Delta)/\Delta^3]$.

IV. APPLICATIONS

Improved bounds on the cost of methods for eigenpath traversal may result in speedups for problems in physics, optimization, and quantum information. In this section, we apply our results to two important examples where polynomial quantum speedups are obtained.

A. Preparation of Projected Entangled Pair States (PEPS)

PEPS, a generalization of matrix product states to space dimensions higher than one [42,43], were conjectured to approximate the ground states of physical systems with local interactions [41]. PEPS also arise in combinatorial optimization and quantum information problems, and their preparation is paramount to solve such problems. For this

reason, methods for the preparation of PEPS on a quantum computer were recently developed [10,40].

An important property of PEPS is that they can be realized as the ground states of frustration-free Hamiltonians. Then, we can analyze the cost of the RM for the preparation of PEPS. That is, if $H(s) = \sum_{k=1}^L \Pi_k(s)$ denotes a frustration-free Hamiltonian path, using the results of Sec. II C we obtain a cost for the RM upper bounded by

$$\max_s \frac{\|\ddot{H}\|}{\varepsilon 2\Delta^2}.$$

Such a cost can be further improved as follows. A remarkable property of frustration-free Hamiltonians is that their spectral gap can be amplified by constructing the related Hamiltonian

$$H' = \sqrt{\|\Pi\|} \sum_{k=1}^L \sqrt{\Pi_k} \otimes [|k\rangle\langle 0| + |0\rangle\langle k|],$$

where $|k\rangle$, $k = 0, 1, \dots, L$ are a basis of states of an ancillary system. H' has $|\psi\rangle \otimes |0\rangle$ as eigenstate of eigenvalue 0, and the spectral gap of H' is $\Delta' \geq \sqrt{\Delta\|\Pi\|}$, where $\|\Pi\| = \max_k \|\Pi_k\|$. These properties and the full spectrum of H' was analyzed in Ref. [40]. Then, if we have access to evolutions under the $\sqrt{\Pi_k(s)}$, the randomized evolution in the RM can be implemented using H' instead, having an average cost of order $1/\Delta' \propto 1/\sqrt{\Delta\|\Pi\|}$ per step. This implies an overall, average cost for the RM upper bounded by

$$\kappa' \max_s \frac{\|\ddot{H}\|}{\varepsilon 2\|\Pi\|^{1/2}} \frac{1}{\Delta^{3/2}}. \quad (20)$$

Similarly, the cost of other methods for eigenpath traversal [31] for this problem will have an improved cost bounded by

$$\kappa' \max_s \frac{\sqrt{\|\ddot{H}\|/2} \times \ln[\sqrt{\|\ddot{H}\|/(2\Delta)}/\varepsilon]}{\varepsilon \|\Pi\|^{1/2}} \frac{1}{\Delta}. \quad (21)$$

Equation (21) follows from Eq. (2) for $c = 1$, replacing Δ by Δ' and L by L^* as in Eq. (8). The cost is almost linear in $1/\Delta$.

We note that for many frustration-free Hamiltonians, the terms Π_k are projectors and $\sqrt{\Pi_k} = \Pi_k$. Otherwise the Π_k may be expressed as a linear combination of projectors, so that the requirement of having access to evolutions with the $\sqrt{\Pi_k}$ is not strong.

B. Quantum simulated annealing

Simulated annealing is a powerful heuristics for solving combinatorial optimization problems. When implemented via Markov Chain Monte Carlo techniques, it generates a stochastic sequence of configurations that converges to the Gibbs distribution determined by the inverse temperature β_q and an objective function E . For sufficiently large β_q , the final sequences are sampled from a distribution mostly weighted on those configurations σ that minimize E . The process is specified by a particular annealing schedule, which consists of a finite increasing sequence of inverse temperatures $\beta_0 = 0 < \beta_1 < \dots < \beta_q$. The cost of the method is the number of Markov steps required to sample from the desired distribution, i.e., q . For constant error, such a number can be upper bounded by $\propto \max_\beta 1/\Delta(\beta)$, where $\Delta(\beta)$ denotes the spectral gap of the stochastic matrix at inverse temperature β .

In Ref. [7] we gave a quantum algorithm that allows us to sample from the same distribution as that approached by the simulated annealing method. The quantum algorithm uses the RM to traverse a path of states $|\psi(\beta)\rangle$. Here $|\psi(\beta)\rangle$ is a *coherent* version of the corresponding Gibbs state, having amplitudes that coincide with the square root of the probabilities. That is,

$$|\psi(\beta)\rangle = \frac{1}{\sqrt{\mathcal{Z}}} \sum_{\sigma} e^{-\beta E[\sigma]/2} |\sigma\rangle, \quad (22)$$

where the sum is over all configurations and $\mathcal{Z} = \sum_{\sigma} \exp(-\beta E[\sigma])$ is the partition function.

In more detail, the cost of the quantum method presented in Ref. [7] is of order

$$\max_{\beta} q \ln q / \sqrt{\Delta(\beta)} \quad (23)$$

with $q = \beta_q^2 E_M^2 / (4\varepsilon)$ and E_M is the maximum of $|E|$. ε denotes the overall error probability of finding the configuration that minimizes E and q is the number of points in the discretization or steps in the RM. As discussed, q is related to the path length so that $q \geq L^2/\varepsilon$, with $L = \int_0^{\beta_q} d\beta \|\partial_{\beta} \psi(\beta)\|$ in this case. In terms of the spectral gap $\Delta(\beta)$, the quantum algorithm of Ref. [7] provides a square root improvement over the classical method, which is important for those hard instances where $\Delta(\beta)$ is small.

We can then use the results in Sec. III to search for a better bound on the path length and, ultimately, a reduction on the cost of the RM for this problem. That is, instead of using q as above, we replace it by q^* , with $L^2 \leq q^*$ and

$$q^* = \frac{\beta_q}{\varepsilon} \int_0^{\beta_q} d\beta \|\partial_{\beta} \psi(\beta)\|^2;$$

see Eq. (11). For such ε , β_q is of order $\ln(d/\varepsilon)/\gamma$, where d is the dimension of the configuration space and γ is the difference between the two smallest values in the range of E (i.e., the spectral gap of E).

In Appendix D, Eq. (D2), we show

$$\|\partial_{\beta} \psi(\beta)\|^2 = -\partial_{\beta} \langle E \rangle / 4,$$

where $\langle E \rangle$ is the expected (thermodynamic) value of E . Then, we obtain

$$q^* = \frac{\beta_q (\langle E \rangle_0 - \langle E \rangle_{\beta_q})}{4\varepsilon}.$$

Without loss of generality, we assume $\langle E \rangle_0 = 0$, as we can always shift the lowest value of E to satisfy the assumption. In fact, the assumption is readily satisfied for many problems of interest, such as those where E describes a so-called Ising model. If $\beta_q \gg 1$, then $\langle E \rangle_{\beta_q} \approx -E_M$ and

$$q^* \leq \frac{\beta_q E_M}{4\varepsilon}.$$

Our improved average cost of the RM for this problem is then

$$T_{\text{QSA}} = \kappa' \max_{\beta} \frac{\beta_q E_M}{4\varepsilon \sqrt{\Delta(\beta)}} \quad (24)$$

(κ' is a small constant). Equation (24) has to be contrasted with the worse cost given by Eq. (23), which in this case is of order

$$\max_{\beta} \frac{\beta_q^2 E_M^2 \ln(\beta_q^2 E_M^2 / \varepsilon)}{\varepsilon \sqrt{\Delta(\beta)}}$$

and much larger than T_{QSA} in the large E_M and β_q limit.

V. CONCLUSIONS

We presented a significantly improved upper bound on L , the length of the path traversed by the continuously related ground states of a family of Hamiltonians. Such a bound is approximately the square root of standard and previously used bounds for L in the literature. It results in an improved average cost of a method for adiabatic state transformations based on evolution randomization, which is a simple extension of AQC. Specifically, we prove an average cost of order $1/\Delta^2$ for the randomization method, whereas AQC has a proven cost of order $1/\Delta^3$ (i.e., the cost of AQC is upper bounded by $1/\Delta^3$, disregarding other quantities). Here Δ is a bound on the spectral gap of the Hamiltonians. When the Hamiltonians satisfy a certain frustration-free property, the average cost of the randomization method is further improved to order $1/\Delta^{3/2}$. The gap Δ is very small for hard instances, and thus the randomization method is a promising alternative to AQC in these cases, as it has a proven lower cost.

We also improved the cost of the randomization method when the simulated measurements are imperfect. We showed that if evolution randomization induces a weak measurement, where the coherences are reduced by a constant, multiplicative factor (e.g., by $1/3$), then the eigenstate of the final Hamiltonian is still prepared at small, bounded error probability. Previous analysis for the randomization method required a reduction on the coherences that depended on the path length.

The randomization method outperforms AQC in certain instances (e.g., Rabi oscillations). Nevertheless, it remains open to show how generic the advantages of the randomization method over AQC are. To understand this problem better, for example, one needs to devise other instances where AQC has a cost dominated by $1/\Delta^3$, so that the cost of AQC is strictly higher than that of the randomization method. Perhaps our most important contribution is a method for eigenpath traversal that has a *proven* lower cost than that provided by quantum adiabatic approximations [25,26,44,45], since rigorously improving the latter cost in terms of the gap, even for simple cases (e.g., linear interpolations), does not seem feasible.

Finally, the improved bound on L can also be used to improve the cost of other methods for eigenpath traversal such as that in Ref. [31]. For the most efficient and known method for eigenpath traversal in the literature, our bound on L implies a cost of order $1/\Delta^{3/2}$ for general Hamiltonians and order $1/\Delta$ for Hamiltonians that satisfy the frustration-free property.

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APPENDIX A: A BOUND ON $\|\dot{\psi}\|$

From $H|\psi\rangle = 0$, where $|\psi\rangle$ is the ground state, we obtain

$$|\dot{\psi}\rangle = -H^{-1}\dot{H}|\psi\rangle.$$

H^{-1} denotes the operator that is inverse to H in the subspace orthogonal to $|\psi\rangle$. We assume the existence of \dot{H} with $\|\dot{H}\| < \infty$. Then,

$$\begin{aligned} \|\dot{\psi}\|^2 &= \langle \psi | \dot{H} H^{-2} \dot{H} | \psi \rangle \\ &\leq \frac{1}{\Delta} \langle \psi | \dot{H} H^{-1} \dot{H} | \psi \rangle \\ &= \frac{-1}{\Delta} \langle \psi | \dot{H} | \dot{\psi} \rangle, \end{aligned} \quad (\text{A1})$$

where we used Cauchy-Schwarz and the assumption that $H \geq 0$. In addition,

$$\dot{H}|\dot{\psi}\rangle = -\frac{1}{2}[\ddot{H}|\psi\rangle + H|\ddot{\psi}\rangle],$$

and using Eq. (A1) we obtain the desired bound as

$$\|\dot{\psi}\|^2 \leq \frac{1}{2\Delta} \langle \psi | \ddot{H} | \psi \rangle. \quad (\text{A2})$$

This assumes the existence of \ddot{H} with $\|\ddot{H}\| < \infty$.

APPENDIX B: A BOUND ON $\sin \alpha_j$

As pointed out, the angles α_j in Sec. III (Fig. 1) can be defined via $\cos \alpha_j = \langle \psi(s_{j-1}) | \psi(s_j) \rangle \in \mathbb{R}$. It follows that

$$\begin{aligned} \sin \alpha_j &= \| |\psi(s_{j-1})\rangle - \cos \alpha_j |\psi(s_j)\rangle \| \\ &\leq \| |\psi(s_{j-1})\rangle - e^{i\phi} |\psi(s_j)\rangle \|. \end{aligned} \quad (\text{B1})$$

The phase $\phi \in \mathbb{R}$ can be arbitrary. Next, we split the interval $[s_{j-1}, s_j]$ into r segments of size $(s_j - s_{j-1})/r$ and define $s_j^n = s_{j-1} + (s_j - s_{j-1})n/r$, with $n = 0, 1, \dots, r$. The corresponding eigenstates are now $|\psi(s_j^n)\rangle$, and, with no loss of generality, we assume $\cos \beta_n = \langle \psi(s_j^{n-1}) | \psi(s_j^n) \rangle \in \mathbb{R}$. In particular, $|\psi(s_j^0)\rangle = |\psi(s_{j-1})\rangle$ and $|\psi(s_j^r)\rangle = e^{i\phi} |\psi(s_j)\rangle$.

From Eq. (B1) we obtain

$$\begin{aligned} \sin \alpha_j &\leq \left\| \sum_{n=0}^{r-1} [|\psi(s_j^n)\rangle - |\psi(s_j^{n+1})\rangle] \right\| \\ &\leq \sum_{n=0}^{r-1} \| |\psi(s_j^n)\rangle - |\psi(s_j^{n+1})\rangle \|, \end{aligned}$$

where we used the triangle inequality. Also,

$$\begin{aligned} \sin \alpha_j &\leq \lim_{r \rightarrow \infty} \sum_{n=0}^{r-1} \frac{\| |\psi(s_j^n)\rangle - |\psi(s_j^{n+1})\rangle \|}{s_j^{n+1} - s_j^n} \frac{n}{r} (s_j - s_{j-1}) \\ &\leq \int_{s_{j-1}}^{s_j} ds \| |\dot{\psi}\rangle \|, \end{aligned} \quad (\text{B2})$$

where the phase of $|\psi\rangle$ must be chosen so that $\langle \dot{\psi} | \psi \rangle \in \mathbb{R}$, and thus $\langle \dot{\psi} | \psi \rangle = 0$ from the normalization condition. The inequality in Eq. (B2) requires existence $|\dot{\psi}\rangle$, i.e., a differentiable path. Since

$$\int_{s_{j-1}}^{s_j} ds \| |\partial_s \psi(s)\rangle \|^2 - \left[\int_{s_{j-1}}^{s_j} ds \| |\partial_s \psi(s)\rangle \| \right]^2 \geq 0$$

from Cauchy Schwarz, we obtain the desired bound as

$$\sin \alpha_j \leq \left(\int_{s_{j-1}}^{s_j} ds \| |\dot{\psi}\rangle \|^2 \right)^{1/2}.$$

APPENDIX C: A BOUND ON THE COHERENCES

As explained in Sec. III B, we let ρ_j be the density matrix for the state after the randomized evolution with $H(s_j)$, i.e., the state output at the j th step of the randomization method:

$$\begin{aligned} \rho_j &= \text{Pr}(j) |\psi(s_j)\rangle \langle \psi(s_j)| + [1 - \text{Pr}(j)] \rho_j^\perp \\ &\quad + |\xi_j\rangle \langle \psi(s_j)| + |\psi(s_j)\rangle \langle \xi_j|. \end{aligned}$$

The coherence factor is defined as

$$c_j = \| |\xi_j\rangle \| = \| P_j^\perp \rho_j | \psi(s_j) \rangle \|,$$

where $P_j^\perp = \mathbb{I} - |\psi(s_j)\rangle \langle \psi(s_j)|$ is the a projector onto the subspace orthogonal to $|\psi(s_j)\rangle$. The coherence factor at the $j+1$ -th step is then

$$\begin{aligned} c_{j+1} &= \| |\xi_{j+1}\rangle \| \\ &= \| P_{j+1}^\perp \rho_{j+1} | \psi(s_{j+1}) \rangle \| \\ &= \left\| P_{j+1}^\perp \int dt f(t) e^{-iH(s_{j+1})t} \rho_j e^{iH(s_{j+1})t} | \psi(s_{j+1}) \rangle \right\|, \end{aligned}$$

where $f(t)$ is the distribution for the random time at that step. Since $e^{iH(s_{j+1})t}$ leaves $|\psi(s_{j+1})\rangle$ invariant (up to a global phase) and

$$\left\| \int dt f(t) e^{-iH(s_{j+1})t} | \bar{\psi}^\perp(s_{j+1}) \rangle \right\| \leq \varepsilon'$$

for any unit state $|\bar{\psi}^\perp(s_{j+1})\rangle$ orthogonal to $|\psi(s_{j+1})\rangle$, we arrive at

$$c_{j+1} \leq \varepsilon' \| P_{j+1}^\perp \rho_j | \psi(s_{j+1}) \rangle \|. \quad (\text{C1})$$

The factor $\varepsilon' < 1$ was defined in Eq. (15) and is the Fourier transform of $f(t)$ at $\Delta \leq \Delta(s_{j+1})$.

We now bound the *rhs* of Eq. (C1). Without loss of generality, we write $|\psi(s_{j+1})\rangle = \cos \alpha_{j+1} |\psi(s_j)\rangle + \sin \alpha_{j+1} |\psi^\perp(s_j)\rangle$, and obtain

$$\begin{aligned} c_{j+1} &\leq \varepsilon' \{ \cos \alpha_{j+1} \| P_{j+1}^\perp [\text{Pr}(j) |\psi(s_j)\rangle + |\xi_j]\| \\ &\quad + \sin \alpha_{j+1} \| P_{j+1}^\perp \rho_j | \psi^\perp(s_j) \rangle \| \}, \end{aligned}$$

where we used the triangle inequality and $\rho_j | \psi(s_j) \rangle = \text{Pr}(j) |\psi(s_j)\rangle + |\xi_j\rangle$. By definition, $\sin \alpha_{j+1} = \| P_{j+1}^\perp | \psi(s_j) \rangle \|$. Also,

$$\begin{aligned} \rho_j | \psi^\perp(s_j) \rangle &= [1 - \text{Pr}(j)] \rho_j^\perp | \psi^\perp(s_j) \rangle + |\psi(s_j)\rangle \langle \xi_j | \psi^\perp(s_j) \rangle. \end{aligned}$$

By using Cauchy-Schwarz and the triangle inequalities, we obtain

$$c_{j+1} \leq \varepsilon' \{ \cos \alpha_{j+1} \Pr(j) \sin \alpha_{j+1} + \cos \alpha_{j+1} c_j + \sin \alpha_{j+1} [1 - \Pr(j)] + \sin^2(\alpha_{j+1}) c_j \}$$

and thus

$$c_{j+1} \leq \varepsilon' \{ \sin \alpha_{j+1} + [1 + \sin^2(\alpha_{j+1})] c_j \}. \quad (\text{C2})$$

Because the initial state (step 0) is exactly $|\psi(s_0)\rangle$, we have $c_0 = 0$ and, by iteration of Eq. (C2),

$$c_{j+1} \leq \varepsilon' \sin \alpha_{j+1} + (\varepsilon')^2 [1 + \sin^2(\alpha_{j+1})] \sin \alpha_j + \dots + (\varepsilon')^{j+1} [1 + \sin^2(\alpha_{j+1})] \dots [1 + \sin^2(\alpha_2)] \sin \alpha_1.$$

In order to relate ε' with the error coming from the discretization (perfect measurements), we recall the condition

$$\sum_{j=1}^q \sin^2(\alpha_j) \leq \varepsilon$$

of Eq. (10). Then,

$$\begin{aligned} & \prod_{j=1}^q [1 + \sin^2(\alpha_j)] \\ & \leq \prod_{j=1}^q [1 + \sin^2(\alpha_j)] \\ & \leq 1 + \sum_{j=1}^q \sin^2(\alpha_j) + \left[\sum_{j=1}^q \sin^2(\alpha_j) \right]^2 + \dots \\ & \leq \sum_{j \geq 0} \varepsilon^j = 1/(1 - \varepsilon), \end{aligned}$$

where the last inequality is due to the geometric series. Then,

$$c_j \leq \frac{1}{1 - \varepsilon} (\varepsilon' \sin \alpha_j + \varepsilon'^2 \sin \alpha_{j-1} + \dots + \varepsilon'^j \sin \alpha_1), \quad (\text{C3})$$

which is the desired bound.

APPENDIX D: EIGENSTATE CHANGE IN QSA

By definition, the eigenstate path in QSA is determined by

$$|\psi(\beta)\rangle = \frac{1}{\sqrt{\mathcal{Z}}} \sum_{\sigma} e^{-\beta E[\sigma]/2} |\sigma\rangle,$$

where $0 \leq \beta \leq \beta_q$, $E[\sigma] \in \mathbb{R}$ is the value of the objective function for (classical) configuration σ , and $\mathcal{Z} = \sum_{\sigma} e^{-\beta E[\sigma]}$ is the partition function. Then, it is simple to show

$$|\partial_{\beta} \psi(\beta)\rangle = \frac{1}{2} \left[\langle E \rangle |\psi(\beta)\rangle - \frac{1}{\sqrt{\mathcal{Z}}} \sum_{\sigma} E[\sigma] e^{-\beta E[\sigma]/2} |\sigma\rangle \right], \quad (\text{D1})$$

where

$$\langle E \rangle = \frac{1}{\mathcal{Z}} \sum_{\sigma} E[\sigma] e^{-\beta E[\sigma]}$$

is the expected (thermodynamic) value of E at inverse temperature β . Because $\{|\sigma\rangle\}$ is an orthogonal basis, Eq. (D1) gives

$$\begin{aligned} \|\partial_{\beta} \psi(\beta)\|^2 &= \frac{1}{4} \sum_{\sigma} (\langle E \rangle - E[\sigma])^2 \frac{e^{-\beta E[\sigma]}}{\mathcal{Z}} \\ &= \frac{1}{4} (\langle E^2 \rangle - \langle E \rangle^2), \end{aligned}$$

relating the rate of change of the state with the thermodynamic fluctuations of E . In addition,

$$\begin{aligned} \partial_{\beta} \langle E \rangle &= \partial_{\beta} \frac{1}{\mathcal{Z}} \sum_{\sigma} E[\sigma] e^{-\beta E[\sigma]} \\ &= \frac{-\partial_{\beta} \mathcal{Z}}{\mathcal{Z}^2} \sum_{\sigma} E[\sigma] e^{-\beta E[\sigma]} - \frac{1}{\mathcal{Z}} \sum_{\sigma} E^2[\sigma] e^{-\beta E[\sigma]} \\ &= \langle E \rangle^2 - \langle E^2 \rangle, \end{aligned}$$

and then

$$\|\partial_{\beta} \psi(\beta)\|^2 = -\frac{\partial_{\beta} \langle E \rangle}{4}. \quad (\text{D2})$$

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