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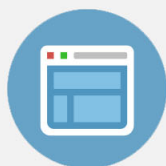
On the efficiency of Hamiltonian-based quantum computation for low-rank matrices

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We present an extension of adiabatic quantum computing (AQC) algorithm for the unstructured search to the case when the number of marked items is unknown. The algorithm maintains the optimal Grover speedup and includes a small counting subroutine. Our other results include a lower bound on the amount of time needed to perform a general Hamiltonian-based quantum search, a lower bound on the evolution time needed to perform a search that is valid in the presence of control error and a generic upper bound on the minimum eigenvalue gap for evolutions. In particular, we demonstrate that quantum speedup for the unstructured search using AQC type algorithms may only be achieved under very rigid control precision requirements. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.3690045]

I. INTRODUCTION AND MAIN RESULTS

A. Introduction

Quantum computing is believed to possess more computational power than classical computing on certain computational tasks. For example, factorization of large numbers can be feasible once a quantum computer is built.[30] The basic paradigm which is usually used in the theoretical works on quantum computing is the so called quantum circuit model (QCM), see, e.g., Ref. 27, although the practical realization of it is yet to be found. Farhi and co-workers[17] had proposed the adiabatic quantum computing (AQC) as an alternative and constructive model for implementing a quantum computer. It was later realized that from a computational complexity point of view AQC is equivalent to all other models for universal quantum computation.[1]

Grover's algorithm,[20] originally derived in the framework of QCM, is one of the milestones in quantum computing. The problem it solves can be formulated as following: Given F: $\{0, 1\}^n \rightarrow \{0, 1\}$ and knowledge that there exists a unique element x such that $F(x) = 1$, find x. It is clear that classically, one needs to check $F(x)$ for all $N = 2^n$ values of x to find the solution, so the time complexity of doing so is $O(N)$. Grover's algorithm uses only $O(\sqrt{N})$ steps to achieve the result, in the framework of QCM. This bound is indeed proven to be optimal for query type of quantum algorithms, see Ref. 7. In the case where there are m (not necessarily 1) values of x for which $F(x) = 1$, a modified version of Grover's algorithm works in QCM if the number m is known.[9] The technique for finding m is called quantum counting and was developed for QCM in Ref. 10.

The original motivation of introducing AQC was to derive the physically attainable algorithm for solving optimization problems such as satisfiability of Boolean formulas by encoding a cost function into the Hamiltonian. One of the (very few) models for which AQC had been shown to produce a speedup is Grover's search problem, addressed first in Ref. 18. The further works in this direction (e.g., Refs. 29 and 31) considered the original problem of Grover (that is the case $m = 1$). The natural question that arises in this context is whether the Grover type running time, e.g. $O(\sqrt{N})$, is still optimal for a more general class of problem Hamiltonian, characterized by $N \gg m > 1$. That means that one wants to derive the analytic lower bound on the runtime of the algorithm, as well

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as to construct the suitable realization of the algorithm for which the running time (being the upper bound on the optimal time) is comparable with this lower bound. The partial result in this direction, namely the lower bound for some class of such models, was established in Ref. 22 (we postpone the more detailed discussion till Sec. I B).

In this paper, we derive the analytic upper and lower bounds on the amount of time needed to perform a (Hamiltonian based but not necessarily adiabatic) unstructured search for the case $N \gg m > 1$. We also present a lower bound on the evolution time needed to perform a search that is valid in the presence of control error and a generic upper bound on the minimum eigenvalue gap for the family of the interpolating Hamiltonians used in AQC. In particular, we show that in general the $O(\ln N/\sqrt{N})$ control precision is necessary in order to achieve quantum speedup over classical computation for the small values of m.

B. Bounds on the running time in Hamiltonian-based quantum computation

In the abstract setting of AQC, we are interested in finding the ground state of the given problem Hamiltonian H_F, in the shortest possible time. To this end, we consider a pair of hermitian $N \times N$ matrices $H_{I,F}$, and will assume that $N \gg 1$. Let $H(s)$ be the interpolating Hamiltonian,

$$H(s) := (1 - f(s))H_I + f(s)H_F , \tag{1}$$

where f is a monotone function on [0, 1] satisfying $f(0) = 0, f(1) = 1$. The idea of AQC is to prepare the initial state of the system $\psi(0)$ in a ground state ψ_I of the Hamiltonian H_I, and let the system evolve according to the (scaled) Schrödinger equation:

$$i\dot{\psi}_\tau(s) = \tau H(s)\psi_\tau(s), \quad \psi_\tau(0) = \psi_I . \tag{2}$$

The adiabatic theorem (AT) of quantum mechanics ensures that under certain conditions (see Theorem 1.4 below for details) the evolution $\psi_\tau(1)$ of the initial state stays close to a ground state of the problem Hamiltonian H_F. For AQC to be efficient, the running (i.e., physical) time τ in (2) must be much smaller than N. One then can ask what choice of the initial Hamiltonian H_I and the parametrization $f(s)$ minimizes τ, and what the optimal value of τ is.

One of the parameters that enters into the upper bound for τ in the standard AT is the minimal value g of the spectral gap $g(s)$ between the ground state energy of $H(s)$ and the rest of its spectrum. Consequently, the traditional approach[17] to AQC involves the estimation of g. Excluding a very short list of interesting situations for which g can be explicitly evaluated (compilation of such examples can be found in Ref. 12), it appears to be a hard problem. In some instances one can get an idea of what size of g could be by using the first-order perturbation theory.[31] In Subsection I C we present rigorous bounds on the size of the gap for the problem at hand, albeit we do not use them explicitly in our study of AQC.

The main purpose of this work is to obtain the rigorous upper and lower bounds on the optimal running time τ for a particular class of problem Hamiltonians, satisfying:

Assumption 1: The problem Hamiltonian is of the small rank:

$$Rank(H_F) := m \ll N .$$

This hypothesis is fulfilled in particular for the generalized unstructured search (GUS) problem, see, e.g., Ref. 10. Since we are interested in the dynamical evolution of the initial state for which shifting the energy results in the overall dynamical phase factor, the above assumption is equivalent to the following condition: Let V denote the largest eigenspace of H_F. Then we require that $N - \dim V \ll N$.

It turns out that for such H_F one can circumvent the standard AT, avoiding the direct estimation of g. We will also see that the (nearly) optimal parametrization $f(s)$ is in fact non-adiabatic.

To formulate our results, we need to introduce some notation first: Let $\{E_n^i\}_{n=1}^N$ ($\{E_n^f\}_{n=1}^N$) be a set of distinct eigenvalues of H_I (respectively H_F), enumerated in the ascending order. It is allowed to the corresponding eigenvalues to be degenerate. In what follows, we will denote by P_I (P_F) the eigenprojection of H_I (H_F) onto $E_I := E_1^i$ ($E_F := E_1^f$), and by Q_I (Q_F) the orthogonal projection

onto the range of H_I (H_F). To AQC to be meaningful in our context we have to impose $E_I \neq 0$. In the typical setup, $E_I = -1$.

Before stating our results, let us note that for AQC to work, it suffices to ensure that $\psi_\tau(1)$ has just the non-trivial overlap with the range of P_F, which we will encode in the requirement $\|P_F\psi_\tau(1)\| \geq \gamma$ for a "reasonable" γ. Indeed, like many quantum algorithms, the AQC algorithm is probabilistic in the sense that it gives the correct answer with the probability γ^2. The probability of failure can be decreased to the desired value (namely $O(1/N)$) by repeating the algorithm $\frac{\ln N}{\gamma^2}$ times. We set $\gamma = 1/5$ throughout this paper. Another issue that we want to settle is normalization of $H(s)$. To that end, we will calibrate $H_{I,F}$ as $\|H_I\| = \|H_F\| = 1$. Note that without loss of generality we can assume that $E_F < 0$ (since otherwise we can interpolate $-H_I$ and $-H_F$ which only changes the solution ψ_τ of (2) into $\bar{\psi}_\tau$). We now introduce some parameters in order to formulate our results. Namely, let $\delta_1 = \|H_F\psi_I\|$, let $\delta_2 = \|P_F\psi_I\|$, and let $\delta_3 = \|Q_F\psi_I\|$, where Q_F is a projection onto $Range\, H_F$. Let $g_F := E_2^f - E_1^f$.

Finally, we introduce the notion of what we will refer to as a generic Hamiltonian H_I. Given an m-dimensional subspace V of $\mathbb{C}^N$, the natural question one can ask is what is a distance from the "typical" vector ψ_I to V. More specifically, suppose one has some reasonable probability distribution function for the vectors ψ_I on the unit sphere S^N in $\mathbb{C}^N$ (say uniform). Then the expected value of $\|\phi_I\|^2$ of the orthogonal projection ϕ_I of the ψ_I on V is equal to m/N. One can check that the probability of the event $\{\psi_I \in \mathbb{C}^N : |\|\phi_I\|^2 - m/N| \geq \alpha m/N\}$ is exponentially small in α (see, e.g., Ref. 13). Note now that $Q_F\psi_I$ is the projection of ψ_I onto the range of Q_F, which is an m-dimensional subspace. We, therefore, will call H_I generic if its ground state ψ_I satisfies $\|Q_F\psi_I\| = O(\sqrt{m/N})$.

Our first assertion is the non-existence result, showing that for any choice of H_I and any function $f(s)$ the running time cannot be smaller than τ_- defined below.

Theorem 1.1 (the lower bound on the running time): *Consider the interpolating family Eq. (1) with an arbitrary f. Then the running time τ_- in Eq. (2) for which $\|P_F\psi_{\tau_-}(1)\| \geq 1/5$ satisfies,*

$$\tau_- \geq \frac{1 - 5\|P_F\psi_I\|}{5\|H_F\psi_I\|}, \quad \text{for} \quad \delta_2 < 1/5. \tag{3}$$

Remark 1:

1. This result shows that it is impossible to construct the family of the interpolating Hamiltonians $H(s)$ such that the evolution of Ψ_I will have a reasonable overlap with P_F if the running time τ is smaller than τ_-. To probe how tight this bound is, one wants to construct a specific family $H(s)$ and the running time τ_+ for which $\|P_F\psi_\tau(1)\|$ is not small, and make a comparison between $\tau_\pm$. As we will see, our bound τ_- is not tight ($\tau_-/\tau_+ - 1 \neq o(1)$), but of the right order of magnitude (meaning $\tau_-/\tau_+ = O(1)$) in terms of the asymptotic dependence on the small parameter m/N.
2. For a generic H_I both $\|H_F\psi_I\|$ and $\|P_F\psi_I\|$ are $O(\sqrt{m/N})$, hence the minimal running time τ cannot be smaller than $O(\sqrt{N/m})$.
3. As we will see, the (nearly) optimizing parametrization $f(s)$ is in fact non adiabatic.

1. Comparison with the Ioannou-Mosca result

In Ref. 22, Ioannou and Mosca established the lower bound on the running time τ for a particular class of problems where the initial Hamiltonian H_I is diagonal in the Hadamard basis while the problem Hamiltonian H_F is diagonal in the standard basis. Their result is non-trivial provided the largest eigenspace of H_I has dimension $N - m$ where $m \ll \sqrt{N}$, and the lower bound they obtained is given by $\tau_- = O(\sqrt{N}/m)$. Since one can always interchange the roles of H_I and H_F and shifts energy so that the largest eigenspace corresponds to the energy 0, their result can be viewed as a slighter weaker version of Theorem 1.1 for this class of Hamiltonians.

In the next assertion we construct a specific family $H(s)$ and determine the runtime τ_+ for which $\|P_F \psi_\tau(1)\| \geq 1/5$:

Theorem 1.2 (The upper bound on the running time): *There exists an explicit rank one H_I and an explicit function f such that $\|P_F \psi_{\tau_+}(1)\| \geq 1/5$ for*

$$\tau_+ = \frac{C(1 - E_F)}{|E_F| \, \|P_F \psi_I\|}, \tag{4}$$

and any value $C \in [1/3, 2/3]$, provided that $\|Q_F \psi_I\|/g_F = O(1/\ln N)$.

Remark 2:

1. For a generic choice of H_I one has $\|Q_F \psi_I\| = O(\sqrt{m/N})$, $\|P_F \psi_I\| = O(\sqrt{m_1/N})$, where $m_1 = Rank\, P_F$. It implies that $\tau_-/\tau_+ = O(1)$ for $m = O(1)$.
2. This assertion can be viewed as an extension of the result obtained in Ref. 18 that considered the original Grover's search problem in the Hamiltonian-based algorithm.
3. The interpolating function f in this construction is similar to the one used in Ref. 18, namely it is a double step function. Since f is discontinuous, we prefer to refer to this particular construction as the Hamiltonian-based algorithm rather than AQC.

Note that *a priori* the values of E_F and δ_2 may be unknown. For instance, the value of the overlap δ_2 has to be determined in the GUS problem with the *unknown* number of marked items. To this end, we prove the following auxiliary result:

Theorem 1.3: *Suppose that the value of E_F is known. Then there is a Hamiltonian-based algorithm that determines $\|P_F \psi_I\|$ with $1/N^2$ accuracy and requires $O((\ln N)^2)$ of the running time.*

Remark 3:

1. The running time for this sub-algorithm is much shorter than τ_+, so it does not significantly affect the total running time.
2. A parallel result in the context of the quantum circuit model was establishes earlier in Ref. 10.

C. Gaps in the spectrum of the interpolating Hamiltonian

Although the size of the gap in the spectrum of $H(s)$ did not play much of the role so far, it is instructive to estimate it for the following reason: The size of the gap manifests itself in the adiabatic theorem of quantum mechanics (AT), on which AQC is build. The following assertion holds, see, e.g., Ref. 5:

Theorem 1.4 (Uniform adiabatic theorem): *Suppose that the $H(s)$ is twice differentiable and bounded family of self-adjoint operators on the interval [0, 1], that is, τ–independent, and suppose in addition that*

$$g := \operatorname{dist}(\lambda_1(s), \sigma(H(s) \setminus \lambda_1(s)) > 0 \quad for\ all\ s \in [0, 1]. \tag{5}$$

Then the solution $\psi_\tau(s)$ of the Initial Value Problem (IVP) (2) satisfies

$$\lim_{\tau \to \infty} \operatorname{dist}(\psi_\tau(s), Range\, P_F) = 0. \tag{6}$$

To AQC to be meaningful, one should choose the initial Hamiltonian H_I in such a way that $Rank\, P_I$ is small. The error in the adiabatic evolution (the right-hand side of (6)) depends on the size of the gap g, with the rough upper bound on the error of the form $\frac{C}{\tau g^3}$.[23]

Theorem 1.5 (The size of the gap): *Let $g_I := E_2^i - E_I$ be a gap between the ground state of the initial Hamiltonian H_I and the rest of its spectrum. Let $\delta_4 := \|P_I Q_F\|$, where Q_F is a projection onto the range of H_F. Then, we have the following estimate on the size of the gap g in (5):*

$$g \leq 10\,\delta_4, \tag{7}$$

provided $g_I > 10\delta_4$.

Remark 4: In fact one can relax the condition $g_I > 10\delta_4$, but to keep the presentation simple we impose this additional constraint.

D. Robust adiabatic quantum computing

In this section we propose a necessary technical requirement on the quantum device for AQC Grover's search to be successful. The $\sqrt{N}$ speedup in AQC algorithm obtained in the tractable problems (cf. Ref. 12 for the Grover's problem or its rigorous treatment in Ref. 23) relies on a special choice of the parametrization $f(s)$ in (1). Namely, it is constructed in such a way that $\dot{f}(s)$ is small at instances $\{s_j\}$ at which the spectral gap $g(s_j) := \lambda_2(s_j) - \lambda_1(s_j)$ of $H(s_j)$ is small. In the AQC jargon, it is usually referred to as the quantum search by local adiabatic evolution. It is interesting to compare this approach with the construction used in Theorem 1.2, where this strategy is pushed to the extreme, namely f used there is actually the constant except for the endpoints $s = 0, 1$ where it jumps. There are two practical problems with this approach:

1. The values $\{s_j\}$ obviously depend on H_F and, in particular, on E_F (even for the Grover's problem, as the simple scaling argument shows). So to choose such an f one has to know the spectral structure of H_F with $o(1/\sqrt{N})$ precision. This is tacitly assumed in Ref. 12. Note that albeit Theorem 1.2 (used in conjunction with Theorem 1.5) represents an improvement with this regard, it still requires knowledge of E_F.
2. Even if this technical obstacle can be overcome, the extreme susceptibility of $\psi_\tau(1)$ to the parametrization f poses a radical problem in practical implementation. Indeed, it is presumably extremely difficult to enforce $\dot{f} = 0$ for a long stretch of the physical time, as the realistic computing device inevitably fluctuates due to the presence of the noise. Some models that try to take into the account the noise were proposed, see e.g. Refs. 4 and 11, but to the best of our knowledge all of the existing constructions contain *ad hoc* parameters and are not derived from the first principles. For some interesting rigorous work in this direction that considers de-phasing open systems see Ref. 6.

Another issue[33] that will motivate our last result below is related to the fact that the adiabatic theorems fall into two categories: Those that describe the solutions for *all* times, including times $s \in [0, 1]$, and those that characterize the solutions at large times $s > 1$ where the Hamiltonian is time-independent again. Interestingly they give more precision for long times. We call the first category, the one that applies to all times, uniform, the second is the long time category.

A representative result from the uniform category is Theorem 1.4 above. A characteristic result (see, e.g., Refs. 8, 25, and 26) which lies in the long-time category is

Theorem 1.6 (Long-time adiabatic theorem): *Suppose that the $H(s)$ is smooth (that is, C^∞ class) and bounded family of self-adjoint operators with $\dot{H}(s)$ supported on [0, 1] that is $\tau-$ independent, and suppose in addition that (5) holds as well. Then the solution $\psi_\tau(s)$ of the IVP (2) satisfies,*

$$\text{dist}\,(\psi_\tau(s), \, Range \; P_F) \; = \; o(\tau^{-n}) \quad \text{for} \quad s \geq 1 \,, \tag{8}$$

for any $n \in \mathbb{N}$.

Remark 5:

1. In words one can say that starting and finishing the interpolation slowly decreases the error in the adiabatic theorem.
2. There is, in general, no uniformity in n; the term on the right-hand side is of order $c_n \tau^{-n}$, where c_n grows rapidly with n (cf. the following discussion).

3. The distinction between the uniform and the long-time AT has an analog in integrals. Suppose that $g(s) \in C^{\infty}([0, 1])$. Then,

$$\int_0^s g(t)e^{it\tau}dt = \begin{cases} o(\tau^{-n}), & \text{if } s \geq 1 \, ; \\ O(\tau^{-1}), & \text{if } s \in (0, 1) \, . \end{cases}$$

In the application to AQC it is natural to investigate the dependence of the coefficients c_n in terms of the gap g and minimize the running time τ in such a way that $c_n\tau^{-n} = o(1)$ for some optimally chosen value n. The recent result in this direction, Ref. 24, gives $\tau = O(g^{-3})$. For the sketch of the argument that uses (truncated) Nenciu's expansion technique[16] and leads to the sharper estimate $\tau = O(g^{-2}|\ln g|^5)$; see Ref. 14. One is then tempted to combine the starting and finishing slowly strategy with the quantum search by local adiabatic evolution strategy in order to minimize the error in the adiabatic theorem. Such analysis was undertaken recently for Grover's search problem in Refs. 28 and 32.

Inspired by the above discussion, we will assume that in the robust setting for any given moment s inside the interval J described below (and which excludes the vicinities of the endpoints $s = 0, 1$) the value $\dot{f}(s)$ is greater than some small but fixed $\kappa > 0$. To motivate the definition of J, suppose that the function f lies in the long-time category, i.e., $\dot{f}$ is supported in $[0, 1]$ and f is smooth. Let $b \in [0, 1]$ be such that $\ddot{f}$ does not change sign on $[b, 1]$ (but it can vanish there). It is not difficult to see that since f is monotone, f has to be concave on $[b, 1]$, hence $\ddot{f} \leq 0$ there. Now let us define the interval J for *any* differentiable function f. Let $a = \min_{s \in [0, 1]}\{f(s) = 1/3\}$. Let $b = \min_{s \in [0, 1]}\{f(s)$ is concave on $[s, 1]\}$. We then define the interval $J := [a, b]$ for $f \in C^1$ provided $a \leq b$, $J = \emptyset$ if $a > b$, and $J := [a, 1]$ if $f \notin C^1$. To illustrate this notion, consider $f \in \mathbb{C}^{\infty}(\mathbb{R})$ constructed as follows:

$$f(t) = \int_{-\infty}^t g(s)ds \, , \quad g(s) = \begin{cases} 0 \, , & \text{if } s \notin [0, 1] \, , \\ \alpha \, e^{\frac{1}{s(s-1)}} & \text{if } s \in (0, 1) \, . \end{cases}$$

The factor α here is a normalization constant, chosen so that $f(1) = 1$. We then have

$$\ddot{f}(t) = \left(\frac{1}{t^2} - \frac{1}{(1-t)^2}\right)g(t) \, , \quad \text{for } t \in [0, 1] \, ,$$

so that the only inflection point is $t = 1/2$. Hence, f is convex on $[0, 1/2]$ and is concave on $[1/2, 1]$. We therefore get $b = 1/2$ and $J = [f^{-1}(1/3), 1/2]$. The convexity of f on $[0, 1/2]$ implies that $f(y) - f(x) \geq \dot{f}(x)(y - x)$ for any $x, y \in [0, 1/2]$. Choosing $x = s, y = 0$, we obtain $\dot{f}(s) \geq f(s)/s$ for $s \in (0, 1/2]$. Since f is monotone, we conclude that $\dot{f}(s) \geq 2/3$ on $[a, 1/2]$. So in this example $\kappa = 2/3$.

The utility of the introduction of the interval J is as follows: On the interval $[a, 1]$ the function f is concave, hence it satisfies $f(y) - f(x) \leq \dot{f}(x)(y - x)$ for any $x, y \in [b, 1]$. In particular, we have

$$1 - f(t) \; \leq \; \dot{f}(t)(1 - t) \; \leq \; \dot{f}(t) \quad \text{for} \quad t \in [b, 1] \, , \tag{9}$$

the relation we are going to exploit.

Our last result establishes that in the case of the small rank initial Hamiltonian, the robust version of AQC does not yield a significant speedup unless κ can be made exponentially small.

Theorem 1.7 (Robust lower bound on the running time): *Suppose that f in Eq. (1) is (piecewise) differentiable and satisfies $\dot{f}(s) \geq \kappa > 0$ for $s \in J$ with the interval J defined above. Also, let us assume that $E_I = -1$. Then, if $\tau < \tau_r = O\left(\frac{\kappa}{m^2\delta^2 \ln \delta}\right)$, we have*

$$|\langle\psi_I|\psi_\tau(1)\rangle| \; > \; \frac{2\sqrt{6}}{5} + 2\delta \, , \tag{10}$$

where $\delta = \|Q_I Q_F\|$. Hence the running time τ for which $\|Q_F\psi_\tau(1)\| \geq 1/5$ cannot be smaller than τ_r.

Remark 6:

1. This theorem tells us that for a generic H_I of the small rank, the robust running time τ_r cannot be smaller than $O(\kappa N/\ln N)$. Hence, unless the control precision κ is on the order of $O(\ln N/\sqrt{N})$, AQC is not much better than its classical counterpart that solves GUS for $\tau = O(N)$.

2. As we remarked earlier, the requirement $E_I = -1$ is a very mild one.

II. PROOF OF THEOREM 1.1

The proof is based on the following observation: Note that ψ_I is an approximate eigenvector of $H(s)$ since $(H(s) - (1 - f(s))E_I I)\psi_I = f(s)H_F\psi_I$, and the norm of the right-hand side is equal to δ_1. So by the first-order perturbation theory, the dynamical evolution of the state ψ_I given by (2) will stay close (up to the dynamical phase) to ψ_I, unless the running time τ is such that the total variation, given by $\tau\delta_1$, is of order 1. The proof below formalizes this argument.

For a solution $\psi_\tau(s)$ of (2), let

$$\phi_\tau(s) := e^{if_\tau(s)}\psi_\tau(s), \quad f_\tau(s) = \tau E_I \int_0^s (1 - f(r))\,dr. \tag{11}$$

Then one can readily check that $\phi_\tau(s)$ satisfies the IVP

$$i\dot\phi_\tau(s) = \tau \hat{H}(s)\psi_\tau(s), \quad \phi_\tau(0) = \psi_I, \tag{12}$$

where

$$\hat{H}(s) = (1 - f(s))(H_I - E_I I) + f(s) H_F.$$

The factor $e^{if_\tau(s)}$ is usually referred to as a dynamical phase.

Let $U_\tau(t, s)$ be a semigroup generated by $\hat{H}(s)$, namely,

$$-i\,\partial_s U_\tau(t, s) = \tau U_\tau(t, s)\hat{H}(s); \quad U_\tau(s, s) = I; \quad t \geq s. \tag{13}$$

Then the solution $\phi_\tau(1)$ of (12) is equal to $U_\tau(1, 0)\,\psi_I$. On the other hand,

$$I - U_\tau(1, 0) = \int_0^1 \partial_s U_\tau(1, s)\,ds = i\tau \int_0^1 U_\tau(t, s)\hat{H}(s)\,ds,$$

hence applying both sides on ψ_I, we obtain

$$\psi_I - \phi_\tau(1) = i\tau \int_0^1 U_\tau(t, s)\hat{H}(s)\psi_I\,ds.$$

We infer

$$\|\psi_I - \phi_\tau(1)\| \leq \tau \int_0^1 \|\hat{H}(s)\psi_I\|\,ds.$$

But,

$$\hat{H}(s)\psi_I = \{(1 - f(s))(H_I - E_I I) + f(s)H_F\}\psi_I = f(s)H_F\psi_I,$$

and we get the bound

$$\|\psi_I - \phi_\tau(1)\| \leq \tau\delta_1 \int_0^1 f(s)\,ds \leq \tau\delta_1,$$

where in the last step we used $0 \leq f(s) \leq 1$. By the triangle inequality,

$$\left| \|P_F\psi_I\| - \|P_F\phi_\tau(1)\| \right| \leq \|P_F\psi_I - P_F\phi_\tau(1)\| \leq \|\psi_I - \phi_\tau(1)\|$$

$$\leq \tau\delta_1,$$

so that

$$\|P_F\phi_\tau(1)\| \leq \tau\delta_1 + \delta_2.$$

On the other hand, by the assumption of the theorem $\|P_F\psi_\tau(1)\| \geq 1/5$, hence $\|P_F\phi_\tau(1)\| \geq 1/5$. As a result, we can bound

$$1/5 \leq \tau\,\delta_1 + \delta_2\,,$$

and the assertion follows.   ∎

III. PROOF OF THEOREM 1.2

We will choose $H_I = -|\psi_I\rangle\langle\psi_I|$, and a non-adiabatic parametrization

$$f(s) = \begin{cases} 0, & \text{if } s = 0\,, \\ \alpha \equiv \frac{1}{1-E_F}, & \text{if } s \in (0,1)\,, \\ 1, & \text{if } s = 1\,. \end{cases}$$

That means we move extremely quickly (instantly in fact) to the middle of the path, stay there for the time τ, and then move quickly again to the end of the path. We first observe that regardless of the choice of $f(s)$ in (1) we have $\psi_\tau(s) \in Y$, where Y is a subspace of the Hilbert space, spanned by the vectors in the range of H_F and ψ_I. Here, we have used the fact that the range of H_I by the assumption of the theorem coincides with $Span\{\psi_I\}$. Let us choose the orthonormal basis $\{e_i\}_{i=1}^{m+1}$ for Y as follows: The first m vectors in the basis are the eigenvectors of H_F corresponding to $\{E_i^f\}$ that differ from zero, and the last vector e_{m+1} is obtained from ψ_I using the Gram-Schmidt procedure. That is,

$$e_{m+1} := \frac{\bar{Q}_F\psi_I}{\|\bar{Q}_F\psi_I\|} = \frac{\bar{Q}_F\psi_I}{\sqrt{1-\delta_3^2}}, \quad \bar{Q}_F = 1 - Q_F\,.$$

We then have

$$\|e_{m+1} - \psi_I\|^2 = \|Q_F e_{m+1} - Q_F\psi_I\|^2 + \|\bar{Q}_F e_{m+1} - \bar{Q}_F\psi_I\|^2$$

$$= \delta_3^2 + \left(\frac{1}{\sqrt{1-\delta_3^2}} - 1\right)^2 \left(1 - \delta_3^2\right)$$

$$\leq \delta_3^2 + \delta_3^4\,. \tag{14}$$

Our choice of g ensures that

$$\psi_\tau(1) = e^{-i\alpha\tau\cdot(E_F P_I + H_F)}\psi_I\,.$$

Here we introduce P_F as the orthogonal projection onto the span of $\{e_i\}$ with $E_i^f = E_1^f$, and P_{m+1} the orthogonal projection onto e_{m+1}. Clearly,

$$P_{m+1} = \frac{\bar{Q}_F P_I \bar{Q}_F}{1 - \delta_3^2}$$

We want to compute the matrix elements of the propagator $e^{-i\alpha\tau(H_I + H_F)}$ in the basis $\{e_i\}$. To this end, we observe that in this basis $H_F = diag(E_F, \ldots, E_m^f, 0)$, and H_I is a block matrix such that

$$\left\| E_F P_I - \begin{bmatrix} 0 & \delta_3 V^* \\ \delta_3 V & E_F \end{bmatrix} \right\| \leq 3\delta_3^2 |E_F|\,, \tag{15}$$

where $\|V\| = |E_F|$. Indeed, we have

$$\|Q_F P_I Q_F\| = \delta_3^2\,,$$

$$\|P_{m+1} P_I P_{m+1}\| = 1 - \delta_3^2\,,$$

$$\|P_{m+1} P_I Q_F\| = \delta_3 (1 - \delta_3^2)^{1/2}\,.$$

Together, we obtain that in this basis

$$\left\| E_F P_I + H_F - \begin{bmatrix} D & \delta_3 V^* \\ \delta_3 V & E_F \end{bmatrix} \right\| \le 3\delta_3^2 |E_F|,$$

where $D = diag(E_F, \dots, E_m^f)$. A simple perturbative argument (cf. Duhamel formula (17) below) shows that

$$\left\| e^{-i\alpha\tau \cdot (E_F P_I + H_F)} - e^{-i\alpha\tau K} \right\| \le 3\delta_3^2 |E_F| \alpha\tau, \tag{16}$$

with

$$K = \begin{bmatrix} D & \delta_3 V^* \\ \delta_3 V & E_F \end{bmatrix}.$$

To this end, we split K into the diagonal and off diagonal parts:

$$K = K_1 + K_2 := \begin{bmatrix} D & 0 \\ 0 & E_F \end{bmatrix} + \begin{bmatrix} 0 & \delta_3 V^* \\ \delta_3 V & 0 \end{bmatrix}.$$

Let

$$\Omega(s) := e^{i\alpha\tau s K_1} e^{-i\alpha\tau s K}; \quad K_2(s) := e^{i\alpha\tau s K_1} K_2 e^{-i\alpha\tau s K_1},$$

then $\dot{\Omega}(s) = -i\alpha\tau K_2(s)\Omega(s)$, and $e^{-i\alpha\tau K}$ is given by the following Duhamel formula:

$$e^{-i\alpha\tau K} = e^{-i\alpha\tau K_1} \left\{ I - i\alpha\tau \int_0^1 K_2(s)\Omega(s)\, ds \right\} \tag{17}$$

$$= e^{-i\alpha\tau K_1} \left\{ I - i\alpha\tau \int_0^1 K_2(s)\, ds \right.$$

$$\left. + (-i\alpha\tau)^2 \int_0^1 K_2(s)\, ds \int_0^s K_2(r)\Omega(r)\, dr \right\}. \tag{18}$$

Observe now that

$$[K_2(s)]_{1,m+1} = [K_2]_{1,m+1},$$

since $e^{-i\frac{\tau}{2}sK_1}$ is diagonal with $(1, 1)$ entry equal to $(m+1, m+1)$ entry. In fact, $[K_2(s)]_{j, m+1} = [K_2]_{j, m+1}$ for all j such that $E_j^f = E_1^f$. Therefore,

$$\left\| P_F \int_0^1 K_2(s)\, ds\, P_{m+1} \right\| = \delta_2 |E_F|, \tag{19}$$

since

$$P_F K_2 P_{m+1} = \frac{|E_F|}{\sqrt{1 - \delta_3^2}} P_F P_I P_{m+1}.$$

To estimate the second term in (18), we note first that the following bound holds.

Lemma 3.1: We have

$$\left\| \int_0^s P_{m+1} K_2(r) Q_F \bar{P}_F \Omega(r)\, dr \right\| \le \frac{8\delta_3}{\tau g_F} + \frac{2\delta_3^2}{g_F}. \tag{20}$$

This estimate is essentially a content of Lemma 3.3 in Ref. 15. The idea is that, since the spectral supports of K_1 for P_{m+1} and $Q_F \bar{P}_F$ are a distance g_F apart, the integral over r has a highly oscillating phase of order τg_F. For completeness, we prove this lemma below.

Armed with this estimate and using the fact that $K_2(s)$ is off diagonal, we get

$$\left\| P_F \int_0^1 K_2(s)\,ds \int_0^s K_2(r)\Omega(r)\,dr\; P_{m+1} \right\|$$

$$= \; \| P_F\, K_2\, P_{m+1} \| \cdot \left\| P_{m+1} \int_0^1 ds \int_0^s K_2(r)\Omega(r)\,dr\; P_{m+1} \right\|$$

$$\leq \; |E_F|\,\delta_2 \cdot \int_0^1 ds \left\| \int_0^s P_{m+1} K_2(r)(P_F + Q_F \bar{P}_F)\Omega(r) P_{m+1}\,dr \right\|$$

$$\leq \; |E_F|\,\delta_2 \cdot \left\{ \int_0^1 \| P_{m+1}\, K_2(r)\, P_F \|\; dr \right.$$

$$\left. + \max_{s \in [0,1]} \left\| \int_0^s P_{m+1}\, K_2(r)\, Q_F\, \bar{P}_F\, \Omega(r)\,dr \right\| \right\},$$

where we have used $\|\Omega(r)\| = \|P_{m+1}\| = 1$ and (19). Applying estimates (19) and (20), we bound

$$\left\| P_F \int_0^1 K_2(s)\,ds \int_0^s K_2(r)\Omega(r)\,dr\; P_{m+1} \right\|$$

$$\leq \; |E_F|\,\delta_2 \cdot \left\{ |E_F|\,\delta_2 + \frac{8\delta_3}{\tau g_F} + \frac{2\delta_3^2}{g_F} \right\}. \tag{21}$$

Multiplying (18) by P_F from the left and by P_{m+1} from the right, and using the estimates (19) and (21), we establish

$$\left\| P_F\, e^{-i\alpha\tau K}\, P_{m+1} \right\| \geq \alpha\tau \left\| P_F \int_0^1 K_2(s)\,ds\; P_{m+1} \right\|$$

$$- (\alpha\tau)^2 \left\| P_F \int_0^1 K_2(s)\,ds \int_0^s K_2(r)\Omega(r)\,dr\; P_{m+1} \right\|$$

$$= \alpha\tau |E_F|\,\delta_2 \cdot \left(1 - \alpha\tau \cdot \left\{ |E_F|\delta_2 + \frac{8\delta_3}{\tau g_F} + \frac{2\delta_3^2}{g_F} \right\} \right). \tag{22}$$

Combining the estimates in (14), (16), and (22) the result will follow provided that

$$\alpha\tau |E_F|\,\delta_2 \cdot \left(1 - \alpha\tau \cdot \left\{ |E_F|\delta_2 + \frac{8\delta_3}{\tau g_F} + \frac{2\delta_3^2}{g_F} \right\} \right)$$

$$\geq 1/5 + \delta_3^2 + \delta_3^4 + 3\delta_3^2 |E_F|\alpha\tau.$$

Note now that for $\tau = O(1/\delta_2)$ the above inequality is satisfied for values of τ and δ_3 such that

$$\alpha\tau |E_F|\,\delta_2 \cdot (1 - \alpha\tau |E_F|\delta_2) \geq 2/9, \quad \delta_3/g_F = O(1/\ln N).$$

The result now follows.   ∎

Proof of Lemma 3.1: Let

$$X := \frac{1}{2\pi i} \oint_\Gamma P_{m+1} (K_1 - zI)^{-1} K_2 (K_1 - zI)^{-1} Q_F \bar{P}_F\, dz, \tag{23}$$

where the contour Γ is a circle $\{ z \in \mathbb{C} : |z - E_F| = g_F/2 \}$. Since

$$\frac{1}{2\pi i} \oint_\Gamma (K_1 - zI)^{-1}\, dz = P_F + P_{m+1},$$

one can readily check that

$$[X,\, K_1] = P_{m+1}\, K_2\, Q_F\, \bar{P}_F.$$

Hence,

$$\int_0^s P_{m+1} \, K_2(r) \, Q_F \, \bar{P}_F \, \Omega(r) \, dr$$

$$= \frac{-2i}{\tau} \int_0^s \frac{d}{dr} \left(e^{-i\frac{\tau}{2}rK_1} \, X \, e^{i\frac{\tau}{2}rK_1} \right) \Omega(r) \, dr \, .$$

Integrating the right-hand side by parts, we obtain

$$\int_0^s P_{m+1} \, K_2(r) \, Q_F \, \bar{P}_F \, \Omega(r) \, dr$$

$$= -\frac{2i}{\tau} \left\{ e^{-i\frac{\tau}{2}rK_1} \, X \, e^{i\frac{\tau}{2}rK_1} \, \Omega(r) \Big|_0^s - \int_0^s e^{-i\frac{\tau}{2}sK_1} \, X \, e^{i\frac{\tau}{2}sK_1} \, \dot{\Omega}(r) \, dr \right\}$$

$$= -\frac{2i}{\tau} e^{-i\frac{\tau}{2}rK_1} \, X \, e^{i\frac{\tau}{2}rK_1} \, \Omega(r) \Big|_0^s - \int_0^s e^{-i\frac{\tau}{2}sK_1} \, X \, e^{i\frac{\tau}{2}sK_1} \, K_2(r)\Omega(r) \, dr \, .$$

The first term is bounded in norm by $4\frac{\|X\|}{\tau}$, while the second one is bounded by $\|X\| \cdot \|K_2\|$. It follows from (23) that $\|X\| \leq \frac{2\|K_2\|}{g_F}$. On the other hand, $\|K_2\| = \delta_3\|V\| = |E_F|\delta_3 \leq \delta_3$ by (15), and the result follows. □

IV. PROOF OF THEOREM 1.3

The algorithm used in the proof is inspired by the mean ergodic theorem and makes use of the fact that the survival probability $c_F(t) = \langle \psi_I | e^{itH_F} | \psi_I \rangle$ is directly measurable in AQC framework. We suggest to measure the survival probability for a number a times specified below to estimate the overlap δ_2, and then to count the total running time spent on this subroutine.

Our starting point is a truncated Taylor's expansion for e^x,

$$e^x = \sum_{k=0}^L \frac{x^k}{k!} + O\left(\frac{|x|^L}{L!} \right).$$

Setting $x = pe^{iw}$, and multiplying both sides by x^{-p}, we obtain the following relation:

$$e^{p(\cos w - 1)}e^{ip\sin w} = e^{-p} \sum_{k=0}^L \frac{p^k e^{iwk}}{k!} + O\left(e^{-p}\frac{p^L}{L!} \right). \tag{24}$$

If $1 - \cos w > g$, then the left-hand side of Eq. (24) is bounded by e^{-pg} and, therefore, is smaller than $1/N^2$, provided $p = 2\ln N/\min(1, g)$. On the other hand, with such choice of p, the remainder term in Eq. (24) is bounded by $O(1/N^2)$ if L is chosen to be equal to ep. Combining these observations, we get

$$e^{-p} \sum_{k=0}^{ep} \frac{p^k e^{ik\omega}}{k!} = \begin{cases} 1 + O(1/N^2), & \text{if } \omega = 0 \\ O(1/N^2), & \text{if } 1 - \cos\omega > g \end{cases}, \tag{25}$$

where $p = 2\ln N/\min(g, 1)$.

Now, using the spectral decomposition of H_F,

$$e^{it(H_F - E_F)} = \sum_{i=1}^N P_i e^{it(E_i^f - E_F)} P_i,$$

where E_i is the i-th distinct eigenvalue of H_F and P_i is the projector onto the spectral subspace associated with E_i. Hence,

$$e^{-p} \sum_{t=0}^{ep} \frac{p^k}{k!} \langle \psi_I | e^{it(H_F - E_F)} \psi_I \rangle = (\delta_2)^2 + O(1/N^2), \tag{26}$$

for $p = 2\ln N/\min(1, 1 - \cos g_F)$ where we have used Eq. (25). The total running time is $\sum_{t=1}^{ep}$ $t = O((\ln N)^2)$. ∎

V. PROOF OF THEOREM 1.5

The main tool we are going to use is the so-called Krein's formula[2] for the rank m perturbation of the initial Hamiltonian H_I. It gives a characterization of the location of m eigenvalues of the perturbed matrix that *differ* from the spectral values of H_I. Specifically, let A and B be two hermitian matrices, with $Rank\, B = m$, and let Q be an orthogonal projection onto $Range\, B$. Suppose that A is invertible (that is, $0 \notin \sigma(A)$). Then Krein's formula tells us that

$$(A + tB)^{-1} = \left(K^{-1} + tBQ\right)^{-1}, \tag{27}$$

with

$$K := QA^{-1}Q,$$

whenever the right-hand side of (27) exists and where $K^{-1} + tBQ$ is interpreted as acting in the m-dimensional space $Range\, B$. In other words, 0 is an eigenvalue of $A + tB$ if and only if the $m \times m$ matrix $K^{-1} + tBQ$ contains 0 in its spectrum.

The Krein's formula follows directly from the Schur complement formula, which says that if C is invertible then

$$QC^{-1}Q = \left(QCQ - QC\bar{Q}(\bar{Q}C\bar{Q})^{-1}\bar{Q}CQ\right)^{-1},$$

where $\bar{Q} := I - Q$ and the inverses on the-right hand side are understood as acting on the ranges of $\bar{Q}$ and Q, respectively.

To apply the Krein's formula in our context, we form a one parameter family

$$H_t := H_I + tH_F, \quad t = \frac{s}{1-s}, \quad t \in [0, \infty).$$

It is then follows that for a fixed $t \in (0, \infty)$ the eigenvalues of H_t that differ from $\sigma(H_I)$ are given by the roots of the equation.

$$\det\left(K^{-1}(E) + tH_FQ_F\right) = 0, \tag{28}$$

where

$$K(E) := Q_F(H_I - E)^{-1}Q_F.$$

Whenever it is clear from the context that we are working with the operators on $Range\, Q_F$, we will suppress the Q_F dependence.

To analyze (28), we start with the following simple observation:

Lemma 5.1: The matrix K(E) can be decomposed as

$$K(E) = \hat{K}(E) + \frac{\delta_4^2 D}{E_I - E}. \tag{29}$$

Here, the matrix D is positive semi-definite, and is bounded in norm by 1. The matrix $\hat{K}(E)$ is holomorphic in the half-plane $Re\, E > E_I - g_I/2$ and is positive definite for $E \in [E_I - g_I/2, E_I + g_I/2]$. Moreover, in this interval we have bounds

$$\frac{2}{4 + g_I} - \delta_4^2 \leq \hat{K}(E) \leq \frac{2}{g_I}; \quad \frac{4}{(4 + g_I)^2} - \delta_4^2 \leq \frac{d\hat{K}(E)}{dE} \leq \frac{4}{g_I^2}. \tag{30}$$

Proof: We decompose

$$K(E) = Q_F(H_I - E)^{-1}Q_F$$
$$= Q_F\bar{P}_I(H_I - E)^{-1}Q_F + Q_FP_I(H_I - E)^{-1}Q_F.$$

The first contribution will correspond to $\hat{K}(E)$ in (29), and the second one to its counterpart in (29). Note now that for $E \in [E_I - g_I/2, E_I + g_I/2]$, we have

$$\frac{g_I}{2} \, \bar{P}_I \; \leq \; \bar{P}_I(H_I - E) \; \leq \; \left(2 + \frac{g_I}{2}\right) \, \bar{P}_I \, ,$$

where the upper bound is a consequence of $\|H_I\| = 1$. Hence, we obtain

$$\frac{2}{4 + g_I} \, Q_F \bar{P}_I Q_F \; \leq \; Q_F \bar{P}_I(H_I - E)^{-1} Q_F \; \leq \; \frac{2}{g_I} \, Q_F \bar{P}_I Q_F \, .$$

Therefore, the first bound in (30) follows now from

$$Q_F \bar{P}_I Q_F \; = \; Q_F \, - \, Q_F P_I Q_F,$$

and

$$0 \; \leq \; Q_F P_I Q_F \; \leq \; \delta_4^2 \, Q_F \, .$$

To obtain the second bound in (30), we note that

$$\frac{d}{dE} \, (H_I \, - \, E)^{-1} \; = \; (H_I \, - \, E)^{-2}$$

for $E \notin \sigma(H_I)$, and then proceed as above.   □

In applications to the AQC, the parameter δ_4 is typically extremely small: $\delta_4^2 = O(1/N)$. Hence, the second contribution in (29) is small provided $|E - E_I| \gg \delta_4$. Therefore for value of E in such intervals, we can first find the roots $\hat{E}_i(t)$ of

$$\det\left(\hat{K}^{-1}(E) \, + \, t H_F\right) \; = \; 0 \, , \tag{31}$$

and then estimate $|\hat{E}_i(t) - E_i(t)|$, where $E_i(t)$ are the corresponding roots of (28). As we will see, the level crossings or the avoided level crossings for H_t occur for values of t such that a pair of eigenvalues $E_k(t), E_l(t)$ is close to E_I. To find these values of t in the first approximation, we fix the value $E = E_I$ in (31) and solve it for t. We have,

Lemma 5.2: The equation

$$\det\left(\hat{K}^{-1}(E_I) \, + \, t H_F\right) \; = \; 0 \, , \tag{32}$$

has exactly m_+ roots $\{t_j\}_{j=1}^{m_+}$ on $(0, \infty)$, where m_+ is a number of negative eigenvalues of H_F.

Proof: Let $A := \hat{K}(E_I)$, then it follows from previous lemma that $0 < A$. Hence,

$$\left(A^{-1} \, + \, t H_F\right) \; = \; t A^{-1/2} \left(t^{-1} \, + \, A^{1/2} H_F A^{1/2}\right) A^{-1/2} \, .$$

The right-hand side is not invertible for values $\{t_j\}$ such that

$$-t_j^{-1} \; \in \; \sigma\left(A^{1/2} H_F A^{1/2}\right) \, ,$$

and the result follows now from Sylvester's law of inertia.[21]   □

We are now in position to estimate the size of the gap g from above. Namely, we consider the gaps g_j for H_t for $t = t_j$. Since $t = \frac{s}{1-s}$ and $H(s) = (1 - s)H_t$, we obtain $g \leq \frac{g_j}{1+t_j} \leq g_j$. Let

$$\beta := 2 \left(\frac{\delta_4^2}{\frac{4}{(4+g_I)^2} - \delta_4^2}\right)^{1/2} \, .$$

To get a bound on g_j, we show that (28) has roots in the intervals $[E_I - \beta, E_I)$ and $(E_I, E_I + \beta]$, at $t = t_j$. We then infer that $g_j \leq 2\beta$, from which the upper bound in (7) follows since $\beta < 5\delta_4$. Observe first that by condition of the Theorem 1.5, $\sigma(H_I) \cap [E_I - \beta, E_I) = \sigma(H_I) \cap (E_I, E_I + \beta] = \emptyset$ (where the latter property follows from the bound $\beta < 5\delta_4 < g_I/2$), hence we are in position to use Lemma 5.1. We only show that for the first interval, the proof is analogous for the second one.

To this end, we will denote by sgn(A) the signature of the matrix A. We observe that since $\frac{\delta_4^2 D}{E_I - E}$ in (29) is positive semidefinite and monotone increasing for the values of E in $[E_I - \beta, E_I)$, we have

$$\text{sgn}(K^{-1}(E_I - 0) + t_j H_F) \leq \text{sgn}(\hat{K}^{-1}(E_I) + t_j H_F). \tag{33}$$

On the other hand, we have

$$\hat{K}(E_I) - \hat{K}(E_I - \beta) = \int_{E_I - \beta}^{E_I} \hat{K}'(E) \, dE \geq \beta \left(\frac{4}{(4 + g_I)^2} - \delta_4^2 \right), \tag{34}$$

where in the last step we have used (30). Hence,

$$K(E_I - \beta) = \hat{K}(E_I - \beta) + \frac{\delta_4^2 D}{\beta}$$

$$\leq \hat{K}(E_I) - \left(\beta \left(\frac{4}{(4 + g_I)^2} - \delta_4^2 \right) I - \frac{\delta_4^2 D}{\beta} \right)$$

$$\leq \hat{K}(E_I) - \frac{\delta_4^2}{\beta} I < \hat{K}(E_I), \tag{35}$$

with a choice of β as above, and where we have used $\|D\| \leq 1$. We infer

$$K^{-1}(E_I - \beta) + t_j H_F > \hat{K}^{-1}(E_I) + t_j H_F,$$

and since the matrix $\hat{K}^{-1}(E_I) + t_j H_F$ has zero eigenvalue by construction, we obtain

$$\text{sgn}(K^{-1}(E_I - \beta) + t_j H_F) < \text{sgn}(\hat{K}^{-1}(E_I) + t_j H_F). \tag{36}$$

Combining (33) and (36) together, we get

$$\text{sgn}(K^{-1}(E_I - \beta) + t_j H_F) < \text{sgn}(K^{-1}(E_I + 0) + t_j H_F). \tag{37}$$

But the family $K^{-1}(E) + t_j H_F$ is continuous on $[E_I - \beta, E_I)$, hence there should be some value of E in this interval for which $K^{-1}(E) + t_j H_F$ has the eigenvalue 0.

VI. PROOF OF THEOREM 1.7

Let us remind the reader that in the context of this assertion $E_I = -1$. As in the proof of Theorem 1.1,

$$\phi_\tau(s) := e^{i f_\tau(s)} \psi_\tau(s), \quad f_\tau(s) = -\tau \int_0^s (1 - f(r)) \, dr,$$

and

$$\hat{H}(s) = (1 - f(s))(H_I + 1) + f(s) H_F.$$

Let us introduce the auxiliary matrix,

$$B(s) = (f(s) H_F + 1 - f(s) + \epsilon i))^{-1},$$

and let $\phi(s) = \psi_I - f(s) H_F B(s) \psi_I$, where ϵ is a small parameter to be chosen later. Omitting the s dependence, we have

$$\hat{H}\phi = -f(1 - f) H_I H_F B \psi_I - i\epsilon f H_F B \psi_I. \tag{38}$$

That means that away from the m values of s for which $B^{-1}(s)$ has zero eigenvalue, $\|\hat{H}\phi\|$ is very small, since $\|H_I H_F \psi_I\| \leq \delta^2$. Note now that by fundamental theorem of calculus, we have

$$\langle \phi(1) | \phi_\tau(1) \rangle = \langle \phi(0) | \phi_\tau(0) \rangle + \int_0^1 \frac{d}{ds} \langle \phi(s) | \phi_\tau(s) \rangle \, ds, \tag{39}$$

where $\phi_\tau(s)$ is defined in (11). But $\phi(0)|\phi_\tau(0) = 1$, and

$$|\langle \phi(1)|\phi_\tau(1)\rangle| = \left| \langle \psi_I|\phi_\tau(1)\rangle - \langle \psi_I| \frac{H_F}{H_F - \epsilon i} |\phi_\tau(1)\rangle \right|$$

$$\leq |\langle \psi_I|\phi_\tau(1)\rangle| + \|Q_F \psi_I\| = |\langle \psi_I|\phi_\tau(1)\rangle| + \delta \,.$$

Substitution into Eq. (39) gives

$$1 - |\langle \psi_I|\phi_\tau(1)\rangle| \leq \left| \int_0^1 \frac{d}{ds} \langle \phi(s)|\phi_\tau(s)\rangle \, ds \right| + \delta \,.$$

Hence, Eq. (10) will follow if

$$\left| \int_0^1 \frac{d}{ds} \langle \phi(s)|\phi_\tau(s)\rangle \, ds \right| < 1 - \frac{2\sqrt{6}}{5} - 3\delta \,. \tag{40}$$

To establish the above bound, we note first that

$$\frac{d}{ds} \langle \phi(s)|\phi_\tau(s)\rangle = \langle \dot{\phi}(s)|\phi_\tau(s)\rangle - i\tau \langle \phi(s)|\hat{H}(s)|\phi_\tau(s)\rangle \,. \tag{41}$$

We bound the first term on the right-hand side by $\|\dot{\phi}\|$ and the second one by $\tau \|\hat{H}\phi\|$. On the other hand, suppressing the s-dependence, we have

$$\dot{\phi} = -\dot{f} H_F B \psi_I - f \dot{f} B(H_F - 1) B H_F \psi_I \,,$$

hence

$$\|\dot{\phi}\| \leq \dot{f} \|B\| \|H_F \psi_I\| + 2\dot{f} \|B\|^2 \|H_F \psi_I\| \,,$$

where we have used $|f| \leq 1$ and $\dot{f} \geq 0$. Let $\mathrm{dist}(S, z)$ be an Euclidean distance from the set S to the point z in $\mathbb{C}$, and let $\sigma(H)$ stand for the spectrum of H. Then we can estimate the right-hand side further as

$$\|\dot{\phi}\| \leq \frac{\dot{f}\delta}{\Delta_\epsilon} + \frac{2\dot{f}\delta}{(\Delta_\epsilon)^2} \,, \tag{42}$$

with

$$\Delta_\epsilon(s) := \mathrm{dist}(f(s)\sigma(H_F), -1 + f(s) + \epsilon i),$$

and where we have used $-Q_F \leq H_F \leq Q_F$. Taking the norm from the both sides of (38), we get that

$$\|\hat{H}\phi\| \leq \|H_I Q_F\| \|f H_F B\| \|Q_F \psi_I\| + \epsilon \|f H_F B\| \|Q_F \psi_I\| \,, \tag{43}$$

where we have used $H_F Q_F = H_F$ and $\|H_I Q_F\| \leq \|Q_I Q_F\|$, with the later relation following from:

$$\|H_I Q_F\| = \|H_I Q_I Q_F\| \leq \|H_I\| \|Q_I Q_F\| \,.$$

To estimate $\|f H_F B\|$, we consider three cases:

1. $s \in [0, a]$: On this interval, we can estimate

$$\|f(s) H_F B(s)\| \leq \max_{s \in [0,a]} \frac{1}{\Delta_\epsilon(s)} \leq 3 \,, \tag{44}$$

    where we have used $\sigma(H_F) \subset [-1, 1]$.
2. $s \in J$: In this case, we bound

$$\|f(s) H_F B(s)\| \leq \frac{1}{\Delta_\epsilon(s)} \leq \frac{\dot{f}(s)}{\kappa \Delta_\epsilon(s)} \tag{45}$$

    using theorem's hypothesis.

3. $s \in [b, 1]$: Here, we estimate

$$\| f(s) H_F B(s) \| = \left\| f(s) H_F \left(f(s) H_F + 1 - f(s) + \epsilon i \right)^{-1} \right\| \leq 1 + \frac{(1 - f(s)) + \epsilon}{\Delta_\epsilon(s)} \leq 2$$

$$+ \frac{\dot{f}(s)}{\Delta_\epsilon(s)} , \tag{46}$$

where in the last step we have used (9).

Plugging (44)–(46) into (43), we obtain

$$\| \hat{H} \phi \| \leq (\delta^2 + \epsilon \delta) \left(3 + \frac{\dot{f}(s)}{\kappa \Delta_\epsilon} \right) . \tag{47}$$

Using (42) and (47) to bound the right-hand side of (41), we get

$$\left| \frac{d}{ds} \langle \phi | \phi_\tau \rangle \right| \leq \frac{\dot{f} \delta}{\Delta_\epsilon} + \frac{2 \dot{f} \delta}{(\Delta_\epsilon)^2} + \tau (\delta^2 + \epsilon \delta) \left(3 + \frac{\dot{f}(s)}{\kappa \Delta_\epsilon} \right) . \tag{48}$$

In what follows we will use:

Lemma 6.1: We have bounds

$$\int_0^1 \frac{\dot{f} \, ds}{\Delta_\epsilon} \leq -2(m+1) \ln \epsilon ; \quad \int_0^1 \frac{\dot{f} \, ds}{(\Delta_\epsilon)^2} \leq \frac{2(m+1)}{\epsilon} . \tag{49}$$

Integrating both sides of (41) over s and using (48) and (49), we arrive at

$$\left| \int_0^1 \frac{d}{ds} \langle \phi(s) | \phi_\tau(s) \rangle \, ds \right| \leq 3\tau (\delta^2 + \epsilon \delta) + 2(m+1) \delta \left(-\ln \epsilon \left(1 + \frac{\tau \delta}{\kappa} + \frac{\tau \epsilon}{\kappa} \right) + \frac{2}{\epsilon} \right) .$$

Hence, the required bound in Eq. (40) follows with the choice $\epsilon = 10^3 (m+1) \delta$, provided $\tau \leq -\frac{C \kappa}{\epsilon^2 \ln \epsilon}$, where C is some generic constant. ∎

Proof of Lemma 6.1: We derive the first bound, the second bound can be shown analogously. To this end, we observe that

$$\frac{\dot{f}}{\Delta_\epsilon} = \max_{E_n \in \sigma(H_F)} \frac{\dot{f}}{|f E_n + 1 - f - \epsilon i|}$$

$$< \sum_{E_n \in \sigma(H_F)} \frac{\dot{f}}{|f(E_n - 1) + 1 - \epsilon i|} .$$

It follows that

$$\int_0^1 \frac{\dot{f} \, ds}{\Delta_\epsilon} < \sum_{E_n \in \sigma(H_F)} \int_0^1 \frac{\dot{f} \, ds}{|f E_n + 1 - f - \epsilon i|}$$

$$\leq (m+1) \max_{E \in [-1,1]} \int_0^1 \frac{\dot{f} \, ds}{|f E + 1 - f - \epsilon i|} ,$$

where $m = Rank \, H_F$. But,

$$\int_0^1 \frac{df}{\sqrt{(f(E-1) + 1)^2 + \epsilon^2}}$$

$$= \left. \frac{1}{E-1} \ln \left((E-1) f + 1 + \sqrt{((E-1) f + 1)^2 + \epsilon^2} \right) \right|_0^1$$

$$= \frac{1}{E-1} \ln \left(\frac{E + \sqrt{E^2 + \epsilon^2}}{1 + \sqrt{1 + \epsilon^2}} \right) .$$

One can check by taking the derivative that the expression on the right-hand side is monotonically decreasing for all $E \in [-1, 1]$. Since it is also positive and continuous, this term achieves its maximum at $E = -1$, with the value

$$-\frac{1}{2} \ln \left(\frac{\sqrt{1+\epsilon^2} - 1}{1 + \sqrt{1+\epsilon^2}} \right) \leq -2 \ln \epsilon,$$

for ϵ small enough. Hence, the first bound in (49) follows.   □

VII. CONCLUSIONS

In this work we derived a number of rigorous results concerning Hamiltonian-based quantum search problems that satisfy Assumption 1. Our results include, in particular, upper and lower bounds on the amount of time needed to perform a general Hamiltonian-based quantum search, a lower bound on the evolution time needed to perform a search that is valid in the presence of control error and a generic upper bound on the minimum eigenvalue gap for evolutions.

The lower bound on the evolution time is to our knowledge the tightest for AQC type problems. It matches exactly the results established in the framework of the quantum circuit algorithm, when applied to Grover's search problem.

We then construct a specific Hamiltonian-based algorithm with the runtime $\tau = O(\sqrt{N/m})$ which nearly recovers the lower bound, and thus close to be optimal, in the case of Grover's search where the final Hamiltonian is a rank m projection. We augment this construction with the Hamiltonian-based quantum counting subroutine, which allows us to compute one input parameter δ_2 to the algorithm. Since the algorithm is robust in a sense that we can allow the running time to vary in the large time interval, it is not very sensitive to the ground state energy E_F. As a result, just an approximate knowledge of E_F is needed to ensure that the algorithm works.

While our methods do not hinge on the knowledge of the gap structure of the underlying interpolating Hamiltonian $H(s)$, we establish an upper bound on the size of the first spectral gap for this family of matrices. For the final Hamiltonian of the Grover's type, i.e. H_F is a rank m projection, the smallest value of the gap cannot exceed $O(\sqrt{m/N})$.

Finally, we address the question of the evolution time for search-Hamiltonians that are also error robust. Namely, we obtain the lower bound on the running time when the velocity $\dot{f}$ is greater than a fixed control parameter κ during the evolution, excluding the vicinities of the endpoints $s = 0, 1$ where it is allowed to be small. We show that the necessary control accuracy requirement should be at least $O(\ln N/\sqrt{N})$ for the algorithm to succeed. In particular, this result implies that starting slow/finishing slow strategy by itself is not sufficient to make AQC better than the classical computer.

For a general form of H_F for which our Assumption 1 is invalid no general lower bounds on the runtime can be obtained, as the examples constructed in Ref. 12 show. It will be very interesting to establish a "typical" lower and upper bounds for the random instances of NP-complete problems, discussed in Ref. 3.

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