Accuracy versus run time in an adiabatic quantum search

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Adiabatic quantum algorithms are characterized by their run time and accuracy. The relation between the two is essential for quantifying adiabatic algorithmic performance yet is often poorly understood. We study the dynamics of a continuous time, adiabatic quantum search algorithm and find rigorous results relating the accuracy and the run time. Proceeding with estimates, we show that under fairly general circumstances the adiabatic algorithmic error exhibits a behavior with two discernible regimes: The error decreases exponentially for short times and then decreases polynomially for longer times. We show that the well-known quadratic speedup over classical search is associated only with the exponential error regime. We illustrate the results through examples of evolution paths derived by minimization of the adiabatic error. We also discuss specific strategies for controlling the adiabatic error and run time.

I. INTRODUCTION

In adiabatic quantum computation (AQC) [1–3] quantum algorithms are implemented by initializing a system in an easily prepared ground state, followed by adiabatic evolution subject to a Hamiltonian whose final ground state represents the solution to a computational problem. It is known that this model is computationally equivalent to the standard circuit model of quantum computation in the sense that each model can simulate the other with polynomial resource overhead [4–6]. While error correction methods have been proposed for AQC [7,8], and arguments have been put forth that AQC is inherently insensitive to certain types of errors [9–11], unlike the circuit model it is still an open question whether AQC can be made fault tolerant subject to realistic noise models pertaining to AQC in an open system setting. Indeed, even what constitutes a consistent picture of adiabatic evolution in open systems is still the subject of some debate [12,13]. Nevertheless, experiments in AQC using superconducting qubits have made great strides recently [14].

The performance of adiabatic quantum algorithms is characterized by the "adiabatic error," i.e., the fidelity loss between the actual time-evolved state (the solution of the Schrödinger equation) and the instantaneous ground state, calculated at the final time T. Since the adiabatic theorem [15–18] guarantees that in the limit of arbitrarily slow evolution the error approaches zero, one expects that a more slowly varying Hamiltonian and/or a longer evolution time should result in higher fidelity or accuracy. This is the *accuracy-time trade-off* in quantum adiabatic algorithms. This trade-off is often formalized by the adiabatic condition, which states (roughly) that the variation rate of the Hamiltonian should be $\ll$ the adiabatic error times the gap squared. A clear disadvantage of this condition is the inherent vagueness of "$\ll$," which makes it difficult to reliably quantify the evolution time vs. the desired accuracy. Moreover, violations of the traditional adiabatic condition have been reported [19–21] in the sense that the condition is neither necessary nor sufficient for adiabatic evolution. While these violations have been explained as being

either due to inconsistent manipulations [22] or due to resonant transitions [23], it appears that there is no single "adiabatic theorem." Rather, a number of different rigorous conditions have been derived, which apply under various mathematical assumptions [24–31]. A rigorous condition which holds for analytic Hamiltonians and exhibits the explicit scaling with system size, needed for AQC resource quantification, was derived in Ref. [32].

In this work we perform a comprehensive analysis of the adiabatic error for the case of an adiabatic quantum search algorithm, in a closed system setting. We focus on quantum search not only because it is an important example of a quantum speedup [33] but also because it is amenable to an exact analytical treatment. Indeed, rather than relying on a particular form of the adiabatic theorem, our approach is based on an exact treatment of the underlying dynamics. We calculate the adiabatic error as an explicit function of the evolution time. We work out the formal $1/T$ expansion of the error—often used in rigorous treatments of the adiabatic theorem—through which we provide a large-T *polynomial* upper bound for the adiabatic error. We shall argue that a leading order truncation of this series expansion can result in misleading estimates for the scaling of the evolution time vs. system size. We draw this conclusion on the basis of a careful study of the adiabatic error, showing that it may exhibit a short-T *exponential* decay, which is hidden in the formal polynomial expansion. We show that this short-time exponential decay heralds the correct scaling for the evolution time vs. system size (a quadratic speedup over classical search), avoiding the overestimation that results from the long-time polynomial decay, and which leads to a loss of the quantum speedup. Additionally, we propose specific adiabatic evolution paths ("interpolations")—inspired by a procedure for minimization of time functionals for adiabatic evolution [34]—and use these to illustrate our results. We also examine the applicability of the traditional measure of the evolution time and contrast this to what we obtain from our analysis. This careful analysis enables us to show explicitly how one can reduce the adiabatic error as a function of the evolution time.

TABLE I. Summary of the notations.

Notation	Definition	Eq. (#)
$T, \tau, \tau_{\mathrm{run}}$	Total, normalized, run time	(1),(26)
$H_T, V_T, \|\psi_T\rangle$	Actual Hamiltonian, evolution, state	(2),(13),(4)
$E_i, \|\Phi_i\rangle$	Eigenvalues, eigenstates	(2)
$(\Delta) D$	(Dimensionless) Ground-state gap	(42) (3)
H_A, A	Adiabatic Hamiltonian, evolution	(12),(10)
h_A	Adiabatic coupling	(67)
$\delta_{\mathrm{ad}}, \delta'_{\mathrm{ad}}$	Adiabatic error	(16),(17) [(18),(19)]
ε	Bound over the adiabatic error	(20)
r	Fraction of marked (M) to all (N) items	(36)
$H_{\mathcal{I}}$	Initial Hamiltonian (all items)	(28)
$H_{\mathcal{M}}$	Final Hamiltonian (marked items)	(29)
$\mathbf{x}$	Adiabatic interpolation	(30)
J	An energy scale	(27)
$\|\widetilde{\psi}\rangle, \widetilde{H}$	2D (unnormalized) state, (non-Hermitian) effective Hamiltonian	(34),(35)
$\|\widehat{\psi}\rangle, \widehat{H}$	2D (normalized) state, (Hermitian) effective Hamiltonian	(51),(46)
$\widehat{}$	Identifies functions, states, operators in the 2D reduced representation (except Δ)	(50),(51)
$\int^\tau g$	Shorthand for $\int_0^\tau g(\tau') \, d\tau'$	(70)
$\mathcal{I}_l$	Dyson matrix elements [Eq. (81)]	(82)
z_0	Pole(s) of Δ in the complex τ plane	(104)
$\varphi\theta$	Identifies a general family of optimal adiabatic interpolations	(117)–(119)

The structure of this article is as follows. We start with some general background in Sec. II by delineating the framework of adiabatic quantum computation, the definition of the adiabatic error, and the adiabatic theorem. Here, Table I summarizes the main notations used throughout the article. In Sec. III, we specialize to the specific problem of quantum search. There we introduce a general Hamiltonian interpolation for the search problem and analytically solve the corresponding Schrödinger equation. Section IV contains the core of our results. We first derive an exact expression for the adiabatic error in Sec. IV A. Next, in Sec. IV B, we approximate this expression and show how the polynomial and exponential behaviors emerge. Since estimation of the adiabatic error requires specific interpolation paths, we derive a general interpolation for the search Hamiltonian in Sec. IV C and investigate in detail three special cases. The adiabatic error for the general interpolation together with the special cases is estimated in Sec. IV D. In Sec. IV E, we discuss a strategy for controllably reducing the adiabatic error. There we show how one can employ a freedom in the interpolation to manipulate the adiabatic error. This accounts for the performance-resource trade-off. We conclude with a summary of the results and an outlook in Sec. V.

II. FRAMEWORK OF ADIABATIC QUANTUM COMPUTATION

We begin by defining the adiabatic error as it arises in the context of AQC. We also provide a brief review of some pertinent facts concerning the "traditional" adiabatic theorem, also in the context of AQC. However, we note that in the sequel we shall not use the adiabatic theorem; rather, we shall treat the dynamics directly by solving the Schrödinger equation and later enforce adiabaticity by means of a $1/T$ expansion.

A. Adiabatic error

Let us treat the total evolution time T as a parameter and define the the scaled (dimensionless) time

$$\tau = t/T \in [0,1]. \qquad (1)$$

Assume that we have an N-dimensional quantum system that evolves for a total time T under the Hamiltonian $H_T(\tau)$ with spectral decomposition

$$H_T(\tau) = \sum_{i=0}^{N-1} E_i(\tau)|\Phi_i(\tau)\rangle\langle\Phi_i(\tau)|, \tau \in [0,1] \qquad (2)$$

where $E_i(\tau) \leqslant E_j(\tau)$ for $i < j$, except that the ground-state energy is separated from the rest of the spectrum by a nonvanishing gap

$$D(\tau) \equiv E_1(\tau) - E_0(\tau) > 0. \qquad (3)$$

Possible level crossing among excited eigenstates $\{|\Phi_i(\tau)\rangle\}_{i>0}$ shall not concern us here because in the following we shall only focus on the ground state $|\Phi_0(\tau)\rangle$. We assume that the system is closed, i.e., the evolution is governed by the Schrödinger equation

$$i|\dot{\psi}_T(\tau)\rangle = T H_T(\tau)|\psi_T(\tau)\rangle, \qquad (4)$$

where from now on dot denotes $d/d\tau$, and we set $\hbar \equiv 1$. The initial state is assumed to be the ground state, i.e.,

$$|\psi_T(0)\rangle = |\Phi_0(0)\rangle. \qquad (5)$$

Remark. We shall use the subscript T to indicate the parametric dependence on T. When symbols already have a subscript we shall avoid the additional T subscript so as not to clutter the notation.

A central quantity of interest to us is the "adiabatic error" $\delta_{\rm ad}(\tau)$, which quantifies the distance between the instantaneous ground state and the actual state:

$$\delta_{\rm ad}(\tau) \equiv \sqrt{1 - |\langle \Phi_0(\tau)|\psi_T(\tau)\rangle|^2}. \qquad (6)$$

Note that $\delta_{\rm ad}(\tau)$ is a distance and (in-)fidelity measure in their rigorous sense. Indeed, the trace distance $\mathcal{D}$ and fidelity $\mathcal{F}$ between two arbitrary density operators ϱ_1 and ϱ_2 are defined as [35]

$$\mathcal{D}(\varrho_1,\varrho_2) \equiv \tfrac{1}{2}\|\varrho_1 - \varrho_2\|_1, \qquad (7)$$

$$\mathcal{F}(\varrho_1,\varrho_2) \equiv \|\sqrt{\varrho_1}\sqrt{\varrho_2}\|_1, \qquad (8)$$

where $\|X\|_1 \equiv {\rm Tr}\sqrt{X^\dagger X}$ is the trace norm (sum of singular values of X). For pure states $\varrho_i = |\psi_i\rangle\langle\psi_i|$ it is not hard to show that $\mathcal{D}(\varrho_1,\varrho_2) = \sqrt{1 - |\langle\psi_1|\psi_2\rangle|^2} \equiv \mathcal{D}(|\psi_1\rangle,|\psi_2\rangle)$ and $\mathcal{F}(\varrho_1,\varrho_2) = |\langle\psi_1|\psi_2\rangle| \equiv \mathcal{F}(|\psi_1\rangle,|\psi_2\rangle)$. Thus

$$\begin{aligned} \delta_{\rm ad}(\tau) &= \mathcal{D}(|\psi_T(\tau)\rangle,|\Phi_0(\tau)\rangle) \\ &= \sqrt{1 - \mathcal{F}(|\psi_T(\tau)\rangle,|\Phi_0(\tau)\rangle)^2}. \end{aligned} \qquad (9)$$

An equivalent and useful formulation of $\delta_{\rm ad}(\tau)$ is the following. Let $P(\tau) \equiv |\Phi_0(\tau)\rangle\langle\Phi_0(\tau)|$ denote the ground-state eigenprojection. The connection between the initial preparation $P(0)$ and the time evolved state $P(\tau)$ is given by

$$P(\tau) = A(\tau)P(0)A^\dagger(\tau), \qquad (10)$$

where the unitary operator $A(\tau)$—called the adiabatic intertwiner [24]—determines the evolution in the eigenspace $P(\tau)$ and its orthogonal complement $\mathbb{1} - P(\tau)$:

$$A(\tau) \equiv \sum_{i=0}^{N-1} |\Phi_i(\tau)\rangle\langle\Phi_i(0)|. \qquad (11)$$

One can assign a (dimensionless) "adiabatic Hamiltonian," $H_A(\tau)$, to this evolution defined via

$$i\dot{A}(\tau) = H_A(\tau)A(\tau). \qquad (12)$$

On the other hand, the evolution operator, generated as

$$i\dot{V}_T(\tau) = TH(\tau)V_T(\tau), \qquad (13)$$

dictates the actual dynamics:

$$|\psi_T(\tau)\rangle\langle\psi_T(\tau)| = V_T(\tau)P(0)V_T^\dagger(\tau). \qquad (14)$$

Thus the error $\delta_{\rm ad}(\tau)$ in fact measures the difference between $V_T(\tau)$ and $A(\tau)$ or, equivalently, how far the unitary operator

$$\Omega_T(\tau) \equiv A^\dagger(\tau)V_T(\tau) \qquad (15)$$

is from $\mathbb{1}$ (identity). Indeed, we have

$$\delta_{\rm ad}(\tau) = \sqrt{1 - |\langle\Phi_0(0)|\Omega_T(\tau)|\Phi_0(0)\rangle|^2}, \qquad (16)$$

which vanishes if and only if $\Omega_T(\tau) = \mathbb{1}$.

The above formulations have presumed that the degeneracy of the ground-state eigensubspace does not change in time. Nonetheless, there may be situations in which this degeneracy preservation assumption does not hold. In fact, as we shall see later, the quantum search problem we study in this article falls into this category. Let us assume that the initial

state is pure, $|\psi_T(0)\rangle = |\Phi_0(0)\rangle$, but the instantaneous ground-state eigenprojection $P(\tau)$ is not necessarily rank 1, accounting for the possibility of degeneracy. Intuitively, if the actual state $|\psi_T(\tau)\rangle$ only has components in the support of $P(\tau)$ the algorithm has achieved its goal at the instant τ, whereas a less than full overlap denotes lack of success at this instant. The overlap of $|\psi_T(\tau)\rangle$ and the support of $P(\tau)$ can be quantified, e.g., with $\langle\psi_T(\tau)|P(\tau)|\psi_T(\tau)\rangle$, whence we define the following performance error:

$$\delta'_{\rm ad}(\tau) \equiv \sqrt{1 - \langle\psi_T(\tau)|P(\tau)|\psi_T(\tau)\rangle}. \qquad (17)$$

It is evident that $0 \leqslant \delta'_{\rm ad}(\tau) \leqslant 1$, with $\delta'_{\rm ad} = 1$ if and only if the actual state has vanishing overlap with the support of the instantaneous ground-state eigenprojection, while $\delta'_{\rm ad} = 0$ if and only if the actual state resides anywhere in the support.

We can write $\langle\Phi_0(0)|\Omega_T(\tau)|\Phi_0(0)\rangle = {\rm Tr}[P(0)\Omega_T(\tau)]$ and $\langle\psi_T(\tau)|P(\tau)|\psi_T(\tau)\rangle = {\rm Tr}[P(\tau)V_T(\tau)P(0)V_T^\dagger(\tau)] = {\rm Tr}[P(0)\Omega_T(\tau)P(0)\Omega_T^\dagger(\tau)]$. Using this, note the difference between

$$\delta_{\rm ad}(\tau) = \sqrt{1 - |{\rm Tr}[P(0)\Omega_T(\tau)]|^2} \qquad (18)$$

and

$$\delta'_{\rm ad}(\tau) = \sqrt{1 - {\rm Tr}[P(0)\Omega_T(\tau)P(0)\Omega_T^\dagger(\tau)]}. \qquad (19)$$

Namely, in the nondegenerate case $\delta_{\rm ad}(\tau) = 0$ if and only if $\Omega_T(\tau) = \mathbb{1}$, indicating that the evolution was perfectly adiabatic. In the degenerate case, on the other hand, algorithmic success does not require the evolution to be perfectly adiabatic since only nonvanishing overlap with the ground-state eigensubspace is required, i.e., $\delta'_{\rm ad} = 0$ if and only if $V_T(\tau)P(0)V_T^\dagger(\tau) \in {\rm supp}[P(\tau)]$, whereas complete failure requires the dynamics to remove any overlap with the ground-state eigensubspace, i.e., $\delta'_{\rm ad} = 1$ if and only if $V_T(\tau)P(0)V_T^\dagger(\tau) \notin {\rm supp}[P(\tau)]$.

While the error as defined in Eq. (17) is not necessarily a distance in the strict sense, it is adequate for quantifying the adiabatic error. Note also that $\delta'_{\rm ad}(\tau)$ reduces to $\delta_{\rm ad}(\tau)$ when the ground state is nondegenerate. From now on we shall be using these various expressions for the adiabatic error as appropriate in the rest of this article.

B. The adiabatic theorem

One variant of the "traditional" adiabatic theorem [17] states that given an $0 < \varepsilon \ll 1$ and a time-dependent Hamiltonian $H(\tau)$ with a nondegenerate ground state, the adiabatic error satisfies $\delta_{\rm ad}(1) \leqslant \varepsilon$, provided that

$$\frac{\max_\tau \|\dot{H}(\tau)\|}{\min_\tau D^2(\tau)} \ll \varepsilon T, \qquad (20)$$

in which $\|\cdot\|$ is the standard operator norm, defined as the maximum singular value, i.e.,

$$\|X\| \equiv \sup_{|v\rangle,\|v\|=1} |\langle v|\sqrt{X^\dagger X}|v\rangle|, \qquad (21)$$

which reduces to $\sup_{|v\rangle,\|v\|=1} |\langle v|X|v\rangle|$ for normal operators. As remarked in the introduction, this condition is hardly

quantitative due to the intrinsic vagueness of "≪," and has been the subject of critique (consistent with its lack of rigor) [19–21], justifications [22,23], and rigorous improvements [24–32]. Nevertheless, it remains a useful rule of thumb, as long as it is applied with appropriate care.

An immediate implication of the adiabatic theorem is that, assuming it is initialized in the ground state, the system remains close to the final ground state at $t = T$. Thus, by choosing the Hamiltonian such that $H(0)$ corresponds to a *simple* ground state $|\Phi_0(0)\rangle$ (simple in the sense that it is easily preparable), and $H(1)$ represents a Hamiltonian whose ground state $|\Phi_0(1)\rangle$ identifies the solution to a computationally *hard* problem, one can devise an adiabatic version for the corresponding algorithmic or computational task. This is precisely the insight that led to the advent of AQC [2,3].

A simple "annealing schedule," or "path," between $H(0)$ and $H(1)$ is the following linear interpolation in τ:

$$H(\tau) = (1 - \tau)H(0) + \tau H(1). \tag{22}$$

In physical situations, however, one often realizes the dynamics by tuning some time-dependent control knobs or couplings $\mathbf{x}(\tau) = \big(x_1(\tau), \dots, x_K(\tau)\big)$ of the Hamiltonian. This suggests that a generalization of Eq. (22) can be introduced by assuming access to a controllable set of noncommuting, linearly independent, primitive Hamiltonians $\{H_i\}_{i=1}^{K \leqslant N}$ combined, e.g., as $H[\mathbf{x}(\tau)] = \sum_{i=1}^{K} x_i(\tau)H_i$. Further generalizations can be introduced as well [2,34,36,37]. However, for our purposes in this article we shall consider the parametrization [34,36]

$$H[\mathbf{x}(\tau)] = x_1(\tau)H(0) + x_2(\tau)H(1), \tag{23}$$

with the boundary conditions

$$\big(x_1(0), x_2(0)\big) = (1, 0), \tag{24}$$

$$\big(x_1(1), x_2(1)\big) = (0, 1). \tag{25}$$

Two remarks are in order regarding AQC. (i) A primary goal in AQC is to make $\delta_{ad}(1)$ decrease more rapidly for a given T and problem size or, alternatively, to make T smaller for a given ε and problem size. Often the problem size is given by N, the dimension of the Hilbert space. However, in the context of many-body quantum systems, where the Hilbert space is a tensor product of subsystems (e.g., qubits), $\log N$ is the correct measure of problem size, coinciding with system size. (ii) The "run time" complexity of a quantum algorithm should be defined as

$$\tau_{run} \equiv T \max_{\tau} \|H(\tau)\|, \tag{26}$$

not T [4]. This *regularization* is required because of the energy-time trade-off in quantum mechanics in the sense that multiplication of $H(\tau)$ in Eq. (20) by some positive factor α manifests itself as dividing T by the same factor, making it possible to decrease T arbitrarily by choosing α sufficiently large. This trade-off can also be understood via the Schrödinger equation (4), in which the final state of a system evolving under Hamiltonian $H(\tau)$ for T is the same as that of a system evolving under $\alpha H(\tau)$ for T/α. This ambiguity is fixed by the definition of τ_{run} as in Eq. (26). Scaling of τ_{run} with system size,

for a given upper bound on the error $\delta_{ad}(1) \leqslant \varepsilon$, determines the run time complexity of the corresponding quantum algorithm.

III. QUANTUM SEARCH HAMILTONIAN

Grover's quantum search algorithm [33] performs a search for M "marked" items among N items of an unsorted database, presuming that there is an "oracle" for distinguishing the marked from the unmarked items. The algorithm in its original form ($M = 1$) comprises the following steps: (i) assign orthonormal quantum states (i.e., labels) $\{|0\rangle, \dots, |N - 1\rangle\}$ to the items, (ii) prepare the quantum system in the equal superposition state $\sum_{i=0}^{N-1} |i\rangle/\sqrt{N}$, and (iii) apply the "Grover operator"—encompassing the oracle—repeatedly [33,35]. The algorithm finds a marked item after $\tau_{run} = O(\sqrt{N/M})$ calls of the oracle—a quadratic speedup over the best classical algorithm—and is provably optimal for any N (not necessarily very large) [38]. Various generalization of the algorithm have been introduced (e.g., Refs. [39–44]), and it has also been implemented experimentally in a number of physical settings (e.g., Refs. [45–49]).

An adiabatic Hamiltonian version of the search algorithm was first introduced in Ref. [2] but failed to display the expected quadratic speedup as it relied on the linear interpolation of Eq. (22). This was fixed in Ref. [36] by using a nonlinear but one-dimensional interpolation with $x_2(\tau) = 1 - x_1(\tau)$ [recall Eq. (23)], which moves fast when away from the minimum gap but slows down near it. As shown in Ref. [34], this result can be further improved, in the sense of a smaller adiabatic error, by adopting a two-dimensional interpolation as in Eq. (23),

$$H(\tau)/J = x_1(\tau)H_{\mathcal{I}} + x_2(\tau)H_{\mathcal{M}}, \tag{27}$$

with the two projective Hamiltonians

$$H_{\mathcal{I}} = \mathbb{1} - |\phi\rangle\langle\phi|, \tag{28}$$

$$H_{\mathcal{M}} = \mathbb{1} - P_{\mathcal{M}}, \tag{29}$$

where $|\phi\rangle \equiv \sum_{i=0}^{N-1} |i\rangle/\sqrt{N}$ is the equal superposition of all of the "label" states (items), $P_{\mathcal{M}} \equiv \sum_{m \in \mathcal{M}} |m\rangle\langle m|$ is the projection over the subspace $\mathcal{M}$ of the marked items ($|\mathcal{M}| = M$), and J is a dimensional constant which sets the energy scale. In other words, the initial state $|\phi\rangle$ is the ground state of the initial Hamiltonian $H_{\mathcal{I}}$, while any state supported fully on $\mathcal{M}$ is a ground state of the final (oracle) Hamiltonian $H_{\mathcal{M}}$. Note that unlike previous treatments of adiabatic quantum search [2,34,36], the Hamiltonian $H_{\mathcal{M}}$ has a degenerate ground eigenspace spanned by $\{|m\rangle\}_{m \in \mathcal{M}}$.

We remark that the search Hamiltonian (27) is a member of the following class of projective Hamiltonians [34,50,51]:

$$H[\mathbf{x}(\tau)] = x_1(\tau)P_{\mathbf{a}}^{\perp} + x_2(\tau)P_{\{\mathbf{b}\}}^{\perp}, \tag{30}$$

where $P_{\mathbf{a}}^{\perp} \equiv \mathbb{1} - |\mathbf{a}\rangle\langle\mathbf{a}|$, $P_{\{\mathbf{b}\}}^{\perp} \equiv \mathbb{1} - \sum_{\mathbf{b}} |\mathbf{b}\rangle\langle\mathbf{b}|$, with $|\mathbf{a}\rangle$ and $\{|\mathbf{b}\rangle\}$ fixed (normalized) vectors in the system Hilbert space, for which $\langle\mathbf{a}|P_{\{\mathbf{b}\}}^{\perp}|\mathbf{a}\rangle$ is a given function of N. In the case of the search problem, we have $|\mathbf{a}\rangle = |\phi\rangle$, $|\mathbf{b}\rangle = |m\rangle$, whence

$|\langle \mathbf{a}|\mathbf{b}\rangle| = 1/\sqrt{N}$. The results of this article can be generalized to other members of the class of projective Hamiltonians.

A. Two-dimensional reduction

In the computational basis, in which $|\psi_T(\tau)\rangle = \sum_{i=0}^{N-1} \psi_i(\tau)|i\rangle$, the Schrödinger equation (4) becomes

$$i\dot{\psi}_i = T\left[\left(x_1 + x_2 - x_2 \sum_{m\in\mathcal{M}} \delta_{mi}\right)\psi_i - \frac{x_1}{N}\sum_{j=1}^{N}\psi_j\right],$$
(31)

with the initial value $\psi_i(0) = 1/\sqrt{N}$. It can be seen from this expression that the marked components all behave similarly, as do the unmarked components. Hence we can rewrite the state $|\psi_T(\tau)\rangle$ as

$$|\psi_T(\tau)\rangle = \psi_u(\tau)\sum_{i\notin\mathcal{M}}|i\rangle + \psi_m(\tau)\sum_{i\in\mathcal{M}}|i\rangle,$$
(32)

where the subscripts u and m denote "unmarked" and "marked," respectively. The normalization condition now reads

$$(N - M)|\psi_u(\tau)|^2 + M|\psi_m(\tau)|^2 = 1.$$
(33)

By defining the (unnormalized) two-dimensional vector

$$|\widetilde{\psi}\rangle = (\psi_u, \psi_m)^T,$$
(34)

and the (non-Hermitian) effective Hamiltonian matrix

$$\widetilde{H}/J = \begin{pmatrix} rx_1 + x_2 & -rx_1 \\ (r-1)x_1 & (1-r)x_1 \end{pmatrix},$$
(35)

in which

$$r = M/N$$
(36)

is the fraction of the marked items, the Schrödinger equation reduces to

$$i|\dot{\widetilde{\psi}}_T(\tau)\rangle = T\widetilde{H}(\tau)|\widetilde{\psi}_T(\tau)\rangle,$$
(37)

with the initial condition $|\widetilde{\psi}(0)\rangle = (1/\sqrt{N}, 1/\sqrt{N})$. Therefore, not only is the parameter space of the problem two dimensional, it is described by an effectively two-dimensional Hamiltonian (in the m-u representation). This reduction from the real Hamiltonian H [Eq. (27)] to the effective Hamiltonian $\widetilde{H}$ [Eq. (35)] will prove useful in our analysis below.

Later in the article we shall need the norm of the Hamiltonian as well. This can be calculated easily from Eqs. (21) and (35) and yields:

$$\|H(\tau)\| = \begin{cases} J|x_1(\tau) + x_2(\tau)| : x_1(\tau) + x_2(\tau) \neq 0, \\ J\sqrt{1-r}|x_1(\tau)| : \text{otherwise}, \end{cases}$$
(38)

and similarly,

$$\|\dot{H}(\tau)\| = \begin{cases} J|\dot{x}_1(\tau) + \dot{x}_2(\tau)| : \dot{x}_1(\tau) + \dot{x}_2(\tau) \neq 0, \\ J\sqrt{1-r}|\dot{x}_1(\tau)| : \text{otherwise}. \end{cases}$$
(39)

B. Diagonalization and unitary interpolation

The Hamiltonian H/J (27) has three distinct dimensionless eigenvalues $E_- \leqslant E_+ \leqslant E_>$, where

$$E_\mp = (x_1 + x_2 \mp \Delta)/2,$$
(40)

$$E_> = x_1 + x_2,$$
(41)

where

$$\Delta \equiv \sqrt{(x_1 - x_2)^2 + 4rx_1x_2},$$
(42)

is the dimensionless gap (hence $D \equiv J\Delta$) and $E_>$ is $(N-2)$-fold degenerate.

Let $\sigma_z = \text{diag}(1, -1)$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ denote the Pauli matrices. Let us define the similarity matrix

$$S \equiv \begin{pmatrix} r/\sqrt{1-r} & \sqrt{r} \\ -\sqrt{1-r} & \sqrt{r} \end{pmatrix},$$
(43)

and the unitary

$$\widehat{A} \equiv e^{-i\sigma_y \arccos\{[x_1 - (1-2r)x_2]/\Delta\}/2}.$$
(44)

Then the effective Hamiltonian $\widetilde{H}(\tau)$ [Eq. (35)] satisfies

$$\widetilde{H}/J = S\widehat{H}(\tau)S^{-1},$$
(45)

where

$$\widehat{H}(\tau) \equiv \widehat{A}\text{diag}(E_+, E_-)\widehat{A}^\dagger$$
(46)

is the Hermitian core of $\widetilde{H}/J$, and we easily find that

$$\widehat{H}(\tau) = \tfrac{1}{2}\{[x_1(\tau) + x_2(\tau)]\mathbb{1} + \Delta(\tau)\widehat{A}(\tau)\sigma_z\widehat{A}^\dagger(\tau)\}.$$
(47)

This last result is remarkable: it states that, up to an overall (time-dependent) shift $[x_1(\tau) + x_2(\tau)]\mathbb{1}$ and a conformal factor $\Delta(\tau)$, the reduced Hamiltonian $\widehat{H}(\tau)$ is a *unitary interpolation* $\widehat{A}(\tau)\sigma_z\widehat{A}^\dagger(\tau)$ [52]. We will exploit this observation below.

The non-Hermitian reduced Hamiltonian $\widetilde{H}(\tau)$ and its Hermitian core $\widehat{H}(\tau)$ have the same set of eigenvalues $\widehat{E}_\mp \equiv E_\mp$, and we have the spectral resolution

$$\widehat{H}/J = \widehat{E}_-|\widehat{\Phi}_-\rangle\langle\widehat{\Phi}_-| + \widehat{E}_+|\widehat{\Phi}_+\rangle\langle\widehat{\Phi}_+|,$$
(48)

where

$$|\widehat{\Phi}_\mp(\tau)\rangle \equiv \widehat{A}(\tau)|z, \mp\rangle,$$
(49)

and $|\widehat{\Phi}_\mp(0)\rangle = |z, \mp\rangle$ are the eigenvectors of σ_z, corresponding to the eigenvalues ∓ 1. The unitary operator $\widehat{A}(\tau)$ acts as a reduced adiabatic intertwiner [Eq. (10)], in the sense that for the reduced projection $\widehat{P}_\mp(\tau) \equiv |\widehat{\Phi}_\mp(\tau)\rangle\langle\widehat{\Phi}_\mp(\tau)|$ we have

$$\widehat{P}_\mp(\tau) = \widehat{A}(\tau)\widehat{P}_\mp(0)\widehat{A}^\dagger(\tau).$$
(50)

Remark. We emphasize that throughout the article the hat and tilde denote states or operators in the reduced representation; the only exception is Δ.

C. Solving the Schrödinger equation

In solving the Schrödinger equation and calculating the adiabatic error $\delta_{\text{ad}}(1)$, it is more convenient to work with the

normalized state

$$|\widehat{\psi}_T(\tau)\rangle \equiv \sqrt{M} S^{-1} |\widetilde{\psi}_T(\tau)\rangle. \qquad (51)$$

Equation (37) now becomes

$$i|\dot{\widehat{\psi}}_T(\tau)\rangle = T\widehat{H}(\tau)|\widehat{\psi}_T(\tau)\rangle, \qquad (52)$$

with $|\widehat{\psi}_T(0)\rangle = |z,-\rangle$. Solving this equation results in

$$|\widehat{\psi}_T(\tau)\rangle = \widehat{V}_T(\tau)|\widehat{\psi}_T(0)\rangle, \qquad (53)$$

in which

$$\widehat{V}_T(\tau) \equiv \mathcal{T} \exp\left[-iT\int_0^\tau \widehat{H}(\tau')\,d\tau'\right] \qquad (54)$$

is the time-ordered reduced evolution operator.

1. General setup: Adiabatic interaction picture and Dyson series

Having observed that the Grover search problem can be cast as a conformal unitary interpolation, we outline a general, systematic approach for solving the corresponding class of Schrödinger equations using the Dyson series expansion [53]. Consider as a specialization of the general time-dependent Hamiltonian of Eq. (2) the "conformal unitary interpolation Hamiltonian"

$$H_T(\tau) = \Delta(\tau)A(\tau)H_T(0)A^\dagger(\tau), \qquad (55)$$

in which

$$H_T(0) = \sum_{i=0}^{N-1} E_i(0)P_i(0), \qquad (56)$$

is the spectral decomposition of the (traceless) initial Hamiltonian $H(0)$, the unitary operator $A(\tau)$ satisfies the adiabatic Schrödinger equation (12) generated by the adiabatic Hamiltonian $H_A(\tau)$ [24,50], and (the dimensionless gap) $\Delta(\tau) > 0$ is a smooth function with the initial value $\Delta(0) = 1$. It is also useful to think of the time-dependent Hamiltonian $H_T(\tau)$ [Eq. (55)] as the "adiabatic interaction picture Hamiltonian," though normally an interaction picture transformation does not involve a time-dependent prefactor such as $\Delta(\tau)$. It is evident that the eigenvalues and eigenprojections of $H_T(\tau)$ satisfy

$$E_i(\tau) = \Delta(\tau)E_i(0), \qquad (57)$$

$$P_i(\tau) = A(\tau)P_i(0)A^\dagger(\tau). \qquad (58)$$

Equation (57) implies that the spectrum of $H_T(\tau)$ evolves conformally with $\Delta(\tau)$, i.e., all the eigenvalues are multiplied by the same factor, while Eq. (58) implies that the eigen-projections are unitarily connected, and the degeneracy is constant in time. Comparison of Eqs. (10) and (58) reveals that $P(\tau) = P_0(\tau)$ and here too, $A(\tau)$ plays the role of the adiabatic intertwiner.

Rather than solving the Schrödinger equation

$$\dot{V}_T(\tau) = TH_T(\tau)V_T(\tau), \qquad (59)$$

we solve the equation of motion for the "adiabatic interaction picture propagator" [cf. Eq. (15)]

$$\Omega_T(\tau) \equiv A^\dagger(\tau)V_T(\tau). \qquad (60)$$

This provides a more direct tool for the calculation of the adiabatic error [Eq. (6)]. Let us define

$$H_0(\tau) \equiv A^\dagger(\tau)H_T(\tau)A(\tau) = \Delta(\tau)H_T(0), \qquad (61)$$

$$H_1(\tau) \equiv A^\dagger(\tau)H_A(\tau)A(\tau). \qquad (62)$$

Note that $H_0(\tau)$ has dimensions of energy while $H_1(\tau)$ is dimensionless. In the adiabatic interaction picture the (dimensionless) "perturbation" is $TH_0(\tau) - H_1(\tau)$, i.e., it follows from Eqs. (12) and (59) that

$$i\dot{\Omega}_T(\tau) = [TH_0(\tau) - H_1(\tau)]\Omega_T(\tau). \qquad (63)$$

We also define the two unitaries $V_0(\tau)$ and $V_1(\tau)$ through the following equations:

$$i\dot{V}_0 = TH_0V_0, \qquad (64)$$

$$i\dot{V}_1 = -V_0^\dagger H_1V_0V_1. \qquad (65)$$

It is easily seen that V_0V_1 also satisfies Eq. (63), so

$$\Omega_T(\tau) = V_0(\tau)V_1(\tau). \qquad (66)$$

To simplify the analysis, we only consider Hamiltonians for which

$$H_A(\tau) = h_A(\tau)\Xi, \qquad (67)$$

in which h_A is an integrable function and Ξ is a constant (τ independent) and traceless operator belonging to the space of linear operators acting on the system Hilbert space. Thus from Eq. (62) we obtain

$$H_1 = H_A. \qquad (68)$$

Note that, from Eqs. (61) and (64),

$$V_0(\tau) = e^{-iTH_T(0)\int^\tau \Delta}, \qquad (69)$$

where $\int^\tau \Delta$ is shorthand for $\int_0^\tau \Delta(\tau')\,d\tau'$—we shall use the similar shorthand

$$\int^\tau g \equiv \int_0^\tau g(\tau')\,d\tau' \qquad (70)$$

wherever convenient. Inserting V_0 into Eq. (65) yields

$$\dot{V}_1 = \mathcal{K}_TV_1, \qquad (71)$$

in which the kernel $\mathcal{K}_T$ is defined as

$$\mathcal{K}_T(\tau) \equiv ih_A(\tau)e^{iTH_T(0)\int^\tau \Delta}\,\Xi\,e^{-iTH_T(0)\int^\tau \Delta}. \qquad (72)$$

Equation (71) or, equivalently, the Volterra equation,

$$V_1(\tau) = \mathbb{1} + \int_0^\tau \mathcal{K}_T(\tau')V_1(\tau')\,d\tau', \qquad (73)$$

can be solved iteratively, yielding the Dyson series

$$V_1(\tau) = \mathbb{1} + \sum_{l=1}^\infty \int_0^\tau \mathcal{K}_T(\tau_1)d\tau_1 \ldots \int_0^{\tau_{l-1}} \mathcal{K}_T(\tau_l)\,d\tau_l. \qquad (74)$$

2. Quantum search

Now we apply the method described above to the adiabatic quantum search problem. Recall that we are working with the reduced states and operators (hence the hat over all reduced

quantities, except the gap Δ [Eq. (42)]). Comparing Eq. (46) with Eq. (55) implies that

$$\widehat{H}(0)/J = \tfrac{1}{2}\sigma_z, \tag{75}$$

after excluding the trivial term $\propto \mathbb{1}$ from $\widehat{H}$. Similarly, Eqs. (44) and (67) yield

$$\widehat{h}_A = \frac{d}{d\tau}\left[\frac{1}{2}\arccos[(x_1 - (1-2r)x_2)/\Delta]\right]$$
$$\stackrel{(42)}{=} \sqrt{r(1-r)}\frac{x_1\dot{x}_2 - \dot{x}_1 x_2}{\Delta^2}, \tag{76}$$

$$\widehat{\Xi} = \sigma_y. \tag{77}$$

As a result, from Eqs. (69) and (72) we obtain

$$\widehat{V}_0 = e^{-i\widehat{\chi}}\mathrm{diag}\big(e^{-\frac{i}{2}JT\int^\tau \Delta}, e^{\frac{i}{2}JT\int^\tau \Delta}\big), \tag{78}$$

$$\widehat{\mathcal{K}}_T = \widehat{h}_A\begin{pmatrix} 0 & e^{iJT\int^\tau \Delta} \\ -e^{-iJT\int^\tau \Delta} & 0 \end{pmatrix}, \tag{79}$$

where the phase factor

$$\widehat{\chi}(\tau) = \frac{1}{2}JT\int_0^\tau [x_1(\tau') + x_2(\tau')]d\tau' \tag{80}$$

compensates for the removal of the trivial term from $\widehat{H}_T(0)$. Some simple algebra then yields

$$\widehat{V}_1(\tau) = \sum_{l=0}^{\infty}(-1)^l\begin{bmatrix} \mathcal{I}_{2l}(\tau) & \mathcal{I}_{2l+1}^*(\tau) \\ -\mathcal{I}_{2l+1}(\tau) & \mathcal{I}_{2l}^*(\tau) \end{bmatrix}, \tag{81}$$

where, for $l \geqslant 1$, the Dyson series terms are

$$\mathcal{I}_l(\tau) \equiv \int_0^\tau \widehat{h}_A(\tau')\mathcal{I}_{l-1}(\tau')e^{i(-1)^l JT\int^{\tau'} \Delta}d\tau', \tag{82}$$

and $\mathcal{I}_0(\tau) \equiv 1$. This completes the derivation of

$$\widehat{\Omega}_T = \widehat{A}^\dagger \widehat{V} = \widehat{V}_0\widehat{V}_1. \tag{83}$$

IV. ADIABATIC ERROR IN THE SEARCH ALGORITHM

In the previous section, we worked out the solution to the Schrödinger equation in the quantum search problem. Having collected the pertinent ingredients, we now return to calculating our main object of interest, $\delta_{\mathrm{ad}}(\tau)$.

After deriving an exact formula for the error, we proceed with approximating it in the large system-size limit, identified with $r \ll 1$. We start with the well-known polynomial expansion of $\delta_{\mathrm{ad}}(1)$ in terms of T, which works well for large times. In refining this result, we show that in fact two regimes are discernible in the behavior of $\delta_{\mathrm{ad}}(1)$ vs. T: (i) the onset of *exponential* decrease, followed by (ii) a *polynomial* tail. This dichotomy will appear to be crucial in a correct characterization of the scaling of the run time of the algorithm with system size.

The exact behavior of the error in the algorithm depends strongly on the form of the interpolation one chooses for the Hamiltonian. Inspired by our earlier study aiming at minimizing the adiabatic error in quantum algorithms [50], we shall suggest a general class of interpolations, which includes three specific cases already studied in the literature. Next, we investigate the specific behavior of the adiabatic error for each interpolation, separately. Finally, we shall suggest methods for suppressing the adiabatic error even further.

A. Exact relation

Recall that the adiabatic quantum search Hamiltonian (27) has a nondegenerate ground state $|\phi\rangle$ at the initial time $\tau = 0$, whereas the ground-state eigenprojection at the final time $\tau = 1$ is $P_{\mathcal{M}}$, which is M-fold degenerate. Here, any full superposition of the form $|\psi_T(1)\rangle = \sum_{i\in\mathcal{M}}\psi_i|i\rangle$ will work equally well, whereas if $|\psi_T(1)\rangle$ does not have complete support over $P_{\mathcal{M}}$ then this indicates that the algorithm has partially failed. Hence, following the discussion in Sec. II [Eq. (17)], the adiabatic error at the final time is determined by

$$\delta'_{\mathrm{ad}}(1) = \sqrt{1 - \langle\psi_T(1)|P_{\mathcal{M}}|\psi_T(1)\rangle}$$
$$= \sqrt{1 - M|\psi_{\mathrm{m}}(1)|^2}$$
$$\stackrel{33}{=} \sqrt{N}\sqrt{1-r}|\psi_{\mathrm{u}}(1)|. \tag{84}$$

An equivalent formulation can be obtained for the two-dimensional reduction we discussed in Sec. III. In this representation $|\psi_T(1)\rangle$ is replaced by $|\widehat{\psi}_T(1)\rangle = \widehat{V}(1)|\widehat{\Phi}_-(0)\rangle$ [Eq. (53)]; similarly, the instantaneous ground state is represented by the nondegenerate state $|\widehat{\Phi}_-(1) = \widehat{A}(1)|\widehat{\Phi}_-(0)\rangle$ [Eq. (49)]. Thus we can employ the error formula appropriate for the nondegenerate case [Eq. (16)], whereby

$$\delta_{\mathrm{ad}}(1) = \sqrt{1 - |\langle\widehat{\Phi}_-(1)|\widehat{\psi}_T(1)\rangle|^2}$$
$$= \sqrt{1 - |\langle z, -|\widehat{\Omega}_T(1)|z, -\rangle|^2}$$
$$= |\langle z, +|\widehat{\Omega}_T(1)|z, -\rangle| = |\langle\widehat{\Phi}_+(1)|\widehat{\psi}_T(1)\rangle|, \tag{85}$$

in which $\widehat{\Omega}_T(1)$ is given by Eq. (83), and in the last line we used the unitarity of $\widehat{\Omega}_T(1)$. The equality of Eqs. (84) and (85) is immediately seen from

$$|\langle\widehat{\Phi}_+(1)|\widehat{\psi}_T(1)\rangle| \stackrel{(51)}{=} \sqrt{M}\left|(1\ 0)\widehat{A}^\dagger(1)S^{-1}\begin{pmatrix}\psi_{\mathrm{u}}(1) \\ \psi_{\mathrm{m}}(1)\end{pmatrix}\right|$$
$$\stackrel{(43),(44)}{=} \sqrt{N}\sqrt{1-r}|\psi_{\mathrm{u}}(1)|. \tag{86}$$

Inserting $\widehat{\Omega}_T(1)$—noting Eqs. (78) and (81)—into Eq. (85) yields the following *exact* expression for the adiabatic error at the final time:

$$\delta_{\mathrm{ad}}(1) = \left|\sum_{l=0}^{\infty}(-1)^l\mathcal{I}_{2l+1}(1)\right|, \tag{87}$$

which is upperbounded by

$$\delta_{\mathrm{ad}}(1) \leqslant \sum_{l=0}^{\infty}\big|\mathcal{I}_{2l+1}(1)\big|. \tag{88}$$

From the above equations we can in principle calculate the adiabatic error or its bound given that we know all $\mathcal{I}_{\mathrm{odd}}(1)$'s.

Remark. The value of $\delta_{\mathrm{ad}}(T=0)$ will be important later. In this case, we have $|\widehat{\psi}_{T=0}(1)\rangle = |\Phi_-(0)\rangle$, thence Eq. (85) yields

$$\delta_{\mathrm{ad}}(0) = \sqrt{1-r}, \tag{89}$$

in which we used the boundary conditions (25) in $\widehat{A}(1)$. This relation is valid for any interpolation that satisfies the boundary conditions.

B. Approximation of the adiabatic error

An exact calculation of the adiabatic error from Eq. (87) can be challenging because of the infinite number of terms in the summand and the fact that each term contains a multiple integral. To alleviate this difficulty, in this subsection we approximate the upper bound on $\delta_{\mathrm{ad}}(1)$ from Eq. (88) from the first few $\mathcal{I}_l$'s and argue that this suffices for most algorithmic purposes. We start from an expansion in powers of $1/T$, based on integration by parts, and explain its limitations. We then provide more careful analyses, based on the residue theorem and on the stationary phase method, both of which lead to an exponential error estimate.

1. Polynomial expansion

The most common rigorous adiabatic approximation employs an expansion in powers of $1/T$, presuming that T is "large" [24,29,32]. Let us now show how one can systematically expand the adiabatic error as a polynomial in $1/T$ by extracting powers of $1/T$ from each term $\mathcal{I}_l(\tau)$ through integration by parts.

From the identity $e^{-iTY(\tau)} = i/\big(T\dot{Y}(\tau)\big)\frac{d}{d\tau}e^{-iTY(\tau)}$ [valid for any differentiable function $Y(\tau)$], we obtain the following relation by integration by parts:

$$\int_0^\tau G(\tau')e^{-iTY(\tau')}d\tau'$$
$$= \frac{i}{T}\left\{ e^{-iTY(\tau')}\frac{G(\tau')}{\dot{Y}(\tau')}\bigg|_0^\tau - \int_0^\tau e^{-iTy(\tau')}\frac{d}{d\tau'}\left[\frac{G(\tau')}{\dot{Y}(\tau')}\right]d\tau' \right\}. \tag{90}$$

Notice how this extracted a $1/T$ in front of the first term. In the second integral on the right-hand side we can iterate the same trick of replacing the exponential with its derivative; which generates $1/T^2$ and higher-order terms. This provides a systematic way for generating poly($1/T$) expansions of exponential integrals, as we shall see more specifically below for the $\mathcal{I}_l(\tau)$'s.

Using Eq. (90), we obtain

$$\mathcal{I}_1(\tau) = \frac{i}{JT}\left\{ e^{-iJT\int^{\tau'}\Delta}\frac{\widehat{h}_A(\tau')}{\Delta(\tau')}\bigg|_0^\tau - e^{-iJT\int^\tau\Delta} \right.$$
$$\left. \times \int_0^\tau \frac{d}{d\tau'}\left[\frac{\widehat{h}_A(\tau')}{\Delta(\tau')}\right]d\tau' \right\}. \tag{91}$$

Applying once more the exponential identity (90) for the second integral above gives rise to $O(1/T^2)$ terms; whence,

$$\mathcal{I}_1(\tau) = \frac{i}{JT}\left[\frac{\widehat{h}_A(\tau)}{\Delta(\tau)}e^{-iJT\int^\tau\Delta} - \widehat{h}_A(0)\right] + O\left(\frac{1}{T^2}\right), \tag{92}$$

i.e., $|\mathcal{I}_1(\tau)| = O(1/T)$. In analogous fashion, for $\mathcal{I}_2(\tau)$ we obtain

$$\mathcal{I}_2(\tau) = \frac{i}{JT}\Bigg\{ \int_0^\tau \frac{\widehat{h}_A^2(\tau')}{\Delta(\tau')}d\tau' - \widehat{h}_A(0)\mathcal{I}_1^*(\tau)$$
$$- \int_0^\tau d\tau'\widehat{h}_A(\tau')e^{iJT\int^{\tau'}\Delta}$$
$$\times \int_0^{\tau'} d\tau''\frac{d}{d\tau''}\left[\frac{\widehat{h}_A(\tau'')}{\Delta(\tau'')}\right]e^{-iJT\int^{\tau''}\Delta} \Bigg\}, \tag{93}$$

from which

$$\mathcal{I}_2(\tau) = \frac{i}{JT}\left[\int_0^\tau \frac{\widehat{h}_A^2(\tau')}{\Delta(\tau')}d\tau'\right] - \frac{\widehat{h}_A(0)}{(JT)^2}$$
$$\times \left[\frac{\widehat{h}_A(\tau)e^{-iJT\int^\tau\Delta}}{\Delta(\tau)} - \widehat{h}_A(0)\right] + O\left(\frac{1}{T^3}\right), \tag{94}$$

and $|\mathcal{I}_2(\tau)| = O(1/T)$. By induction, one can conclude from Eq. (82) that [24,25]

$$|\mathcal{I}_{2l-1}(\tau)| = |\mathcal{I}_{2l}(\tau)| = O\left(\frac{1}{T^l}\right), \tag{95}$$

for $l \in \mathbb{N}$. Thus, from Eq. (88) the adiabatic error bound becomes

$$\delta_{\mathrm{ad}}(1) \leqslant |\mathcal{I}_1(1)| + O\left(\frac{1}{T^2}\right)$$
$$= \frac{1}{JT}\left[|\widehat{h}_A(0)| + |\widehat{h}_A(1)|\right] + O\left(\frac{1}{T^2}\right). \tag{96}$$

This relation can be simplified further. From the boundary conditions (24) and (25), we obtain $\Delta(0) = \Delta(1) = 1$ [Eq. (42)], $\widehat{h}_A(0) = \sqrt{r(1-r)}\dot{x}_2(0)$ and $\widehat{h}_A(1) = -\sqrt{r(1-r)}\dot{x}_1(1)$ [Eq. (76)]. Thus Eq. (96) reduces to

$$\delta_{\mathrm{ad}}(1) \leqslant \frac{\sqrt{r(1-r)}}{JT}[|\dot{x}_2(0)| + |\dot{x}_1(1)|] + O\left(\frac{1}{T^2}\right). \tag{97}$$

Proceeding in a similar manner, one can in principle obtain the exact form of the coefficient of each $1/T^l$ term, for arbitrary $l \in \mathbb{N}$.

Remarks. Let us make some remarks regarding the polynomial expansion, and in particular Eq. (97).

(i) Note that often the poly($1/T$) series is *truncated* after the first- or at most the second-order term, on the basis of the assumption that for sufficiently large T the first couple of terms should give a reliable and accurate upper bound. However, without correctly defining what "large" T means, a truncation after the first few terms might be unjustifiable. In fact, in addition to T, the system size $\log N$ (introduced here through r) and the gap $\Delta(\tau)$ are also key players in the estimation of $\delta_{\mathrm{ad}}(\tau)$. The minimum (system-size dependent) gap $\Delta_{\min} \equiv \min_\tau \Delta(\tau)$ works in general as a bottleneck for the performance of quantum algorithms (e.g., Refs. [2,3,34,54,55]). Specifically, where the gap closes or becomes small, the adiabatic approximation may not hold, indicative of a "quantum phase transition" (in the thermodynamic limit) [54,56–59]. This implies that the coefficients of some high order $1/T^l$ terms might have a stronger gap dependence than those of lower-order terms. With this caveat, neglecting those higher-order terms is not always possible. In fact, it is not difficult to see

that the coefficient of the $1/T^2$ has a Δ^{-6} dependence (see also Ref. [29]) stronger than the Δ^{-2} dependence of the coefficient of the $1/T$ term in $\delta_{ad}(\tau)$ [Eq. (76)].

(ii) For similar reasons, an estimate of T arising from $\delta_{ad}(1) \leqslant \varepsilon$ (for a given ε) along with a truncated poly$(1/T)$ expansion is not always reliable. We shall see this explicitly later in this section.

(iii) One might argue that $\delta_{ad}(1) = O(1/T)$ results from an energy-time uncertainty relation such as $\delta_{ad}(1) \times T \approx 1$ [presuming $\delta_{ad}(1)$ is directly related to the uncertainty in measurement of energy]. However, this argument is not rigorous and should not be considered as a replacement for the analysis leading to the poly$(1/T)$ expansion (unless justified carefully). A rigorous energy-time uncertainty relation is given, for example, by the Mandelstam-Tamm inequality

$$\Delta_\psi[H] \times T_\psi[K] \geqslant 1/2, \qquad (98)$$

in which $T_\psi[K] \equiv \Delta_\psi[K]/|d\langle\psi|K|\psi\rangle/dt|$, K is any observable, and $\Delta_\psi[X] \equiv \sqrt{\langle\psi|X^2|\psi\rangle - \langle\psi|X|\psi\rangle^2}$ [60]. Hence, as is well known the naive relation $\Delta_\psi[H] \times T \approx 1$ should be treated with care. Strictly, a relation between $\Delta_{\widehat\psi_T(1)}[\widehat H(1)]$ and $\delta_{ad}(1)$ can be constructed as the following. Note that we can write

$$|\widehat\psi_T(\tau)\rangle = \sqrt{1 - \delta_{ad}(\tau)}|\widehat\Phi_-(\tau)\rangle + \delta_{ad}(\tau)|\widehat\Phi_-^\perp(\tau)\rangle, \quad (99)$$

where $|\widehat\Phi_-^\perp(\tau)\rangle$ is orthogonal to $|\widehat\Phi_-(\tau)\rangle$ [Eq. (85)]. Hence, after some algebra we obtain

$$\Delta_{\widehat\psi_T(1)}\widehat H(1) \approx \delta_{ad}(1)$$
$$\times \sqrt{2\widehat E_- [\widehat E_- \langle\widehat\Phi_-^\perp|H^2|\widehat\Phi_-^\perp\rangle - \langle\widehat\Phi_-^\perp|H|\widehat\Phi_-^\perp\rangle]|_{\tau=1}}$$
$$+ O(\delta_{ad}^2). \qquad (100)$$

Despite this relation, connecting T and $T_{\widehat\psi_T(1)}[K]$ is not straightforward. Although using different versions of the energy-time uncertainty relation [61–63] may provide additional insights, we shall not further pursue this here.

2. Exponential estimate

Residue theorem analysis. In the previous subsection we used integration by parts to arrive at a polynomial expansion. Let us now show that an alternative, more careful analysis based on the residue theorem of complex analysis reveals that the adiabatic error decays *exponentially* for sufficiently short times. In some sense, this exponential behavior is reminiscent of the well-known Landau-Zener formula for two-state quantum systems [64], which—in its simplest form—states that the *tunneling probability* $p_T(1) \equiv |\langle\psi(0)|V_T^\dagger(1)|\Phi_1(1)\rangle|^2$ from $|\psi(0)\rangle = |\Phi_0(0)\rangle$ to $|\Phi_1(1)\rangle$, for the Hamiltonian $H(\tau)/J = (\tau\sigma_z + D\sigma_x)/2$, is

$$p_T(1) = e^{-\pi JTD^2/2}. \qquad (101)$$

We note that $p_T(1)$ is in fact intimately related to $\delta_{ad}(1)$ in this simple two-state case, as

$$p_T(1) = 1 - \delta_{ad}^2(1). \qquad (102)$$

The exponentiality of the adiabatic error vs. time and (some power of) the gap has been previously established in generality

in rigorous treatments of the adiabatic theorem [26–28,32] (see also Ref. [55] in a more restricted setting).

In what follows we focus on $\mathcal{I}_1(\tau)$; higher-order terms can be treated similarly. We start from Eq. (88), whence

$$\delta_{ad}(1) \leqslant \left|\int_0^1 \widehat h_A(\tau) e^{iJT\int^\tau \Delta} d\tau\right| + \cdots \qquad (103)$$

Here "..." denotes the higher-order terms $|\mathcal{I}_{2l+1}(1)|$ ($l \geqslant 1$), whose neglect we justify below in the specific examples we discuss. Note that above we have used the property $|\mathcal{I}_1(1)| = |\mathcal{I}_1^*(1)|$ (for $\tau \in \mathbb{R}$), hence the positive sign for the exponent within the integral. This permissible change enables—as will be clear in the following—extraction of an exponentially *decreasing* factor for $\delta_{ad}(1)$. More explicitly, an exponential error term can be obtained, for example, by extending the integral to the complex time plane and using an appropriate closed contour for the application of the residue theorem [65]. A precursor to this treatment of the adiabatic error can be found, e.g., in Ref. [55].

If $\widehat h_A(z)$ ($z \in \mathbb{C}$) is not constant it has poles at points z_0 where the gap vanishes: $\Delta(z_0) = 0$ [Eq. (76)]. From Eq. (42), we obtain $x_1(z_0) = x_2(z_0) = 0$ or [assuming $x_1(z_0) \neq 0$]

$$x_{21}(z_{0\pm}) = 1 - 2r \pm 2i\sqrt{r(1-r)}, \qquad (104)$$

where $x_{21} \equiv x_2/x_1$. The poles z_0 can in principle be obtained by inverting this relation for a given interpolation $x_{21}(\tau)$. Note, however, that there might exist other singularities (typically at infinity) arising from the exponential $e^{-iJT\int^z \Delta}$ in Eq. (103). Therefore, estimating the integral (103) requires finding all contributing singularities in a suitably chosen contour $\mathcal{C}$ in the complex τ plane.

The value of the integral $|\int_0^1 \widehat h_A(\tau) e^{iJT\int^\tau \Delta} d\tau|$ can now be obtained by calculating the residues of the integrand at the poles enclosed inside the contour,

$$|\mathcal{I}_1(1)| = \left|2\pi i \sum_{z_0 \in \text{inside}(\mathcal{C})} \text{Res}[\widehat h_A(z)e^{iJT\int^z \Delta}, z_0]\right.$$
$$\left. - \int_{\mathcal{C}-[0,1]} \widehat h_A(z)e^{iJT\int^z \Delta} dz\right|. \qquad (105)$$

For example, if the poles z_0 are *simple* and arise from $\Delta(z_0) = 0$, calculating the integral becomes straightforward. Recall that $\widehat h_A \propto 1/\Delta^2$ [Eq. (76)] and the residue of a rational function $P(z)/Q(z)$ at a simple pole $z^\star$ is given by $P(z^\star)/\partial_z Q(z^\star)$ [65]. Thus, in this case we obtain

$$\text{Res}[\widehat h_A(z)e^{iJT\int^z \Delta}, z_0]$$
$$= \frac{\sqrt{r(1-r)}\dot x_{21}(z_0)e^{iJT\int^{z_0}\Delta}}{\frac{d}{dz}[[1-x_{21}(z)]^2 + 4rx_{21}(z)]|_{z_0}} \approx \frac{1}{4i}e^{iJT\int^{z_0}\Delta}, \quad (106)$$

where in the last line we assumed $\dot x_{21}(z_0) \neq 0$. Note that this computation of the residues does not necessarily hold when $\widehat h_A = \text{const}$ or when z_0 is at infinity.

Now we substitute $\int^{z_0} \Delta = \text{Re}[\int^{z_0} \Delta] + i\text{Im}[\int^{z_0} \Delta]$. Calculating the absolute value of the residue [Eq. (103)] annihilates the phase factor resulting from $\text{Re}[\int^{z_0} \Delta]$, and an exponentially decreasing contribution emerges from $\text{Im}[\int^{z_0} \Delta]$ of the exponential within the integrand—perhaps in addition to

a generically non-exponentially-decreasing term. Thus, from Eq. (106) we find

$$\delta_{\text{ad}}(1) \lessapprox \sum_{z_0 \in \text{inside}(\mathcal{C})} R_T(z_0) e^{-JT\text{Im}[\int^{z_0} \Delta]} + R'_T(1), \quad (107)$$

where $R_T(z_0) \in \mathbb{R}^+$ results from the nonexponential contribution of the residue at z_0 and $R'_T(1) \in \mathbb{R}^+$ encapsulates the collective nonvanishing contribution of other segments of the contour as well as other non-exponentially-decreasing contributions emerging from the "..." terms in Eq. (103).[1]

Stationary phase analysis. An alternative and complementary approach for obtaining the exponential contribution to the adiabatic error is to use the stationary phase method. This method is appropriate for obtaining asymptotic value of complex integrals of the form $\int_\gamma F(z) e^{iTG(z)} dz$, where $T > 0$ is a large number and γ is a path for the integration. Assuming $F(z)$ is a slowly varying function over γ and $G(z)$ is an analytic function, one can argue that the major contribution to the integral comes from the point(s) z_0 at which $G(z)$ has a minimum, whence [66]

$$\int_\gamma F(z) e^{iTG(z)} dz \approx \sqrt{\frac{2\pi}{T \ddot{G}(z_0)}} F(z_0) e^{i\pi/4} e^{iTG(z_0)}. \quad (108)$$

To apply this result to Eq. (103), we replace $G(z)$ and $F(z)$ with $J \int^z \Delta$ and $\widehat{h}_A(z)$, respectively. Accordingly, z_0 is where $\dot{G}(z_0) = \Delta(z_0) = 0$. The minimum point z_0 is often a complex number. In fact, in quantum many-body situations, the gap Δ is a non-negative function, often with a nonvanishing minimum, which becomes zero in the thermodynamic limit [56]. In such cases, $G(z)$ does indeed have a minimum. It is also required that $\widehat{h}_A(z_0)$ be finite (this, of course, is not satisfied when $\widehat{h}_A$ has a pole or singularity at z_0). If all these conditions are satisfied, Eqs. (103) and (108) yield

$$\delta_{\text{ad}}(1) \lessapprox \left| \widehat{h}_A(z_0) \sqrt{\frac{2\pi}{JT \dot{\Delta}(z_0)}} \right| e^{-JT\text{Im}[\int^{z_0} \Delta]}, \quad (109)$$

as we wished. This relation complements Eq. (106) in that it may be applicable when Eq. (106) is not.

Discussion. The emergence of the exponential dependence of δ_{ad} on T [Eqs. (107) and (109)] in contrast to the polynomial dependence [Eq. (97)] is remarkable, as it indicates a much faster decay of the adiabatic error than what is suggested by the standard $1/T$ expansion. In the exponential regime it suffices that T be large compared to $1/\text{Im}[\int^{z_0} \Delta]$ or roughly [55]:

$$T \gg \frac{1}{J\Delta}. \quad (110)$$

This is a less stringent condition than the standard condition (20) or its more rigorous counterparts [24–32], involving higher powers of the gap. The crossover point $T^\star$ between

the exponential and the polynomial regimes can be estimated by solving

$$R_{T^\star}(r) e^{-JT^\star \text{Im}[\int^{z_0} \Delta]} \approx \frac{\sqrt{r}}{JT^\star} (|\dot{x}_1(1)| + |\dot{x}_2(0)|), \quad (111)$$

in which $R_T(r)$ is a nonexponential prefactor given by Eq. (107) or (109). If $T \lesssim T^\star$ ($T \gtrsim T^\star$) the exponential (polynomial) behavior prevails. Later in this section, we show explicitly that the expected run time for the quantum search algorithm is often given by the exponential contribution; the polynomial regime may *overestimate* the minimum run time required for reasonable accuracy.

Since the scaling of the run time depends on which interpolation we choose for the Hamiltonian, in the following we shall obtain specific interpolations by employing some recently developed results for (partial) minimization of the adiabatic error [34,50].

C. Hamiltonian interpolation

The set of available control knobs ($\mathbf{x}$), as well as the way one varies them, determine the specific Hamiltonian interpolation implemented in a laboratory setting. Theoretically, though, there are various ways by which one can obtain families of Hamiltonians for an adiabatic quantum algorithm. One natural choice is interpolations which minimize "physical" cost. For example, in the setting of Refs. [34,36], time functionals were constructed from a *local* version of the adiabatic condition (20), whose minimization resulted in a set of Euler-Lagrange equations for the underlying interpolations. A different method was suggested in Ref. [50], where it was shown that in the standard poly($1/T$) expansion of the adiabatic error $\delta_{\text{ad}}(\tau)$ [general counterpart of Eq. (96) or (97)], the coefficient of the $1/T$ term has a *geometric* part, in a differential geometric sense. Specifically, this geometric coefficient, in terms of the ground-state eigenprojection, $P(\tau)$, is

$$\int_0^\tau \|[\dot{P}[\mathbf{x}(\tau')], P[\mathbf{x}(\tau')]]\| d\tau'. \quad (112)$$

Minimizing this coefficient yields adiabatic "geodesic" interpolations, which partially decrease $\delta_{\text{ad}}(\tau)$ for a given T. It follows from standard variational calculus [65,67] that the geodesic interpolations satisfy the following equation

$$\|[\dot{P}[\mathbf{x}(\tau)], P[\mathbf{x}(\tau)]]\| |_{\mathbf{x}_{\text{geo}}(\tau)} = \text{const}, \quad (113)$$

where the constant is chosen to satisfy boundary conditions. We adopt this method in the following and derive geodesic interpolations for the adiabatic quantum search.

1. General case

In the reduced two-dimensional representation, P is replaced with $\widehat{P}_- = |\widehat{\Phi}_-\rangle\langle\widehat{\Phi}_-|$. Thus we have

$$[\dot{\widehat{P}}_-, \widehat{P}_-] = |\dot{\widehat{\Phi}}_-\rangle\langle\widehat{\Phi}_-| - |\widehat{\Phi}_-\rangle\langle\dot{\widehat{\Phi}}_-| + |\widehat{\Phi}_-\rangle\langle\widehat{\Phi}_-|$$
$$\times (\langle\dot{\widehat{\Phi}}_-|\widehat{\Phi}_-\rangle - \langle\widehat{\Phi}_-|\dot{\widehat{\Phi}}_-\rangle). \quad (114)$$

Noting, with the help of Eqs. (44), (49), and (76), that

$$\langle\widehat{\Phi}_-|\dot{\widehat{\Phi}}_-\rangle = i\widehat{h}_A\langle z, -|\widehat{A}^\dagger \sigma_y \widehat{A}|z, -\rangle = 0, \quad (115)$$

---

[1]In the case of Eq. (106), and from Eq. (105), we obtain: $R_T = \pi/2$. This is in good agreement with Eq. (89) when $T = 0$ and $r \ll 1$.

we find

$$\|[\hat{\dot{P}}_-, \hat{P}_-]\| = \sqrt{2\langle \hat{\dot{\Phi}}_- | \hat{\dot{\Phi}}_- \rangle}$$
$$\overset{(49)}{=} \sqrt{2}|\hat{h}_A|. \tag{116}$$

Hence, according to Eq. (113), a class of adiabatic geodesics can be obtained from

$$\hat{h}_A[\mathbf{x}(\tau)] = \text{const} \equiv \varphi, \tag{117}$$

which implies that the adiabatic Hamiltonian $\hat{H}_A(\tau)$ is in fact constant. In other words, from $\hat{A}(\tau) = e^{-i\int^\tau \hat{H}_A}$ [Eq. (44)] we can see that

$$\hat{A}(\tau) = e^{-i\varphi\tau\sigma_y}. \tag{118}$$

This equation suggests that a more general choice for the intertwiner $\hat{A}$ can be obtained by $\varphi\tau \to \varphi\theta(\tau)$, for some arbitrary differentiable θ; i.e., $\hat{A}(\tau) = e^{-i\varphi\theta(\tau)\sigma_y}$. In terms of $\hat{h}_A$, this translates into choosing $\hat{h}_A[\mathbf{x}(\tau)] = \varphi\dot{\theta}(\tau)$. In terms of the geometric factor (112), this simply means that on the geodesic, the time is determined by $\theta(\tau)$ rather than τ. To see this, note that

$$\int_0^\tau \|[\dot{P}(\tau'), P(\tau')]\| d\tau' = \int_0^{\theta(\tau)} \|[\partial_\theta P(\theta), P(\theta)]\| d\theta, \quad (119)$$

which, in turn, from variational calculus, gives the following equation for the geodesics:

$$\|[\partial_\theta P(\mathbf{x}[\theta(\tau)]), P(\mathbf{x}[\theta(\tau)])]\| |_{\mathbf{x}_{\text{geo}}(\theta(\tau))} = \text{const}. \tag{120}$$

Hence,

$$\|[\partial_\theta \hat{P}_-, \hat{P}_-]\| = \frac{1}{\dot\theta} \|[\hat{\dot{P}}_-, \hat{P}_-]\|$$
$$= \sqrt{2}\frac{|\hat{h}_A|}{\dot\theta}$$
$$= \text{const}, \tag{121}$$

where we assumed $\dot\theta(\tau) > 0$, $\theta(0) = 0$, and $\theta(1) = 1$. As a result, we choose the adiabatic geodesic satisfying

$$\hat{h}_A(\mathbf{x}[\theta(\tau)]) = \varphi\dot\theta(\tau). \tag{122}$$

We remark that introducing an arbitrary nondecreasing function $\theta(\tau)$ will serve as more than a generalization. In fact, we show below that θ allows us to substantially enhance the suppression of the adiabatic error. For example, choosing a θ such that it is a differentiable function of τ (up to some controllable order, say, k), with vanishing derivatives (up to the same order k) at the initial and final times, can suppress the adiabatic error [up to poly$(1/T^{k+1})$]. This property—which comes at the relatively small price of sufficient control at the beginning and end of the dynamics—may have immediate applications in experimental realizations of quantum annealing and AQC.

The above geodesic equation can be solved analytically. Recall that $x_{21} = x_2/x_1$, with the boundary values $x_{21}(0) = 0$ and $x_{21}(1) = \infty$ [Eqs. (24) and (25)]. Then from Eq. (76) we find

$$\frac{\sqrt{r(1-r)}\dot{x}_{21}(\tau)}{[1 - x_{21}(\tau)]^2 + 4r x_{21}(\tau)} = \varphi\dot\theta(\tau). \tag{123}$$

The solution to this equation can be written as follows:

$$x_{21}[\theta(\tau)] = \frac{\sin[2\theta(\tau)\varphi]}{\sin[2(1 - \theta(\tau))\varphi]}, \tag{124}$$

where we must choose

$$\varphi = \arctan[\sqrt{(1-r)/r}]. \tag{125}$$

Observe that $x_{21}[\theta(\tau)]$ has the following symmetry:

$$x_{21}[1 - \theta(\tau)] = 1/x_{21}[\theta(\tau)], \tag{126}$$

which is satisfied, for example, by requiring

$$x_2[\theta(\tau)] = x_1[1 - \theta(\tau)]. \tag{127}$$

Equations (124) and (127) identify a two-dimensional interpolation for the quantum search Hamiltonian.

Note that, given Eq. (124), we can also add another relation (satisfying the boundary conditions) to find other classes of interpolation. For example, we can choose

$$x_1[\theta(\tau)] + x_2[\theta(\tau)] = a(\tau), \tag{128}$$

in which $a(\tau)$ can be a smooth function with the boundary values $a(0) = a(1) = 1$; e.g., $a(\tau) = 1 + \tau(1 - \tau)$ or $a(\tau) = 1 + \sin(\pi\tau)$. Choosing a form for $a(\tau)$ corresponds to assuming a given $\|H(\tau)\|$ [Eq. (38)], which implies a given control over the maximum amount of the available energy in the system. Thus, Eqs. (124) and (128) yield

$$x_1[\theta(\tau)] = \frac{a(\tau)\sin\{2[1 - \theta(\tau)]\varphi\}}{2\sin(\varphi)\cos\{[1 - 2\theta(\tau)]\varphi\}}$$
$$= \frac{a(\tau)}{2}(1 + \cot(\varphi)\tan\{[1 - 2\theta(\tau)]\varphi\}), \tag{129}$$

$$x_2[\theta(\tau)] = \frac{a(\tau)\sin[2\theta(\tau)\varphi]}{2\sin(\varphi)\cos\{[1 - 2\theta(\tau)]\varphi\}}$$
$$= \frac{a(\tau)}{2}(1 - \cot(\varphi)\tan\{[1 - 2\theta(\tau)]\varphi\}). \tag{130}$$

Note that this interpolation also satisfies the symmetry (127).

It is clear that one can consider other auxiliary or control conditions over the Hamiltonian different from Eq. (128). In the following, we address three special cases: (i) The Hamiltonian interpolation is linear in time, namely $x_1(\tau) = 1 - x_2(\tau) = 1 - \tau$; (ii) Hamiltonians with constant norm, specifically $\|H(\tau)\|/J = 1$; and (iii) Hamiltonians with constant gap, specifically $\Delta(\tau) = 1$.

2. Linear interpolation

If we choose

$$\theta(\tau) = \frac{1}{2} - \frac{1}{2\varphi}\arctan[(1 - 2\tau)\tan\varphi], \tag{131}$$

and assume $a(\tau) = 1$, from Eqs. (129) and (130) we obtain the simple linear interpolation

$$x_1(\tau) = 1 - \tau, \tag{132}$$
$$x_2(\tau) = \tau. \tag{133}$$

3. Constant-norm interpolation

Let us assume $0 \leqslant x_1, x_2 \leqslant 1$. The constraint $\|H(\tau)\|/J = 1$ implies that $x_1 + x_2 = 1$ [Eq. (38)] or, equivalently, $a(\tau) = 1$ [Eq. (128)]. Hence, in this case from Eqs. (129) and (130) we obtain

$$x_1[\theta(\tau)] = \frac{1}{2} + \frac{\sqrt{r}}{2\sqrt{1-r}} \tan\{[1 - 2\theta(\tau)]\varphi\}, \quad (134)$$

$$x_2[\theta(\tau)] = \frac{1}{2} - \frac{\sqrt{r}}{2\sqrt{1-r}} \tan\{[1 - 2\theta(\tau)]\varphi\}. \quad (135)$$

This interpolation is a generalization of the interpolation obtained in Refs. [34,36,50] by using a local adiabatic condition.

4. Constant-gap interpolation

Rather than assuming condition (128), here we consider the case in which the gap is constant, e.g., $\Delta(\tau) = D(\tau)/J = 1$. Hence combining the following relation [Eq. (42)]:

$$\big(x_1[\theta(\tau)] - x_2[\theta(\tau)]\big)^2 + 4r x_1[\theta(\tau)] x_2[\theta(\tau)] = 1 \quad (136)$$

and Eq. (124) yields

$$x_1[\theta(\tau)] = \frac{1}{2\sqrt{r(1-r)}} \sin\{2[1 - \theta(\tau)]\varphi\}, \quad (137)$$

$$x_2[\theta(\tau)] = \frac{1}{2\sqrt{r(1-r)}} \sin[2\theta(\tau)\varphi]. \quad (138)$$

D. Error estimation for different interpolations

Having given a general recipe for adiabatic interpolations and having obtained three particular interpolations, we proceed to compute the adiabatic error for each of these interpolations. Our main interest here is to analyze how the run time scales with system size for each of these three interpolations. We shall also contrast the result for each case with the estimate obtained from the traditional adiabatic theorem. As a result, we will demonstrate that the traditional adiabatic condition is not always reliable for estimation of the minimum run time (given an error threshold), whereas the time we obtain from the exponential regime of the adiabatic error is in fact accurate. A remarkable feature of this result is that the estimated times (in an appropriate sense) need not be very large.

1. Linear interpolation

In this case, $\big(x_1(\tau), x_2(\tau)\big) = (1 - \tau, \tau)$, so we have

$$\|H(\tau)\|/J \overset{(38)}{=} 1, \quad (139)$$

$$\|\dot{H}(\tau)\|/J \overset{(39)}{=} 1, \quad (140)$$

$$\Delta_{\min} \overset{(42)}{=} \sqrt{r}. \quad (141)$$

Hence the traditional adiabatic condition (20) implies that, for $\delta_{\text{ad}}(1) \leqslant \varepsilon$, we should have

$$T \gg \frac{1}{J\varepsilon r}, \quad (142)$$

or, equivalently, from Eq. (26),

$$\tau_{\text{run}} = O\left(\frac{1}{\varepsilon r}\right). \quad (143)$$

That is, that the adiabatic quantum search with a linear interpolation Hamiltonian requires a run time $O(N)$ [recall $r = M/N$], hence performing no better than a classical search algorithm [36].

Note, however, that if we truncate the poly $(1/T)$ expansion (97) after the first term, in the $r \ll 1$ limit we obtain

$$T \gtrsim \frac{2\sqrt{r}}{J\varepsilon}, \quad (144)$$

i.e., $\tau_{\text{run}} = O(\sqrt{N})$, which is not the right estimate. This illustrates the caveat we discussed in Sec. IV.

Now we employ the results we developed in Sec. IV for estimating the exponential regime of $\delta_{\text{ad}}(1)$ [Eq. (107)]. It is obvious that for this case there exist no point at which both $x_1(\tau) = 1 - \tau$ and $x_2(\tau) = \tau$ vanish. Thus, the pole z_0 (where the gap vanishes) is obtained simply by inverting Eq. (104), i.e.,

$$z_{0\pm} = \frac{1}{2} \pm \frac{i\sqrt{r}}{2\sqrt{1-r}}. \quad (145)$$

The integral over the gap can be evaluated explicitly as

$$\text{Im}\left[\int_0^{z_{0+}} \Delta(z)\,dz\right] = \frac{\pi r}{8\sqrt{1-r}}. \quad (146)$$

For the integral (106), we choose the contour $\mathcal{C}$ to be a rectangle composed of (i) $\mathcal{C}_1$, the real line $[0,1]$; (ii) $\mathcal{C}_2$, the line connecting $z = 1$ to $z = 1 + i\infty$; (iii) $\mathcal{C}_3$, the line connecting $z = 1 + i\infty$ to $z = i\infty$; and (iv) $\mathcal{C}_4$, the line connecting $z = 1 + i\infty$ to $z = 0$. From the form of $\widehat{h}_A$, we can easily see that $\int_{\mathcal{C}_3} = 0$ [because $\lim_{z\to\infty} \Delta(z) \to \infty$] and $\int_{\mathcal{C}_2} = -\int_{\mathcal{C}_4}$ [because $\Delta(z) = \Delta(1 - z)$]. This means that for $r \ll 1$ and in the regime in which $|\mathcal{I}_1(1)|$ gives the dominant contribution to $\delta_{\text{ad}}(1)$, the error exhibits an exponentially decreasing behavior as

$$\delta_{\text{ad}}(1) \overset{(106)}{\lesssim} \frac{\pi}{2} e^{-\pi J T r/8}. \quad (147)$$

In this regime, for $\delta_{\text{ad}}(1) \leqslant \varepsilon$ it is sufficient to have

$$T \gtrsim \frac{8\ln(1/\varepsilon)}{\pi J r} + \frac{8\ln(\pi/2)}{\pi J r}, \quad (148)$$

whereby we can estimate the following run time:

$$\tau_{\text{run}} = O\left(\frac{1}{r}\ln(1/\varepsilon)\right). \quad (149)$$

This result agrees perfectly with the expected $O(N)$ scaling, with a *logarithmic* (rather than inverse) dependence on the error ε. Figure 1 depicts the adiabatic error vs. time, calculated by solving the corresponding Schrödinger equation numerically. It illustrates the exponential and polynomial regimes.

Remark. Here we could not use Eq. (109) because $\widehat{h}_A$ has poles $z_{0\pm}$.

2. Constant-norm interpolation

Here for simplicity, we assume $\theta(\tau) = \tau$. From Eqs. (134) and (135), the gap (42) is

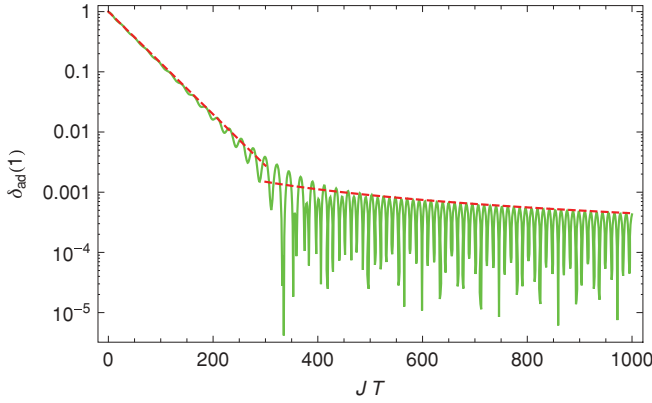$$\Delta(\tau) = \sqrt{r}\sec[(1 - 2\tau)\varphi], \quad (150)$$

FIG. 1. (Color online) $\delta_{\text{ad}}(1)$ for the linear interpolation $\mathbf{x}(\tau) = (1 - \tau, \tau)$, obtained by numerically solving the corresponding Schrödinger equation for $r = 0.05$. The dashed lines represent the exponential fits $e^{-\pi JTr/8}$ [Eq. (147)] and the polynomial fit $2\sqrt{r}/(JT)$ [Eq. (144)], from left to right, respectively.

with the minimum value $\min_\tau \Delta = \sqrt{r}$ at $\tau_{\min} = 1/2$, and Eqs. (38) and (39) yield

$$\|H(\tau)\|/J = 1, \tag{151}$$

$$\|\dot{H}(\tau)\|/J = \sqrt{r}\varphi \sec^2[(1 - 2\tau)\varphi], \tag{152}$$

the latter with the maximum value $\max_\tau \|\dot{H}(\tau)\| = \varphi/\sqrt{r}$ at $\tau_{\max} = 0, 1$. Thus, according to the traditional adiabatic condition (20), in order to have $\delta_{\text{ad}}(1) \leqslant \varepsilon$, we should require

$$T \gg \frac{1}{J\varepsilon r\sqrt{r}}, \tag{153}$$

and, in turn,

$$\tau_{\text{run}} = O\left(\frac{1}{\varepsilon r\sqrt{r}}\right), \tag{154}$$

which is larger than the expected $O(\sqrt{N/M})$ Grover-like scaling [34,36].

On the other hand, truncation of the corresponding $\text{poly}(1/T)$ expansion (97) results in

$$T \gtrapprox \frac{2\varphi}{J\varepsilon}, \tag{155}$$

in which we used $|\dot{x}_1(1)| = |\dot{x}_2(0)| = \varphi/\sqrt{r(1 - r)}$ [Eqs. (134) and (135)] and $\varphi \approx \pi/2$. Hence,

$$\tau_{\text{run}} = O(1), \tag{156}$$

which of course is incorrect.

Now we show that a careful treatment of $\mathcal{I}_1(\tau)$, as in Sec. IV, results in an exponential adiabatic error and gives the correct scaling for the run time. Here, we note that $\hat{h}_A(\tau) = \varphi$ [Eq. (76)], from which

$$\mathcal{I}_1(\tau) = \varphi \int_0^\tau e^{-iJT \int^{\tau'} \Delta} d\tau' = \varphi e^{-i\frac{JT\sqrt{r}}{\varphi}\text{arctanh}\sqrt{1-r}}$$

$$\times \int_0^\tau \left[\frac{1 - \sin(\varphi) + \cos(\varphi)\tan(\varphi\tau')}{1 + \sin(\varphi) - \cos(\varphi)\tan(\varphi\tau')}\right]^{-i\frac{JT\sqrt{r}}{2\varphi}} d\tau', \tag{157}$$

where we used the identity $\text{arctanh}(x) = \frac{1}{2}\ln\left|\frac{1+x}{1-x}\right|$. For $r \ll 1$ $[\sin(\varphi) \approx 1]$, this gives rise to

$$|\mathcal{I}_1(\tau)| \lessapprox \varphi \left|\int_0^\tau [\tan(\varphi\tau')]^{-i\frac{JT\sqrt{r}}{2\varphi}} d\tau'\right|$$

$$\approx \frac{\pi}{2} \int_0^1 [\tan(\pi\tau'/2)]^{-i\frac{JT\sqrt{r}}{2\varphi}} d\tau' + O(\sqrt{r}). \tag{158}$$

Further simplification can be obtained by using the identity $\int_0^1 [\tan(\pi\tau')]^{-i\alpha} d\tau' = \text{sech}(\pi\alpha/2)$ (for $\alpha \geqslant 0$) and the inequality $\text{sech}(y) \leqslant 2e^{-y}$ (for $y \geqslant 0$); hence,

$$\delta_{\text{ad}}(1) \lessapprox \pi e^{-JT\sqrt{r}/2} + O(\sqrt{r}). \tag{159}$$

This is the corresponding *exponential* behavior for the constant-norm Hamiltonian interpolation. It implies that for $\delta_{\text{ad}}(1) \leqslant \varepsilon$ it is sufficient to have

$$T \gtrapprox \frac{2\ln(1/\varepsilon)}{J\sqrt{r}} \tag{160}$$

or, equivalently,

$$\tau_{\text{run}} = O\left(\frac{\ln(1/\varepsilon)}{\sqrt{r}}\right), \tag{161}$$

which is the expected Grover-like $O(\sqrt{N/M})$ scaling [34,36] but with a logarithmic dependence on the error.

Although Eq. (106) may not be applicable to the case of constant-norm interpolation (for $\hat{h}_A$ does not have any singularity), we can apply Eq. (109) instead. In fact, Eq. (150) implies that

$$z_{0\pm} = \pm i\infty. \tag{162}$$

Hence,

$$\text{Im}\left[\int_0^{z_{0+}} \Delta(z) dz\right] = \frac{\pi\sqrt{r}}{4\varphi} \overset{r \ll 1}{\approx} \frac{\sqrt{r}}{2}, \tag{163}$$

and in turn [Eq. (109)]

$$\delta_{\text{ad}}(1) \lessapprox R(1) e^{-JT\sqrt{r}/2}, \tag{164}$$

with some nonexponentially decreasing $R(1)$. This results in a scaling similar to Eq. (161). Figure 2 contrasts the above analytical results with numerics.

3. Constant-gap interpolation

In this case $[\Delta(\tau) = 1]$, from Eqs. (38), (39), (137), and (138) we obtain

$$\|H(\tau)\|/J = |\cos[(1 - 2\tau)\varphi]|/\sqrt{r}, \tag{165}$$

$$\|\dot{H}(\tau)\|/J = \varphi|\sin[(1 - 2\tau)\varphi]|/\sqrt{r}. \tag{166}$$

Hence, according to the traditional adiabatic condition (20), in order to have $\delta_{\text{ad}}(1) \leqslant \varepsilon$, it is sufficient to have

$$T \gg \frac{\varphi}{J\varepsilon\sqrt{r}}, \tag{167}$$

whereby

$$\tau_{\text{run}} = O\left(\frac{1}{\varepsilon r}\right), \tag{168}$$

which is quadratically larger than the Grover-like $O(\sqrt{N/M})$ scaling.
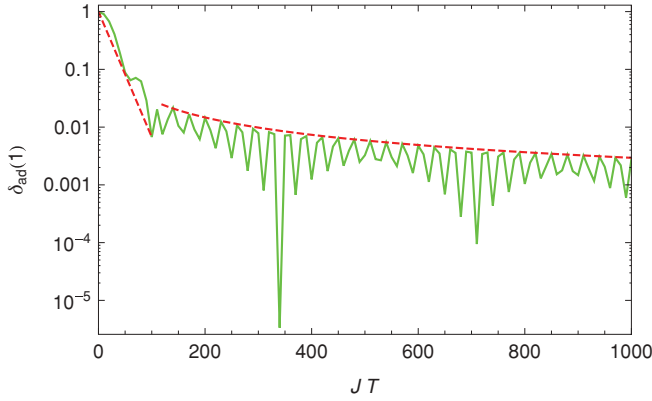
FIG. 2. (Color online) $\delta_{\text{ad}}(1)$ for the constant-norm interpolation [Eqs. (134) and (135)], obtained by numerically solving the corresponding Schrödinger equation for $r = 0.01$. The dashed lines represent the exponential fit $e^{-JT\sqrt{r}/2}$ [Eq. (159)] and the polynomial fit $2\varphi(r)/(JT)$ [Eq. (155)].

On the other hand, noting that $|\dot{x}_1(1)| = |\dot{x}_2(0)| = \varphi/\sqrt{r(1-r)}$ [Eqs. (137) and (138)], the truncation of the corresponding poly$(1/T)$ expansion after the first term yields

$$T \gtrsim \frac{2\varphi}{J\varepsilon} \qquad (169)$$

or, equivalently,

$$\tau_{\text{run}} = O\left(\frac{1}{\varepsilon\sqrt{r}}\right). \qquad (170)$$

Clearly, Eqs. (168) and (170) are not in agreement.

It is interesting to note that here one can in fact solve the Schrödinger equation exactly. The operator $\widehat{\Omega}_T(\tau)$ [Eq. (83)] satisfies the following equation:

$$\dot{\widehat{\Omega}} = -i\widehat{W}\widehat{\Omega}, \qquad (171)$$

in which

$$\widehat{W} = T\widehat{A}^\dagger \widehat{H}\widehat{A} - \widehat{A}^\dagger \widehat{H}_A \widehat{A}$$
$$\stackrel{(137),(138),(76)}{=} \frac{JT}{2}\left\{\frac{\cos[(1-2\tau)\varphi]}{\sqrt{r}}\mathbb{1} + \sigma_z\right\} - \varphi\sigma_y. \qquad (172)$$

Since $\widehat{W}$ is time independent, integration of Eq. (171) is straightforward:

$$\widehat{\Omega}_T(\tau) = e^{-i\int_0^\tau \widehat{W}(1)d\tau'} = e^{-\frac{i\tau JT\sqrt{1-r}}{2\varphi\sqrt{r}}}$$
$$\times \frac{\sin\left[\tau\sqrt{\varphi^2 + (JT)^2/4}\right]}{\sqrt{\varphi^2 + (JT)^2/4}}\left\{\sqrt{\varphi^2 + (JT)^2/4}\right.$$
$$\times \cot[\tau\sqrt{\varphi^2 + (JT)^2/4}]\mathbb{1} + i\varphi\tau\sigma_y - \left.\frac{iJT}{2}\sigma_z\right\}. \qquad (173)$$

Thus, from Eq. (85) the adiabatic error is exactly

$$\delta_{\text{ad}}(1) = \varphi\frac{|\sin\sqrt{\varphi^2 + (JT)^2/4}|}{\sqrt{\varphi^2 + (JT)^2/4}}. \qquad (174)$$

Figure 3 depicts $\delta_{\text{ad}}(1)$ for two different values of r. Note that for large evolution times $T \gg 2\varphi/J$, we obtain

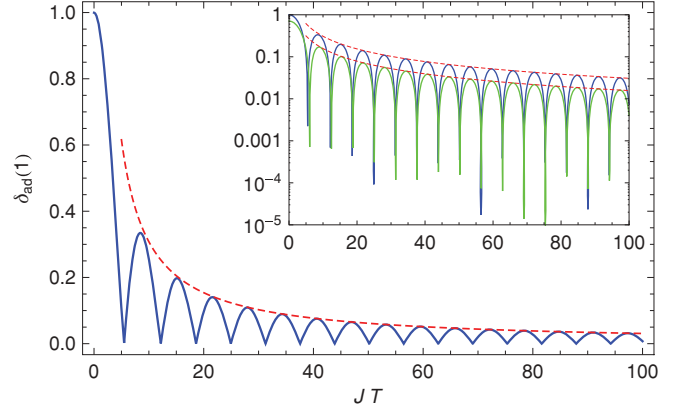$$\delta_{\text{ad}}(1) \leqslant \frac{2\varphi}{JT}. \qquad (175)$$

FIG. 3. (Color online) $\delta_{\text{ad}}(1)$ for the constant-gap interpolation [Eqs. (137) and (138)]. Here, $r = 0.001, 0.5$ (blue and green, respectively), and the dashed lines (red) show the $2\varphi(r)/(JT)$ envelopes. The points T_k, where $\delta_{\text{ad}}(1)|_{T_k} = 0$, are given by Eq. (177).

This implies that, in the $r \ll 1$ limit, in order for $\delta_{\text{ad}}(1) \leqslant \varepsilon$ it is sufficient to have

$$\tau_{\text{run}} = O\left(\frac{1}{\varepsilon\sqrt{r}}\right), \qquad (176)$$

which is the Grover-like scaling $O(\sqrt{N/M})$. Note that in this limit the adiabatic error behaves inverse linearly, $\delta_{\text{ad}}(1) \leqslant 2\varphi/JT$, which is in perfect agreement with Eq. (169). In addition, we observe that there exist Ts less than the above limit in which the adiabatic error can vanish (hence instantaneous full adiabaticity). According to Eq. (174), we have $\delta_{\text{ad}}(1)|_{T_k} = 0$, where

$$JT_k = 2\sqrt{k^2\pi^2 - \varphi^2} \stackrel{r \ll 1}{\approx} 2\pi\sqrt{k^2 - 1/4}, \qquad (177)$$

for $k \in \mathbb{N}$. The existence of such T_ks is in agreement with Ref. [64]. Figure 3 shows $\delta_{\text{ad}}(1)$ for two different values of r.

Remark. As is evident here the adiabatic error does not show any exponential behavior. In fact, neither of the methods we discussed in Sec. IV B 2 is applicable.

4. General interpolation

Here, we discuss the behavior of the exponential $e^{-JT\text{Im}[\int^{z_0}\Delta]}$ for the general interpolation we derived in Sec. IV C 1. Our analysis is based on a formal power series expansion of $x_1[\theta(\tau)]$ and $x_2[\theta(\tau)]$ in terms of r—recall that we are interested in the regime $r \ll 1$. We further assume that $\theta(\tau)$ does not depend explicitly on r.

Consider the following formal expansions:

$$x_1[\theta(\tau)] = f_1[\theta(\tau)] + g_1[\theta(\tau)]r^{\alpha_1} + O(r^{\alpha_1+\epsilon_1}), \qquad (178)$$
$$x_2[\theta(\tau)] = f_2[\theta(\tau)] + g_2[\theta(\tau)]r^{\alpha_2} + O(r^{\alpha_2+\epsilon_2}), \qquad (179)$$

in which α_1 and α_2 are some non-negative numbers (to be determined later), $\epsilon_1, \epsilon_2 > 0$, and $f_1, f_2 \neq 0$. We notice that the linear and constant-gap interpolations (Secs. IV C 2 and IV C 4) do not admit expansions as in Eqs. (178) and (179). Equation (42) hence yields

$$\Delta^2 = (f_1 - f_2)^2 + 2(f_1 - f_2)(g_1r^{\alpha_1} - g_2r^{\alpha_2}) + 4f_1f_2r$$
$$+ (g_1r^{\alpha_1} - g_2r^{\alpha_2})^2 + O(r^{\alpha_1+\alpha_2+\epsilon_1+\epsilon_2}). \qquad (180)$$

Similarly, inserting Eqs. (178) and (179) into $x_{21} = x_2/x_1$ gives

$$x_{21} = \frac{f_2}{f_1} - \frac{f_2 g_1}{f_1^2} r^{\alpha_1} + \frac{g_2}{f_1} r^{\alpha_2} + O(r^{\alpha_1 + \alpha_2 + \epsilon_1 + \epsilon_2}). \quad (181)$$

On the other hand, Eq. (124) yields

$$x_{21}(\tau) = 1 - 2\sqrt{r} \cot[\pi\theta(\tau)] + O(r). \quad (182)$$

The symmetry $x_2[\theta(\tau)] = x_1[1 - \theta(\tau)]$ [Eq. (127)] requires that

$$g_1[\theta(\tau)] = g_2[1 - \theta(\tau)], \quad (183)$$

which in turn implies $\alpha_1 = \alpha_2 = 1/2$. Comparing the terms with the same powers of r in Eqs. (181) and (182), we conclude that

$$f_1[\theta(\tau)] = f_2[\theta(\tau)] \equiv f[\theta(\tau)] \quad (184)$$

and

$$\frac{g_1[\theta(\tau)] - g_2[\theta(\tau)]}{f[\theta(\tau)]} = 2\cot[\pi\theta(\tau)]. \quad (185)$$

After inserting the above relations back into Eq. (180) and using Eq. (185), we obtain

$$\Delta(\tau) = 2f[\theta(\tau)] \csc[\pi\theta(\tau)]\sqrt{r} + O(r). \quad (186)$$

Now we assume that $f[\theta(\tau)] \neq 0$ everywhere, or if there exist points at which f vanishes, their contribution to the integral $\mathrm{Im}[\int^{z_0} \Delta]$ is not substantial. Note that the previous condition is in fact a condition on the norm of the Hamiltonian—because from Eq. (38)

$$\|H\|/J = 2f + O(\sqrt{r}). \quad (187)$$

Therefore, provided that for large times the adiabatic error asymptotically behaves as in Eq. (106) or (109), we obtain

$$\delta_{\mathrm{ad}}(1) \lessapprox R(1) e^{-2\sqrt{r} JT |\mathrm{Im}[\int_0^{z_0} f[\theta(z)] \csc[\pi\theta(z)] dz]|}, \quad (188)$$

where $R(1)$ is a nonexponential function of T (which may also depend weakly on r). Hence, in the $r \ll 1$ limit for $\delta_{\mathrm{ad}}(1) \leqslant \varepsilon$, it is sufficient to have

$$T \gtrapprox \frac{\ln(1/\varepsilon)}{2J\sqrt{r}} \left| \mathrm{Im}\left[\int_0^{z_0(r)} f[\theta(z)] \csc[\pi\theta(z)] dz \right] \right|. \quad (189)$$

This in turn implies the following scaling for the run time:

$$\tau_{\mathrm{run}} = O\left(\frac{\ln(1/\varepsilon)}{\sqrt{r}} \left| \mathrm{Im}\left[\int_0^{z_0(r)} f[\theta(z)] \csc[\pi\theta(z)] dz \right] \right| \right). \quad (190)$$

The overall r dependence here comes from $\sqrt{r}$ and $z_0(r)$; e.g., we recover the Grover-like $O(\sqrt{N/M})$ scaling if z_0 does not depend on r. This analysis then highlights in a fairly general way the interplay between r, T, and $\delta_{\mathrm{ad}}(1)$ in the quantum search algorithm.

E. A strategy for reducing the adiabatic error

For most applications it is desirable to make the adiabatic error as small as possible. We have seen that $\delta_{\mathrm{ad}}(1)$ contains exponential terms, suppressed by the polynomially decaying terms. Therefore, it is useful to somehow extend the dominance

of the exponential term by reducing the contribution of the polynomial term, e.g., by prolonging the dominance of the exponential regime or by enforcing higher-order polynomial behavior. In the following we shall discuss a control strategy for reducing the adiabatic error by manipulation of the boundary conditions (see, e.g., Refs. [28,32]).

1. A general strategy: Control via boundary conditions

Equation (97) demonstrates explicitly how the adiabatic error depends on the boundary conditions, up to $O(1/T)$. Interestingly, if we choose $\dot{x}_2(0) = \dot{x}_1(1) = 0$, the prefactor of the $1/T$ vanishes, whence $\delta_{\mathrm{ad}}(1) = O(1/T^2)$. In a similar fashion, one can see that by enforcing suitable (extra) boundary conditions on the interpolation $\mathbf{x}(\tau)$, the prefactor of the $1/T^2$ or even higher-order terms can be made zero. This implies that by manipulating the boundary conditions of the interpolation, one may achieve smaller adiabatic errors. This observation is a manifestation of the following general theorem: If the Hamiltonian $H(\tau)$ is sufficiently differentiable, forcing *all* time derivatives of the Hamiltonian up to some order k to vanish at the boundaries,

$$\left. \frac{d^l H(\tau)}{d\tau^l} \right|_{\tau \in \{0,1\}} = 0 \ \forall l \in \{1, \ldots, k\}, \quad (191)$$

is sufficient for $\delta_{\mathrm{ad}}(1) = O(1/T^{k+1})$ [28,29,32,53]. It is interesting to note that the very same condition together with the assumption of the *analyticity* of $H(\tau)$ in a small strip around the real axis in the *complex* τ plane give rise to $\delta_{\mathrm{ad}}(1) = O[e^{-c(r)JT}]$, where $c(r) \equiv \Delta_{\min}^3 / \max_\tau \|\dot{H}(\tau)\|^2$ [up to an $O(1)$ prefactor] [32].[2]

This is a remarkable result in that it guarantees that with sufficient smoothness at two points one can substantially suppress the adiabatic error. This is a fairly low price to pay for higher accuracy. In particular, in experimental realizations, manipulating Hamiltonian interpolations only at the beginning and the end (as opposed to from the beginning to the end) may offer a less demanding control strategy than one seeking to control the dynamics instantaneously along the entire evolution.

Now we show that, in the framework we developed earlier, enforcing the required smoothness properties can be achieved by choosing an appropriate $\theta(\tau)$ function. We recall that this function was fairly arbitrary; we required that it be a monotonically increasing differentiable function ($\dot{\theta}(\tau) > 0$) satisfying the boundary conditions $\theta(0) = 0$ and $\theta(1) = 1$. We require further that $\theta(\tau) \equiv \theta_k(\tau)$ (for a given $k \in \mathbb{N}$) have the following property:

$$\left. \frac{d^l \theta_k(\tau)}{d\tau^l} \right|_{\tau \in \{0,1\}} = 0 \ \forall l \in \{1, \ldots, k\}, \quad (192)$$

namely the first k derivatives should vanish at the boundaries. This property is sufficient for fulfilling Eq. (191) because $\dot{H} = \dot{\theta} \partial_\theta H$. An example of such $\theta_k(\tau)$ is the regularized incomplete

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[2]Note that the conditions $\dot{x}_2(0) = \dot{x}_1(1) = 0$ we obtained above are in fact weaker than requiring $\dot{x}_1(\{0,1\}) = \dot{x}_2(\{0,1\}) = 0$ [sufficient for $\dot{H}(\tau)|_{\tau \in \{0,1\}} = 0$].

β function,

$$\theta_k(\tau) = \frac{B_\tau(1+k, 1+k)}{B_1(1+k, 1+k)}, \tag{193}$$

in which $B_\tau(a,b) \equiv \int_0^\tau y^{a-1}(1-y)^{b-1}dy$, with Re$(a)$, Re$(b) > 0$, and $|\tau| \leqslant 1$ [65,66].

2. Polynomial reduction

To demonstrate explicitly how the conditions (191) affect the adiabatic error, we employ the method developed in Refs. [28,32] for approximating the coefficients in the poly($1/T$) expansion of $\delta_{\mathrm{ad}}(1)$. One can construct an approximate (unnormalized) ansatz for the solution to the Schrödinger equation (4) in the powers of $1/T$ as follows:

$$
|\Psi_n(\tau)\rangle
= e^{-iJT \int_0^\tau E_0}\left[|\Phi_0(\tau)\rangle + \sum_{l=1}^n \frac{1}{(JT)^l}|\psi_l(\tau)\rangle + \frac{|\psi_{n+1}^\perp(\tau)\rangle}{(JT)^{n+1}} \right], \tag{194}
$$

with the error

$$\||\psi_T(1)\rangle - |\Psi_n(1)\rangle\| \leqslant \frac{\max_\tau \||\psi_{n+1}^\perp(\tau)\rangle\|}{(JT)^{n+1}}. \tag{195}$$

Here, $\{|\psi_l(\tau)\rangle\}$ and $\{|\psi_l^\perp(\tau)\rangle\}$ are given as follows [32]:

$$|\psi_l\rangle = a_l|\Phi_0\rangle + |\psi_l^\perp\rangle, \tag{196}$$

$$|\psi_l^\perp\rangle = G_r(f_{l-1}|\dot\Phi_0\rangle + |\dot\psi_{l-1}^\perp\rangle), \tag{197}$$

$$a_l = -\int_\tau^1 \langle\Phi_0|\dot\psi_l^\perp\rangle d\tau', \quad a_0 \equiv 1, \tag{198}$$

$$G_r = i(H - E_0)^{-1}(\mathbb{1} - |\Phi_0\rangle\langle\Phi_0|). \tag{199}$$

It is evident that $|\psi_T(\tau)\rangle = |\Psi_\infty(\tau)\rangle/\|\Psi_\infty(\tau)\|$.

Provided that all n derivatives of $H(\tau)$ vanish at the boundaries, Eq. (191), all the terms except $|\Phi_0(1)\rangle$ and $|\psi_{n+1}^\perp(1)\rangle/(JT)^{n+1}$ will vanish [53] (see also Ref. [32], where with a condition differing from Eq. (198) all the terms except $|\Phi_0\rangle$ vanish).

Let us define

$$\delta_1(1) \equiv \sqrt{1 - |\langle\widehat\psi_T(1)|\widehat\Psi_n(1)\rangle|^2/\|\widehat\Psi_n(1)\|^2}, \tag{200}$$

$$\delta_2(1) \equiv \sqrt{1 - |\langle\widehat\Psi_n(1)|\widehat\Phi_-(1)\rangle|^2/\|\widehat\Psi_n(1)\|^2}, \tag{201}$$

in which the normalized state $|\widehat\psi_T(\tau)\rangle$ has been defined as [Eq. (51)]

$$|\widehat\psi_T(\tau)\rangle \equiv \sqrt{M}S^{-1}|\widetilde\psi_T(\tau)\rangle. \tag{202}$$

Since $\delta(a,b) \equiv \sqrt{1 - |\langle a|b\rangle|^2}$ (for normalized $|a\rangle$ and $|b\rangle$) is a distance [Eq. (9)], from the triangle inequality $\delta(a,b) \leqslant \delta(a,c) + \delta(b,c)$ we have:

$$\delta_{\mathrm{ad}}(1) \leqslant \delta_1(1) + \delta_2(1). \tag{203}$$

Notice that $\delta_1(1)$ can also be written as follows:

$$
\begin{aligned}
\delta_1(1) &= \sqrt{1 - \frac{|\langle\widehat\Psi_n(1)|\widehat\Psi_\infty(1)\rangle|^2}{\|\widehat\Psi_n(1)\|^2\|\widehat\Psi_\infty(1)\|^2}} \\
&= \sqrt{1 - \frac{|\langle\widehat\Psi_n(1)|(|\widehat\Psi_n(1)\rangle + |\widehat R_n(1)\rangle)|^2}{[1 + O(1/T)]^2[1 + O(1/T)]^2}} \\
&\approx \sqrt{1 - (1 + 2\mathrm{Re}[\langle\widehat\Psi_n(1)|\widehat R_n(1)\rangle])} \\
&= O\left(\frac{1}{T^{n+2}}\right),
\end{aligned} \tag{204}
$$

where

$$|\widehat R_n(1)\rangle \equiv |\widehat\Psi_\infty(1)\rangle - |\widehat\Psi_n(1)\rangle. \tag{205}$$

On the other hand, a straightforward calculation (supplemented with induction) shows that

$$
\begin{aligned}
\delta_2(1) &= \sqrt{1 - |\langle\widehat\Psi_n(1)|\widehat\Phi_-(1)\rangle|^2/\|\widehat\Psi_n(1)\|^2} \\
&= \frac{\sqrt{r(1-r)}|1-2r|}{(JT)^{n+1}}\big(|\dot x_2(0)\theta_n^{(n+1)}(0)| \\
&\quad + |\dot x_1(1)\theta_n^{(n+1)}(1)|\big) + O\left(\frac{1}{T^{n+2}}\right).
\end{aligned} \tag{206}
$$

This bound holds true for any interpolating paths $\mathbf{x}(\tau)$ for which $x_1(1-\tau) = x_2(\tau)$. As can be seen, $\delta_1(1)$ is negligible in comparison to $\delta_2(1)$, hence we obtain

$$
\begin{aligned}
\delta_{\mathrm{ad}}(1) \leqslant &\frac{\sqrt{r(1-r)}|1-2r|}{(JT)^{n+1}}\big(|\dot x_1(1)\theta_n^{(n+1)}(1)| \\
&+ |\dot x_2(0)\theta_n^{(n+1)}(0)|\big) + O\left(\frac{1}{T^{n+2}}\right).
\end{aligned} \tag{207}
$$

This result is a generalization of Eq. (97). For example, in the case of the constant-gap interpolation (Sec. IV C 4), this error reduces to

$$\delta_{\mathrm{ad}}(1) \lessapprox \frac{2\varphi|\theta_n^{(n+1)}(1)|}{(JT)^{n+1}}, \tag{208}$$

in comparison with Eq. (175). Figure 4 depicts $\delta_{\mathrm{ad}}(1)$ for the constant-norm interpolation [Eqs. (134) and (135)]. It can be seen that by increasing k the exponential regime dominates longer, while the polynomial regime is pushed farther away to the region of large evolution times. However, this improvement comes at a price. The rate of exponentiality decreases with increasing k; that is, if $k_1 < k_2$ and $\delta_{\mathrm{ad}}(1) \leqslant \varepsilon$ for an ε in the exponential regime for the larger k, then $T_1(\varepsilon) > T_2(\varepsilon)$ (see the inset of Fig. 4). In other words, for some values of ε, increasing k might give rise to an increased run time. Of course, if ε is such that the polynomial regimes dominate for both values of k_1 and k_2, the interpolation with the larger k (k_2) results in a smaller run time.

3. Exponential reduction

Since choosing a $\theta_k(\tau)$ with a larger k benefits the accuracy of the adiabatic evolution, it is natural to investigate cases with $k = \infty$. An example of such $\theta_\infty(\tau)$ is

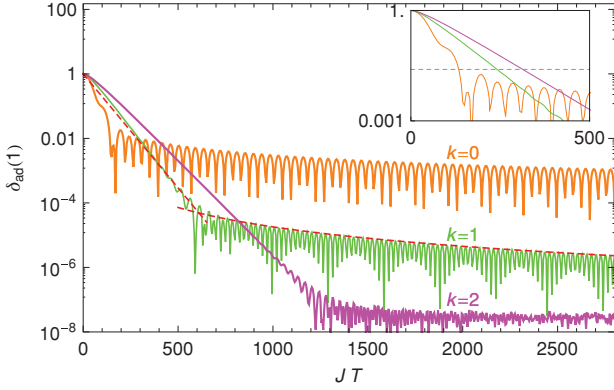$$\theta_\infty(\tau) = \frac{\int_0^\tau b_{\alpha\beta}(\tau')d\tau'}{\int_0^1 b_{\alpha\beta}(\tau')d\tau'}, \tag{209}$$

FIG. 4. (Color online) $\delta_{ad}(1)$ obtained by numerically solving the Schrödinger equation corresponding to the constant-norm interpolation with $\theta_k(\tau)$ the regularized β function [Eq. (193)], for $k \in \{0, 1, 2\}$ (here $r = 2^{-8}$). The dashed (red) lines represent $e^{-\pi JT\sqrt{r}/(8\varphi)}$ and $2\varphi|\theta_1^{(2)}(1)|/(JT)^2$ [Eq. (208)].

where

$$b_{\alpha\beta}(\tau) = e^{-\beta/[\tau^\alpha(1-\tau)^\alpha]} \quad 0 < \alpha, \quad \beta \leqslant 1, \qquad (210)$$

is a symmetric "bump function." We notice that $b_{\alpha\beta}(\tau)$ is compactly supported and infinitely differentiable in $\tau \in [0, 1]$ (the "Schwartz class" [68]); in particular,

$$\left.\frac{d^l b_{\alpha\beta}(\tau)}{d\tau^l}\right|_{\tau \in \{0,1\}} = 0 \quad \forall l \in \mathbb{N}. \qquad (211)$$

However, it is not an *analytic* function of τ, which implies that $H[\mathbf{x}[\theta_\infty(\tau)]]$ is not analytic either. Despite this infinite smoothness, the very lack of analyticity in fact prevents the adiabatic error from being identically zero [28,29].

Nevertheless, $\theta_\infty(\tau)$ helps remove the polynomial terms arbitrarily, hence extending the exponential regime farther. Additionally, the exponent of the exponential term is controllable through varying the parameters α and β. In this case, asymptotic evaluation of the integral (82) with the stationary phase method results in a faster-than-polynomial convergence to zero. For example, with $\alpha = 1$ and $\beta \ll 1$ for the constant-norm interpolation, we can approach an exponential convergence similarly to the case with $k = 0$. The achievement of an exponentially small $\delta_{ad}(1)$ for such functions may be understood as an instance of rigorously derived exponentially small errors for a general class of functions called the Gevrey class [26,27].

It is evident that manipulating the $\theta(\tau)$ function may also affect the exponent $\text{Im}[\int_0^{z_0} \Delta(\theta(\tau'))d\tau']$. This can be observed in Fig. 4 (the inset) through the change of the slope of the exponential lines in the log plot. A side consequence of using a $\theta(\tau)$ with the desired boundary conditions (192) is that increasing k may adversely increase the value of T for which $\delta_{ad}(1) \leqslant \varepsilon$ (in the exponential regime). To quantify how choosing a $\theta_k(\tau)$ for the Hamiltonian interpolation affects the performance of the algorithm, we propose the following measure:

$$\eta_k(1) \equiv \frac{1}{T} \int_0^T \delta_{ad}(1)|_{\mathbf{x}[\theta_k(\tau)]} \, dT, \qquad (212)$$

namely the average adiabatic error up to time T for a given k. A larger average error may be interpreted as less efficient performance.

The above problem with the effect of k on exponentiality may be partially alleviated in some cases. Recall that in Sec. IV C 1 we found a fairly general interpolation, which resulted in the parametrization $x_{12}(\tau)$ [Eq. (124)]—it was later that we added further conditions so as to find $x_1(\tau)$ and $x_2(\tau)$ separately. Rather than assuming the condition (128), let us impose

$$2f[\theta(\tau)] = 1 + \zeta\dot{\theta}(\tau), \qquad (213)$$

for some $\zeta \neq 0$. We should be mindful of the fact that, from Eq. (187), modifying f leads to a modification of the norm of the Hamiltonian or, equivalently, the maximum energy of the system; this is a cost which should be taken care of in the correct estimation of τ_{run} [Eq. (26)]. Additionally, from Eq. (186) it is seen that—since we assumed $f \neq 0$ (up to the leading order in r)—the gap Δ vanishes where $\sin[\theta(z_0)] \propto \infty$; i.e., $\theta(z_{0\pm}) = \pm i\infty$. In this case, the exponent $\text{Im}[\int_0^{z_0} \Delta[\theta(\tau')]d\tau']$ [Eq. (107)] becomes

$$\text{Im}\left\{\int_0^{z_{0+}} [1 + \zeta\dot{\theta}(\tau')] \csc[\pi\theta(\tau')]d\tau'\right\}$$
$$= \text{Im}\left[\int_0^{z_{0+}} \csc[\pi\theta(\tau')] \, d\tau'\right] + \frac{\zeta}{2}. \qquad (214)$$

Therefore, by appropriately choosing ζ—subject to the condition $1 + \zeta\dot{\theta} > 0$—we can tune the exponent of the exponential term in $\delta_{ad}(1)$. This in turn gives us control over the run time in the exponential regime. Furthermore, as we argued earlier, replacing $\theta(\tau) \to \theta_k(\tau)$ causes the polynomial terms of $\delta_{ad}(1)$ to be $O(1/T^{k+1})$. Thus, we are now in possession of two control parameters k [more precisely $\theta_k(\tau)$] and ζ with which we can manipulate how the adiabatic error behaves in either of the exponential and polynomial regimes. This type of control may have applications in experiments in which adiabaticity plays a role.

As an example, let $\theta_k(\tau)$ be the regularized β function [Eq. (193)]. For $k \gg 1$ and after employing Stirling's approximation for the factorial function ($k! \approx \sqrt{2\pi k}(k/e)^k$ [65]), we obtain

$$\max_\tau \dot{\theta}(\tau) = \dot{\theta}(1/2) \approx \frac{2(2+k)^{-\frac{5}{2}-k}\left(\frac{5}{2}+k\right)^{3+k}}{\sqrt{\pi e}} \approx \sqrt{k}, \qquad (215)$$

whereby

$$\max_\tau \|H(\tau)\|/J \approx 1 + \sqrt{k}|\zeta_k|. \qquad (216)$$

As a result, for example, in order to keep the maximum energy constant, while having the advantages of θ_k, we should choose $|\zeta_k| = O(1/\sqrt{k})$.

V. SUMMARY AND CONCLUSIONS

Adiabatic evolution is characterized by a trade-off between the total time taken and the error in the final state reached, relative to the desired adiabatic state. Motivated by a desire to understand and optimize this trade-off, in this work we performed a detailed analysis of the adiabatic error for the

case of an adiabatic quantum search algorithm. Rather than using the traditional adiabatic condition, with its associated pitfalls, we chose to calculate the adiabatic error directly by solving the Schrödinger equation. This enabled us to derive an exact relation for the adiabatic error. Building on this exact result, we employed a formal polynomial series expansion in $1/T$ for calculating the error term by term. This also allowed us to bound the adiabatic error. We showed that the polynomial expansion should be truncated carefully if we aim to obtain a reliable estimate for the run time of the algorithm.

We demonstrated that employing a different technique based on complex analysis reveals, in fairly general situations, a regime of exponential time-dependent decay of the adiabatic error, preceding a polynomial regime. The latter has been shown to be a general feature of adiabatic Hamiltonians, whereas the existence of an exponential precursor is not always guaranteed. We showed how, in case these two regimes both exist, one can estimate the crossover region—i.e., the time at which a transition between the two regimes takes place. Equipped with this, we provided an estimate for the minimum time required for the algorithm to achieve a given accuracy threshold. Discerning the exponential regime enabled us to give an improved total time estimate, circumventing the overestimate arising from the error bound using only the polynomial expansion. Indeed, the total time estimated from the exponential regime always gave the correct scaling with system size (the well-known quadratic speedup over classical search), while the estimate resulting from the polynomial regime resulted in unreliable and even erroneous results.

We also obtained a specific class of Hamiltonian interpolations for the search problem. To this end, we employed a recently developed theory, based on the geometry of adiabatic evolutions, for obtaining suitable adiabatic interpolations. This theory separates the adiabatic error into geometric and nongeometric parts and minimizes the former. We discussed three special cases of the resulting class of interpolations in detail: (i) linear, (ii) constant-norm, and (iii) constant-gap interpolations.

Finding strategies for minimizing the required total time as a function of a given resource (system size, for example) is a desirable goal for many applications and is also of fundamental importance for the control of quantum systems. We demonstrated explicitly how by imposing fairly general controllability assumptions, which should be experimentally straightforward to realize in certain scenarios, one can achieve a significant reduction of the adiabatic error and hence improve algorithmic performance. The method we used relied on a polynomial expansion of the adiabatic error and resulted in the suppression of polynomial terms in $1/T$ by requiring smoothness for interpolations at the initial and final times. It is evident that controlling the interpolation in this manner, at only two points, has a substantial advantage over instantaneous control of the Hamiltonian along the entire evolution. However, we demonstrated that there is an extra price to pay for this error reduction: the exponential regime (if it exists) is extended but with a slower rate of decay. This, in turn, may result in an overestimation of the run time of the algorithm for some values of the error threshold. We proposed a measure for quantifying the performance of an adiabatic interpolation with various controllability properties. In some cases, we also suggested a remedy for the above problem. This fix necessitated further control over the Hamiltonian interpolation, directly related to the amount of accessible energy in the system. The interplay between the degree of required control over Hamiltonian interpolations and the run time needed for achieving a given accuracy was thus clearly exhibited.

Although we focused on the quantum search problem, our methods and most of our results are applicable (perhaps with minor modifications) to a wider class of problems—as discussed in the text. Since a principal goal in adiabatic quantum algorithms, adiabatic quantum transport, quantum annealing, and other applications of the adiabatic theorem is the design of algorithms with favorable performance-resource trade-off, we hope that our results will be of use in related physical applications.

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