Error-run-time trade-off in the adiabatic approximation beyond scaling relations

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The use of the adiabatic approximation in practical applications, as in adiabatic quantum computation, demands an assessment of the errors made in finite-time evolutions. Aiming at such scenarios, we derive bounds relating error and evolution time in the adiabatic approximation that go beyond typical scaling relations. Using the Adiabatic Perturbation Theory, we obtain leading-order expressions valid for long evolution time $T$, while explicitly determining the shortest time $T$ and the largest error $\varepsilon$ for which they are valid. Restricting our considerations to this validity regime, we can make clear and precise statements about the evolution time necessary to reach a given error and vice-versa. As an example of practical importance, we apply these results to the adiabatic version of Grover’s quantum search algorithm and obtain highly accurate trade-off relations between run time and error for several evolution schedules. Their examination indicates that different strategies are required to optimize for either shorter time or minimal error.

I. INTRODUCTION

The quantum adiabatic theorem [1, 2] is a fundamental result derived early in the development of quantum mechanics. It states that a system submitted to the action of a time-dependent Hamiltonian which changes sufficiently slowly in time will remain in an instantaneous eigenstate of that Hamiltonian throughout its evolution. Since its appearance, it has played an important role in quantum mechanics and has found application in a wide range of subjects [3–6]. More recently, the adiabatic theorem has been used as the basis for a new method of quantum computation, known as adiabatic quantum computing (AQC) [7–9], generating a renewed interest in the quantum adiabatic approximation. In AQC, one chooses an initial Hamiltonian whose ground state can be easily prepared, whereas the corresponding eigenstate of the final Hamiltonian encodes some information of interest (such as the answer to a computational problem). The time-dependent Hamiltonian is free to interpolate between the two so as to adiabatically drive the simple initial eigenstate into the information-encoding eigenstate at the final time $T$ as well as possible. AQC is as powerful as the circuit version of quantum computation and is featured prominently in proposals for quantum machine learning [10], quantum chemistry simulations [11], as well as in several other examples of adiabatic quantum algorithms [9]. Quantum annealing [12, 13] also bears a close relationship to AQC [14].

As seen in its original form [2] or in standard textbook approaches [15], however, the quantum adiabatic theorem only applies to infinitely slow system driving. Whereas in early applications it was not decisive to have a rigorous bound on the shortest driving time $T$ necessary for the adiabatic approximation be reliable, in AQC it is of fundamental importance. Since the main goal of adiabatic quantum computing is to perform computations in a time scale shorter than its classical counterparts, it becomes peremptory to have accurate estimates of the time necessary for an adiabatic behavior. This has taken the form of trade-off relations between the total time $T$ allowed for the system to be driven, which is called the run time of the algorithm, and the error made by applying the adiabatic theorem as an approximation for determining the final state of the system at time $T$ [16–20]. The focus is to find an interpolation between initial and final Hamiltonians which minimizes the run time $T$ and the error $\varepsilon$, measured by the distance between the actual state of the system at time $T$ and the ground state of the Hamiltonian at that time. One, typically, seeks to minimize the run time $T$ for a fixed error $\varepsilon$ and problem size or, alternatively, to minimize the error $\varepsilon$ for a given run time $T$ and problem size.

Since the appearance of AQC, bounds to the relation between the run time $T$ and the error $\varepsilon$ have been presented [9]. However, as such bounds typically rely on some type of approximation based on an expansion in $1/T$ of the error $\varepsilon$, they are not valid for arbitrary values of $T$. The lack of clear quantitative statements about the domain of validity of those approximations precludes one to establish the range of values of $T$ and $\varepsilon$ to which those bounds in fact apply, leading, in some cases, to wrong estimations of the complexity of quantum adiabatic algorithms. One of our main goals here is to provide asymptotically tight bounds to the relation between the run time $T$ and the error $\varepsilon$, whereas explicitly determining a lower limit on the value of $T$ and/or an upper limit on
the value of $\varepsilon$ for which these bounds still apply.

In this article we use the adiabatic perturbation theory (APT) [21] to obtain general results for the trade-off relation between the run time $T$ and the error $\varepsilon$ of the adiabatic approximation. Going beyond scaling relations, we obtain leading-order expressions valid for large time $T$. More importantly, we are able to explicitly determine the shortest time $T$ and the largest error $\varepsilon$ for which these results are valid. Restricting our considerations to times larger than that time and/or errors smaller than that error, we can make clear and correct statements about the run time necessary to reach a given error and vice-versa. As a figure of merit for the error, we employ the Bures angle between the actual state of the system and the instantaneous ground state of the Hamiltonian at time $T$. This angle satisfies all the desired properties of a distance between quantum states, and also depends only on the fidelity between the states in question, being a genuine measure of error with direct physical interpretation. We apply our results to the quantum adiabatic search algorithm [7, 22] and show that they produce correct trade-off relations between the run time $T$ and error $\varepsilon$, beyond scaling relations.

This article is organized as follows. In Sec. II we outline the framework of the adiabatic approximation and derive general results for the trade-off relation between run time $T$ and error $\varepsilon$. In Sec. III, these results are applied to the adiabatic quantum search algorithm, which, besides being of practical importance for AQC, admits an exact analytical treatment; Sect IV is left to final remarks.

II. ADIABATIC ERRORS AND VALIDITY CONDITIONS

We treat the evolution of a closed system from an initial time $t = 0$ to a final time $t = T$ governed by a driven Hamiltonian of the form $H(t/T)$. This dependence solely on $s := t/T (\in [0, 1])$ includes Hamiltonians of interest for most applications, most notably adiabatic quantum computation (AQC), but excludes those with more than one independent timescale. Importantly, this excludes Hamiltonians which can lead to so-called resonances [23–27], which happen when two different timescales of the Hamiltonian coincide [28–31] and results in far-from-adiabatic evolution.

Besides being the final time, $T$ serves as a global parameter which rescales the total driving time, hence allows an adjustment of the speed of change of the Hamiltonian. The evolution obeys the Schrödinger equation, which, in terms of dimensionless time $s$, reads

$$\frac{i\hbar}{T}|\Psi(s, T)\rangle = H(s)|\Psi(s, T)\rangle,$$

where $|\Psi(s, T)\rangle$ is the physical state of the system at $s$ and $T$ is convenient to our discussion of long times $T$.

At each time $s$, there is an instantaneous eigenbasis $\{|\phi_n(s)\rangle\}$ of $H(s)$ with eigenenergies $E_n(s)$ nondecreasing with $n$ ($E_0(s)$ being the ground-state energy). The time dependence of each $|\phi_n(s)\rangle$ reflects the driving program and does not obey the Schrödinger equation. Assuming an evolution that starts on the $j$-th eigenstate $|\Psi(0, T)\rangle = |\phi_j(0)\rangle$, however, the adiabatic theorem in its traditional form [15] states that, for infinitely long driving time $T$, the physical state coincides with the corresponding eigenstate along the evolution, $|\Psi(s, T)\rangle = e^{i\alpha} |\phi_j(s)\rangle$ for some phase $e^{i\alpha}$, given that $E_j(s)$ is non-degenerate throughout. The results of this paper will be valid for any initial eigenstate, but to fix the notation, we will consider, in the remainder of the text, the system to be initially in the ground state ($j = 0$) — and $E_0(s)$ will be assumed to be non-degenerate.

The error of the adiabatic theorem amounts to precising how distant the physical state $|\Psi(s, T)\rangle$ is from the instantaneous ground state $|\phi_0(s)\rangle$. Illustrative of their different roles is the fact that $|\phi_0(s)\rangle$ does not depend on $T$. Several figures of merit for this error $\varepsilon$ have been used in the literature [19, 20, 32]. We will use an explicit well-known distance, the Bures angle:

$$\varepsilon = D[|\Psi(s, T)\rangle, |\phi_0(s)\rangle] := \arccos (|\langle \phi_0(s)|\Psi(s, T)\rangle|).$$

The Bures angle has the advantage of being a genuine, Riemannian distance between the two states, defined from the Fubini-Study metric [33–37], and, importantly, it depends on the fidelity between the two states, having a maximum value of $\pi/2$ for orthogonal states and a minimum of zero if, and only if, the two states are the same. This is particularly relevant in that we want not only to describe the scaling of the error, but to obtain numerical values.

In order to estimate the error made by using the adiabatic approximation, we make use of the Adiabatic Perturbation Theory [21], which relies on an expansion well-suited for long evolution times. First, the physical state of the system is decomposed in terms of the energy eigenbasis:

$$|\Psi(s, T)\rangle = \sum_{n=0} e^{-iT\omega_n(s)} b_n(s, T)|\phi_n(s)\rangle,$$
where the dynamical phase \( \omega_n(s) := \frac{1}{\hbar} \int_0^s E_n(s') ds' \) and the sum extends over all eigenstates. The geometric phase usually appearing in this expansion is absent here because, without loss of generality, it will be taken as zero by assuming a choice of eigenvector phases such that \( \langle \phi_n(s) | \phi_n(s) \rangle = 0 \).

To treat the long-run-time regime, each complex coefficient \( b_n(s, T) \) is written \([21]\) as a sum of powers of \( \frac{\hbar}{T} \). Due to \( T \)-dependency of Eq.(1), it is convenient to write it in terms of powers of \( i\hbar/T \):

\[
b_n(s, T) = \sum_{p=0}^{\infty} \frac{(i\hbar)^p}{T^p} b_n^{(p)}(s) .
\] (4)

In a slight abuse of notation, coefficients \( b_n^{(p)}(s) \) may still depend on \( T \) (usually in the form of a complex phase), but are upper- and lower-bounded by \( T \)-independent expressions. The (zero-order) adiabatic approximation amounts to taking \( b_n(s) = b_n^{(0)}(s) = \delta_{n0} \), formally equivalent to the \( T \to \infty \) limit. We will be interested in leading-order expressions beyond \( b_n^{(0)}(s) \).

Importantly, any analysis based on a perturbative expansion requires validity conditions — in our case, conditions for it to be truncated at the first nonvanishing term. To this end, we will obtain closed-form expressions for leading and next-to-leading order coefficients. This is essential for a correct analysis of the perturbative results.

### A. General results

Let us begin to state our main results. The Bures angle can be expanded as

\[
D[\Psi(s, T), |\phi_0(s)\rangle] = \frac{\hbar}{T} \sqrt{\sum_{n \neq 0} |b_n^{(1)}|^2} - \frac{\hbar^2}{2T^2} \left( \frac{\sum_{n \neq 0} \text{Im} \left( b_n^{(1)} b_n^{(2)} \right)}{\sqrt{\sum_{n \neq 0} |b_n^{(1)}|^2}} - i \left( \sum_{n \neq 0} |b_n^{(1)}|^2 \text{Im} \left( b_0^{(1)} \right) \right) + O \left( \frac{1}{T^3} \right) \right),
\] (5)

where, as before, the terms may have additional \( T \) dependences, as long as they are both upper- and lower-bounded by \( T \)-independent expressions; \( \sum_{n \neq 0} \) indicates a sum that runs over all excited levels (proof in Appendix A). By calculating the first-order terms \( b_n^{(1)} \), we can write a closed-form expression for the error:

\[
\varepsilon = D[\Psi(s, T), |\phi_0(s)\rangle] = \frac{\hbar}{T} \sqrt{\sum_{n \neq 0} \left| e^{iT\omega_n} \frac{\langle \phi_n | H | \phi_0 \rangle}{\Delta_{n0}} \right|^2} + O \left( \frac{1}{T^3} \right),
\] (6)

where \( \Delta_{n0}(s) := E_n(s) - E_0(s) \), \( \omega_{n0}(s) := \omega_n(s) - \omega_0(s) \) and the notation \( f|_a^b := f(s=b) - f(s=a) \) has been used — in this case, \( f \) involves the gaps, inner products, phases.

For numerical applications, it is interesting to avoid the instability of calculating the oscillating exponential. This can be done by upper- and lower-bounding the leading-order term above:

\[
\varepsilon = D[\Psi(s, T), |\phi_0(s)\rangle] \leq \frac{\hbar}{T} \sum_{n \neq 0} \left( \left| \frac{\langle \phi_n | H | \phi_0 \rangle}{\Delta_{n0}} \right| \pm \left| \frac{\langle \phi_n | H | \phi_0 \rangle}{\Delta_{n0}} \right|_0 \right)^2 + O \left( \frac{1}{T^3} \right),
\] (7)

where the +/- sign gives the upper/lower bound. These bounds also have the advantage of only depending on initial- and final-time parameters, since they do away with \( \omega_{n0}(s) \).

The \( 1/T^2 \) term in Eq.(5) can be used to establish a reasonable, practical validity condition for Eqs.(6,7): they will be valid as long as \( T \) is large enough that the second term is negligible compared to the first. This happens when

\[
T \geq T_{val} = C \frac{\hbar}{\sum_{n \neq 0} \left| b_n^{(1)}(s) \right|^2},
\] (8)

where \( C \) is a large constant, e.g. with a value of \( \sim 100 \), and the fact that \( b_n^{(1)} \in \mathbb{R} \) has been used. For \( n \neq 0 \), \( b_n^{(1)} \) can be
derived here are valid only for \( T \) long enough, in accordance with previous results [21, 32, 38]. The coefficient \( b_{n}^{(2)} \), in turn, equals [21]

\[
b_{n}^{(2)}(s) = e^{iT\omega n s} J_{n}(s) \lambda_{n0}(s) - J_{n}(s) \lambda_{n0}(0) + \left[ e^{iT\omega n s} \right] \left( \frac{\lambda_{n0}(s)}{\Delta_{n0}(s)} + \sum_{k \neq 0} \lambda_{k0}(s) \frac{\langle \phi_{n}(s') | \phi_{k}(s') \rangle}{\Delta_{n0}(s')} \right) \nonumber \\
- \sum_{k \neq 0} e^{iT\omega n k s} \lambda_{k0}(0) \lambda_{n k}(s') \right|_{s'=0}^{s}, \tag{10}
\]

where \( J_{n}(s) := \sum_{k \neq n} \int_{s}^{s'} |\langle \phi_{k}(s') | \phi_{n}(s') \rangle|^{2} / \Delta_{n0}(s') ds' \).

The calculation of these coefficients is found in Appendices B and C.

Importantly, from \( T_{\text{val}} \) one can obtain an upper bound \( \tilde{\varepsilon} \) on the error \( \varepsilon \) for which these expressions are valid, given by \( \tilde{\varepsilon} = D[|\Psi(s, T_{\text{val}})|, |\phi_{0}(s)|] \).

Substituting \( T_{\text{val}} \) from Eq.(8) in Eq.(5) to first order,

\[
\tilde{\varepsilon} = \frac{1}{C} \left( \frac{\sum_{n \neq 0} \left| b_{n}^{(1)}(s) \right|^{2}}{\sum_{n \neq 0} \text{Im} \left( b_{n}^{(1)}(b_{n}^{(2)}(s)) \right)} \right)^{3/2}. \tag{11}
\]

Since we know that error-run-time relations of the type we derived here are valid only for \( T \geq T_{\text{val}} \) and/or \( \varepsilon \leq \tilde{\varepsilon} \), we rewrite these relations as

\[
T \geq \frac{T_{\text{val}}}{\alpha} \text{ for } \varepsilon \leq \alpha \tilde{\varepsilon} \quad (0 < \alpha \leq 1), \tag{12}
\]

and refrain from making any statement for \( \varepsilon > \tilde{\varepsilon} \) and/or \( T < T_{\text{val}} \). Doing so, we guarantee that these relations are correct for any value of \( 0 < \alpha \leq 1 \).

### B. Boundary cancelation

There are cases of interest, however, where the above expressions are not the most useful, such as when \( \hat{H}(0) = 0 = \hat{H}(s) \), which makes \( b_{n}^{(1)}(s) = 0 \). Especially relevant is the use of boundary cancelation [9, 20, 32, 39], which is known to reduce the scale of the error with \( T \) in the asymptotic limit of long times. Therefore, we now tackle Hamiltonian evolutions obeying the boundary-cancelation condition,

\[
H^{(j)}(0) = 0 = H^{(j)}(1) \text{ forall } 1 \leq j \leq p, \tag{13}
\]

where \( H^{(j)} := (\partial / \partial s)^{j} H \). The study of these boundary-cancelation conditions is especially relevant for quantum computation, since the freedom to impose them is typically within the experimenter’s reach. Unlike previous boundary-cancelation results [20, 32, 39, 40], we go beyond the scaling of the error with \( T \) and express the distance in terms of quantities with clear physical interpretations, with concise bounds that only depend on the initial- and final-time Hamiltonian, facilitating numerical approximations.

The expansion of the Bures angle in parameter \( 1/T \) at the final time \( s = 1 \) is altered, since \( b_{n}^{(1)}(1) = 0 \). In fact, all coefficients \( b_{n}^{(j)}(1) \) vanish up to \( j = p \) and this expansion reads

\[
D[|\Psi(1, T)|, |\phi_{0}(1)|] = \frac{\hbar^{p+1}}{T^{p+1}} \sum_{n \neq 0} \left| b_{n}^{(p+1)}(1) \right|^{2} - \frac{\hbar^{p+2}}{T^{p+2}} \sum_{n \neq 0} \text{Im} \left( b_{n}^{(p+1)} b_{n}^{(p+2)}(1) \right) + O \left( \frac{1}{T^{p+3}} \right), \tag{14}
\]

where \( b_{0}^{(1)} \in \mathbb{R} \) has been used. This demonstrates the boundary-cancelation effect of producing an error-run-time tradeoff of \( \varepsilon \sim 1 / T^{p+1} \) from the perturbative analysis. Calculating the first non-vanishing coefficient \( b_{n}^{(p+1)}(1) \) and substituting in the expansion, we find

\[
\varepsilon = D[|\Psi(1, T)|, |\phi_{0}(1)|] = \frac{\hbar^{p+1}}{T^{p+1}} \times \nonumber \\
- \frac{1}{\Delta_{n0}^{p+2}} \sum_{n \neq 0} \left| e^{iT\omega n} \langle \phi_{n} | H^{(p+1)} | \phi_{0} \rangle \right|_{0}^{1} + O \left( \frac{1}{T^{p+2}} \right). \tag{15}
\]
Bounds without the oscillating exponentials can again be found, up to $O(1/T^2)$

$$\varepsilon = D[|\Phi(1, T)|, |\phi_0(1)|] \leq \frac{b^{p+1}}{T^{p+1}} \times \left( \sum_{n \neq 0} \left( \frac{\langle \phi_n | H^{(p+1)} | \phi_0 \rangle}{\Delta_n^{p+2}} \pm \frac{\langle \phi_n | H^{(p+1)} | \phi_0 \rangle}{\Delta_n^{p+2}} \right) \right)^2.$$  

A validity condition is obtained from the comparison of the second term of Eq.(14) with the first, leading to

$$T_{val} = C \hbar \sum_{n \neq 0} \text{Im} \left( b_n^{(p+1)}(1) b_n^{(p+2)}(1) \right).$$  

Assuming $p \geq 1$ and $n \neq 0$, $b_n^{(p+1)}$ is given by

$$b_n^{(p+1)}(1) = e^{iT\omega_0(1)} \frac{\lambda_n^{(p)}(0)}{\Delta_n^{p+2}} - \frac{\lambda_n^{(p+1)}(0)}{\Delta_n^{p+2}},$$  

and $b_n^{(p+2)}$, by

$$b_n^{(p+2)}(1) = e^{iT\omega_0(1)} \frac{\lambda_n^{(p+1)}(1)}{\Delta_n^{p+2}} - \frac{\lambda_n^{(p+2)}(0)}{\Delta_n^{p+2}} \quad \text{or} \quad e^{iT\omega_0(1)} J_0(1) \lambda_n^{(p)}(1) - J_n(1) \lambda_n^{(p+2)}(0).$$

and we remark that the conditions for boundary cancelation of Eq.(13) allow us to write $\lambda_n^{(j)} = -\langle \phi_n | H^{(j+1)} | \phi_0 \rangle / \Delta_n$ for $s = 0$ or 1 and $j + 1$. The error value $\tilde{\varepsilon}$ that upper-bounds the validity of these expressions is given by substituting Eq.(17) in Eq.(14) up to leading order:

$$\tilde{\varepsilon} = \frac{1}{C^{p+1}} \left( \sum_{n \neq 0} \left| b_n^{(p+1)}(1) \right|^2 \right)^{p+3/2} \left| \sum_{n \neq 0} \text{Im} \left( b_n^{(p+1)}(1) b_n^{(p+2)}(1) \right) \right|^{p+T}.$$  

Given that $b_n^{(p+1)}$ and $b_n^{(p+2)}$ are of the same order of magnitude — as will be the case in our example — this expression shows a general, disadvantageous feature of boundary cancelation: although a very favorable scaling of the error with the run time is eventually obtained, that scaling is only reached for extremely low values of the error ($\propto 1/C^{p+1}$ for large $C$). As will be clear in our application to Grover search, practical error tolerances will often be above this bound, and, other drivings present acceptably low errors in a time shorter than $T_{val}$. Notice also that the trade-off is now valid for

$$T \geq \frac{T_{val}}{\alpha} \quad \text{for} \quad \varepsilon \leq \alpha^{p+1}\tilde{\varepsilon} \quad (0 < \alpha \leq 1).$$

Finally, a comment on the quantity $J_n$, which is present in $T_{val}$ [compare Eqs.(17,19), or Eqs.(8,10)]. This quantity is upper-bounded by

$$J_n(s) \leq \int_0^s \frac{\mathcal{F}_{\Phi_n}(s') ds'}{4 \text{min}_k \Delta_{kn}(s')},$$

where $\mathcal{F}_{\Phi_n}(s)$ is the quantum Fisher information of eigenstate $|\phi_n(s)\rangle$ with respect to $s$. It has been established that $\sqrt{\mathcal{F}_{\Phi_n}(s)}$ constitutes a speed for the evolution of the state $|\phi_n(s)\rangle$ when using the Fubini-Study metric [35, 41] and therefore is a figure of merit for the driving speed of the Hamiltonian $H(s)$. This relation establishes a connection between the adiabatic theorem and the differential geometry of the quantum state space, which will be explored as we apply these results to the Grover search.

### III. APPLICATION: ADIABATIC QUANTUM SEARCH

In the following, we apply the general results presented in the previous section to a concrete example given by the adiabatic quantum search algorithm, first presented in Ref. [7] and later modified in Ref. [22]. It is an adiabatic version of Grover’s original discrete quantum search algorithm [42]. Grover’s algorithm searches for a marked item in an unstructured database composed of $N$ items. It finds the marked item after $O(\sqrt{N})$ queries to a quantum “oracle”, whereas a classical algorithm has to query an “oracle”, on average, $N/2$ times in order to find the marked item. This means that the quantum algorithm leads to a quadratic speedup in solving this problem when compared to the best classical algorithm.

#### A. The adiabatic quantum search algorithm

The adiabatic quantum search algorithm is an important example of quantum speedup obtained via AQC. It uses $n = \log_2 N$ q-bits to represent the $N$ items of the database. Each item is represented by one of the elements $|x\rangle$ of the computational basis, with $x = 0, \cdots, N - 1$, while the
marked item is represented by $|m\rangle$. The oracle Hamiltonian is given by $H_f = 1 - |m\rangle\langle m|$, which has $|m\rangle$ as ground state with eigenvalue 0. The $n$ q-bits are initialized in the uniform superposition state $|\sigma\rangle = 1/\sqrt{N} \sum_{x=0}^{N-1} |x\rangle$ and are submitted to the action of a time-dependent Hamiltonian which interpolates between the initial Hamiltonian $H_i = 1 - |\sigma\rangle\langle \sigma|$ which has $|\sigma\rangle$ as ground state with eigenvalue 0, and the final Hamiltonian $H_f$:

$$H(s)/\mathcal{E} = (1-f(s)) H_i + f(s) H_f$$

$$= (1-f(s)) (1-|\sigma\rangle\langle \sigma|) + f(s) (1-|m\rangle\langle m|),$$

where $\mathcal{E}$ is a dimensional constant that establishes the energy scale and $f(s)$ is a monotonically increasing function with $f(0) = 0$ and $f(1) = 1$. Since the system is initialized in the state $|\sigma\rangle$, its evolution will remain in the subspace spanned by $|\sigma\rangle$ and $|m\rangle$. The problem may, then, be studied in the two-dimensional subspace spanned by $|m\rangle$ and $|m_\perp\rangle = \sqrt{N-1} / \sqrt{N} (|\sigma\rangle - 1/\sqrt{N}|m\rangle)$. In this subspace, the Hamiltonian $H(s)/\mathcal{E}$ reduces to

$$H(s)/\mathcal{E} |_{|m\rangle,|m_\perp\rangle} = \begin{pmatrix} (N-1)/N & \sqrt{N-1}/N (f(s)-1) \\ \sqrt{N-1}/N (f(s)-1) & (N-1)/N f(s) + 1/N \end{pmatrix}.$$  

Its dimensionless eigenvalues inside this subspace are given by

$$E_0(s) = \frac{1}{2} (1 - \Delta(s)),$$

$$E_1(s) = \frac{1}{2} (1 + \Delta(s)),$$

where

$$\Delta(s) = \sqrt{1 - 4 \left( \frac{N-1}{N} \right) f(s) (1-f(s))}.$$  

is the dimensionless gap between the two eigenvalues. The corresponding eigenstates can be written as

$$|\phi_0(s)\rangle = \sin \frac{\theta(s)}{2} |m\rangle + \cos \frac{\theta(s)}{2} |m_\perp\rangle$$

$$|\phi_1(s)\rangle = \cos \frac{\theta(s)}{2} |m\rangle - \sin \frac{\theta(s)}{2} |m_\perp\rangle,$$

where

$$\sin \frac{\theta(s)}{2} = \frac{1}{\sqrt{2}} \left( 1 - \frac{2(N-1)}{N} (1-f(s)) - \frac{1}{\Delta(s)} \right)^{1/2}$$

$$\cos \frac{\theta(s)}{2} = \frac{1}{\sqrt{2}} \left( 1 + \frac{2(N-1)}{N} (1-f(s)) - \frac{1}{\Delta(s)} \right)^{1/2}.$$  

The remaining $N-2$ eigenstates of $H(s)/\mathcal{E}$ outside the two-dimensional subspace have a common constant eigenvalue $E_2 = 1$.

Later in this section we shall need the transition matrix element $\langle \phi_1(s)|\dot{H}(s)/\mathcal{E} |\phi_0(s)\rangle$, which can be determined straightforwardly from Eqs. (23) and (27)-(30):

$$\langle \phi_1(s)|\dot{H}(s)/\mathcal{E} |\phi_0(s)\rangle = -\sqrt{N-1} \frac{\dot{f}(s)}{\Delta(s)}.$$  

**B. Error-run-time relations**

We apply now the general results of Section II A to the adiabatic quantum search algorithm in order to obtain a tradeoff relation between the error $\varepsilon$ and the run time $T$ for this problem. First we shall consider the traditional interpolation schedules, which do not require that derivatives of $H(s)$ vanish at $s = 0$ and $s=1$. We begin by adapting the expression for the upper bound to the error $\varepsilon$ in Eq. (7) and the expression for $T_{\text{opt}}$ in Eq. (8) to the two-dimensional problem. They become
\[ \varepsilon \leq \frac{h}{\mathcal{E}T} \left( \left| \frac{\langle \phi_1(1)|\dot{H}(1)/\mathcal{E}|\phi_0(1)\rangle}{\Delta^2(1)} \right| + \frac{\left| \langle \phi_1(0)|\dot{H}(0)/\mathcal{E}|\phi_0(0)\rangle \right|}{\Delta^2(0)} \right) + O\left( \frac{1}{T^2} \right) \]  

(32)

\[ T_{\text{val}} = C \frac{h}{\mathcal{E}} \left| \text{Im} \left( \frac{b_1^{(1)}(1) b_1^{(2)}(1)}{|b_1^{(1)}(1)|^2} \right) \right| = C \frac{h}{\mathcal{E}} \left| \text{Im} \left( \frac{b_1^{(2)}(1)}{b_1^{(1)}(1)} \right) \right|. \]  

(33)

The coefficients \( b_1^{(1)}(1) \) and \( b_1^{(2)}(1) \) can be obtained from Eqs. (9) and (10), respectively. They read

\[ b_1^{(1)}(1) = e^{iT\omega_1(1)} \lambda_1(1) - \lambda_1(0) \]  

(34)

\[ b_1^{(2)}(1) = e^{iT\omega_1(1)} \left[ J_0(1) \lambda_1(1) + \lambda_1(0) \right] + \left[ J_1(1) \lambda_1(0) + \lambda_1(0) \right], \]  

(35)

where

\[ \lambda_1(s) = \frac{\langle \phi_1(s)|\dot{\phi}_1(0)\rangle}{\Delta(s)} = -\frac{\langle \phi_2(s)|\dot{H}(s)/\mathcal{E}|\phi_0(s)\rangle}{\Delta^2(s)} \]  

(36)

\[ J_0(1) = -J_1(1) = \int_0^1 \left| \frac{\langle \phi_1(s)|\dot{\phi}_0(0)\rangle}{\Delta(s)} \right|^2 ds, \]  

(37)

and we have used that \( \Delta(0) = \Delta(1) = 1 \). In the two interpolation examples which we shall consider in the following, the properties of \( f(s) \) are such that \( \lambda_1(0) = \lambda_1(1) \) and \( \lambda_1(0) = -\lambda_1(1) \). For these most common choices of \( f(s) \), we have

\[ b_1^{(1)}(1) = \lambda_1(1) \left( e^{iT\omega_1(1)} - 1 \right) \]  

(38)

\[ b_1^{(2)}(1) = \left( J_0(1) \lambda_1(0) + \lambda_1(0) \right) \left( e^{iT\omega_1(1)} + 1 \right). \]  

(39)

Notice that for \( T = T_n = 2n\pi/\omega_{\text{ad}}(1) \), where \( n = 1, 2, \ldots \), the coefficient \( b_1^{(1)}(1) \) vanishes. This means that at those specific run times the leading term of \( D[|\Psi(1, T)|] \), \( |\phi_0(1)| \) is of order of \( 1/T_n \), and the leading term becomes of the order of \( 1/T_n^2 \). This happens because of a boundary symmetry of the Hamiltonian \( H(s) \), which is manifest in the condition \( \lambda_3(1) = \lambda_1(0) \). The use of such classes of symmetries as a technique to improve the scaling of the error \( \varepsilon \) with \( T \), at certain discrete values of \( T \), was proposed in Ref. [32] and applied to the adiabatic search problem. While the authors of Ref. [32] could only confirm the improvement of the scaling of \( \varepsilon \) with \( T \) from numerical evidence, we can easily calculate the error \( \varepsilon(T_n) \) at the times \( T_n \) via Eqs. (5),(6),(38) and (39):

\[ \varepsilon(T_n) = -\frac{h^2}{(\mathcal{E}T_n)^2} \text{Im} \left( \frac{b_1^{(1)}(1) b_1^{(2)}(1)}{|b_1^{(1)}(1)|^2} \right) + O\left( \frac{1}{T_n^3} \right) \]  

(40)

Since the change in the scaling of \( \varepsilon \) will happen only at discrete values of \( T \), we shall ignore this oscillatory behavior and use an upper bound to the value of \( \varepsilon \) given by Eq. (32), which can be rewritten as

\[ \varepsilon \leq \frac{h}{\mathcal{E}T^2} |\lambda_1(1)| + O\left( \frac{1}{T^2} \right), \]  

(41)

where we made use of Eq. (36) and of the relation \( \lambda_1(1) = \lambda_1(0) \). Due to the boundary symmetries of \( H(s) \), the coefficient \( b_1^{(2)}(1) \) will also vanish at times \( T = T_n = (2n + 1)\pi/\omega_{\text{ad}}(1) \), where \( n = 0, 1, \ldots \), which are all different from the times \( T_n \) at which the coefficient \( b_1^{(1)}(1) \) vanishes. At the discrete set of times \( T_n \), the term of order \( 1/T^2 \) in \( D[|\Psi(1, T)|] \), \( |\phi_0(1)| \) vanishes [Eq. (5)] and the next to leading order term is of order of \( 1/T^3 \). At those times, Eq. (33) cannot be applied without modifications, but they constitute a zero-measure set of discrete points. In order to correctly handle the oscillatory behaviors of \( b_1^{(1)}(1) \) and \( b_1^{(2)}(1) \) in the evaluation of \( T_{\text{val}} \), we shall take the contributions of the oscillatory terms to \( b_1^{(1)}(1) \) and \( b_1^{(2)}(1) \) in Eqs. (38) and (39) at their point of maximum absolute value. Under these conditions, we reach

\[ T_{\text{val}} = \frac{h}{\mathcal{E}} \left| C J_0(1) + \frac{\lambda_1(1)}{\lambda_1(0)} \right|. \]  

(42)
We are now in a position to derive explicit trade-off relations between the error \( \varepsilon \) and the run time \( T \). Let us first consider the second term in Eq. (42). This term depends only on the ground state, the Hamiltonian \( H(s) \), and the instantaneous speed \( \dot{f}(s) \) of the path. Let us consider the second term in Eq. (10). This term depends only on the value of the parameters \( s \) and \( \lambda(s) \). Making use of Eqs. (26) and (36), we can write

\[
\frac{\lambda_{10}(1)}{\lambda_{10}(1)} = \frac{\tilde{f}(1)}{f(1)} - 6 \left( \frac{N - 1}{N} \right) f(1). \tag{43}
\]

Let us now consider more closely the term \( J_0(1) \). Using Eq. (37), \( J_0(1) \) can be rewritten as

\[
J_0(1) = \frac{1}{4} \int_0^1 \frac{F_{\phi_0}(s)}{\Delta(s)} ds, \tag{44}
\]

where

\[
F_{\phi_0}(s) = 4 \left| \langle \phi_1(s) | \phi_0(s) \rangle \right|^2 = 4 \left| \langle \phi_1(s) | H(s)/\mathcal{E} | \phi_0(s) \rangle \right|^2 / \Delta^2(s) = \left[ \frac{\sqrt{N - 1}}{N} \frac{\tilde{f}(s)}{\Delta^2(s)} \right]^2. \tag{45}
\]

is the quantum Fisher information of the instantaneous ground state \( |\phi_0(s)\rangle \) with respect to \( s \). As stated previously, \( \sqrt{F_{\phi_0}(s)} \) is proportional to the instantaneous speed of separation between two neighboring states \( |\phi_0(s)\rangle \) and \( |\phi_0(s + ds)\rangle \) when using the Fubini-Study metric [35, 41]. That is, \( \sqrt{F_{\phi_0}(s)} \) is proportional to the instantaneous speed of the ground state \( |\phi_0(s)\rangle \) when moving along the path joining the states \( |\phi_0(0)\rangle \) and \( |\phi_0(1)\rangle \) in the state space. This shows that \( J_0(1) \) is a geometrical quantity, in a differential geometric sense. It is natural, then, to investigate the properties of the path, determined by \( f(s) \), which minimizes \( J_0(1) \) and, consequently, \( T_{val} \). For this purpose, consider the quantity

\[
K = \frac{1}{4} \int_0^1 F_{\phi_0}(s) ds, \tag{46}
\]

which is called the action of the path followed by \( |\phi_0(s)\rangle \) when moving from \( |\phi_0(0)\rangle \) to \( |\phi_0(1)\rangle \). Using the Cauchy-Schwarz inequality, it is straightforward to show that

\[
K \geq \left( \int_0^1 \sqrt{F_{\phi_0}(s)/2} ds \right)^2 = \mathcal{L}^2, \tag{47}
\]

where \( \mathcal{L} \) is the Bures length, as defined by Uhlmann [43], of the path in the state space followed by \( |\phi_0(s)\rangle \). Equality in the above expression occurs when the integrand is constant, that is, when \( F_{\phi_0}(s) \) is constant. We shall minimize \( J_0(1) \) by minimizing the action \( K \). This happens when

\[
\sqrt{F_{\phi_0}(s)} = L_{sh} = D(|\phi_0(0)\rangle, |\phi_0(1)\rangle) = \arccos \left( 1/\sqrt{N} \right), \tag{48}
\]

where \( L_{sh} \) is the Bures length of the shortest path between \( |\phi_0(0)\rangle \) and \( |\phi_0(1)\rangle \). By definition, this is equal to the distance \( D \) [Eq. (2)] between \( |\phi_0(0)\rangle \) and \( |\phi_0(1)\rangle \) — i.e., between \( |\sigma\rangle \) and \( |\nu\rangle \) —, which is in fact attained by this interpolation. Notice that this choice of \( F_{\phi_0}(s) \) forces the state \( |\phi_0(s)\rangle \) to move with constant speed along a geodesic in the state space. From Eq. (45), one can see that, in order to maintain \( F_{\phi_0}(s) \) constant along the whole evolution, the rate of change of the Hamiltonian \( H(s) \) has to be adapted to the local value of the gap \( \Delta(s) \). When the gap decreases, the Hamiltonian \( H(s) \) has to change slower, whereas, when the gap increases, \( H(s) \) changes faster.

We look now for the interpolation \( f(s) \) which satisfies condition (48). Using Eq. (45), one can show that, in order to satisfy condition (48), \( f(s) \) has to be the solution of

\[
f(s) = \frac{N}{\sqrt{N - 1}} \arccos \left( 1/\sqrt{N} \right) \Delta^2(s), \tag{49}
\]

with the conditions \( f(0) = 0 \) and \( f(1) = 1 \) [notice that \( \Delta \) depends on \( s \) through \( f(s) \), see Eq. (26)]. The solution is given by

\[
f(s) = \frac{1}{2} \left[ 1 + \frac{1}{\sqrt{N - 1}} \tan \left( \arctan \left( \sqrt{N - 1} \right)(2s - 1) \right) \right], \tag{50}
\]

where we used \( \arccos \left( 1/\sqrt{N} \right) = \arctan \sqrt{N - 1} \). This interpolation was first proposed in Ref. [22] as a solution to a “local adiabatic condition” and was found to be optimal. More recently, in Refs. [40, 44, 45], the authors used differential geometric techniques to obtain the same interpolation as an adiabatic geodesic.

We determine now the value of \( T_{val} \) when the interpolation in \( H(s) \) is given by Eq. (50). Using Eqs. (43) and (49), we obtain

\[
\frac{\lambda_{10}(1)}{\lambda_{10}(1)} = -2 \arccos \left( 1/\sqrt{N} \right) \sqrt{N - 1}. \tag{51}
\]

In order to evaluate \( J_0(1) \), we may make use of Eq. (49) to perform a change of variables in the integration. The result is

\[
J_0(1) = \arccos \left( 1/\sqrt{N} \right) \sqrt{N - 1}. \tag{52}
\]
Substituting these expressions in Eq. (42), we get finally

\[ T_{\text{val}} = \frac{\hbar}{\varepsilon} C \arccos \left( \frac{1}{\sqrt{N}} \right) \sqrt{N - 1}. \]  

(53)

The upper bound to the error \( \varepsilon \) [Eq. (41)], for the interpolation (50), can be straightforwardly calculated with the use of Eq. (36):

\[ \varepsilon \leq \frac{\hbar}{\sqrt{N}} 2 \arccos \left( \frac{1}{\sqrt{N}} \right) + O \left( \frac{1}{T^2} \right). \]  

(54)

Substituting \( T_{\text{val}} \) in the above expression, we obtain \( \tilde{\varepsilon} \), which is the upper bound to \( \varepsilon \) at \( T = T_{\text{val}} \) and establishes the largest value of \( \varepsilon \) for which the error-run-time relations in Eqs. (32), (41) and (54) are still valid:

\[ \tilde{\varepsilon} = \frac{2}{C \sqrt{N^2} - 1}. \]  

(55)

At this point, it is important to stress the meanings of \( T_{\text{val}} \) and \( \tilde{\varepsilon} \). Since bounds on the error \( \varepsilon \) like those in Eqs. (7), (32), and (41) result from a truncation in first order of an expansion of the error \( \varepsilon \) in powers of \( 1/T \), they are not valid for arbitrary values of \( T \) and/or \( \varepsilon \). Instead of relying on the vagueness of conditions like \( T \gg 1 \) and/or \( \varepsilon \ll 1 \), we are able to specify, via the value of \( T_{\text{val}} \), the values of \( T \) for which those relations are valid, namely \( T \geq T_{\text{val}} \), and, consequently, \( \varepsilon \leq \tilde{\varepsilon} \).

Notice that, for \( N \gg 1 \), \( \tilde{\varepsilon} \approx \frac{2}{C \sqrt{N}} = O \left( \frac{1}{\sqrt{N}} \right) \) and \( T_{\text{val}} \approx \frac{2}{C \varepsilon^2} \sqrt{N} = O \left( \sqrt{N} \right) \). This means that, in order to reach an error of \( O(1/\sqrt{N}) \) with the use of interpolation (50), the adiabatic search algorithm will need a run time of \( O(\sqrt{N}) \). This is precisely the trade-off relation between error and run time of the original Grover’s algorithm [22] in the limit of \( N \gg 1 \). Until now, evidence that, with the use of interpolation (50), a run time of \( O(\sqrt{N}) \) leads to a small error \( \varepsilon \) has been only numerical [9]. Here, we show analytically that this, in fact, happens, beside presenting a tight bound on the value of \( \varepsilon \).

In order to show that the use of relations like Eq. (54), without a clear statement about their domain of validity, can be problematic, let us consider the first result concerning the run time necessary to reach an error \( \varepsilon \) (for \( \varepsilon \ll 1 \)) with the use of interpolation (50) [22, 46]. There, it was found that, in order to reach an error \( \varepsilon \), the run time of the algorithm should be \( T \approx (\pi/2\varepsilon) \sqrt{N} \), for \( N \gg 1 \). Since this time scales with \( \sqrt{N} \), the same scaling of the original Grover’s algorithm, it was concluded that the adiabatic search algorithm, when using interpolation (50), is equivalent to the original circuit algorithm. However, for an error \( \varepsilon = O(1/\sqrt{N}) \), that relation would predict a run time \( T = O(N) \), which does not correspond to the run time of Grover’s algorithm for this error. On the other hand, Eq. (53) shows that, for fixed \( \varepsilon \ll \tilde{\varepsilon} \), the run time \( T \) scales, in fact, with \( \sqrt{N} \). This was also checked numerically by the authors of [22]. The same happens for the run time estimate obtained in [40] without relying on a truncation at first order of an expansion in powers of \( 1/T \) of the error \( \varepsilon \). It states that, in order to reach an error \( \varepsilon \), the run time should be \( T = O(\sqrt{N} \ln(1/\varepsilon)) \). For an error \( \varepsilon = O(1/\sqrt{N}) \), this relation would predict a run time \( T = O(\sqrt{N} \ln N) \). The problem in these relations is the presence of the “free” parameter \( \varepsilon \). For this reason, we use instead Eq. (12) for establishing a trade-off relation between error and run time and refrain of making any statement for \( \varepsilon > \tilde{\varepsilon} \) and/or \( T < T_{\text{val}} \).

To check the correctness of our results, we solved numerically the Schrödinger equation corresponding to the Hamiltonian \( H(s) \) [Eq. (23)] and compared the distance between the physical state of the system \( |\Psi(1, T)\rangle \), evolved via the Schrödinger equation, and the instantaneous ground state \( |\phi_0(T)\rangle \) with the upper bound on the error \( \varepsilon \), given in Eq. (54), for different values of \( T \). This comparison is shown in Fig. 1 and corroborates the correctness of the trade-off relation between \( \varepsilon \) and \( T \) we derived for interpolation (50).
We turn our attention now to the linear interpolation presented in the first proposal of the adiabatic search algorithm [7]. Although it has been shown that this interpolation leads to a run time of $O(N)$ and, for this reason, did not bring any advantage when compared to a classical search algorithm, it remains the unsolved issue of the value of the error $\varepsilon$ reached at this run time.

For this interpolation, $f(s) = s$. We begin with the determination of $T_{val}$. Using Eq. (43), we obtain

$$\frac{\dot{\lambda}(1)}{\lambda(1)} = -6 \left( \frac{N-1}{N} \right),$$

where we used $\dot{f}(s) = 1$ and $\ddot{f}(s) = 0$. The use of Eqs. (44) and (45) leads to

$$J_0(1) = \left( \frac{N-1}{N} \right) \int_0^1 \frac{ds}{\Delta^3(s)} = \frac{1}{3} \left( \frac{N-1}{N} \right) + \frac{2}{3} (N-1).$$

Putting these two expressions into into Eq. (42), produces finally

$$T_{val} = \frac{\hbar}{\tilde{\varepsilon}} \left[ \frac{1}{3} \left( \frac{N-1}{N} \right) \right] C \left[ 2(N-1) - 17 \left( \frac{N-1}{N} \right) \right].$$

The upper bound to the error $\varepsilon$ [Eq. (41)] can be obtained with the use of Eq. (36):

$$\varepsilon \leq \frac{\hbar}{\tilde{\varepsilon} 2 N - 1} + O\left( \frac{1}{T^2} \right).$$

Substituting $T_{val}$ in the above expression, we obtain $\tilde{\varepsilon}$ [Eq. (11)], which is the upper bound to $\varepsilon$ at $T = T_{val}$:

$$\tilde{\varepsilon} = \frac{6}{C \left( 2N - 17 \right) \sqrt{N - 1}}.$$

Now, for $N \gg 1$, $\tilde{\varepsilon} \approx 3/(CN^{3/2}) = O(1/N^{3/2})$ and $T_{val} \approx \frac{\hbar}{\tilde{\varepsilon}} C 2N/3 = O(N)$. This means that, to reach an error $\varepsilon = O(1/N^{3/2})$, the use of the linear interpolation requires a run time $T = O(N)$. This is the well known linear scaling of the run time with $N$ for the linear interpolation. It has been derived already in Refs. [7, 22] as $T = O(N/\varepsilon)$ and in Ref. [40] as $T = O(N \ln(1/\varepsilon))$. Notice that, if one requires an error $\varepsilon = O(1/N^{3/2})$, both these relations predict a run time very different from $O(N)$, showing, once more, the problem of having the error $\varepsilon$ playing the role of a free parameter.

Fig.2 compares our analytical results with the corresponding quantities produced by a numerical solution of the Schrödinger equation, confirming the validity of our results.

For fixed value of $N$, the linear interpolation has a larger value of $T_{val}$ than interpolation (50). This means that, when the relations derived here for the linear interpolation are
valid, the same happens for the relations derived for interpolation (50). One could then ask about the run time required by interpolation (50) to reach the same error as the linear interpolation reaches with a run time \( T = O(N) \). This can be easily answered with the use of Eq. (12), with \( \alpha \) set as the ratio of the values of \( \varepsilon \) for both interpolations. For \( N \gg 1 \), this gives
\[
T = \frac{T_{\text{val}}}{\alpha} = \frac{2N}{3}T_{\text{val}} = \frac{\hbar}{\mathcal{E}}C\frac{\pi N^{1/2}}{3},
\] (61)
where we used the value of \( T_{\text{val}} \) for interpolation (50). Interestingly, this time is \( \sqrt{N} \) larger than the time required by the linear interpolation (cf. Fig.2), although interpolation (50) is considered optimal in the sense that its run time scales with \( \sqrt{N} \). This shows that optimality of a given interpolation has to be stated carefully, taking into account the final error one wants to reach.

We consider now Hamiltonian evolutions obeying the boundary-cancelation condition (13). A Hamiltonian \( H(s) \) which obeys this boundary-cancelation condition can be built with a function \( f(s) \) obeying \( f^{(j)}(0) = 0 = f^{(j)}(1) \) for \( j = 1, \ldots, p \). The minimal-order polynomial that satisfies these conditions up to order \( p \) can be written as \([32, 40]\)
\[
f_p(s) := \int_0^s x^p(1-x)^p dx = I_s(p + 1, p + 1),
\] (62)
where \( I_s(p + 1, p + 1) \) is the regularized incomplete \( \beta \) function. Notice that \( f_p(s) \) satisfies the following relations:
\[
f_p^{(p+1)}(0) = (-1)^p f_p^{(p+1)}(1); f_p^{(p+2)}(0) = (-1)^{p+1} f_p^{(p+2)}(1).
\] (63)
These relations imply that
\[
\lambda_{10}^{(p)}(1) = (-1)^p \lambda_{10}^{(p)}(0) = \frac{\sqrt{N-1}}{N} f_p^{(p+1)}(1).
\] (64)
Now, using the results of Sec. II B and proceeding in the same way as in the previous cases, it is straightforward to show that
\[
T_{\text{val}} = \frac{\hbar}{\mathcal{E}} C \left| J_0(1) + \frac{f_p^{(p+2)}(1)}{f_p^{(p+1)}(1)} \right| = \frac{\hbar}{\mathcal{E}} C |J_0(1)+p(p+1)|,
\] (65)
with
\[
J_0(1) = \frac{N-1}{N^2} \int_0^1 \frac{f_p^2(s)}{\Delta^3(s)} \, ds
\] (66)
\[
\approx \frac{N}{2} \left( 1 + \sqrt{p} + \frac{p}{20} \right),
\] (67)
where the \( O(N) \) dependence is valid in general for \( N \gg 1 \), and the approximate value including the dependence on \( p \) is correct up to 5\% error. One can then write:
\[
T_{\text{val}} \approx \frac{\hbar}{\mathcal{E}} C \frac{N}{2} \left( 1 + \sqrt{p} + \frac{p}{20} \right) + p(p+1).
\] (68)
Notice that \( T_{\text{val}} \) for this case has the same scaling with \( N \) as \( T_{\text{val}} \) for the linear interpolation case.

The upper bound on the error \( \varepsilon \) can be obtained via the same proceeding:
\[
\varepsilon \leq \frac{\hbar^{p+1}}{(\mathcal{E}T)^{p+1}} \frac{2\sqrt{N-1}}{N} \frac{2^p + 1}{p!},
\] (69)
where we used \( |f_p^{(p+1)}(1)| = (2p+1)!/p! \). Using Eqs. (68) and (69), we can determine \( \varepsilon \), the upper bound to \( \varepsilon \) at \( T = T_{\text{val}} \) for \( N \gg 1 \):
\[
\varepsilon \approx \frac{1}{C^{p+1}} \frac{2^{p+2}(2p+1)!}{1 + \sqrt{p} + p/20} \frac{1}{N^{p+3/2}}.
\] (70)
Therefore, in order to reach an error \( \varepsilon = O(N^{p+3/2}) \), the use of an interpolation which satisfies the boundary-cancelation condition (13) requires a run time \( T = O(N) \), with a prefactor increasing with \( p \). This means that this interpolation reaches a much smaller final error than the linear one, but requires a longer run time, although with the same scaling in \( N \). Notice that this also happens in comparison with interpolation (50): for run times larger or equal to \( T = O(N) \), the error reached by the current interpolation is much smaller than the error reached by interpolation (50), showing that, besides the scaling with the size of the problem, it is important to take into account the error reached by each interpolation for a given value of the run time \( T \). Fig. 3 compares the behavior of the error \( \varepsilon \) with the run time \( T \) for the different interpolation we have considered here. The smaller asymptotic error typically comes at the price of a longer necessary convergence time.

**IV. FINAL COMMENTS**

We have obtained errors of the adiabatic approximation for finite driving times \( T \) beyond scaling relations. Using the Bures angle between the actual state of the system and the instantaneous ground state of the Hamiltonian at time \( T \) as a figure of merit for the error, we derived general results for the trade-off relation between the run time \( T \) and the error \( \varepsilon \).
linear interpolation \( p = 0 \)

\[
p = 1 \quad p = 2
\]

\( N = 32 \)

Figure 3. Behavior of the error in adiabatic search using boundary cancelation. Upper bounds [from Eq.(69)], distance up to leading order [from Eq.(6)] and direct numerical calculation are displayed as in Figs. 1, 2. With each successive order \( p \) a smaller error value is attained, as seen in Eq.(70), at the cost of a longer \( T_{val} \). These validity times are obtained from Eq.(68) by setting \( C = 50 \) for \( p = 1 \) and \( C = 70 \) for \( p = 2 \).

in terms of quantities with very clear physical interpretations. With the use of the Adiabatic Perturbation Theory (APT), we performed an expansion of the error \( \epsilon \) for small values of \( 1/T \) up to next-to-leading-order terms. This allowed us to delimit the domain of validity of the trade-off relations obtained via leading-order approximations and, consequently, to explicitly determine the shortest time \( T = T_{val} \) and the largest error \( \tilde{\epsilon} = \epsilon \) for which these relations are valid. When the use of these relations is restricted to values of \( \epsilon \leq \tilde{\epsilon} \) and/or \( T \geq T_{val} \), they give correctly the value of the error \( \epsilon \) for a given run time \( T \) or the value of the run time \( T \) required for reaching a given error \( \epsilon \), going, in this way, beyond scaling only relations. In our opinion, this approach corrects some problems which are present in several trade-off relations derived so far, where the error \( \epsilon \) appears as a “free” parameter, although those relations rely on some truncated expansion of \( \epsilon \) in powers of \( 1/T \) and, for this reason, are not valid for arbitrary values of \( \epsilon \).

We applied these results to the adiabatic quantum search algorithm, which, besides being of practical importance for AQC, admits an exact analytical treatment. With our approach, we were able to reobtain the interpolation which is considered optimal for this algorithm via a minimization of the functional for the shortest time \( T_{val} \) for which the relations we derived still apply. More importantly, apart from getting the right scaling of the run time with the system size \( N \), we could determine for the first time the actual value of the final error for that interpolation. We also investigated other classes of interpolations recently proposed in the literature and obtained for them, in the same way, the value of the errors reached at a given run time. In doing so, we could show that traditional scaling-only trade-off relations, although showing the right scaling of the run time with \( N \), do not produce the correct value of the run time \( T \) for a given value of the error \( \epsilon \).

We believe that our approach offers a viable alternative for deriving trade-off relations between error and run time for quantum adiabatic algorithms, relations which allow for precise estimations of the run time required for an algorithm to be performed with a given error.

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Appendix A: Expansion of the distance in the parameter \( 1/T \)

In this Appendix, we demonstrate the expansion of the Bures angle in the small parameter \( 1/T \) up to second nonvanishing order [Eqs.(5,14)]. In fact, there is a two-fold dependence of the Bures angle on \( T \). On one hand, there is the dependence expressed in the expansion of Eq.(4),

\[
b_n(s, T) = \sum_{p=0}^{\infty} \frac{(i\hbar)^p}{T^p} b_n^{(p)}(s). \tag{A1}
\]

On the other hand, \( b_n^{(p)}(s) \) may still depend on \( T \) (through a complex exponential). We will make a perturbative expansion of \( D[|\Psi(s, T)|, |\phi_0(s)|] \) in the small parameter \( 1/T \), which should not be confused with a genuine power-series expansion. This means that the expansion is made as if \( b_n^{(p)}(s) \) did not depend on \( T \). We assume \( b_n^{(0)} = \delta_{n0} \) (recovering the infinite-time result), and also that we calculate the distance at a time \( s \) at which the coefficients \( b_n^{(q)}(s) = 0 \) for \( n \neq 0 \) and \( q = 1, 2, ..., p \). Eq. (5) will correspond to \( p = 0 \) (for any value of \( s \)), and for the boundary-cancelation case \( (p \geq 1) \), this assumption will be proven for \( s = 1 \) in Appendix B.

Let us express the Bures angle between the instantaneous ground state \( |\phi_0(s)\rangle \) and the state of the system \( |\psi(s, T)\rangle \). Because a truncated expression for \( |\psi(s, T)\rangle \) does not preserve normalization [21] (as usual in perturbation theories), we replace Eq.(2), written for normalized states, for an expression not assuming a normalized \( |\Psi(s, T)\rangle \) [34, 37],

\[
D[|\Psi(s, T)|, |\phi_0(s)|] := \arccos \left( \frac{1}{\sqrt{|\Psi(s, T)|}_{\Psi(s, T)}} \right),
\tag{A2}
\]

where \( |\phi_0(s)\rangle \) is still assumed normalized. In terms of the coefficients in Eq.(3),

\[
D[|\Psi(s, T)|, |\phi_0(s)|] = \arccos \left( \frac{1}{\sqrt{1 + \sum_{n \neq 0} |b_n(s, T)|^2}} \right). \tag{A3}
\]

We define \( w := \sum_{n \neq 0} |b_n(s, T)|^2/|b_0(s, T)|^2 \), which, together with a trigonometric identity, allows us to write

\[
D[|\Psi(s, T)|, |\phi_0(s)|] = \arctan \sqrt{w}. \tag{A4}
\]

We can expand (A4) in a power series as

\[
D[|\Psi(s, T)|, |\phi_0(s)|] = w^{1/2} - \frac{1}{3} w^{3/2} + O(w^{5/2}), \tag{A5}
\]

which converges absolutely for \(|w| < 1 \) or \( D[|\Psi(s, T)|, |\phi_0(s)|] < \pi/4 \).
From Eq.(A1), we find that

\[ w = \left( \frac{\hbar}{T} \right)^{2p+2} \sum_{n \neq 0} \left| b_n^{(p+1)} \right|^2 + \frac{\hbar}{T} 2 \text{Re}(i b_n^{*(p+1)} b_n^{(p+2)}) + O(1/T^2) \]

\[ w = \frac{\hbar^{2p+2}}{T^{2p+2}} \sum_{n \neq 0} \left( \left| b_n^{(p+1)} \right|^2 + \frac{\hbar}{T} \left[ 2 \text{Re}(i b_n^{*(p+1)} b_n^{(p+2)}) - \left| b_n^{(p+1)} \right|^2 2 \text{Re}(i \hbar/T b_n^{(1)}) \right] + O(1/T^2) \right), \tag{A6} \]

where \( b_n^{(p+1)} \) is the first nonvanishing coefficient for \( n \neq 0 \), but \( b_0^{(1)} \neq 0 \) in general. We see that \( w^{1/2} = O(1/T^{p+1}) \)

and the two leading terms will be of order \( 1/T^{p+1} \), \( 1/T^{p+2} \), with \( w^{3/2} = O(1/T^{3p+3}) \) being neglected (since \( 1/T^{3p+3} \) is higher-order than \( 1/T^{p+2} \) for any \( p \geq 0 \)). Then,

\[ D[|\Psi(s, T)|, |\phi_0(s)|] = \frac{\hbar^{p+1}}{T^{p+1}} \sqrt{\sum_{n \neq 0} \left| b_n^{(p+1)} \right|^2} \]

\[ + \frac{\hbar^{p+2}}{T^{p+2}} \left[ \sum_{n \neq 0} \text{Re}(i b_n^{*(p+1)} b_n^{(p+2)}) \right] - \frac{\hbar}{T} \sqrt{\sum_{n \neq 0} \left| b_n^{(p+1)} \right|^2} \text{Re} \left( \frac{\hbar}{T} b_0^{(1)} \right) + O \left( \frac{1}{T^{p+3}} \right), \tag{A7} \]

which yields Eq.(5) for \( p = 0 \). For \( p \neq 0 \), Eq.(14) is reached by using that \( b_0^{(1)} \) is real (proven in Appendix B).

**Appendix B: Leading coefficients**

In this Appendix, we calculate the leading coefficients of expansion (4) both for the general case, \( b_n^{(1)}(s) \), and with boundary cancelation, \( b_n^{(p+1)}(1) \) — both for \( n \neq 0 \). Along the way we demonstrate that the assumptions made in the previous Appendix are valid \( b_n^{(0)} = \delta_{n0} \) and \( b_n^{(q)}(s) = 0 \) for \( n \neq 0 \) up to \( q = p \).

**1. General Case**

We now need to calculate \( b_n^{(1)}(s) \) for \( n \neq 0 \). We begin by writing the coefficients in Eq.(4) as

\[ b_n^{(p)}(s) = \sum_{m=0} e^{iT \omega m(s)} b_m^{(p)}(s). \tag{B1} \]

Inserting Eqs. (4), (B1) into Eq.(3) we get

\[ |\Psi(s, T)| = \sum_{p=0}^{\infty} \sum_{n, m=0}^{\infty} \frac{(i \hbar)^p}{T^p} e^{-iT \omega m(s)} b_m^{(p)}(s) |\phi_n(s)|. \tag{B2} \]

At this point we impose that all the contributions higher than the zeroth order vanish at \( s = 0 \), i.e. \( b_n(0, T) = b_n^{(0)}(0) \) and

\[ b_n^{(p)}(0) = \sum_{m=0} b_m^{(p)}(0) = 0, \quad (p \geq 1). \tag{B3} \]
Furthermore we also impose that the zeroth order contribution is the adiabatic approximation,
\[ b_n^{(0)}(s) = b_n^{(0)}(0) = \delta_{n0} \Rightarrow b_{nm}^{(0)}(s) = b_n^{(0)}(0) = \delta_{n0}\delta_{nm}. \]  
(B4)

We now substitute (B2) into the Schrödinger Equation (Eq.1) and left-multiply it by \( \langle \phi_k(s) \rangle \), leading to the general recurrence relation
\[ \Delta_{nm}(s)b_{nm}^{(p+1)}(s) = b_{nm}^{(p)}(s) + \sum_{k \neq n} M_{nk}(s)b_{kn}^{(p)}(s), \]  
(B5)

where \( M_{nk}(s) := \langle \phi_n(s) | \phi_k(s) \rangle \) and \( M_{nn}(s) \) has been taken as zero without loss of generality.

Let us then calculate the terms \( b_{nm}^{(1)}(s) \), starting by the off-diagonal terms \( (n \neq m) \). From Eq.(B4) and Eq.(B5) with \( p = 0 \),
\[ b_{nm}^{(1)}(s) = \frac{M_{nm}(s)}{\Delta_{nm}(s)} \delta_{m0} = \lambda_{nm}(s)\delta_{m0}, \quad (n \neq m). \]  
(B6)

The recurrence relation (B5) furnishes a first-order differential equation for the diagonal terms,
\[ \ddot{b}_{nm}^{(1)}(s) + \sum_{k \neq n} M_{nk}(s)b_{kn}^{(1)}(s) = 0, \]  
(B7)

which can be integrated
\[ \dot{b}_{nm}^{(1)}(s) = \dot{b}_{nm}^{(1)}(0) - \int_0^s \sum_{k \neq n} M_{nk}(s')b_{kn}^{(1)}(s')ds' \]  
(B8)

and, for \( n \neq 0 \), solved using Eqs.(B6), (B3):
\[ \dot{b}_{nm}^{(1)}(s) = \dot{b}_{nm}^{(1)}(0) = -\sum_{m \neq n} b_{mn}^{(1)}(0) = -\lambda_{n0}(0). \]  
(B9)

From (B1), (B6) and (B9), one obtains the first-order contribution \( b_{nm}^{(1)}(s) \) as in Eq.(9), in accordance with [21]. One then substitutes that in Eq.(5) and, taking into account that
\[ M_{nm}(s) = -\frac{\langle \phi_n(s) | \hat{H}(s) | \phi_m(s) \rangle}{\Delta_{nm}(s)}, \]  
(B10)

Equation (6) is obtained. (Notice that equality (B10) is demonstrated by differentiating the eigenvalue equation.)

We take the opportunity to calculate \( b_{00}^{(1)}(s) \) from (B8), which will be necessary for a later result. We first note that, due to (B3) and (B6),
\[ b_{00}^{(1)}(0) = -\sum_{m \neq 0} b_{m0}^{(1)}(0) = 0. \]  
(B11)

Substituting (B6) in (B8) then gives
\[ \dot{b}_{00}^{(1)}(s) = -\int_0^s \sum_{k \neq 0} M_{0k}(s')\frac{M_{k0}(s')}{\Delta_{k0}(s')}ds' = J_0(s), \]  
(B12)

where \( M_{0k} \) has been used and
\[ J_n(s) = \sum_{k \neq n} \int_0^s \frac{|M_{kn}(s')|^2}{\Delta_{kn}(s')}ds', \]  
as defined in the main text.

2. Boundary cancelation

We will introduce several Lemmas to show that \( b_{n}^{(r)}(1) \) vanish up for \( r = 1, 2, ..., p \) and to calculate the value of \( b_{n}^{(p+1)}(1) \).

Lemma 1. For \( n \neq m \) the general form of the coefficients \( b_{nm}^{(p)}(s) \) is given by
\[ b_{nm}^{(p)}(s) = \sum_{q=0}^{p-1} \sum_{k \neq 0} \lambda_{nkm}(s)\chi_{kq}(s). \]  
(B14)

where \( \chi_{kq}(s) := \frac{d^q\lambda_{km}(s)}{ds^q} \) and \( \lambda_{nkm}(s) \) are coefficients to be obtained recursively.

Proof. The proof is by induction as follows: the statement holds for \( p = 1 \),
\[ b_{nm}^{(1)}(s) = \sum_{q=0}^{0} \sum_{k \neq 0} \lambda_{nkm}(s)\chi_{kq}(s), \]  
(B15)

if we set \( \lambda_{0}^{(0)} = \delta_{n0}\delta_{nm} \). Now we prove that if the statement holds for some \( p \), then it holds for \( (p + 1) \). We substitute (B14) into the right-hand side of the recurrence relation (B5) to obtain
\[ \Delta_{nm}(s)b_{nm}^{(p+1)}(s) = \sum_{q=0}^{p-1} \sum_{k \neq 0} \left( \lambda_{nkm}(s)\chi_{kq}(s) + \chi_{nkm}^{(1)}(s)\lambda_{km}^{(q+1)}(s) + \right) + \sum_{k \neq n,m} M_{nt}(s)\chi_{nt}(s)\lambda_{km}^{(q)}(s) + M_{nm}(s)b_{nm}^{(p)}(s). \]  
(B16)
The last term in (B16) can be rewritten as

\[ M_{nm}(s) b_{nm}^{(p)}(s) = \sum_{q=0}^{p-1} \sum_{k \neq m} \Delta_{nm}(s) \lambda_{km}^{(q)}(s) b_{nm}^{(p)}(s) \delta_{q0}\delta_{kn}, \quad (B17) \]

so that this term can be reincorporated into the sum (B16) as

\[ \Delta_{nm} b_{nm}^{(p+1)} = \sum_{q=0}^{p-1} \sum_{k \neq m} \left( \lambda_{km}^{(q)} + \lambda_{km}^{(q+1)} \right) b_{nm}^{(p)}(s) + \sum_{l \neq n,m} M_{nl} \chi_{lmk}^{p,q} + \Delta_{nm} b_{nm}^{(p)} \delta_{q0}\delta_{kn}, \quad (B18) \]

in which we have omitted the \( s \)-dependence. On the other hand, if we make \( q \to q - 1 \), then

\[ \sum_{q=0}^{p-1} \sum_{k \neq m} \lambda_{nmk}^{q}(s) \lambda_{km}^{(q+1)}(s) = \sum_{q=0}^{p-1} \sum_{k \neq m} \lambda_{nmk}^{q-1}(s) \lambda_{km}^{(q)}(s)(1 - \delta_{q0}) + \sum_{k \neq m} \lambda_{nmk}^{p-1}(s) \lambda_{km}^{(p)}(s) \]

which allows us to rewrite (B18) as

\[ \Delta_{nm} b_{nm}^{(p+1)} = \sum_{k \neq m} \lambda_{nmk}^{p-1}(s) \lambda_{km}^{(p)} + \sum_{q=0}^{p-1} \sum_{k \neq m} \left( \lambda_{nmk}^{q} + \lambda_{nmk}^{q-1}(1 - \delta_{q0}) + \right) + \sum_{l \neq n,m} M_{nl} \chi_{lmk}^{p,q} + \Delta_{nm} b_{nm}^{(p)} \delta_{q0}\delta_{kn}. \quad (B20) \]

Finally after the preceding rearrangements we can compare (B20) with the general form

\[ b_{nm}^{(p+1)} = \sum_{q=0}^{p} \sum_{k \neq m} \lambda_{nmk}^{q+1}(s) \lambda_{km}^{(q)}(s), \quad (B21) \]

which fits perfectly if we set

\[ \lambda_{nmk}^{p+1,p}(s) = \frac{\lambda_{nmk}^{p-1}(s)}{\Delta_{nm}(s)}, \quad (B22) \]

and, for \( q = 0, 1, ..., p - 1, \)

\[ \chi_{nmk}^{p+1,q}(s) = \frac{1}{\Delta_{nm}(s)} \left( \chi_{nmk}^{p,q}(s) + \chi_{nmk}^{p,q-1} \delta_{q0} (1 - \delta_{q0}) + \right) + \sum_{l \neq n,m} M_{nl}(s) \chi_{lmk}^{p,q} + \Delta_{nm}(s) b_{nm}^{(p)}(s) \delta_{q0}\delta_{kn}. \quad (B23) \]

which concludes the proof.

Lemma 1 leads to a Corollary.

**Corollary 2 (Off-diagonal terms).** The condition

\[ H^{(1)}(\bar{\bar{s}}) = H^{(2)}(\bar{\bar{s}}) = \cdots = H^{(p)}(\bar{\bar{s}}) = 0 \quad (B24) \]

at some time \( \bar{\bar{s}} \in [0, 1] \) implies, for \( n \neq m, \)

\[ b_{nm}^{(1)}(\bar{\bar{s}}) = b_{nm}^{(2)}(\bar{\bar{s}}) = \cdots = b_{nm}^{(p)}(\bar{\bar{s}}) = 0. \quad (B25) \]

**Proof.** First notice that the Leibniz rule for derivatives provides

\[ \lambda_{nm}^{q}(s) = \sum_{j=0}^{q} \frac{q!}{(q-j)!j!} \frac{d^j M_{nm}(s)}{ds^j} \frac{d^{q-j}}{ds^{q-j}} \left( \frac{1}{\Delta_{nm}(s)} \right), \quad (B26) \]

an expression in which, due to (B10), every term involves a derivative of \( H(s) \) of order 1 through \( (q+1) \). By setting such derivatives of \( H(s) \) to zero as in the statement, \( \lambda_{nm}^{q}(\bar{\bar{s}}) = 0 \) for \( q = 0, 1, ..., p - 1 \). Due to Lemma 1, the coefficients \( b_{nm}^{(p)}(\bar{\bar{s}}) \) also become zero.

At this point we turn to the diagonal terms \( b_{nn}^{(p)}(s) \) and to the conditions imposed on the Hamiltonian at the initial time.

**Lemma 3.** The condition

\[ H^{(1)}(0) = H^{(2)}(0) = \cdots = H^{(p)}(0) = 0, \quad (B27) \]

implies \( \chi_{nmk}^{r,q}(s) \sim \delta_{m0} \) for every coefficient \( \chi_{nmk}^{r,q}(s) \) in (B14) with \( r \in \{1, 2, ..., p+1\} \).

**Proof.** The proof is by induction, beginning with the assertion that, for \( r = 1 \), the coefficients are \( \chi_{nmk}^{1,q}(s) = \chi_{nmk}(s) = \delta_{kn}\delta_{m0} \), as mentioned after Eq.(B15). The recurrence relations (B22) and (B23) show that if \( \chi_{nmk}^{r,q} \sim \delta_{m0} \) \( (r \leq p) \) holds for some value \( r \), then it holds for all terms of
The induction breaks down for \( q \) power of contribution in these conditions, namely, the one in lowest Lemma 1, so are \( b^{(r)}_{km}(s') \). The initial condition (B3) provides

\[
b^{(r)}_{mm}(0) = -\sum_{k \neq m} b^{(r)}_{mk}(0) = 0,
\]

(B29)

where the last equality follows from Corollary 2 with \( \bar{s} = 0 \). As such, \( b^{(r)}_{mm}(s) \sim \delta_{m0} \), therefore, \( \chi^{r,q}_{nmk}(s) \sim \delta_{m0} \). The induction breaks down for \( \chi^{p+2,q}_{nmk} \) because the initial condition \( b^{(p+1)}_{mm}(0) \neq 0 \).

We now highlight a result on the diagonal terms \( b^{(p)}_{mm}(s) \) that appeared in this demonstration.

**Corollary 4** (Diagonal terms). The condition

\[
H^{(1)}(0) = H^{(2)}(0) = \ldots = H^{(p)}(0) = 0
\]

implies, for \( m \neq 0 \),

\[
b^{(1)}_{mm}(s) = b^{(2)}_{mm}(s) = \ldots = b^{(p)}_{mm}(s) = 0.
\]

(B31)

Corollaries 2 and 4, when substituted in the expansion (B1), lead to an important conclusion:

**Lemma 5** (Vanishing coefficients). If, for any \( \bar{s} \in [0,1] \) and all \( r \in \{1,2,\ldots,p\} \),

\[
H^{(r)}(0) = 0 = H^{(r)}(\bar{s}),
\]

then, for \( n \neq 0 \),

\[
b^{(1)}_{n}(\bar{s}) = b^{(2)}_{n}(\bar{s}) = \ldots = b^{(p)}_{n}(\bar{s}) = 0.
\]

(B33)

We are then left with the task of calculating the leading contribution in these conditions, namely, the one in lowest power of \( 1/T \) not identically zero. Since \( \lambda_{nm}(\bar{s}) = 0 \) for \( q = 0,1,\ldots,p-1 \) as mentioned in the proof of Corollary 2, the expansion (B4) for \( b^{(p+1)}_{nm}(\bar{s}) \) \((n \neq m)\) reads

\[
b^{(p+1)}_{nm}(\bar{s}) = \sum_{k \neq m} \lambda^{p+1}_{nmk}(\bar{s}) \chi_{km}(\bar{s}).
\]

(B34)

The coefficients \( \chi^{p+1}_{nmk}(\bar{s}) \) can be obtained by iterating (B22) up to \( \chi^{1}_{nmk}(\bar{s}) = \delta_{kn} \delta_{m0} \).

\[
\chi^{p+1}_{nmk}(\bar{s}) = \delta_{kn} \delta_{m0} \Delta_{nm}(\bar{s}),
\]

(B35)

For \( n = m \neq 0 \), Eq. (B28) and Lemma 3 show that

\[
b^{(p+1)}_{nn}(\bar{s}) = b^{(p+1)}_{nn}(0),
\]

(B36)

and employing (B3) together with (B34) and (B35) at \( \bar{s} = 0 \), we have

\[
b^{(p+1)}_{nn}(0) = -\sum_{m \neq n} b^{(p+1)}_{nm}(0) = -\frac{\lambda^{(p)}_{m0}(0)}{\Delta_{n0}(0)}.
\]

(B37)

Eq.(18) for the leading term \( b^{(p+1)}_{nn}(\bar{s}) = 1 \) then follows from substituting (B34), (B35) and (B37) into (B1). In order to obtain Eq.(15), one must use

\[
\lambda^{(p)}_{n0}(\bar{s}) = -\frac{\phi_{n}(\bar{s}) H^{(p+1)}(\bar{s})}{\phi_{n}(\bar{s})} \frac{\Delta_{n0}(\bar{s})}{\Delta_{n0}^{p+2}(\bar{s})},
\]

(B38)

at \( \bar{s} = 0 \) and 1, valid due to the vanishing derivatives of \( H(s) \).

**Appendix C: Next-to-leading coefficients**

Our last proof tackles the next-order coefficients, using the results from App B above.

1. General Case

Let us obtain \( b^{(2)}_{nm}(s) \). Lemma 1 provides, for \( n \neq m \),

\[
b^{(2)}_{nm}(s) = \sum_{k \neq m} \lambda^{2}_{nmk}(s) \lambda^{(0)}_{km}(0) + \lambda^{2}_{nmk}(s) \lambda^{(1)}_{km}(s).
\]

(C1)

The first order coefficient \( \chi^{1}_{nmk}(s) = \delta_{nk} \delta_{m0} \) and the recurrence relations (B22) allow us to obtain the coefficients

\[
\chi^{2}_{nmk}(s) = \frac{\lambda^{1}_{nmk}(s)}{\Delta_{nm}(s)} = \frac{\delta_{nk} \delta_{m0}}{\Delta_{nm}(s)},
\]

(C2)

while (B23), (B9) and (B12) lead to

\[
\chi^{2}_{nmk}(s) = \frac{1}{\Delta_{nm}(s)} \sum_{l \neq m} M_{nl}(s) \delta_{lk} \delta_{m0} + J_{0}(s) \delta_{kn} \delta_{m0} - \lambda_{m0}(0) \delta_{kn}(1 - \delta_{m0})
\]

(C3)
The nondiagonal term $b_{nm}^{(2)}(s)$ can be written from (C1), (C2) and (C3) as

$$b_{nm}^{(2)}(s) = \frac{\dot{\lambda}_n(0)(s)}{\Delta_{nm}(s)} + \sum_{k \neq n} \frac{M_{nk}(s)\lambda_{kn}(s)}{\Delta_{nm}(s)} + J_0(s)\lambda_{n0}(s)$$

where

$$J_0(s)\lambda_{n0}(s)$$

is identically zero for $n \neq 0$, and the only remaining contribution comes from $\chi_{knk}^{(p+2)} = b_{nm}^{(p+2)}(s)$:

$$b_{kn}^{(p+2)}(s) = \lambda_{n0}^{(p+1)}(\tilde{s})\delta_{kn}\delta_{m0}$$

where (B7) was used. Substituting (C13) and (C14) in (C12) and using (B13), we find, for $n \neq 0$,

$$b_{nm}^{(p+2)}(0) = -\sum_{k \neq n} b_{kn}^{(p+2)}(0) = -\frac{\lambda_{n0}^{(p+1)}(0)}{\Delta_{nm}^{p+1}(0)}$$

The nondiagonal term $b_{nm}^{(p+2)}(\tilde{s})$ can be written from (C7), (C8) and (C10) as

$$b_{nm}^{(p+2)}(\tilde{s}) = \left(\frac{\lambda_{n0}^{(p+1)}(\tilde{s})}{\Delta_{n0}^{p+1}(\tilde{s})} + J_0(\tilde{s})\frac{\lambda_{n0}^{(p)}(\tilde{s})}{\Delta_{n0}^{p}(\tilde{s})}\right)\delta_{nm}.$$ (C11)

Now we obtain the diagonal terms $b_{nn}^{(p+2)}(\tilde{s})$ for $n \neq 0$. We need to solve

$$b_{nn}^{(p+2)}(\tilde{s}) = b_{nn}^{(p+2)}(0) - \sum_{k \neq n} \int_0^\infty M_{nk}(s')b_{kn}^{(p+2)}(s')ds'$$

where

$$b_{nn}^{(p+2)}(0) = -\sum_{k \neq n} b_{kn}^{(p+2)}(0) = -\frac{\lambda_{n0}^{(p+1)}(0)}{\Delta_{nm}^{p+1}(0)},$$

and $\lambda^{p+1\pm\infty}_{nm}(\tilde{s})$ can be obtained by iterating (B22) and (B23) (except for $\Delta_{nm}^{p+2}(0)$). The former can be found for any time $s$, not just those times $\tilde{s}$ when derivatives of the Hamiltonian vanish, as in (C11). Due to (B14), it depends on $\chi_{knk}^{p+1\infty}(s)$, which is obtained from $\chi_{knk}^{p+1\infty}(s)$ through (B22) and (B23) (except for $\chi_{knk}^{p+2\infty}(s)$). But Lemma 3 guarantees that $\chi_{knk}^{p+1\infty}(s)$ is identically zero for $n \neq 0$, and the only remaining contribution comes from $\chi_{knk}^{p+2\infty} = b_{nm}^{(p+2)}(s)$:

$$b_{kn}^{(p+2)}(s) = b_{kn}^{(p+1)}(s)\lambda_{kn}(s) = \frac{\lambda_{n0}^{(p)}(0)}{\Delta_{n0}^{p}(0)}\lambda_{kn}(s),$$

where (B3) was used. Substituting (C13) and (C14) in (C12) and using (B13), we find, for $n \neq 0$,

$$b_{nn}^{(p+2)}(0) = -\frac{\lambda_{n0}^{(p+1)}(0)}{\Delta_{nm}^{p+1}(0)} - J_n(s)\frac{\lambda_{n0}^{(p)}(0)}{\Delta_{n0}^{p}(0)}.$$ (C15)

The expression for $b_{kn}^{(p+2)}(\tilde{s})$ in Eq.(19) follows from (B1), (C11) and (C15) with $\tilde{s} = 1$, concluding the proof.