

Large time-step discretization of adiabatic quantum dynamics

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Adiabatic quantum computing is a general framework for preparing eigenstates of Hamiltonians on quantum devices. However, its digital implementation requires an efficient Hamiltonian simulation subroutine, which may introduce extra computational overhead or complicated quantum control logic. In this work, we show that the time-step sizes in time discretization can be much larger than expected, and the overall complexity is greatly reduced. Remarkably, regardless of the general convergence order of the numerical method, we can choose a uniform time-step size independent of tolerated error and evolution time for sufficiently accurate simulation. Furthermore, with the boundary cancellation condition where the continuous diabatic errors are exponentially suppressed, we provide strong evidence for a superpolynomial convergence of first-order Trotter with uniform time-step size. We apply our analysis to the example of adiabatic unstructured search and show several preferable features of the Trotterized adiabatic approach: It can match the Grover lower bound, it does not require *a priori* knowledge of the number of marked states, and its performance can be asymptotically comparable with that of the quantum approximate optimization algorithm.

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I. INTRODUCTION

Preparing eigenstates of Hamiltonians is a fundamental task in quantum physics, quantum chemistry, and quantum information. Classical algorithms have a cost that scales polynomially with the dimension of the Hilbert space, which motivates the exploration of quantum algorithms for potential speedup. An approach to solving the eigenstate preparation problem is adiabatic quantum computing (AQC) [1]. In the framework of AQC, we consider the dynamics of a time-dependent Hamiltonian given by

$$i\partial_t|\psi(t)\rangle = H(t/T)|\psi(t)\rangle, \quad 0 \leq t \leq T, \quad (1)$$

where $H(s) = (1 - f(s))H_0 + f(s)H_1$ is an interpolating Hamiltonian that smoothly evolves from an initial Hamiltonian H_0 to a target Hamiltonian H_1 , and $f(s)$ is called the scheduling function such that $f(0) = 0$ and $f(1) = 1$. Typically, H_0 is designed to be simple with easily preparable eigenstates. Then, under the gap condition that the desired eigenpath of $H(s)$ is separated from the rest of the spectrum, the dynamics of Eq. (1) will approximately drive the system from the eigenstate of H_0 to that of H_1 , as $T \rightarrow \infty$.

While AQC is a promising technique for solving general eigenstate preparation problems, its implementation on

digital quantum devices requires an efficient subroutine for simulating Eq. (1), which may introduce nonoptimal asymptotic scalings. Commonly used methods include the first-order exponential integrator [2,3] and the first-order product formula [4–7]. Both methods, despite their simplicity, have only first-order convergence, and thus make the number of discrete evolution steps superlinear in the evolution time T (for first-order methods, it is specifically quadratic in T). This can be expensive since T is usually large to minimize diabatic excitation in AQC dynamics. Alternatively, high-order time-dependent Hamiltonian simulation algorithms, such as the high-order Trotter-Suzuki formula [6,8] and the truncated Dyson series method [9,10], can reduce the number of evolution steps to almost linear in T . However, these methods may still introduce extra computational complication. The number of exponentially many local operators in the product formulas may grow rapidly as the convergence order increases, and the truncated Dyson series method requires complicated quantum control logic [11,12].

In this work, we develop a general methodology of analyzing numerical discretization methods for digitally simulating near-adiabatic dynamics and obtain greatly improved error bounds. According to our analysis, the time-step sizes in discretizing near-adiabatic dynamics can be much larger than expected, and the overall complexity is greatly reduced. Specifically, we consider the first-order exponential integrator and the product formula for time discretization. We show that, as long as the time-step size is smaller than a uniform threshold independent of tolerated error ϵ and evolution time T , time discretization errors will be nondominant and the digital simulation can achieve sufficient accuracy. Furthermore, under an additional assumption called the boundary cancellation

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condition, which has been well studied for continuous-time adiabatic quantum dynamics [13–18], we provide strong evidence that in practice even a first-order product formula with uniform time-step size can achieve superpolynomial convergence, which achieves a superpolynomial speedup in precision over previous results.

Our analysis is based on the discrete adiabatic theorem, which is a discrete analog of the continuous adiabatic theorem and guarantees that sequentially applying a set of slowly varying gapped unitary walk operators can approximately drive the system from the eigenstate of the initial walk operator to the connected eigenstate of the final walk operator. In our analysis, we treat the numerical integrators as the set of discrete walk operators and show that the discretized dynamics indeed follows an adiabatic path with the same initial and final eigenstates as the continuous one but different in the middle. This not only allows us to obtain the aforementioned improved error bounds, but also shows that the discretized evolution can potentially solve eigenstate preparation problems that are beyond the reach of the original continuous formulation. For example, if the Hamiltonian $H(s)$ becomes gapless, then the continuous AQC based on Eq. (1) cannot follow the desired eigenpath. However, through a toy model, we find that, even for a gapless Hamiltonian, it is possible that the first-order Trotterized operator with large time-step size satisfies the gap condition, so the corresponding discretized evolution may still succeed in preparing the desired eigenstates.

As an application, we use our analysis to design a discrete adiabatic algorithm for the unstructured search problem with multiple marked items. Our algorithm has several preferable features: It can match the Grover lower bound, it does not require *a priori* knowledge on the number of marked states, and it can achieve a logarithmic scaling in the inverse precision numerically. Additionally, we contribute to the active discussions on the relation between AQC and quantum approximate optimization algorithm (QAOA) [19], by showing that our discrete-adiabatic-based algorithm gives a set of QAOA angles that can achieve the optimal query complexity $\mathcal{O}(\sqrt{N})$ for finding the single marked state among N states.

There have been a few recent efforts on improving the analysis of discretizing AQC. For instance, Ref. [20] demonstrates the robustness of digital adiabatic simulation using first-order Trotter formula with large time-step sizes by applying continuous adiabatic theorems to an effective Hamiltonian. Additionally, a more recent work [21] proves a similar result by relating the first-order Trotter error estimate to its second-order counterpart. Our results improve over prior work in the following ways:

(1) Our analysis is applicable to the first-order exponential integrator and product formulas of any order. As a comparison, previous works [20,21] only focus on the first-order Trotter formula, and their analysis heavily relies on its specific structure.

(2) Under the boundary cancellation condition, our analysis explains why first-order methods with large time-step sizes are very likely to have a superpolynomial time convergence in this case, while previous works [20,21] still only show a linear convergence as it is unclear how their approaches can be naturally combined with the additional boundary cancellation condition.

(3) Our analysis uncovers the intrinsic property of time discretization of the AQC as following another (discrete) adiabatic path. This is not only conceptually different from the standard numerical analysis that views time discretization only as introducing numerical errors and driving the dynamics away from the adiabatic path, but also the key for revealing new findings. For example, with the discrete adiabatic point of view, we are able to show that Trotterized adiabatic evolution may still succeed even for a gapless Hamiltonian on certain occasions using a toy model. Thus, our work makes a first step toward exploring the power of digital simulation to perform adiabatic state preparation for gapless Hamiltonians, which was not covered in Refs. [20,21].

The rest of this paper is organized as follows. We first summarize our main results in Sec. II. In Sec. III, we show our improved complexity estimates based on the discrete adiabatic theorem in the general case, and Sec. IV is devoted to the case with the boundary cancellation condition. Section V discusses the possibility of using the first-order product formula with large step for gapless Hamiltonians. In Sec. VI, we present our results for robust adiabatic Grover search and compare it with QAOA. Section VII summarizes this work and discusses potential further work.

II. SUMMARY OF THE RESULTS

A. Setup and numerical methods

We first formally restate the state preparation problem.

Problem 1 (State preparation). Let H_1 be a Hamiltonian and $|\phi\rangle$ be a target eigenstate of H_1 . For $\varepsilon > 0$, the goal of the state preparation problem is to prepare a quantum state $|\tilde{\phi}\rangle$ such that $\| |\tilde{\phi}\rangle\langle\tilde{\phi}| - |\phi\rangle\langle\phi| \| \leq \varepsilon$.

In the framework of AQC, given another simple Hamiltonian H_0 with known eigenstate, we consider the dynamics of Eq. (1) with interpolating Hamiltonian

$$H(s) = (1 - f(s))H_0 + f(s)H_1 \quad (2)$$

and the scheduling function $f(s)$. Under the gap condition, starting from the eigenstate of H_0 , the solution of Eq. (1) at the final time will be a good approximation of the corresponding eigenstate of H_1 .

The AQC dynamics of Eq. (1) needs further time discretization to be implemented on a digital quantum device. The most commonly used strategy for numerical propagation is to divide the time interval into T_d equidistant subintervals and approximate the exact local evolution operator by a local unitary numerical propagator. Specifically, a p th-order local unitary evolution operator U_{num} is constructed such that for any $0 \leq j \leq T_d - 1$, it approximates the time-ordering operator from jh to $(j+1)h$ as follows:

$$\mathcal{T}e^{-i \int_{jh}^{(j+1)h} H(t/T)dt} = U_{\text{num}}((j+1)h, jh) + \mathcal{O}(h^{p+1}), \quad (3)$$

and the global exact evolution operator can be approximated as

$$\mathcal{T}e^{-i \int_0^T H(t/T)dt} \approx \prod_{j=0}^{T_d-1} U_{\text{num}}((j+1)h, jh), \quad (4)$$

where T_d is the number of discrete time steps and $h = T/T_d$ is the step size.

TABLE I. Summary of the complexity estimates on discretizing Eq. (1). Query complexity is measured by the number of time propagation steps required in the evolution. We assume the gap condition only for the time-dependent Hamiltonian $H(t)$, and that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded. Here, $\alpha = \|H_0\| + \|H_1\|$, $\tilde{\alpha}_p = \sum_{\gamma_0, \dots, \gamma_p \in \{0,1\}} \| [H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]] \|$, T is the evolution time, ϵ is the tolerated error, and Δ_* represents the minimum gap of $H(s)$.

Method	Error bound	Time-step size	Scaling
First-order exponential integrator	Standard	$\mathcal{O}(\epsilon \alpha^{-1})$	$\mathcal{O}(\alpha^3 \Delta_*^{-3} \epsilon^{-2})$
First-order product formula	Standard	$\mathcal{O}(\epsilon \alpha^{-2} T^{-1})$	$\mathcal{O}(\alpha^6 \Delta_*^{-6} \epsilon^{-3})$
p th-order product formula	Standard	$\mathcal{O}(\epsilon^{1/p} \alpha^{-1-1/p} T^{-1/p})$	$\mathcal{O}(\alpha^{3+3/p} \Delta_*^{-3-3/p} \epsilon^{-1-2/p})$
First-order exponential integrator	Corollary 1	α^{-1}	$\mathcal{O}(\alpha^3 \Delta_*^{-3} \epsilon^{-1})$
First-order product formula	Corollary 2	$\mathcal{O}(\min\{\alpha^{-1}, \Delta_*^{1/2} \tilde{\alpha}_2^{-1/2}\})$	$\mathcal{O}(\alpha^3 \Delta_*^{-3} \epsilon^{-1} \max\{1, \tilde{\alpha}_2^{1/2} \Delta_*^{-1/2} \alpha^{-1}\})$
p th-order simplified product formula	Corollary 3	$\mathcal{O}(\min\{\alpha^{-1}, \Delta_*^{1/p} \tilde{\alpha}_p^{-1/p}\})$	$\mathcal{O}(\alpha^3 \Delta_*^{-3} \epsilon^{-1} \max\{1, \tilde{\alpha}_p^{1/p} \Delta_*^{-1/p} \alpha^{-1}\})$

In practice, there are two common classes of numerical methods, namely, the first-order exponential integrator and the product formulas. They differ in the level of time discretization. If we only approximate the time-ordering operator by a time-independent Hamiltonian simulation problem, we obtain the first-order exponential integrator, which is given by

$$U_{\text{exp}}(t+h, t) = \exp(-ihH(t/T)). \quad (5)$$

In this method, each propagation step only involves one matrix exponential but the exponent is still an interpolation of the Hamiltonians H_0 and H_1 . If we further split the evolution of $H(t/T)$ into exponentials of H_0 and H_1 separately, we obtain the product formulas. The first- and second-order product formulas are given as

$$U_{\text{pf},1}(t+h, t) = \exp(-ihf(t/T)H_1) \times \exp(-ih(1-f(t/T))H_0) \quad (6)$$

and

$$U_{\text{pf},2}(t+h, t) = \exp(-ih/2(1-f((t+h/2)/T))H_0) \times \exp(-ihf((t+h/2)/T)H_1) \times \exp(-ih/2(1-f((t+h/2)/T))H_0). \quad (7)$$

Arbitrary p th-order formulas can be constructed via several approaches, such as Trotter-Suzuki recursion [8,22], Yoshida method [23], and their improved versions [24,25]. The resulting p th-order formula can be written in the general form as

$$U_{\text{pf},p}(t+h, t) = \prod_{k=0}^{K_p} \exp(-i\beta_{p,k}hf((t+\delta_{p,k}h)/T)H_1) \times \exp(-i\alpha_{p,k}h(1-f((t+\gamma_{p,k}h)/T))H_0) \quad (8)$$

for some real parameters $\alpha_{p,k}$, $\beta_{p,k}$, $\gamma_{p,k}$, and $\delta_{p,k}$. We will also consider a simplified higher-order product formula

$$U_{\text{spf},p}(t+h, t) = \prod_{k=0}^{K_p} \exp(-i\beta_{p,k}hf(t/T)H_1) \times \exp(-i\alpha_{p,k}h(1-f(t/T))H_0). \quad (9)$$

Equation (9) is obtained by replacing all the discrete time points [Eq. (8)] with the fixed initial time. If the function f is

a constant function (which is not the case for the adiabatic dynamics), then Eq. (9) represents a p th-order time-independent product formula.

B. Main results

1. Improved complexity

In this work, we propose a general framework for analyzing algorithms to simulate near-adiabatic dynamics and obtain greatly improved error bounds in Sec. III. Our results and a comparison with previous results are summarized in Table I.

We first state our results for the first-order exponential integrator. In Sec. III C 1, we demonstrate that this first-order method can utilize a time-step size as large as α^{-1} without introducing significant discretization errors, where $\alpha = \|H_0\| + \|H_1\|$. In comparison, the standard error bound typically requires a time-step size of $\mathcal{O}(\epsilon \alpha^{-1})$, where ϵ is the tolerated level of errors (see Appendix D). Therefore, our analysis greatly increases the allowed time-step size for sufficiently accurate simulation by fully excluding the error dependence in the time-step size. Since the overall evolution time T should be $\mathcal{O}(\alpha^2 \Delta_*^{-3} \epsilon^{-1})$ to mitigate diabatic errors [26], where Δ_* is the minimum gap of $H(s)$, our result reduces the number of the total propagation steps from $\mathcal{O}(\alpha^3 \Delta_*^{-3} \epsilon^{-2})$ to $\mathcal{O}(\alpha^3 \Delta_*^{-3} \epsilon^{-1})$.

Our analysis is built upon the discrete AQC framework, which has been investigated in several works [27–29] although the literature remains much smaller than that on continuous-time AQC. The main theoretical tool in our analysis is the discrete adiabatic theorem, which can be viewed as a discrete analog of the continuous adiabatic theorem. The theorem was first established in Ref. [30], and an improved version with explicit gap dependence was introduced in the recent work [31]. In the discrete adiabatic theorem, we are provided with a set of slowly varying unitary operators, along with a promise of the gap condition of these unitary operators. Sequentially applying these operators allows us to steer the system from the eigenstate of the initial unitary to the eigenstate of the final unitary, with a diabatic error bounded by $\mathcal{O}(1/T_d)$, where T_d is the number of unitary operators. In our analysis, we treat the numerical integrators as a set of discrete walk operators. This allows us to directly apply the discrete adiabatic theorems to bound the error between the actual state and the exact eigenstates, making our approach tighter and

more straightforward compared to standard analyses where errors are typically bounded by the sum of continuous diabatic errors and time discretization errors. The gap condition of the numerical integrator $e^{-ihH(t/T)}$ can be guaranteed from the gap condition of $H(s)$, as long as the step size $h \leq \alpha^{-1}$. The changes between adjacent numerical integrators are determined by the scheduling function $f(t/T)$, which is already sufficiently slow with large evolution time T and suppresses the discrete adiabatic errors. This is why further reduction of the time-step size is unnecessary.

Our analysis based on the discrete adiabatic theorem also applies to the high-order product formula. However, unlike the first-order exponential integrator case, now the gap condition of the Trotter numerical integrators can be very different from the gap condition of the Hamiltonian $H(s)$. For example, even for the first-order Trotter method $e^{-ihf(s)H_1}e^{-ih(1-f(s))H_0}$, it is not clear how its gap is related to the gap condition of the Hamiltonian $H(s)$ when the step size h is large. It becomes even more complicated when we consider higher-order Trotter in Eq. (8), because the exponentials are the time evolution of Hamiltonian $H(s)$ evaluated at different times. Therefore, in Sec. III C 2, we instead consider the simplified higher-order product formula in Eq. (9) with all the Hamiltonians evaluated at the same time. Our strategy is to reduce the step size h such that the numerical operator $U_{\text{spf},p}$ is close to the walk operator $e^{-ihH(t/T)}$ by the distance at most $ch\Delta_*$ for a small constant c , then the gap of $H(s)$ would imply the gap of $U_{\text{spf},p}$. Such a step size can be determined using the time-independent Trotter error bound in Ref. [6]. An important observation is that the sole purpose of reducing the time-step size is to ensure the gap condition, so the time-step size depends only on the norms and gaps of the Hamiltonians, but is independent of the overall evolution time T and the tolerated error ϵ .

Combining this with the discrete adiabatic theorem, we show in Sec. III C 2 that, in a simplified p th-order product formula, a sufficiently accurate simulation may be obtained with time-step size $h = \mathcal{O}(\min\{\alpha^{-1}, \Delta_*^{1/p}\tilde{\alpha}_p^{-1/p}\})$, where $\tilde{\alpha}_p = \sum_{\gamma_0, \dots, \gamma_p \in [0,1]} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\|$ is the scaling of nested commutators of depth p . Again, our analysis shows that the time-step size can be independent of T and ϵ , while the best previous analysis [22] gives the estimate of $h = \mathcal{O}(\epsilon^{1/p}\alpha^{-1-1/p}T^{-1/p})$, which still depends on ϵ and T . As a result, our results still improve the standard complexity estimate by suggesting a larger time-step size and a smaller number of propagation steps for accurate simulation. Another interesting remark is that our analysis implies the advantage of higher-order methods from a completely different perspective—The advantage is because higher-order methods can better match the gap condition with larger time-step sizes, instead of better ϵ and T dependence, as suggested by the standard numerical analysis.

It is crucial to emphasize that the time-step size h in our analysis should be bounded by $\mathcal{O}(\alpha^{-1})$. If h is too large such that $h\alpha > \pi$, the eigenvalues of the unitary walk operators $W(s)$ might wrap around the unit circle even if the Hamiltonian $H(s)$ is gapped, causing high-energy excited states to hybridize with the instantaneous ground states and destroying the discrete adiabatic computation. While α is $\mathcal{O}(1)$ in some applications such as Grover search and linear systems of

equations [31–33], it generally grows with the system size for many-body physical systems. Thus, the physical difficulties associated with large energy scales are entirely absorbed into α , and our approach is efficient only when α has mild growth (e.g., polynomial in terms of the number of qubits).

However, it is important to recognize that this extensive dependence is not unique to our discrete approach. It is a fundamental limitation of digital quantum simulation. As shown in Table I, time-step sizes based on standard analysis all scale at least inverse linearly in α . Additionally, an established theoretical lower bound (called the no-fast-forwarding theorem [34]) indicates that the computational complexity of simulating a general Hamiltonian must scale $\Omega(\alpha)$. Therefore, any generic digital implementation must confront this scaling bottleneck, and our algorithmic advantage lies in allowing the time step to remain independent of the evolution time T and the tolerated error ϵ .

2. Improved complexity with boundary cancellation condition

We have shown that the overall complexity of simulating near-adiabatic dynamics using the first-order exponential integrator or product formula is $\mathcal{O}(1/\epsilon)$, omitting dependence on other parameters. This linear dependence is due to the scaling of the adiabatic error in general case, namely, $\mathcal{O}(1/T)$ in the continuous adiabatic theorem and $\mathcal{O}(1/T_d)$ in the discrete adiabatic theorem. In Sec. IV, we show how the overall complexity can be further improved by taking advantage of high-order adiabatic theorems, under an additional assumption, which is known as the boundary cancellation condition.

The boundary cancellation condition assumes the scheduling function $f(s)$ has vanishing derivatives of any order at the boundary $s = 0, 1$. Note that such a condition can be satisfied for any Hamiltonians H_0 and H_1 provided the scheduling function $f(s)$ is chosen appropriately. In the continuous case, the boundary cancellation condition and its effect have been well studied: The diabatic error can be suppressed by the high-order adiabatic theorems to a superpolynomial scaling $\mathcal{O}(1/T^k)$ for any positive integer k [26], or even an exponential convergence $\mathcal{O}(e^{-cT})$ [13,18]. In the discrete case, the work [30] also claims a high-order discrete adiabatic theorem, which has the error scaling $\mathcal{O}(1/T^k)$ for any positive integer k . Again, in the time discretization of Eq. (1), we view the numerical integrators as a set of discrete walk operators. Then, the high-order discrete adiabatic theorem would guarantee that, if the Hamiltonian has constant spectral norm and gap, then it suffices to use an $\mathcal{O}(1)$ time-step size and the overall number of steps is $\mathcal{O}(1/\epsilon^{\mathcal{O}(1)})$. Such a high-order convergence holds for any numerical methods, even including first-order ones like the first-order exponential integrator and the first-order product formula.

However, we remark that the improved scaling $\mathcal{O}(1/\epsilon^{\mathcal{O}(1)})$ we find here is not mathematically rigorously proved yet. This is because our analysis is based on the high-order discrete adiabatic theorem claimed in Ref. [30], but we find a missing step in its proof and this missing step seemingly cannot be fixed in a simple way (see Appendix F 2 for details). Nevertheless, in Appendix F 2, we show numerical evidence that supports the correctness of the high-order discrete adiabatic theorem, so our improved complexity holds numerically.

3. Advantage of Trotterized evolution over continuous AQC

So far, we have given improved complexity estimates of discretized AQC for gapped Hamiltonian $H(s)$. Notice that in order to apply the discrete adiabatic theorem, what we need is the gap condition of the numerical integrators rather than the Hamiltonian $H(s)$. In the first-order product formula with large time-step size, these two types of gap conditions can be very different. Our strategy so far is to moderately reduce the time-step size h such that the Trotter operator $e^{-ihf(s)H_1} e^{-ih(1-f(s))H_0}$ is sufficiently close to the walk operator $e^{-ihH(s)}$, whose spectral gap is closely related to that of the Hamiltonian $H(s)$.

It seems that the difference of the gap conditions between the interpolating Hamiltonian $H(s)$ and the unitary numerical operators only introduces extra computational overheads, as reduced time-step size is required to match the gap conditions. However, in Sec. V, we discuss an interesting phenomenon that such difference of the gap conditions can actually be advantageous when the interpolating Hamiltonian has an exponentially small spectral gap or becomes gapless. In such cases, Trotterized evolution with large time-step size may significantly outperform the continuous AQC and even become the only way for adiabatic state preparation. More specifically, we consider the case where the gap of $H(s)$ is exponentially small or just becomes 0. Then, continuous AQC requires an exponentially large evolution time or may even fail [35]. However, numerical discretization with a large time-step size, such as the first-order Trotter method with time-step size 1 (i.e., $e^{-if(s)H_1} e^{-i(1-f(s))H_0}$), may still have a large gap. Thus, discrete adiabatic theorems suggest that the large-step-size evolution may be able to find the desired eigenstates with much lower complexity. Notice that in this case, reducing the time-step size further could make the situation worse, as the discrete evolution would be forced to approximate the continuous AQC that does not work. Such a potential difference between these two gap conditions might lead to a surprising speedup of large-step-size discretization compared to continuous AQC. We provide numerical evidence for this phenomenon using a toy model in Sec. V.

We would like to highlight that all of the findings about the gapless Hamiltonians are based on a toy model. It is also important to emphasize that we do not claim large-step time discretization will generally lift level crossings or resolve the proliferation of small gaps often seen in complex quantum dynamics. Increasing the time-step size may either improve the gap in special cases or introduce additional quasienergy resonances and avoided crossings. The gap condition of the walk operator must therefore be verified for the chosen time-step size. The gapless toy model presented here serves solely as a proof of principle to demonstrate that time discretization is not always detrimental. Rather than necessarily decreasing the gap, it is possible for large-step discretization to fortuitously open a gap in specific instances. Whether and how this purely algorithmic discretization negatively or positively affects the gap condition in practical many-body systems remains an interesting open question.

4. Discrete adiabatic Grover search and implication on QAOA

All of our aforementioned results have superlinear spectral gap dependence, as they hold generically and in the worst-case scenario. However, in continuous AQC, a linear gap dependence can be achieved by carefully designing an interpolation function that takes into account simultaneous gap information [1,26,33,36]. We observe that the linear gap dependence can be preserved with the same interpolating function when discretizing the dynamics using a large time-step size.

To illustrate this, in Sec. VI, we consider the example of adiabatic Grover search [36], where we aim to find a uniform superposition of M target states in an N -dimensional Hilbert space. We consider two possible interpolation functions: one generalized from Refs. [36,37] that changes speed proportional to the gap size, and the second, a smooth connection of two identical glue functions, used in Ref. [33] to construct adiabatic quantum linear system solvers. The latter simultaneously slows down when the gap closes and satisfies the boundary cancellation condition. We show that the AQC dynamics with either interpolation function can be discretized using a time-step size 1 without incurring extra discretization errors, and the overall number of steps using the second interpolation function can be $\tilde{O}(\sqrt{N/M})$ in dimension, almost recovering the quadratic Grover speedup, and $\mathcal{O}(1/\epsilon^{o(1)})$ in precision assuming the correctness of high-order discrete adiabatic theorems. Our second scheduling function provides a superpolynomial improvement in precision compared to previous work on adiabatic quantum search [37]. A remarkable feature of our algorithm is that it is robust against the estimations of M in two aspects. First, constructing the interpolation functions does not require an estimate of M (and for the second interpolation function, not even information about N). Additionally, increasing the number of propagation steps improves accuracy, similar to fixed-point iteration [37,38], instead of “overcooking” the problem as in the original Grover algorithm [39].

Another powerful approach for eigenstate preparation is the QAOA [19]. In QAOA, an ansatz is considered that alternately evolves an input state with the target Hamiltonian H_1 and a mixing Hamiltonian H_0 . The goal is to optimize the evolution times, also called QAOA angles, such that the final output state approximates the desired eigenstate. QAOA is closely related to AQC and especially discretized AQC, since for gapped Hamiltonian the Trotterization of AQC directly gives a candidate of the QAOA angles, yet QAOA is believed to have the potential to outperform AQC by resulting in a shorter overall evolution time and having better gap dependence. Even for the simple example of the Grover search problem, it was previously believed that the performance and analysis of QAOA should involve a very different process from estimating the gap dependence in the AQC approach [40]. However, our improved AQC results demonstrate the existence of a Trotterized AQC with time-step size 1, which can readily solve the Grover search problem with a cost of $\mathcal{O}(\sqrt{N})$ in the case of a single marked state. Therefore, the performance of discretized AQC can match that of QAOA for this task.

III. IMPROVED TIME-STEP SIZE AND COMPLEXITY ESTIMATE

A. Key idea

We first explain the key components in our improved analysis. The first observation is that, unlike the standard analysis that uses the triangle inequality and bounds both the continuous adiabatic error and the time discretization error, we directly view the numerical propagation operator $U_{\text{num}}((j+1)h, jh)$ as the discrete adiabatic walk operator. Then, as long as U_{num} satisfies the assumptions in the discrete adiabatic theorems and the eigenstate of the last numerical propagation operator coincides with our target eigenstate, the overall approximation error can be directly bounded using the discrete adiabatic theorems. This is a more straightforward and tighter way to bound the overall error. The second observation is that numerical operators with relatively large time-step size suffice to fulfill the assumption of slow changes in the discrete adiabatic theorems. This is because the Hamiltonian $H(t/T)$ varies on the rescaled time $s = t/T$, which already controls the change of the walk operators at a low level and thus smaller time-step sizes are not necessary.

A further result from our analysis is a better time discretization error bound for the first-order exponential integrator and the product formula. We may use the triangle inequality in a different way to bound the numerical discretization error by the sum of the continuous and discrete adiabatic errors, which are both well bounded even with large time-step sizes.

B. A review of the discrete adiabatic theorem

Discrete adiabatic evolution is a discrete analog of continuous adiabatic evolution. In continuous adiabatic evolution (see Appendix A for a detailed discussion), we are given a time-dependent Schrödinger equation. If the time-dependent Hamiltonian varies slowly and there is a gap in its spectrum, then propagating the Schrödinger equation approximately drives the state from an eigenstate of the initial Hamiltonian to an eigenstate of the final Hamiltonian. In the discrete setting, we are given a set of unitary walk operators and sequentially apply those on an input quantum state. If two adjacent walk operators are close and satisfy the gap condition, then such discrete evolution will approximately drive the quantum state from the eigenstate of the first walk operator to the eigenstate of the final walk operator.

The discrete adiabatic theorem bounds the distance between the output of the discrete evolution and the ideal eigenspace of the final walk operator. It was first proved in Ref. [30], and a recent work [31] improved the linearly convergent discrete adiabatic theorem to an explicit form with clear gap dependence. Here, we briefly review the result in Ref. [31].

Let $W(s)$ be a set of parametrized unitary walk operators for $s \in [0, 1]$. For an input quantum state $|\psi\rangle$ and a positive integer T_d , consider the discrete evolution $U(n/T_d)$ defined as

$$U(n/T_d)|\psi\rangle = \prod_{j=0}^{n-1} W(j/T_d)|\psi\rangle, \quad 1 \leq n \leq T_d. \quad (10)$$

Suppose that the discrete evolution satisfies the following conditions.

(1) For $k = 1, 2$, there exist real-valued functions $c_k(s)$ such that

$$\|D^{(k)}W(s)\| \leq \frac{c_k(s)}{T_d^k} \quad (11)$$

for $0 \leq s \leq 1 - k/T_d$, where $D^{(k)}W(s)$ represents the k th-order finite difference of $W(s)$ with step size $1/T_d$.

(2) The eigenvalues of $W(s)$ can be separated into two groups $\sigma_P(s)$ and $\sigma_Q(s)$, such that for any $k = 0, 1, 2$ and $0 \leq s \leq 1 - k/T_d$, the angular distance between the arcs $\sigma_P^{(k)}(s)$ and $\sigma_Q^{(k)}(s)$ is bounded from below by $\Delta_k(s) > 0$, where

$$\sigma_P^{(k)}(s) \supseteq \bigcup_{l=0}^k \sigma_P(s + l/T_d), \quad \sigma_Q^{(k)}(s) \supseteq \bigcup_{l=0}^k \sigma_Q(s + l/T_d). \quad (12)$$

(3) The input state $|\psi\rangle$ is within the eigenspace corresponding to $\sigma_P(0)$.

The first of these conditions means that the rate of variation of the walk operator is bounded and is a similar condition to the bound on the first and second time derivatives in the continuous case. The second condition is ensuring that there is a gap. For generality, it is allowed to be a gap between eigenspaces, rather than just a ground state and excited states. There is a further subtlety in the discrete case that the gap is considered between successive steps as well; that is, the eigenspace σ_P at one step cannot overlap with σ_Q at the next step. This is accounted for by considering the union of the eigenspaces at three successive steps as in Eq. (12). However, we remark that if T_d is large enough, then this multistep gap condition can be guaranteed by a uniformly bounded spectral gap of each $W(s)$. Intuitively, this is because the eigenvalues of $W(s)$ do not change much from one step to another, and thus different arcs of the spectrum at different time steps will not overlap. We discuss this with more technical details in Appendix B. The third condition just specifies σ_P as the eigenspace that the state should remain within during the discrete adiabatic evolution.

For reference, we also need to define an ideal adiabatic evolution operator $U_A(n/T_d)$, which drives the input state to the ideal final eigenspace without any leakage. The operator $U_A(n/T_d)$ is defined through a set of ideal adiabatic walk operators $W_A(s)$ such that

$$U_A(n/T_d)|\psi\rangle = \prod_{j=0}^{n-1} W_A(j/T_d)|\psi\rangle, \quad 1 \leq n \leq T_d. \quad (13)$$

The ideal adiabatic walk operators $W_A(s)$ include a counterdiabatic correction of the original walk operators $W(s)$. For technical simplicity, we omit the explicit definition of $W_A(s)$ here and refer to Refs. [30,31]. An important proposition involving $U_A(n/T_d)$ is that for all $1 \leq n \leq T_d$,

$$U_A(n/T_d)P(0) = P(n/T_d)U_A(n/T_d), \quad (14)$$

where $P(s)$ denotes the spectral projection onto the eigenspace $\sigma_P(s)$. The left-hand side corresponds to projecting onto the desired initial eigenspace, then evolving for n steps, which should give the eigenspace at step n if the evolution is adiabatic. That is indeed what the right-hand side shows, because it has the evolution for n steps followed by the projection onto

the eigenspace, so acting with this operator on any state must yield a state in the correct eigenspace. Therefore, $U_A(n/T_d)$ exactly preserves the instantaneous eigenspace of $W(n/T_d)$ corresponding to $\sigma_P(n/T_d)$.

Now, we are ready to state the first discrete adiabatic theorem proved in Ref. [31].

Lemma 1. Suppose that $T_d \geq \sup_{s \in [0,1]} (4\hat{c}_1(s)/\check{\Delta}_2(s))$, where the hat (check) notations of a function at s represent the maximum (minimum) of its function values at neighboring points $\{s - 1/T_d, s, s + 1/T_d\}$ whenever well defined. Then, for any $1 \leq n \leq T_d$, there exists an absolute constant C such that

$$\begin{aligned} & \|U(n/T_d) - U_A(n/T_d)\| \\ & \leq \frac{C}{T_d} \left(\frac{\hat{c}_1(0)}{\check{\Delta}_2(0)^2} + \frac{\hat{c}_1(n/T_d)}{\check{\Delta}_2(n/T_d)^2} + \sum_{j=0}^{n-1} \frac{\hat{c}_1(j/T_d)^2}{T_d \check{\Delta}_2(j/T_d)^3} \right. \\ & \quad \left. + \sum_{j=0}^{n-1} \frac{\hat{c}_2(j/T_d)}{T_d \check{\Delta}_2(j/T_d)^2} \right). \end{aligned} \quad (15)$$

Because $U_A(n/T_d)$ is exact adiabatic evolution, it would map an initial state in the initial eigenspace to one in the desired final eigenspace. The bound on the difference of operators therefore gives a bound on how much the state can leak outside the eigenspace under the true evolution $U(n/T_d)$.

C. Our results

1. First-order exponential integrator

Now, we consider walk operators that are given by Hamiltonian evolution for time h , $W(s) = e^{-ihH(s)}$, where $H(s)$ is varied in an adiabatic way as in Eq. (2). We can then use this form to determine $c_k(s)$ and provide a theorem for the error in terms of the properties of the Hamiltonians H_0, H_1 . For this theorem, the gap is still given for the walk operator, though it will be implicitly dependent on h .

In general cases, we can obtain a linear convergence in the evolution time. By directly leveraging Lemma 1, we first obtain the following result for arbitrary time-step size h under the multistep gap assumption for the walk operator. Its detailed proof can be found in Appendix E 1.

Theorem 1. Consider Problem 1 using digital adiabatic simulation with first-order exponential integrator $W(s) = e^{-ihH(s)}$, where $H(s)$ is given as Eq. (2). Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Let $\Delta(s)$ denote the multistep spectral gap of $U_{\text{exp}}(sT + h, sT)$, and $\tilde{\Delta}_* = \min_{s \in [0, 1-h/T]} \Delta(s)$. Then, the overall error between the actual and the ideal evolution can be bounded by

$$\begin{aligned} & \mathcal{O} \left(\frac{h}{T} \left(\frac{h(\|H_0\| + \|H_1\|)}{\tilde{\Delta}_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{\tilde{\Delta}_*^2} \right. \right. \\ & \quad \left. \left. + \frac{h^2(\|H_0\| + \|H_1\|)^2}{\tilde{\Delta}_*^3} \right) \right). \end{aligned} \quad (16)$$

Theorem 1 assumes the multistep gap condition for the first-order exponential integrator. While this may be established independently in some applications, a more common

assumption is the (fixed-time) gap condition for the Hamiltonian $H(s)$. When the time-step size is small enough, we may relate the multistep gap condition for $W(s)$ to the fixed-time gap condition for $H(s)$ and show the following result, whose proof can be found in Appendix E 1.

Corollary 1. Consider Problem 1 using digital adiabatic simulation with the first-order exponential integrator [Eq. (5)], $W(s) = e^{-ihH(s)}$. Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Let $\Delta(s)$ denote the spectral gap of $H(s)$, and $\Delta_* = \min_{s \in [0,1]} \Delta(s)$. Then, in order to bound the overall error by $\epsilon \in (0, 1)$, it suffices to choose

$$T = \mathcal{O} \left(\frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon} \right) \quad (17)$$

and

$$h = \frac{1}{\|H_0\| + \|H_1\|}, \quad (18)$$

and the overall number of steps becomes

$$T_d = \mathcal{O} \left(\frac{(\|H_0\| + \|H_1\|)^3}{\Delta_*^3 \epsilon} \right). \quad (19)$$

So far, we have shown an improved estimate on the number of steps in the first-order exponential integrator. However, it is still not straightforward to implement the first-order exponential integrator $e^{-ihH(s)}$ from the input models of H_0 and H_1 . Here, we briefly describe how to implement $e^{-ihH(s)}$. Suppose that we are given unitaries V_0 and V_1 such that, for $j = 0, 1$, V_j is a $(\eta_j, n_a, 0)$ block encoding of H_j , i.e.,

$${}_a \langle 0 | V_j | 0 \rangle_a = \frac{1}{\eta_j} H_j. \quad (20)$$

Here, η_j represents the block-encoding factor such that $\eta_j \geq \|H_j\|$. The number of the ancilla qubits for both block encodings is the same as n_a without loss of generality (if the numbers of ancilla qubits are not the same, then we may define n_a to be the larger one and supplement the other unitary with extra trivial ancilla qubits). We further assume that the block-encoding factors are asymptotically optimal in the sense that $\eta_j = \mathcal{O}(\|H_j\|)$ as well.

For every fixed $s \in [0, 1]$, we first block encode $H(s) = (1 - f(s))H_0 + f(s)H_1$. This can be done using the linear combination of unitaries technique supplemented with an extra ancilla qubit. Let the rotation be

$$\begin{aligned} R(s) &= \frac{1}{\sqrt{(1 - f(s))^2 \eta_0^2 + f(s)^2 \eta_1^2}} \\ & \times \begin{pmatrix} (1 - f(s))\eta_0 & f(s)\eta_1 \\ f(s)\eta_1 & -(1 - f(s))\eta_0 \end{pmatrix}, \end{aligned} \quad (21)$$

and the select oracle be

$$\text{SEL} = |0\rangle\langle 0| \otimes V_0 + |1\rangle\langle 1| \otimes V_1. \quad (22)$$

Then, according to Lemma 52 of Ref. [41], the operator $(H \otimes I_{n_a} \otimes I_n) \text{SEL}(R(s) \otimes I_{n_a} \otimes I_n)$ is a $(1, n_a + 1, 0)$ block encoding of

$$\frac{1}{\sqrt{2} \sqrt{(1 - f(s))^2 \eta_0^2 + f(s)^2 \eta_1^2}} H(s). \quad (23)$$

To implement $e^{-ihH(s)}$, we may use the qubitization [42] or the quantum singular value transformation technique [41]. In particular, write

$$e^{-ihH(s)} = \exp \left(-ih\sqrt{2}\sqrt{(1-f(s))^2\eta_0^2 + f(s)^2\eta_1^2} \right. \\ \left. \times \frac{1}{\sqrt{2}\sqrt{(1-f(s))^2\eta_0^2 + f(s)^2\eta_1^2}} H(s) \right), \quad (24)$$

so we need to evolve the rescaled Hamiltonian $\frac{1}{\sqrt{2}\sqrt{(1-f(s))^2\eta_0^2 + f(s)^2\eta_1^2}} H(s)$ to time $h\sqrt{2}\sqrt{(1-f(s))^2\eta_0^2 + f(s)^2\eta_1^2}$, which is still $\mathcal{O}(1)$. This is because $h\sqrt{2}\sqrt{(1-f(s))^2\eta_0^2 + f(s)^2\eta_1^2} \leq \sqrt{2}h(\eta_0 + \eta_1)$, which is $\mathcal{O}(1)$ due to the choice of h in Corollary 1. Then, by Corollary 60 of Ref. [41], we may obtain a $(1, n_a + 3, \epsilon')$ block encoding of $e^{-ihH(s)}$, using the unitaries V_0 and V_1 a total number of times $\mathcal{O}(\ln(1/\epsilon'))$. Finally, the overall numerical propagator can be obtained by multiplying all the block-encoded unitaries, which, by Corollary 55 of Ref. [41], yields a $(1, n_a + 3, 4(T/h)^2\epsilon')$ block encoding of it. To bound the overall error by ϵ , it suffices to choose $\epsilon' = \epsilon h^2/T^2$, and this contributes to an extra factor of $\ln((\|H_0\| + \|H_1\|)/(\epsilon\Delta_*))$ in the complexity of the gate-based implementation.

2. Product formula

We now consider the product formula

$$U_{pf,p}(t+h, t) = \prod_{k=0}^{K_p} \exp(-i\beta_{p,k} h f((t + \delta_{p,k}h)/T) H_1) \\ \times \exp(-i\alpha_{p,k} h (1 - f((t + \gamma_{p,k}h)/T)) H_0) \quad (25)$$

and its simplified version

$$U_{spf,p}(t+h, t) = \prod_{k=0}^{K_p} \exp(-i\beta_{p,k} h f(t/T) H_1) \\ \times \exp(-i\alpha_{p,k} h (1 - f(t/T)) H_0). \quad (26)$$

We start with the simplest case where we assume the multi-step gap condition for the product walk operator. Similarly to the exponential integrator, we can obtain the following result by directly applying the discrete adiabatic theorem in Lemma 1. Detailed proofs of the following result and all the other results being presented in this subsection are shown in Appendix E2.

Theorem 2. Consider Problem 1 using digital adiabatic simulation with the product formula $U_{pf,p}$ or the simplified product formula $U_{spf,p}$. Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Let $\tilde{\Delta}(s)$ denote the multistep spectral gap of $U_{pf,p}(sT+h, sT)$ or $U_{spf,p}(sT+h, sT)$, and $\tilde{\Delta}_* = \min_{s \in [0, 1-h/T]} \tilde{\Delta}(s)$. Then, the overall error between

the actual and the ideal evolution can be bounded by

$$\mathcal{O} \left(\frac{h}{T} \left(\frac{h(\|H_0\| + \|H_1\|)}{\tilde{\Delta}_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{\tilde{\Delta}_*^2} \right. \right. \\ \left. \left. + \frac{h^2(\|H_0\| + \|H_1\|)^2}{\tilde{\Delta}_*^3} \right) \right). \quad (27)$$

Theorem 2 assumes the gap condition for the product walk operator, which is not natural when the time-step size h is large. When the gap condition is not assumed, we can indeed decrease the time-step size to make the walk operator closer to the evolution $e^{-ihH(s)}$, of which the gap is closely related to that of $H(s)$. Here, we only consider the simplified product formula Eq. (9).

We first show the result for first- and second-order product formulas. An interesting phenomenon is that the first- and second-order formulas share the same eigenvalues, so the results revealed by our analysis for the first- and second-order product formulas are the same. This is because $U_{spf,2}$ is just a rotation of $U_{spf,1}$ according to a unitary, i.e.,

$$U_{spf,2}(t+h, t) = V U_{spf,1}(t+h, t) V^\dagger, \quad V = e^{-ih(1-f(t/T))H_0/2}, \quad (28)$$

and such a rotation does not change eigenvalues. We formally state this result in the following lemma.

Lemma 2. Consider the simplified first-order product formula $U_{spf,1}(t+h, t) = e^{-ihf(t/T)H_1} e^{-ih(1-f(t/T))H_0}$ and the simplified second-order product formula $U_{spf,2}(t+h, t) = e^{-ih(1-f(t/T))H_0/2} e^{-ihf(t/T)H_1} e^{-ih(1-f(t/T))H_0/2}$. The eigenvalues of $U_{spf,1}(t+h, t)$ and $U_{spf,2}(t+h, t)$ are exactly the same.

Now, we can estimate the gap of the product walk operators by reducing the time-step size and using perturbation theory. An important observation is that the time-step size will not depend on the tolerated error ϵ , because the only reason to reduce the time-step size is for the gap condition, which is independent of the numerical error. We state this result formally in the next lemma.

Lemma 3. For $s \in [0, 1-h/T]$ and a scheduling function $f(s)$, let $H(s) = (1-f(s))H_0 + f(s)H_1$ be the interpolating Hamiltonian, and $U_{spf,1}$ and $U_{spf,2}$ be the simplified time-dependent product formulas as $U_{spf,1}(sT+h, sT) = e^{-ihf(s)H_1} e^{-ih(1-f(s))H_0}$ and $U_{spf,2}(sT+h, sT) = e^{-ih(1-f(s))H_0/2} e^{-ihf(s)H_1} e^{-ih(1-f(s))H_0/2}$. Let $\Delta_H(s)$ and $\Delta_{U,p}(s)$ denote the spectral gap of $H(s)$ and $U_{spf,p}$, respectively. Then, for any $h \leq 1/(\|H_0\| + \|H_1\|)$ and $p = 1, 2$, we have

$$h\Delta_H(s) - \frac{h^3}{95} (2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|) \\ \leq \Delta_{U,p}(s) \leq h\Delta_H(s) + \frac{h^3}{95} (2\|[H_1, [H_1, H_0]]\| \\ + \|[H_0, [H_0, H_1]]\|). \quad (29)$$

Now, we are ready to state the following complexity estimate for the product formula without assuming the gap condition of the product walk operator.

Corollary 2. Consider Problem 1 using digital adiabatic simulation with the simplified first- and second-order product formulas as in Eq. (9). Suppose that both $|f'(s)|$ and $|f''(s)|$

are uniformly bounded over $[0, 1]$. Let $\Delta(s)$ denote the spectral gap of $H(s)$, and $\Delta_* = \min_{s \in [0, 1]} \Delta(s)$. Then, in order to bound the overall error between the actual and the ideal evolution by $\epsilon \in (0, 1)$, it suffices to choose

$$T = \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon}\right) \quad (30)$$

and

$$h = \min \left\{ \frac{1}{\|H_0\| + \|H_1\|}, \sqrt{\frac{95}{2}} \sqrt{\frac{\Delta_*}{2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|}} \right\}, \quad (31)$$

and the overall number of steps becomes

$$T_d = \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^3}{\Delta_*^3 \epsilon} \max \left\{ 1, \sqrt{\frac{2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|}{\Delta_* (\|H_0\| + \|H_1\|)^2}} \right\}\right). \quad (32)$$

For high-order product formulas, we can estimate the complexity by the same strategy as the first- and second-order formulas. Specifically, we use the high-order Trotter error analysis in Theorem 11 of Ref. [6] to bound the distance between the walk operator $U_{\text{spf},p}(s)$ and the operator $e^{-ihH(s)}$. By shrinking the size of h , we can close this distance to at most $ch\Delta_*$ to ensure the gap condition of $U_{\text{spf},p}(s)$ from the gap condition of $e^{-ihH(s)}$ or equivalently $H(s)$, where Δ_* is the minimum gap of $H(s)$ and $c \in (0, 1)$. As a result, the time-step size h remains independent of the overall evolution time T and the target error ϵ of the adiabatic state preparation. Then,

a complete complexity estimate can be obtained by applying Theorem 2. We formally state the choices of the step size h and the complexities in the next two results, and their proofs can be found in Appendix E2.

Lemma 4. For $s \in [0, 1 - h/T]$ and a scheduling function $f(s)$, let $H(s) = (1 - f(s))H_0 + f(s)H_1$ be the interpolating Hamiltonian and $U_{\text{spf},p}(sT + h, sT)$ be the simplified product formula as in Eq. (9). Let $\Delta_H(s)$ and $\Delta_{U,p}(s)$ denote the spectral gap of $H(s)$ and $U_{\text{spf},p}(s)$, respectively. Then, for any $h \leq 1/(\|H_0\| + \|H_1\|)$ and $p \geq 1$, there exist p -dependent constants c_p such that

$$h\Delta_H(s) - c_p h^{p+1} \sum_{\gamma_0, \dots, \gamma_p \in \{0, 1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\| \leq \Delta_{U,p}(s) \leq h\Delta_H(s) + c_p h^{p+1} \sum_{\gamma_0, \dots, \gamma_p \in \{0, 1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\|. \quad (33)$$

Corollary 3. Consider Problem 1 using digital adiabatic simulation with simplified p th-order product formulas as in Eq. (9). Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Let $\Delta(s)$ denote the spectral gap of $H(s)$, and $\Delta_* = \min_{s \in [0, 1]} \Delta(s)$. Then, for any $p \geq 1$,

(1) the overall error between the actual and the ideal evolution can be bounded by

$$\mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{T \Delta_*^3}\right); \quad (34)$$

(2) in order to bound the overall error by ϵ , it suffices to choose

$$T = \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon}\right) \quad (35)$$

and

$$h = \Theta\left(\min \left\{ \frac{1}{\|H_0\| + \|H_1\|}, \frac{\Delta_*^{1/p}}{\left(\sum_{\gamma_0, \dots, \gamma_p \in \{0, 1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\|\right)^{1/p}} \right\}\right), \quad (36)$$

and the overall number of steps becomes

$$T_d = \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^3}{\Delta_*^3 \epsilon} \max \left\{ 1, \frac{\left(\sum_{\gamma_0, \dots, \gamma_p \in \{0, 1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\|\right)^{1/p}}{\Delta_*^{1/p} (\|H_0\| + \|H_1\|)} \right\}\right). \quad (37)$$

IV. IMPROVED TIME-STEP SIZE AND COMPLEXITY ESTIMATE WITH BOUNDARY CANCELLATION

A. A review of the high-order discrete adiabatic theorem

The high-order discrete adiabatic theorem aims to establish a superpolynomial convergence in $1/T_d$ under further assumptions. In particular, we suppose the discrete evolution satisfies the following conditions.

(1) For $k \geq 1$, there exist real-valued functions $c_k(s)$ such that $\|D^{(k)}W(s)\| \leq c_k(s)/T_d^k$ for $0 \leq s \leq 1 - k/T_d$, where $D^{(k)}W(s)$ represents the k th-order finite difference of $W(s)$ with step size $1/T_d$.

(2) The eigenvalues of $W(s)$ can be separated into two groups $\sigma_P(s)$ and $\sigma_Q(s)$ such that each continuous eigenpath $\lambda(s)$ of $W(s)$ consistently belongs to one of the two groups and the distance between $\sigma_P(s)$ and $\sigma_Q(s)$ is bounded from below by $\Delta(s) > 0$.

(3) The input state $|\psi\rangle$ is within the eigenspace corresponding to $\sigma_P(0)$.

Under these conditions, Ref. [30] claims an upper bound of the discrete diabatic error, achieving $\mathcal{O}(1/T_d^k)$ for any positive integer k . Unfortunately, after a careful examination, we find a missing step in the proof provided in Ref. [30], so the claimed high-order discrete adiabatic theorem is not rigorously supported. Nevertheless, we also perform a numerical test, suggesting that the conclusion on the high-order convergence is numerically correct. Therefore, to be precise, here we present the result in Ref. [30] as a conjecture that we strongly believe to be correct, and refer to Appendix F for more details on the missing step in the proof and our numerical validation.

Conjecture 1. Suppose that $W(s)$ satisfies the boundary cancellation condition in the sense that $W^{(k)}(0) = W^{(k)}(1) = 0$ for all $k \geq 1$. Then, for any integer T_d and any positive integer k , we have

$$\|U(1)|\psi\rangle - P(1)U(1)|\psi\rangle\| \leq \frac{C_k}{T_d^k}, \quad (38)$$

where $U(s)$ is the discrete evolution defined in Eq. (10), $P(s)$ is the spectral projection of $W(s)$ onto $\sigma_P(s)$, and C_k is a constant independent of T_d .

Similar to the continuous case, Conjecture 1 bounds the leakage rate of the actual state out of the desired eigenspace. Compared with Lemma 1, Conjecture 1 might give an error bound with superpolynomial convergence in T_d under an additional assumption analogous to the continuous boundary cancellation condition. However, Conjecture 1 does not give an explicit dependence on the spectral gap. It does not show how the preconstant depends on the order k either, which prevents us from obtaining an exponentially small error because there might be an exponential dependence on k hidden in the constant C_k .

B. Our results

We now focus on the scenario with the additional boundary cancellation condition and establish the superpolynomial convergence result. Due to the lack of a discrete adiabatic theorem with superpolynomial convergence and explicit gap dependence at the same time, it is hard to simultaneously establish both the gap dependence and the precision dependence.

Notice that if we want to track only the gap dependence, we can assume the tolerated error to be at a constant level and directly use Corollary 1 or 3 in the general case, which gives an $\mathcal{O}(\Delta_*^{-3})$ dependence. Throughout this section, we assume that the spectral norms of the Hamiltonians H_0 and H_1 are bounded by 1 and the minimum spectral gap is bounded from below by a constant, and we focus on the dependence on ϵ .

For the first-order exponential integrator and product formulas, we can obtain the following two propositions, which show that for any method it suffices to choose an $\mathcal{O}(1)$ time-step size and the number of steps can be $\mathcal{O}(1/\epsilon^{o(1)})$. The idea is to directly apply Conjecture 1 to the numerical integrators, and technical details of the proofs can be found in Appendix G. Remarkably, such results also hold even for first-order numerical methods.

Proposition 1. Consider Problem 1 using exponential propagators [Eq. (5)]. Suppose that Conjecture 1 is true, both $\|H_0\|$ and $\|H_1\|$ are bounded by 1, $H(s)$ satisfies the gap condition with constant-level minimum gap, and the smooth interpolation function has $f^{(k)}(0) = f^{(k)}(1) = 0$ for all $k \geq 1$. Then, in order to prepare an ϵ approximation of the eigenstate of H_1 , it suffices to choose $h = 1$, and the evolution time and overall number of steps as

$$T = T_d = \mathcal{O}\left(\frac{1}{\epsilon^{1/k}}\right) \quad (39)$$

for any $k \geq 1$.

Proposition 2. Consider Problem 1 using simplified product formula as in Eq. (9). Suppose that Conjecture 1 is true, both $\|H_0\|$ and $\|H_1\|$ are bounded by 1, $H(s)$ satisfies the gap condition with constant-level minimum gap, and the smooth interpolation function $f(s)$ has $f^{(k)}(0) = f^{(k)}(1) = 0$ for all $k \geq 1$. Then, in order to prepare an ϵ approximation of the eigenstate of H_1 , it suffices to choose $h = \mathcal{O}(1)$, and the evolution time and overall number of steps as

$$T = \mathcal{O}\left(\frac{1}{\epsilon^{1/k}}\right), \quad T_d = \mathcal{O}\left(\frac{1}{\epsilon^{1/k}}\right) \quad (40)$$

for any $k \geq 1$.

As a side product, we can obtain an improved error bound on the numerical discretization errors as well. The idea is to use the triangle inequality to bound the numerical discretization error by the sum of the continuous and discrete adiabatic errors. Here, we state an error bound for the first-order product formula and give the proof in Appendix G. Similar results for other numerical methods can be established in the same way.

Corollary 4. Let $|\psi(T)\rangle$ be the solution of Eq. (1) at the final time and $|\tilde{\phi}\rangle$ be the numerical solution obtained by the first-order product formula with step size $\mathcal{O}(1)$. Suppose that Conjecture 1 is true, both $\|H_0\|$ and $\|H_1\|$ are bounded by 1, the Hamiltonian $(1-s)H_0 + sH_1$ satisfies the gap condition, the spectrum of interest only consists of one simple eigenvalue, and the smooth interpolation function $f(s)$ has $f^{(k)}(0) = f^{(k)}(1) = 0$ for any $k \geq 1$. Then, for any $k \geq 1$, we have

$$\| |\tilde{\phi}\rangle \langle \tilde{\phi}| - |\psi(T)\rangle \langle \psi(T)| \| \leq \mathcal{O}\left(\frac{1}{T^k}\right). \quad (41)$$

We compare Corollary 4 with the standard Trotter error bound in two aspects. First, standard Trotter error bounds are

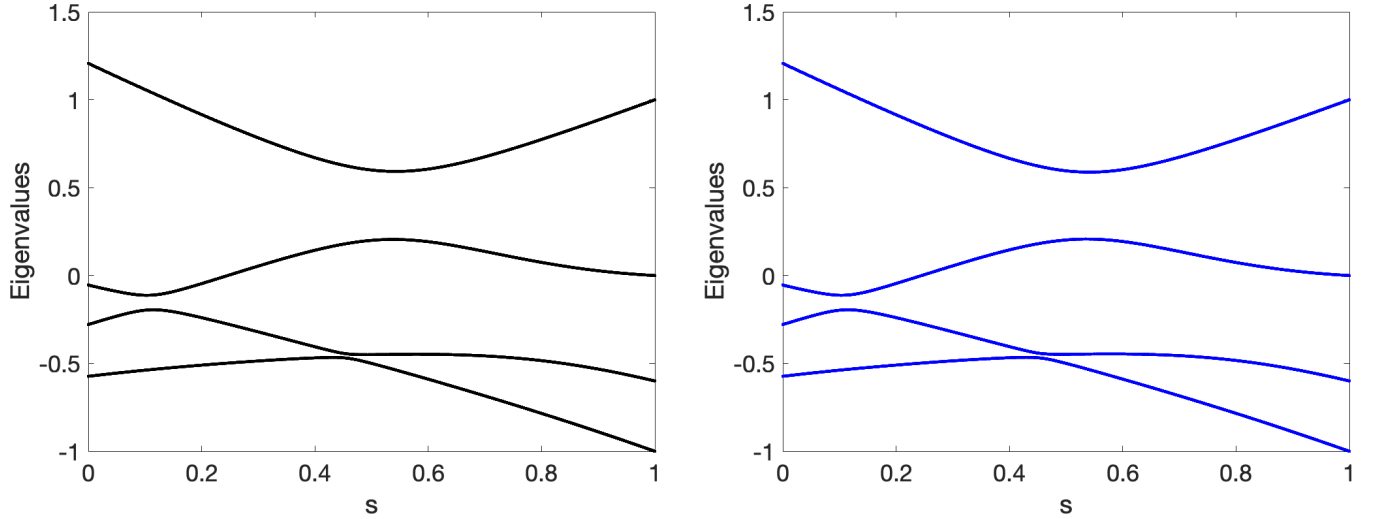


FIG. 1. Left: Spectrum of $H(s)$. Right: Spectrum of $i \ln(W(s))$. Here, $\epsilon = 0.05$.

typically in terms of operator norm, and thus simultaneously bound the fidelity error and the phase error. However, our result in Corollary 4 only bounds the difference in the density matrix, and there is nothing we can conclude from Corollary 4 about the error within the phase. Nevertheless, in the scenario of near-adiabatic evolution, the phase factor is usually not of importance and our bound on the density matrices is usually sufficient. Second, in terms of the density matrices, our error bound significantly improves the standard ones. Our Trotter error bound for near-adiabatic evolution is $\mathcal{O}(T^{-k})$ for an arbitrarily large k , while the standard error bound of first-order Trotter with time-step size $\mathcal{O}(1)$ is only $\mathcal{O}(1)$. We remark that such an improvement requires additional conditions, including the regularity conditions and the Hamiltonian gap conditions specified in Corollary 4.

V. GAP CONDITIONS OF PRODUCT FORMULA AND DISCRETE ADIABATIC EVOLUTION FOR GAPLESS HAMILTONIAN

Our analysis requires the gap condition of the local numerical propagator due to the usage of the discrete adiabatic theorems. For product formula, if only the gap in the Hamiltonian $H(s)$ is assumed rather than the product walk operator, we can reduce the time-step size h to make sure that the product walk operator also has a spectral gap (as shown in Lemma 4 and Corollary 3).

However, when the time-step size is large (i.e., as large as $\mathcal{O}(1)$), the relation between the gap of the product walk operator and the gap of the Hamiltonian is not straightforward yet since the perturbation theory does not directly apply. We show by toy numerical examples that, in the worst case, even if $\|H_0\|$ and $\|H_1\|$ are bounded, the gap condition of the Hamiltonian does not necessarily imply that of the first-order Trotter operator, and vice versa.

The first example is that the gap of $H(s)$ remains constant while the gap of $W(s)$ closes. We consider a four-dimensional system, and H_0 and H_1 are constructed as follows. Let Q be

the eigenbasis of the matrix

$$\begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}, \quad (42)$$

$D = \text{diag}(-0.5, -0.5 + \epsilon, 0.2, 0.6)$ for a small parameter $\epsilon \geq 0$, and define $\tilde{W} = Qe^{-iD}Q^\dagger$. Then, we choose $H_1 = \text{diag}(-1, -0.6, 0, 1)$, $H_0 = 2i \ln(e^{iH_1/2}\tilde{W})$, and the scheduling function is linear (i.e., $f(s) = s$). By definition, $W(0.5)$ is exactly $\tilde{W}$, so we can control the gap of $W(s)$ by tuning ϵ . In particular, the gap vanishes when we choose $\epsilon = 0$. As an illustration, the spectra of $H(s)$ and $W(s)$ are shown in Fig. 1. Notice that the gap of $W(s)$ is measured using the distance in $\mathbb{S}^1$ (i.e., the spectral gap of $i \ln(W(s))$). At a first glance of Fig. 1, the spectra of $H(s)$ and $i \ln(W(s))$ are surprisingly very similar. However, a careful computation yields small differences. We numerically compute the spectral gap between ground and first excited states, and results with different ϵ are shown in Table II. As ϵ decreases, the gap of $W(s)$ decreases, but the gap of $H(s)$ remains at a constant level (although as small as $\sim 10^{-3}$) when ϵ is small enough. In the extreme case where $\epsilon = 0$, the gap of $W(s)$ becomes 0 as expected (numerical gap is $\sim 10^{-16}$, reaching machine epsilon), while the gap of $H(s)$ is still $\sim 10^{-3}$.

Similarly, we can construct a second example where the gap of $W(s)$ remains constant while the gap of $H(s)$ closes. Let Q and $D = \text{diag}(-0.5, -0.5 + \epsilon, 0.2, 0.6)$ be the same as in the first example. Define $\tilde{H} = QDQ^\dagger$, $H_1 = \text{diag}(-1, -0.6, 0, 1)$, $H_0 = 2\tilde{H} - H_1$, and the scheduling function $f(s) = s$. Again by definition, $H(0.5)$ is exactly $\tilde{H}$ and thus can be gapless when $\epsilon = 0$. Table III shows the spectral gaps with different ϵ , and we can observe that, as ϵ decreases, the gap of $H(s)$ vanishes while the gap of $W(s)$ remains at a constant level.

The second example where the gap of $H(s)$ closes while the gap of $W(s)$ of the first-order Trotter operator remains constant suggests the possibility of efficient adiabatic optimization for systems with exponentially small gap or even

TABLE II. Spectral gaps of $H(s)$ and $W(s)$ in the first example. Here, the gap reported is the minimal gap over equidistant points with step size 10^{-4} .

ϵ	10^{-1}	5×10^{-2}	2×10^{-2}	10^{-2}	5×10^{-3}	2×10^{-3}	10^{-3}	5×10^{-4}	2×10^{-4}	10^{-4}	0
Gap of $H(s)$	5.1×10^{-2}	2.3×10^{-2}	7.9×10^{-3}	3.0×10^{-3}	5.6×10^{-4}	8.9×10^{-4}	1.4×10^{-3}	1.6×10^{-3}	1.8×10^{-3}	1.8×10^{-3}	1.9×10^{-3}
Gap of $W(s)$	5.2×10^{-2}	2.5×10^{-2}	9.7×10^{-3}	4.8×10^{-3}	2.6×10^{-3}	9.5×10^{-4}	4.8×10^{-4}	2.4×10^{-4}	1.0×10^{-4}	5.2×10^{-5}	1.1×10^{-16}

gapless systems. Specifically, for gapless systems, we can try first-order Trotter with time-step size 1. Thanks to the discrete adiabatic theorems, such an approach will work and approximate the desired eigenstate if the product walk operators satisfy the gap condition, which is possible even for gapless systems (and we have observed this in our second example). Meanwhile, decreasing the time-step sizes might worsen the computation because it makes the numerical evolution closer to the continuous dynamics, which is known to be away from the desired eigenstate.

We illustrate this phenomenon using our second toy model again. Here, we directly choose $\epsilon = 0$, so the Hamiltonian $H(s)$ is gapless and the walk operator $W(s)$ of first-order Trotter with time-step size 1 still satisfies the gap condition. Figure 2 shows the spectrum of $H(s)$ and $W(s)$, and confirms that $H(s)$ is gapless and $W(s)$ is gapped (though the gap is indeed very small). We choose time $T = 10^k$ for $k = 3, 4, 5, 6, 7$, and implement first-order Trotter method with time-step sizes $h = 2^{-k}$ for $k = 0, 1, 2, 3, 4, 5$. In Fig. 3, we plot the fidelity $|\langle \phi | e_j \rangle|$ for $j = 0, 1$, where $|\tilde{\phi}\rangle$ is our final actual state and $|e_j\rangle$ is the j th eigenstate of the final Hamiltonian H_1 . When the time-step size is fixed to be 1, the actual state will better approximate the ground state of H_1 as T becomes larger. This can be explained by the discrete adiabatic theorems and the analysis we establish in this work. However, if we decrease the time-step size, then the numerical solution will go away from the ground state and tend to the first excited state instead. This is because, as the time-step size decreases, the numerical solution will be closer to the solution of the continuous dynamics governed by $H(s)$, which is gapless and does not even approximately follow the ground eigenpath. The observation that it goes to the first excited state can be explained according to the adiabatic theorem without gap condition [35] since the ground state of the initial Hamiltonian H_0 and the first excited state of the final Hamiltonian H_1 are smoothly connected. In summary, this toy example shows that for gapless Hamiltonian, continuous adiabatic evolution does not approximate the ground state but the Trotterization with $\mathcal{O}(1)$ time-step size may still work as long as the product walk operator satisfies the gap condition.

We highlight that all of the above findings on the gapless systems are based on the toy model. Exploring useful applications beyond the artificial four-level example is an

important open question and can be of significant practical relevance. We believe that similar phenomenon might occur for more physically realistic gapless systems, which could be understood by the correspondence between the discretized evolution and its effective Hamiltonian. Specifically, for the unitary walk operator $U_{\text{num}}((j+1)h, jh)$, there exists a time-dependent version of the effective Hamiltonian $H_{\text{eff}}(s)$ such that $U_{\text{num}}((j+1)h, jh)$ is the time evolution operator of $H_{\text{eff}}(s)$ over the time interval $[jh, (j+1)h]$. The effective Hamiltonian can then be split as $H_{\text{eff}}(s) = (1 - f(s))H_0 + f(s)H_1 + H_2(s)$, where the additional $H_2(s)$ term is not necessarily small due to the use of large step size. However, in the continuous adiabatic quantum computing literature, it has been shown that adding an additional term (usually called a ‘‘catalyst’’ Hamiltonian) can open up the spectral gap of the Hamiltonian in many applications, including instances of MAX 2SAT [43] and 3SAT [44], quadratic unconstrained binary optimization problems [45], fully connected Ising model [46], and infinite-range Ising models with ferromagnetic or antiferromagnetic interactions [47–50]. Then, one potential direction is to relate our $H_2(s)$ in the effective Hamiltonian to any of the existing catalysts, or show that it has similar mechanics as the catalysts.

VI. OPTIMIZED GAP DEPENDENCE WITH APPLICATION TO GROVER SEARCH AND COMPARISON WITH QAOA

We have shown that the time-step size in discretizing near-adiabatic dynamics can be larger than previously expected by viewing the numerical integrator as the set of discrete adiabatic walk operators. In our analysis, we mainly focus on the improved scalings in ϵ , and we simply bound the time-dependent spectral gap by the minimal gap, resulting in a generally superlinear dependence on the gap. However, the gap dependence can be improved to be linear if we are given sufficient information of the simultaneous gap and carefully choose the scheduling function $f(s)$ according to the size of the gap. This has been observed in several applications of the continuous adiabatic evolution as well as using the first-order exponential integrator to construct optimal linear system solver. Here, we demonstrate by the adiabatic Grover search example that the linear gap dependence can also be achieved in first-order Trotter method as well.

TABLE III. Spectral gaps of $H(s)$ and $W(s)$ in the second example. Here, the gap reported is the minimal gap over equidistant points with step size 10^{-4} .

ϵ	10^{-1}	5×10^{-2}	2×10^{-2}	10^{-2}	5×10^{-3}	2×10^{-3}	10^{-3}	5×10^{-4}	2×10^{-4}	10^{-4}	0
Gap of $H(s)$	5.1×10^{-2}	2.5×10^{-2}	9.6×10^{-3}	4.7×10^{-3}	2.4×10^{-3}	9.4×10^{-4}	4.7×10^{-4}	2.3×10^{-4}	1.0×10^{-4}	5.1×10^{-5}	3.3×10^{-16}
Gap of $W(s)$	5.3×10^{-2}	2.6×10^{-2}	1.1×10^{-2}	6.6×10^{-3}	4.2×10^{-3}	2.8×10^{-3}	2.4×10^{-3}	2.1×10^{-3}	2.0×10^{-3}	1.9×10^{-3}	1.9×10^{-3}

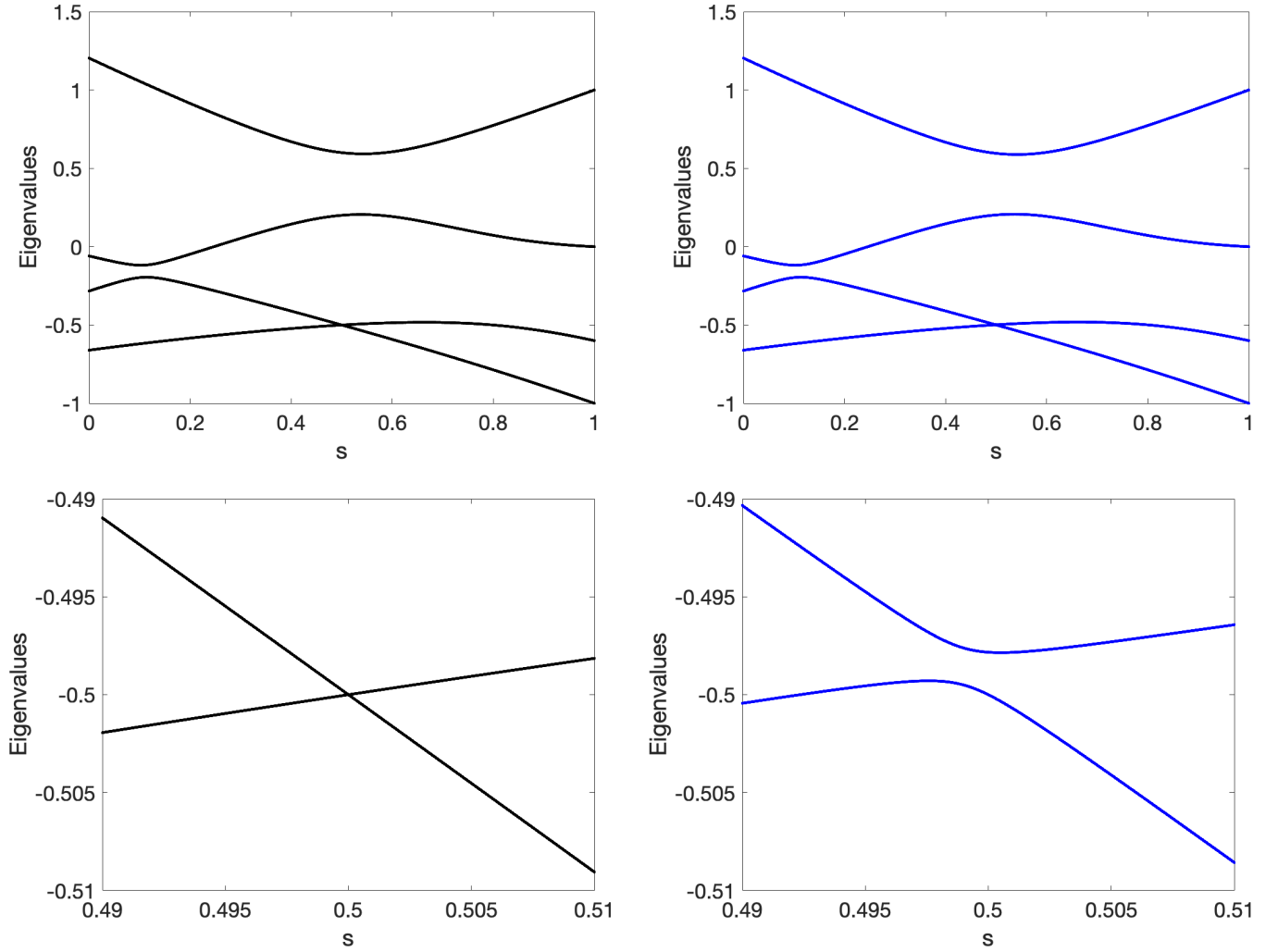


FIG. 2. Spectrum of $H(s)$ and $i \ln(W(s))$ of first-order Trotter with time-step size 1 in the second toy example with $\epsilon = 0$. Here, the top left is of $H(s)$, the top right is of $i \ln(W(s))$, and the bottom two are enlarged views.

We consider the unstructured search problem in N -dimensional Hilbert space. Let $\{|j\rangle\}_{j=0}^{N-1}$ denote the computational basis and let $\mathcal{M} \subset \{|j\rangle\}_{j=0}^{N-1}$ be the set of the marked

states with $|\mathcal{M}| = M$. We assume $N \geq 2M$. Starting with the uniform superposition of the computational basis, our goal is to find the uniform superposition of all marked states. Here, we do not assume *a priori* knowledge on M since estimating

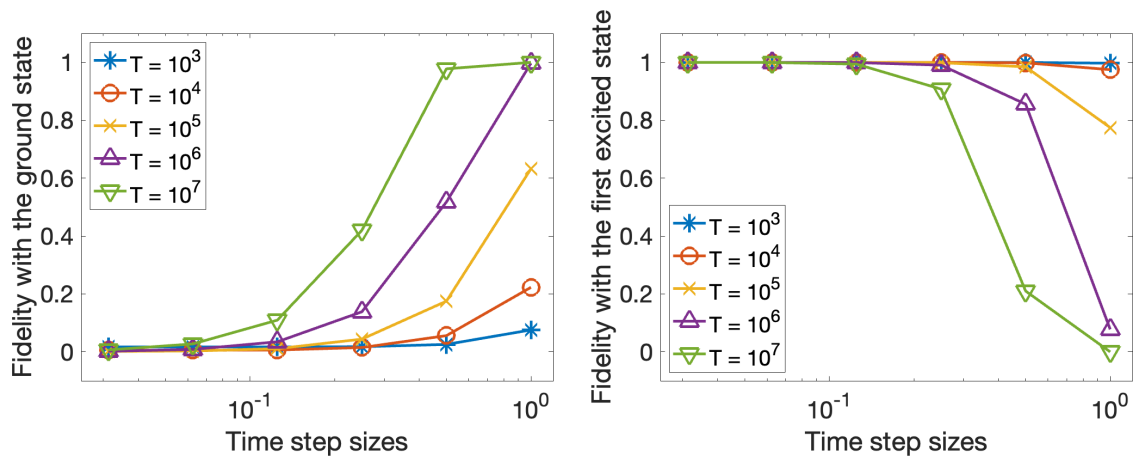


FIG. 3. Fidelity with the ground state (left) and the first excited state (right) of the numerical solutions from first-order Trotter method with different time T and time-step sizes h .

the bound of M can be costly—Instead, we are interested in designing robust algorithm that does not use the information of M in implementing the algorithm and automatically becomes more accurate when M is larger.

Adiabatic formulation [1] takes the initial Hamiltonian to be

$$H_0 = I - |u\rangle\langle u|, \quad (43)$$

where $|u\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} |j\rangle$ is the uniform superposition, and the final Hamiltonian to be

$$H_1 = I - \sum_{j \in \mathcal{M}} |j\rangle\langle j|. \quad (44)$$

Notice that both H_0 and H_1 only effectively act on a two-dimensional subspace. The orthonormal basis of this subspace is $\{|e_0\rangle, |e_1\rangle\}$, where

$$|e_0\rangle = \frac{1}{\sqrt{M}} \sum_{j \in \mathcal{M}} |j\rangle, \quad |e_1\rangle = \frac{1}{\sqrt{N-M}} \sum_{j \notin \mathcal{M}} |j\rangle, \quad (45)$$

and the corresponding matrix representations of H_0 and H_1 are

$$H_0 = \begin{pmatrix} 1 - M/N & -\sqrt{M(N-M)}/N \\ -\sqrt{M(N-M)}/N & M/N \end{pmatrix}, \quad (46)$$

$$H_1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Furthermore, $|u\rangle$ is the ground state of H_0 and our target state $|e_0\rangle$ is the ground state of H_1 . Let $H(s) = (1 - f(s))H_0 + f(s)H_1$, where $f(s)$ is the scheduling function such that $f(0) = 0$ and $f(1) = 1$. We may solve the time evolution governed by $H(s)$ with the initial state $|u\rangle$ to approximate the target state. The corresponding digital simulation algorithm, using first-order Trotter method with time-step size 1 (so $T = T_d$ in this case), goes as

$$\prod_{j=0}^{T-1} \exp(-if(j/T)H_1) \exp(-i(1 - f(j/T))H_0)|u\rangle. \quad (47)$$

For time-dependent Hamiltonian $H(s) = (1 - f(s))H_0 + f(s)H_1$, straightforward computations yield that two relevant eigenvalues that determine the diabatic errors are [1]

$$\lambda_{\pm} = \frac{1}{2} \pm \frac{1}{2} \sqrt{(1 - 2f(s))^2 + \frac{4M}{N} f(s)(1 - f(s))}. \quad (48)$$

The gap of $H(s)$ is

$$\Delta_H(s; N, M, f) = \sqrt{(1 - 2f(s))^2 + \frac{4M}{N} f(s)(1 - f(s))}. \quad (49)$$

However, in the discrete evolution, the gap of the walk operator $W(s) = \exp(-if(s)H_1) \exp(-i(1 - f(s))H_0)$ is what determines the scaling of T . Since $W(s)$ is represented by a two-dimensional matrix, it is possible to explicitly compute its eigenvalues and spectral gap (see Appendix H). However, the explicit expression of the gap turns out to be complicated for us to estimate the adiabatic error using Lemma 1. To facilitate further computations, we alternatively relate the gap of $W(s)$ to that of $H(s)$ in the following lemma, for which the proof can be found in Appendix H.

Lemma 5. Consider the adiabatic Grover search problem. Let $H(s)$ be the Hamiltonian with the gap $\Delta_H(s; N, M, f)$ specified in Eq. (49), and $\Delta_W(s; N, M, f)$ denote the gap of the walk operator $W(s)$. Then,

$$\Delta_W(s; N, M, f) \geq \frac{2}{3} \Delta_H(s; N, M, f). \quad (50)$$

The minimum gap appears when $s = f^{-1}(1/2)$ and $\sim \sqrt{M/N}$. As a result, a linear interpolation ($f(s) = s$) leads to the nonoptimal scaling $T \geq N/M$, which is at least quadratically worse than Grover's algorithm. To recover the Grover speedup, we need to choose a carefully designed scheduling function such that it slows down when the gap closes.

We consider two options. The first one is to use the scheduling function designed for $M = 1$, so the scheduling function is independent of general values of M . The intuitive reason why this may work is that the case $M = 1$ is the hardest one with smallest gap near $s = f^{-1}(1/2)$, so the resulting scheduling function is also sufficiently slow near the smallest gap for general $M > 1$. One example is defined through the differential equation

$$\partial_s f(s) = d_{N,p} \Delta_H(s; N, 1, f(s))^p, \quad f(0) = 0, \quad (51)$$

where the normalization constant $d_{N,p}$ is chosen such that $f(1) = 1$ and has the expression

$$d_{N,p} = \int_0^1 \Delta_H(s; N, 1, s)^{-p} ds. \quad (52)$$

Such a scheduling function was originally proposed in Ref. [36] with $p = 2$ and generalized in Ref. [26] with $1 < p < 2$ for continuous AQC. The work [37] considers the time discretization error with $p = 2$ and shows that the time-step size can be as large as 1 via efficient Hamiltonian approach. For $1 \leq p < 2$, we give the error bound in the following theorem, and the proof can be found in Appendix I.

Theorem 3. Consider solving the Grover search problem in N dimensions with M marked states using AQC discretized by first-order product formula with time-step size 1. Suppose that M is unknown.

(1) Suppose that $T \geq \mathcal{O}(\ln(N))$ and the scheduling function is defined in Eq. (51) with $p = 1$. Then, the overall error is bounded by

$$\mathcal{O}\left(\frac{\ln(N)}{T} \sqrt{\frac{N}{M}}\right). \quad (53)$$

(2) Suppose that $T \geq \mathcal{O}(N^{\frac{p-1}{2}})$ and the scheduling function is defined in Eq. (51) with $1 < p < 2$. Then, the overall error is bounded by

$$\mathcal{O}\left(\frac{1}{T} \frac{\sqrt{N}}{M^{1-\frac{p}{2}}} + \frac{N^{p-1}}{T^2} \max\left\{1, \frac{N^{3/2-p}}{M^{3/2-p}}\right\}\right). \quad (54)$$

Theorem 3 implies that, to achieve an ϵ error, the smallest number of Trotter steps required is $\mathcal{O}(\frac{\sqrt{N} \ln(N)}{M \epsilon})$ for $p = 1$ and $\mathcal{O}(\frac{\sqrt{N}}{M^{1-p/2}} \frac{1}{\epsilon})$ for $1 < p < 2$. The discrete adiabatic evolution with $p = 1$ is nearly optimal (up to a logarithmic factor) in both N and M , and that with $1 < p < 2$ is optimal in N but not optimal in M . Notice that these critical points are only for comparison with other algorithms and not for designing

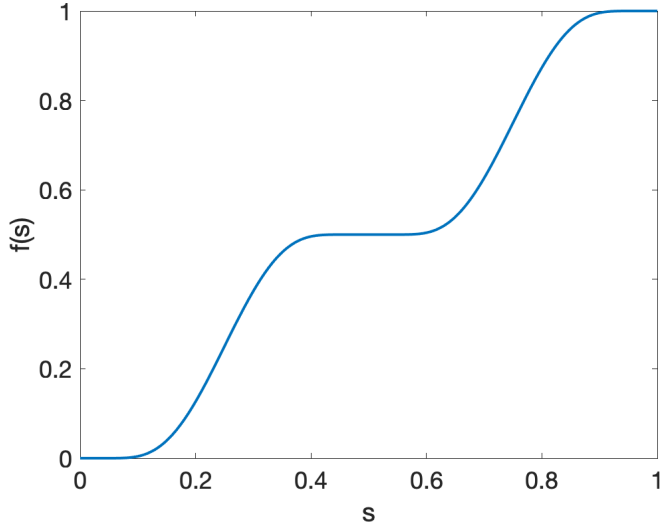


FIG. 4. The scheduling function in robust Grover search with boundary cancellation.

algorithms since we do not know M *a priori*—Instead, we will use sufficiently large T and the error becomes automatically smaller if T is too large.

Now, we consider another scheduling function satisfying boundary cancellation condition. We also want it to slow down at $s = 1/2$ to preserve the Grover speedup. We start with the function

$$g(s) = c_e^{-1} \int_0^s \exp\left(-\frac{1}{s'(1-s')}\right) ds', \quad (55)$$

where

$$c_e = \int_0^1 \exp\left(-\frac{1}{s'(1-s')}\right) ds'. \quad (56)$$

One can show that $g(0) = 0$, $g(1) = 1$, and $g^{(k)}(0) = g^{(k)}(1) = 0$ for all $k \geq 1$. Consider

$$f(s) = \begin{cases} \frac{1}{2}g(2s), & s \in [0, \frac{1}{2}], \\ \frac{1}{2} + \frac{1}{2}g(2s-1), & s \in (\frac{1}{2}, 1], \end{cases} \quad (57)$$

which is illustrated in Fig. 4. Intuitively, we symmetrically connect two g 's and the resulting function $f(s)$ is smooth, satisfies the boundary cancellation, and becomes slow in the middle. With this scheduling function Eq. (57), we can bound the error as follows, and the proof can be found in Appendix J.

Theorem 4. Consider solving the Grover search problem in N dimensions with M marked states using AQC with the scheduling function [Eq. (57)], discretized by first-order product formula with time-step size 1. Suppose that Conjecture 1 is true, and $T \geq \mathcal{O}(\sqrt{N/M})$. Then, for any integer $k \geq 1$, the overall error can be bounded by

$$\min \left\{ \frac{C}{T} \sqrt{\frac{N}{M}} \left(\ln \frac{N}{M} \right)^4, \frac{C_k(N, M)}{T^k} \right\}. \quad (58)$$

Here, C is an absolute constant and $C_k(N, M)$ is a constant that depends on k, N, M .

Theorem 4 can be understood from two angles. On the one hand, for constant level of error ϵ , we use the first error bound

and the number of Trotter steps required scales $\tilde{\mathcal{O}}(\sqrt{N/M})$, achieving the Grover scaling up to logarithmic factors. On the other hand, for fixed N and M , we use the second error bound to conclude that the convergence in T is superpolynomial and T scales $\tilde{\mathcal{O}}(1/\epsilon^{o(1)})$. Notice that the scheduling function Eq. (57) is independent of both M and N .

Finally, we compare our results with QAOA. Our results imply an approach to construct the angles in QAOA via adiabatic evolution for Grover search problem. Specifically, QAOA for Grover search takes the ansatz

$$|\psi\rangle = \prod_{j=0}^{p-1} e^{-i\gamma_j H_1} e^{-i\beta_j H_0} |\psi_0\rangle, \quad (59)$$

where the parameters (β_j, γ_j) are optimized to minimize $\langle \psi | H_1 | \psi \rangle$. According to our discrete adiabatic result, the first-order Trotter method with time step 1 outputs

$$|\tilde{\phi}\rangle = \prod_{j=0}^{T-1} e^{-if(j/T)H_1} e^{-i(1-f(j/T))H_0} |u\rangle, \quad (60)$$

and $|\tilde{\phi}\rangle$ is a good approximation of the ground state of H_1 . This implies a set of near-optimal QAOA parameters

$$\beta_j = 1 - f(j/T), \quad \gamma_j = f(j/T), \quad (61)$$

where $f(s)$ is the scheduling function in Eq. (51) with $1 < p < 2$. When $M = 1$, the depth and time complexity of QAOA are both $p = T \sim \sqrt{N}$, which already matches the Grover lower bound. Therefore, our result shows that discrete adiabatic evolution can asymptotically match the performance of optimized QAOA for Grover search problem, and the speedup of QAOA is at most a constant factor.

VII. CONCLUSIONS

In this work, we establish improved error bounds and complexity analysis for the first-order exponential integrator and product formula when applied to simulating near-adiabatic quantum dynamics. The key step in our analysis is to view the numerical integrator as the set of slowly varying unitary walk operators, and to directly bound the distance between the actual output state and the ideal eigenstate. Compared to the standard error analysis that combines the continuous adiabatic theorem and the bounds for time discretization error in the general setting, our method provides a much more direct point of view and thus yields improvements. In the first-order exponential integrator or product formula of any order, for accurate simulation, it suffices to choose a uniform time-step size independent of the error ϵ and the evolution time T . This greatly improves the previous estimate that scales as $\epsilon^{1/p}/T^{1/p}$ for a p th-order product formula. Remarkably, when the Hamiltonian is bounded by 1, a first-order method with unit time-step size would suffice. Furthermore, under the boundary cancellation condition, even first-order methods with uniform time-step size can achieve superpolynomial convergence.

The key technical tool in our analysis is the discrete adiabatic theorem. In particular, under the boundary cancellation condition, we use a high-order discrete adiabatic theorem to

show strong evidence of superpolynomial convergence for first-order methods. However, there are two open questions in the high-order discrete adiabatic theorem. First, as discussed in Appendix F2, although the conclusion of the high-order discrete adiabatic theorem is numerically correct, the proof presented in Ref. [30] seems not valid due to a missing step. It is our future work to fix this gap and establish a rigorous proof for the high-order discrete adiabatic theorem. Another drawback of the current high-order discrete adiabatic theorem is that it only analyzes the scaling of errors in terms of the evolution time T . It would be interesting and practically useful to enhance the result with explicit dependence on the spectral gap as well, similar to what has been done for the first-order discrete adiabatic theorem in Ref. [31].

To apply the discrete adiabatic theorems, we require the numerical integrator to satisfy the gap condition as well. When analyzing high-order product formula, we match the gap condition for the numerical integrator with that of the time-dependent Hamiltonian $H(s)$, as long as the time-step size is smaller than a threshold that only depends on the Hamiltonian $H(s)$ itself. However, when the time-step size is large, there is no clear relation between the gap of the numerical integrator and the gap of the Hamiltonian, as shown in Sec. V via toy models. Remarkably, it is possible that, even if the Hamiltonian $H(s)$ has small gap or becomes gapless, its Trotterization with large time step might regain the gap condition, indicating that adiabatic evolution with suitable discretization might possibly achieve exponential speedup over the standard AQC framework. It is very interesting to find if there is any application of practical interest that has such feature in its gap condition.

We apply our analysis to the example of adiabatic Grover search problem. For this problem, we find that the QAOA approach does not yield better asymptotic scaling compared to the Trotterized adiabatic approach. Relation and comparison between AQC and QAOA for eigenstate preparation and optimization is a long-standing topic, and a thorough and comprehensive understanding may significantly advance the theoretical study on QAOA or even more general variational quantum algorithms. Our work here is the first step to bridge the connection, in the scenario where the Hamiltonian is bounded and well gapped. The next step would be to further explore AQC (and especially discrete AQC) and QAOA for gapped Hamiltonian but with large spectral norm, and then even for gapless Hamiltonian.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: CONTINUOUS ADIABATIC THEOREMS

Here, we briefly review the previous results about continuous adiabatic theorems, which aim to bound the distance between the dynamics in Eq. (1) and the ideal eigenspace.

For a general interpolation function $f(s)$, the continuous adiabatic error can be bounded linearly in the inverse evolution time. Here, we present a result from Ref. [26]. Let $U(t)$ denote the exact evolution operator of Eq. (1) and $P(s)$ denote the spectral projection onto the eigenspace of $H(s)$ of interest. Suppose that $\Delta(s)$ is the spectral gap of the Hamiltonian $H(s)$.

Lemma A1 (Continuous adiabatic theorem). Suppose that $H(s)$ is second-order continuously differentiable. Let $\Delta(s)$ denote the spectral gap of $H(s)$. Then, for any $t \in [0, T]$ and $s = t/T$, we have

$$\begin{aligned} & \| |\psi(t)\rangle - P(s)|\psi(t)\rangle \| \\ & \leq \frac{C}{T} \left(\frac{\|H'(0)\|}{\Delta(0)^2} + \frac{\|H'(s)\|}{\Delta(s)^2} + \int_0^s \frac{\|H''(\tau)\|}{\Delta(\tau)^2} d\tau \right. \\ & \quad \left. + \int_0^s \frac{\|H'(\tau)\|^2}{\Delta(\tau)^3} d\tau \right) \end{aligned} \quad (\text{A1})$$

for a constant $C > 0$, which only depends on the number of the eigenstates contained in $P(s)$.

When the Hamiltonian $H(s)$ satisfies the boundary cancellation condition, namely, that the derivatives of $H(s)$ of any order vanish at the boundary, convergence of the final adiabatic error can be improved to be exponential in time. Such a high-order adiabatic theorem was rigorously proved in Ref. [13] without explicit gap dependence and in Ref. [18] with cubic inverse gap dependence. Based on their approaches, a recent work [51] improved the gap dependence to be quadratic. Here, we present the main result in Ref. [51].

Definition A1 (Gevrey class). A function $g(s)$ defined on $[0, 1]$ is in the Gevrey class G^α for $\alpha > 0$ if there exist constants $C, D > 0$ such that for all $k \geq 0$,

$$\max_{s \in [0, 1]} \|g^{(k)}(s)\| \leq CD^k \frac{(k!)^{1+\alpha}}{(k+1)^2}. \quad (\text{A2})$$

Here, $\|\cdot\|$ represents the absolute value if g is scalar valued and the spectral norm if g is operator valued.

Lemma A2 (Continuous adiabatic theorem with boundary cancellation; Theorem 7 of Ref. [51]). Suppose that $H(s)$ is in the Gevrey class G^α for $\alpha > 0$ and assume that $H^{(k)}(0) = H^{(k)}(1) = 0$ for all $k \geq 1$. Let $\Delta(s)$ denote a lower bound of the spectral gap of $H(s)$ and let $\Delta_* = \min_{s \in [0, 1]} \Delta(s)$. Then, we have

$$\| |\psi(T)\rangle - P(1)|\psi(T)\rangle \| \leq \frac{c}{\Delta_*} \exp\left(- (c'T \Delta_*^2)^{\frac{1}{1+\alpha}}\right), \quad (\text{A3})$$

where c and c' are positive constants only depending on C, D (specified according to Definition A1), and α .

Both Lemmas A1 and A2 bound the leakage of the dynamics out of the desired eigenspace. We remark that, up to a constant factor 2, it can also serve as the upper bound of

the distance between the dynamics and an ideal eigenstate $P(s)|\psi(t)\rangle/\|P(s)|\psi(t)\rangle\|$ using a linear algebra result that

$$\left\| |\psi(t)\rangle - \frac{P(s)|\psi(t)\rangle}{\|P(s)|\psi(t)\rangle\|} \right\| \leq 2\| |\psi(t)\rangle - P(s)|\psi(t)\rangle \| \quad (\text{A4})$$

APPENDIX B: MULTISTEP GAP CONDITION

The discrete adiabatic theorem in Lemma 1 (Sec. III B) needs the multistep gap condition; i.e., the gap is assumed between successive steps, which is a further subtlety. Here, we show that, if the number of steps T_d is large enough and each $W(s)$ has a uniformly bounded spectral gap, then the multistep gap condition can be guaranteed.

Lemma B1. Let $W(s)$ be the walk operator, T_d be the number of discrete walk steps, and $c_1(s)$ be the function such that $\|DW(s)\| \leq c_1(s)/T_d$. Suppose that the gap between two groups $\sigma_P(s)$ and $\sigma_Q(s)$ of the eigenvalues of $W(s)$ is bounded from below by $\Delta_* > 0$. Then, as long as $T_d \geq (2\pi/\Delta_*) \sup_{\tilde{s} \in \{s, s+1/T_d\} \cap [0, 1]} c_1(\tilde{s})$, the multistep gap between the arcs $\sigma_P^{(2)}(s)$ and $\sigma_Q^{(2)}(s)$ is bounded from below by $\Delta_*/2$.

Proof. Let $\lambda(s)$ and $\mu(s)$ denote the two eigenvalues of $W(s)$ that determine the gap, i.e., at the corresponding boundary of the arcs. For any $s', s'' \in \{s, s+1/T_d, s+2/T_d\} \cap [0, 1]$, according to Ref. [52] and the definition of $c_1(s)$, we have

$$\begin{aligned} |\lambda(s') - \lambda(s'')| &\leq \|W(s') - W(s'')\| \\ &\leq \frac{2}{T_d} \sup_{\tilde{s} \in \{s, s+1/T_d\} \cap [0, 1]} c_1(\tilde{s}). \end{aligned} \quad (\text{B1})$$

Let $\mathbb{S}^1$ denote the unit circle, and define $|z_1 - z_2|_{\mathbb{S}^1}$ to be the angular distance between $z_1, z_2 \in \mathbb{S}^1$. Using $|z_1 - z_2|_{\mathbb{S}^1} \leq \frac{\pi}{2}|z_1 - z_2|$, we have

$$|\lambda(s') - \lambda(s'')|_{\mathbb{S}^1} \leq \frac{\pi}{T_d} \sup_{\tilde{s} \in \{s, s+1/T_d\} \cap [0, 1]} c_1(\tilde{s}). \quad (\text{B2})$$

We have required that $T_d \geq \frac{2\pi}{\Delta_*} \sup_{\tilde{s} \in \{s, s+1/T_d\} \cap [0, 1]} c_1(\tilde{s})$, which gives

$$|\lambda(s') - \lambda(s'')|_{\mathbb{S}^1} \leq \frac{\Delta_*}{2}. \quad (\text{B3})$$

Therefore, by the triangle inequality, we have

$$\begin{aligned} |\lambda(s') - \mu(s'')|_{\mathbb{S}^1} &\geq |\lambda(s'') - \mu(s'')|_{\mathbb{S}^1} - |\lambda(s') - \lambda(s'')|_{\mathbb{S}^1} \\ &\geq \frac{\Delta_*}{2}, \end{aligned} \quad (\text{B4})$$

which means that the multistep gap is at least $\Delta_*/2$. ■

APPENDIX C: BOUNDS FOR FINITE DIFFERENCES

To apply the discrete adiabatic theorem stated in Lemma 1, we need to estimate the scalings of $c_1(s)$ and $c_2(s)$. Here, we show how to bound $c_1(s)$ and $c_2(s)$ by the derivatives of the walk operator $W(s)$ and derive explicit estimates for the first-order exponential integrator and the product formula.

We first show that for each k , $c_k(s)$ is closely related to the k th-order derivative of $W(s)$.

Lemma C1. Let $W(s)$ be a set of parametrized unitary walk operators for $s \in [0, 1]$, and let $D^{(k)}$ represent the k th-order finite difference of $W(s)$ with step size $1/T_d$ for an integer T_d . For any positive integer k , if $W(s)$ is k th-order continuously differentiable, then we have

$$\|D^{(k)}W(s)\| \leq \frac{c_k(s)}{T_d^k}, \quad (\text{C1})$$

where

$$c_k(s) = \max_{s' \in [s, s+k/T_d]} \|W^{(k)}(s')\|. \quad (\text{C2})$$

Proof. For $k = 1$, using the fundamental theorem of calculus, we have

$$DW(s) = W(s + 1/T_d) - W(s) = \int_s^{s+1/T_d} W'(s') ds'. \quad (\text{C3})$$

More generally,

$$\begin{aligned} D^{(k)}W(s) &= \int_0^{1/T_d} ds_1 \int_0^{1/T_d} ds_2 \cdots \\ &\quad \times \int_0^{1/T_d} ds_k W^{(k)}(s + s_1 + s_2 + \cdots + s_k). \end{aligned} \quad (\text{C4})$$

This is the matrix form of a standard result for scalar finite differences (page 10 of Ref. [53]), and is easily found by induction with

$$\begin{aligned} D^{(k)}W(s) &= D^{(k-1)}W(s + 1/T_d) - D^{(k-1)}W(s) \\ &= \int_0^{1/T_d} ds_1 \int_0^{1/T_d} ds_2 \cdots \int_0^{1/T_d} ds_{k-1} W^{(k-1)}(s + 1/T_d + s_1 + s_2 + \cdots + s_{k-1}) \\ &\quad - \int_0^{1/T_d} ds_1 \int_0^{1/T_d} ds_2 \cdots \int_0^{1/T_d} ds_{k-1} W^{(k-1)}(s + s_1 + s_2 + \cdots + s_{k-1}) \\ &= \int_0^{1/T_d} ds_1 \int_0^{1/T_d} ds_2 \cdots \int_0^{1/T_d} ds_{k-1} DW^{(k-1)}(s + s_1 + s_2 + \cdots + s_{k-1}) \\ &= \int_0^{1/T_d} ds_1 \int_0^{1/T_d} ds_2 \cdots \int_0^{1/T_d} ds_k W^{(k)}(s + s_1 + s_2 + \cdots + s_k). \end{aligned} \quad (\text{C5})$$

This expression gives, by the triangle inequality,

$$\|D^{(k)}W(s)\| \leq \int_0^{1/T_d} ds_1 \int_0^{1/T_d} ds_2 \cdots \int_0^{1/T_d} ds_k \|W^{(k)}(s + s_1 + s_2 + \cdots + s_k)\| \leq \frac{1}{T_d^k} \max_{s' \in [s, s+k/T_d]} \|W^{(k)}(s')\|. \quad (\text{C6})$$

Therefore, $\|D^{(k)}W(s)\|$ is upper bounded with c_k as in Eq. (C2). ■

Now, we give explicit choices of $c_1(s)$ and $c_2(s)$ for the first-order exponential integrator and the product formula.

Lemma C2. Let $W(s) = U_{\text{exp}}(sT + h, sT)$ be the first-order exponential integrator defined in Eq. (5), where $h = T/T_d$ is the time-step size. Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Then, we can choose

$$c_1(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|)), \quad c_2(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \quad (\text{C7})$$

Proof. First, using the formula that for any operator $X(s)$,

$$\frac{d}{ds} e^{X(s)} = \int_0^1 e^{\alpha X(s)} \frac{dX(s)}{ds} e^{(1-\alpha)X(s)} d\alpha, \quad (\text{C8})$$

we can compute that

$$W'(s) = -ihf'(s) \int_0^1 e^{-i\alpha hH(s)} (H_1 - H_0) e^{-i(1-\alpha)hH(s)} d\alpha, \quad (\text{C9})$$

and, according to the chain rule,

$$\begin{aligned} W''(s) &= -ihf''(s) \int_0^1 e^{-i\alpha hH(s)} (H_1 - H_0) e^{-i(1-\alpha)hH(s)} d\alpha \\ &\quad - h^2 f'(s)^2 \int_0^1 \int_0^1 \alpha e^{-i\alpha \beta hH(s)} (H_1 - H_0) e^{-i\alpha(1-\beta)hH(s)} (H_1 - H_0) e^{-i(1-\alpha)hH(s)} d\beta d\alpha \\ &\quad - h^2 f'(s)^2 \int_0^1 \int_0^1 (1-\alpha) e^{-i\alpha hH(s)} (H_1 - H_0) e^{-i(1-\alpha)\beta hH(s)} (H_1 - H_0) e^{-i(1-\alpha)(1-\beta)hH(s)} d\beta d\alpha. \end{aligned} \quad (\text{C10})$$

Therefore, using the bound $\|H_1 - H_0\| \leq (\|H_0\| + \|H_1\|)$, we have

$$\|W'(s)\| \leq h|f'(s)| \int_0^1 \|H_1 - H_0\| d\alpha \leq \mathcal{O}(h(\|H_0\| + \|H_1\|)) \quad (\text{C11})$$

and

$$\begin{aligned} \|W''(s)\| &\leq h|f''(s)| \int_0^1 \|H_1 - H_0\| d\alpha + h^2|f'(s)|^2 \int_0^1 \int_0^1 \alpha \|H_1 - H_0\|^2 d\beta d\alpha + h^2|f'(s)|^2 \int_0^1 \int_0^1 (1-\alpha) \|H_1 - H_0\|^2 d\beta d\alpha \\ &\leq \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \end{aligned} \quad (\text{C12})$$

Then, we can choose $c_1(s)$ and $c_2(s)$ as stated according to Lemma C1 and Eqs. (C11) and (C12). ■

Lemma C3. Let

$$W(s) = U_{\text{pf},p}(sT + h, sT) = \prod_{k=0}^{K_p} \exp(-i\beta_{p,k} h f((sT + \delta_{p,k}h)/T) H_1) \exp(-i\alpha_{p,k} h (1 - f((sT + \gamma_{p,k}h)/T)) H_0) \quad (\text{C13})$$

be the product formula defined in Eq. (8), where $h = T/T_d$ is the time-step size. Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Then, we can choose

$$c_1(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|)), \quad c_2(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \quad (\text{C14})$$

Proof. Let

$$V_{k,0}(s) = \exp(-i\alpha_{p,k} h (1 - f((sT + \gamma_{p,k}h)/T)) H_0), \quad V_{k,1}(s) = \exp(-i\beta_{p,k} h f((sT + \delta_{p,k}h)/T) H_1), \quad (\text{C15})$$

and

$$V_k(s) = V_{k,1}(s) V_{k,0}(s), \quad (\text{C16})$$

so that $W(s) = \prod_{k=0}^{K_p} V_k(s)$. By the product rule, we have

$$W'(s) = \sum_{k=0}^{K_p} \left(\prod_{k'=k+1}^{K_p} V_{k'}(s) \right) V'_k(s) \left(\prod_{k'=0}^{k-1} V_{k'}(s) \right) = \sum_{k=0}^{K_p} \left(\prod_{k'=k+1}^{K_p} V_{k'}(s) \right) (V'_{k,1}(s) V_{k,0}(s) + V_{k,1}(s) V'_{k,0}(s)) \left(\prod_{k'=0}^{k-1} V_{k'}(s) \right) \quad (\text{C17})$$

and

$$\|W'(s)\| = \mathcal{O}\left(\sum_{k=0}^{K_p} (\|V'_{k,1}(s)\| + \|V'_{k,0}(s)\|)\right). \quad (\text{C18})$$

Because the exponent of each operator $V_{k,j}$, $j = 0, 1$, involves a single operator, they commute with their derivatives, so we can use

$$\frac{d}{ds} e^{X(s)} = e^{X(s)} X'(s), \quad (\text{C19})$$

so

$$\frac{d}{ds} V_{k,0}(s) = V_{k,0}(s)(i\alpha_{p,k} h f'(\phi_k(s)) H_0), \quad \frac{d}{ds} V_{k,1}(s) = V_{k,1}(s)(-i\beta_{p,k} h f'(\phi_k(s)) H_1), \quad (\text{C20})$$

where $\phi_k(s) = (sT + \gamma_{p,k}h)/T$ and $\phi_k(s) = (sT + \delta_{p,k}h)/T$. So we have $\|V'_{k,0}(s)\| = \mathcal{O}(h\|H_0\|)$ and $\|V'_{k,1}(s)\| = \mathcal{O}(h\|H_1\|)$, and

$$\|W'(s)\| = \mathcal{O}(h(\|H_0\| + \|H_1\|)). \quad (\text{C21})$$

Then, according to Lemma C1, we can choose $c_1(s) = \max \|W'(s)\| = \mathcal{O}(h(\|H_0\| + \|H_1\|))$.

Now, we estimate the second-order derivative of $W(s)$. Using the product rule again, we can compute

$$\begin{aligned} W''(s) &= \sum_{k=0}^{K_p} \left(\prod_{k'=k+1}^{K_p} V_{k'}(s) \right) V''_k(s) \left(\prod_{k'=0}^{k-1} V_{k'}(s) \right) + 2 \sum_{0 \leq k_0 < k_1 \leq K_p} \left(\prod_{k'=k_1+1}^{K_p} V_{k'}(s) \right) V'_{k_1}(s) \left(\prod_{k'=k_0+1}^{k_1-1} V_{k'}(s) \right) V'_{k_0}(s) \left(\prod_{k'=0}^{k_0-1} V_{k'}(s) \right) \\ &= \sum_{k=0}^{K_p} \left(\prod_{k'=k+1}^{K_p} V_{k'}(s) \right) (V''_{k,1}(s) V_{k,0}(s) + 2V'_{k,1}(s) V'_{k,0}(s) + V_{k,1}(s) V''_{k,0}(s)) \left(\prod_{k'=0}^{k-1} V_{k'}(s) \right) \\ &\quad + 2 \sum_{0 \leq k_0 < k_1 \leq K_p} \left(\prod_{k'=k_1+1}^{K_p} V_{k'}(s) \right) (V'_{k_1,1}(s) V_{k_1,0}(s) + V_{k_1,1}(s) V'_{k_1,0}(s)) \\ &\quad \times \left(\prod_{k'=k_0+1}^{k_1-1} V_{k'}(s) \right) (V'_{k_0,1}(s) V_{k_0,0}(s) + V_{k_0,1}(s) V'_{k_0,0}(s)) \left(\prod_{k'=0}^{k_0-1} V_{k'}(s) \right). \end{aligned} \quad (\text{C22})$$

Then,

$$\begin{aligned} \|W''(s)\| &= \mathcal{O}\left(\sum_{k=0}^{K_p} (\|V''_{k,1}(s)\| + \|V'_{k,1}(s)\| \|V'_{k,0}(s)\| + \|V''_{k,0}(s)\|)\right) \\ &\quad + \mathcal{O}\left(\sum_{0 \leq k_0 < k_1 \leq K_p} (\|V'_{k_1,1}(s)\| + \|V'_{k_1,0}(s)\|) (\|V'_{k_0,1}(s)\| + \|V'_{k_0,0}(s)\|)\right). \end{aligned} \quad (\text{C23})$$

Notice that

$$\begin{aligned} V''_{k,0}(s) &= (i\alpha_{p,k} h f''((sT + \gamma_{p,k}h)/T)) H_0 \\ &\quad \times \exp(-i\alpha_{p,k} h (1 - f((sT + \gamma_{p,k}h)/T)) H_0) \\ &\quad + (i\alpha_{p,k} h f'((sT + \gamma_{p,k}h)/T)) H_0^2 \\ &\quad \times \exp(-i\alpha_{p,k} h (1 - f((sT + \gamma_{p,k}h)/T)) H_0), \end{aligned} \quad (\text{C24})$$

$$\begin{aligned} V''_{k,1}(s) &= (-i\beta_{p,k} h f''((sT + \delta_{p,k}h)/T)) H_1 \\ &\quad \times \exp(-i\beta_{p,k} h f((sT + \delta_{p,k}h)/T) H_1) \\ &\quad + (-i\beta_{p,k} h f'((sT + \delta_{p,k}h)/T)) H_1^2 \\ &\quad \times \exp(-i\beta_{p,k} h f((sT + \delta_{p,k}h)/T) H_1), \end{aligned} \quad (\text{C25})$$

so we have $\|V''_{k,0}(s)\| = \mathcal{O}(h\|H_0\| + h^2\|H_0\|^2)$ and $\|V''_{k,1}(s)\| = \mathcal{O}(h\|H_1\| + h^2\|H_1\|^2)$. Together with $\|V'_{k,0}(s)\| =$

$\mathcal{O}(h\|H_0\|)$ and $\|V'_{k,1}(s)\| = \mathcal{O}(h\|H_1\|)$, we have

$$\|W''(s)\| = \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \quad (\text{C26})$$

Then, we can choose $c_2(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2)$ according to Lemma C1. ■

For the simplified product formula, the same bound also holds because the simplified product formula is just a special case of the general product formula.

Lemma C4. Let

$$\begin{aligned} W(s) &= U_{\text{spf},p}(sT + h, sT) \\ &= \prod_{k=0}^{K_p} \exp(-i\beta_{p,k} h f(s) H_1) \\ &\quad \times \exp(-i\alpha_{p,k} h (1 - f(s)) H_0) \end{aligned} \quad (\text{C27})$$

be the simplified product formula defined in Eq. (9), where $h = T/T_d$ is the time-step size. Suppose that both $|f'(s)|$ and $|f''(s)|$ are uniformly bounded over $[0, 1]$. Then, we can choose

$$\begin{aligned} c_1(s) &= \mathcal{O}(h(\|H_0\| + \|H_1\|)), \\ c_2(s) &= \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \end{aligned} \quad (\text{C28})$$

APPENDIX D: NUMERICAL METHODS AND THEIR STANDARD COMPLEXITY ESTIMATES

In the main text, we focus on two types of numerical methods for discretizing Eq. (1), namely, the first-order exponential integrator [Eq. (5)] and the product formula [Eq. (8)]. Here, we present their standard time discretization error bounds and complexity estimates.

1. Standard time discretization error bounds

For the first-order exponential integrator, its standard error bound is given as follows.

Lemma D1. Let $U_{\text{exp}}(t+h, t)$ be the first-order exponential integrator defined in Eq. (5). Suppose that $|f'(s)|$ is uniformly bounded over $[0, 1]$. Then, we have $\|U_{\text{exp}}(t+h, t) - \mathcal{T} \exp(-i \int_t^{t+h} H(\tau/T) d\tau)\| \leq C_{1,H} h^2$, where

$$C_{1,H} = \mathcal{O}\left(\frac{\|H_0\| + \|H_1\|}{T}\right). \quad (\text{D1})$$

Proof. For a fixed time t and a step size h , let $\tau \in [0, h]$. The exact evolution operator from t to $t+\tau$ is

$$U(t+\tau, t) = \mathcal{T} \exp\left(-i \int_0^\tau H(t/T + \tau'/T) d\tau'\right), \quad (\text{D2})$$

and the first-order exponential integrator can be written as

$$U_{\text{exp}}(t+\tau, t) = \exp(-i\tau H(t/T)). \quad (\text{D3})$$

These two operators satisfy the differential equations, respectively,

$$\frac{d}{d\tau} U(t+\tau, t) = -iH(t/T + \tau/T)U(t+\tau, t), \quad U(t, t) = I \quad (\text{D4})$$

and

$$\frac{d}{d\tau} U_{\text{exp}}(t+\tau, t) = -iH(t/T)U_{\text{exp}}(t+\tau, t), \quad U_{\text{exp}}(t, t) = I. \quad (\text{D5})$$

According to the variation of parameters formula (also known as Duhamel's principle), we may write U_{exp} as a perturbation of U , that is,

$$\begin{aligned} U_{\text{exp}}(t+\tau, t) &= U(t+\tau, t) + i \int_0^\tau U(t+\tau, t+\tau') (H(t/T + \tau'/T) - H(t/T)) U_{\text{exp}}(t+\tau', t) d\tau' \\ &= U(t+\tau, t) + i \int_0^\tau U(t+\tau, t+\tau') \\ &\quad \times \int_0^{\tau'} \frac{1}{T} H^{(1)}(t/T + \tau''/T) U_{\text{exp}}(t+\tau', t) d\tau'' d\tau'. \end{aligned} \quad (\text{D6})$$

In the second line, we use the fundamental theorem of calculus, and we are getting an extra $1/T$ scaling because the Hamiltonian is changing slowly on the scale of T (technically, we are taking the derivative with respect to τ' for the function $H(t/T + \tau'/T)$, in which the argument τ' is divided by T). Since $\|H^{(1)}(s)\| = |f'(s)|\|H_1 - H_0\| \leq \mathcal{O}(\|H_0\| + \|H_1\|)$, we have

$$\|U_{\text{exp}}(t+h, t) - U(t+h, t)\| \leq \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)h^2}{T}\right). \quad (\text{D7})$$

We show an error bound for the Trotter-Suzuki formula in the next result, which is a direct corollary of the general analysis in Ref. [22]. We also expect a similar error bound for general product formulas based Trotter-Suzuki.

Lemma D2. Let $U_{\text{pf},p}(t+h, t)$ denote the p th-order time-dependent product formula obtained by Suzuki recursion. Suppose that the scheduling function $f(s)$ is smooth with uniformly bounded derivatives of any order, and $\|H_0\| + \|H_1\| \geq 1$. Then, for any $p \geq 1$ and $T \geq 1$, we have

$$\begin{aligned} &\left\| U_{\text{pf},p}(t+h, t) - \mathcal{T} \exp\left(-i \int_t^{t+h} H(\tau/T) d\tau\right) \right\| \\ &\leq C_p (\|H_0\| + \|H_1\|)^{p+1} h^{p+1}, \end{aligned} \quad (\text{D8})$$

where C_p is a constant that depends on p and the derivatives of $f(s)$.

Proof. According to Theorem 3 of Ref. [22], there exists a p -dependent constant $\tilde{C}_p$ such that

$$\begin{aligned} &\left\| U_{\text{pf},p}(t+h, t) - \mathcal{T} \exp\left(-i \int_t^{t+h} H(\tau/T) d\tau\right) \right\| \\ &\leq \tilde{C}_p \Lambda_p^{p+1} h^{p+1}. \end{aligned} \quad (\text{D9})$$

Here, Λ_p is a constant such that

$$\Lambda_p \geq \max_{\tau \in [t, t+h]} \left\| \frac{d^m H(\tau/T)}{d\tau^m} \right\|^{1/(m+1)}, \quad \forall 0 \leq m \leq p. \quad (\text{D10})$$

By $H(s) = (1-f(s))H_0 + f(s)H_1$ and the triangle inequality, it suffices to choose

$$\begin{aligned} \Lambda_p &\geq \max_{\tau \in [t, t+h]} \left(\left\| \frac{d^m (1-f(\tau/T))}{d\tau^m} H_0 \right\| + \left\| \frac{d^m f(\tau/T)}{d\tau^m} H_1 \right\| \right)^{1/(m+1)}, \quad \forall 0 \leq m \leq p. \end{aligned} \quad (\text{D11})$$

Let F_m be the upper bound of $|f^{(m)}(s)|$ for all $s \in [0, 1]$, then we have

$$\begin{aligned} &\left(\left\| \frac{d^m (1-f(t/T))}{dt^m} H_0 \right\| + \left\| \frac{d^m f(t/T)}{dt^m} H_1 \right\| \right)^{1/(m+1)} \\ &\leq \left(\frac{F_m}{T^m} (\|H_0\| + \|H_1\|) \right)^{1/(m+1)} \\ &\leq F_m^{1/(m+1)} (\|H_0\| + \|H_1\|). \end{aligned} \quad (\text{D12})$$

So, we can choose $\Lambda_p = \max_{0 \leq m \leq p} F_m^{1/(m+1)}(\|H_0\| + \|H_1\|)$, and the claimed error bound can be obtained by defining $C_p = \max_{0 \leq m \leq p} F_m^{(p+1)/(m+1)} \tilde{C}_p$. ■

2. Standard complexity estimates

Now, we show the standard approach to analyze the complexity of using discretized AQC to prepare an eigenstate. Specifically, let $|\phi\rangle$ denote the exact target eigenstate and

$$|\tilde{\phi}\rangle = \prod_{j=0}^{T_d-1} U_{\text{num}}((j+1)h, jh)|\psi(0)\rangle, \quad (\text{D13})$$

where U_{num} is a p th-order local numerical propagator in the sense that the local truncation error can be bounded by

$$\text{LTE}_p \leq C_{p,H} h^{p+1}, \quad (\text{D14})$$

where $C_{p,H}$ is a constant that might depend on p and certain norms of H , H_0 , and H_1 , but is independent of the time-step size h . Notice that in the first-order exponential integrator, this C parameter also depends on T . We would like to study how the number of local numerical propagators, namely, T_d , scales if we want $\| |\tilde{\phi}\rangle \langle \tilde{\phi}| - |\phi\rangle \langle \phi| \| \leq \epsilon$ for some $0 < \epsilon < 1$.

A standard approach for estimating the final eigenstate error ε_{Eig} is by using ε_{AQC} as the upper bound from the continuous adiabatic theorem plus the error from the time discretization $\varepsilon_{\text{Disc}}$:

$$\varepsilon_{\text{Eig}} \leq \varepsilon_{\text{AQC}} + \varepsilon_{\text{Disc}}. \quad (\text{D15})$$

To bound the overall approximation error by $\mathcal{O}(\epsilon)$, it suffices to bound both the continuous adiabatic error and the time discretization error by $\mathcal{O}(\epsilon)$. In order to bound the time discretization error, which is $C_{p,H} T h^p$ for a p th-order method, we can choose

$$h = \mathcal{O}\left(\frac{\epsilon^{1/p}}{C_{p,H}^{1/p} T^{1/p}}\right). \quad (\text{D16})$$

Therefore, the overall number of queries to U_{num} can be bounded by

$$T_d = \frac{T}{h} = \mathcal{O}\left(\frac{C_{p,H}^{1/p} T^{1+1/p}}{\epsilon^{1/p}}\right), \quad (\text{D17})$$

and we only need to further study the scaling of the evolution time T , which needs to be chosen large enough such that the adiabatic error is bounded as well. For the general second-order continuously differentiable interpolation function $f(s)$, which is independent of the Hamiltonians, Lemma A1 implies that the adiabatic error is bounded by

$$\begin{aligned} & \mathcal{O}\left(\frac{1}{T} \left(\frac{\|H_0\| + \|H_1\|}{\Delta_*^2} + \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3} \right)\right) \\ & \leq \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{T \Delta_*^3}\right), \end{aligned} \quad (\text{D18})$$

then the evolution time should be chosen as

$$T = \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon}\right). \quad (\text{D19})$$

The overall number of steps is thus

$$T_d = \mathcal{O}\left(\frac{C_{p,H}^{1/p} (\|H_0\| + \|H_1\|)^{2+2/p}}{\Delta_*^{3+3/p} \epsilon^{1+2/p}}\right). \quad (\text{D20})$$

Now, we consider the boundary cancellation condition. Here, we further assume that both $\|H_0\|$ and $\|H_1\|$ are bounded by 1. We can use Lemma A2 to bound the adiabatic error, which implies the choice of evolution time to be

$$T = \mathcal{O}\left(\frac{1}{\Delta_*^2} \left(\ln\left(\frac{1}{\Delta_* \epsilon}\right)\right)^{1+\alpha}\right) \quad (\text{D21})$$

and thus the overall number of steps to be

$$T_d = \mathcal{O}\left(\frac{1}{\Delta_*^{2+2/p} \epsilon^{1/p}} \left(\ln\left(\frac{1}{\Delta_* \epsilon}\right)\right)^{(1+\alpha)(1+1/p)}\right). \quad (\text{D22})$$

APPENDIX E: TECHNICAL DETAILS OF THE COMPLEXITY ANALYSIS

In this Appendix, we provide full technical details on the results we present in the main text.

1. First-order exponential integrator

Proof of Theorem 1. Let $T_d = T/h$. For $s \in [0, 1]$ and any $0 \leq j \leq T_d - 1$, we have

$$W(j/T_d) = e^{-ihH(j/T_d)} = e^{-ihH(jh/T)} = U_{\text{exp}}((j+1)h, jh). \quad (\text{E1})$$

We show in Lemma C2 that, for this walk operator $W(s)$, we can choose its corresponding $c_1(s)$ and $c_2(s)$ [defined in Eq. (11)] as

$$\begin{aligned} c_1(s) &= \mathcal{O}(h(\|H_0\| + \|H_1\|)), \\ c_2(s) &= \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \end{aligned} \quad (\text{E2})$$

Then, we can apply Lemma 1 to obtain the desired error bound. ■

Proof of Corollary 1. Following the notations in the proof of Theorem 1, we use $T_d = T/h$ to denote the number of steps and define the walk operator $W(s) = e^{-ihH(s)}$. Notice that when $h = 1/(\|H_0\| + \|H_1\|)$, we always have $\|hH(s)\| \leq 1$, so the gap of $W(s)$ is exactly the same as that of $hH(s)$, which is bounded from below by $h\Delta_*$. Suppose that our choice of T is

$$T = C \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon} \quad (\text{E3})$$

for a constant $C > 0$. Then, we have

$$T_d = T/h = C \frac{(\|H_0\| + \|H_1\|)^3}{\Delta_*^3 \epsilon} \geq C \frac{(\|H_0\| + \|H_1\|)^3}{\Delta_*^3}. \quad (\text{E4})$$

Notice that $\Delta_* \leq 2\|H(s)\| \leq 2(\|H_0\| + \|H_1\|)$, so we have

$$T_d \geq \frac{C}{4} \frac{\|H_0\| + \|H_1\|}{\Delta_*} = \frac{C}{4h\Delta_*}. \quad (\text{E5})$$

According to Lemma C2, we have $c_1(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|)) = \mathcal{O}(1)$, so we can choose a sufficiently large constant C such that $T_d \geq \frac{2\pi}{h\Delta_*} \sup c_1(s)$. Then, Lemma B1 ensures that the multistep gap of $W(s)$ is bounded from below by $h\Delta_*/2$.

Plugging this back into Theorem 1 yields the error bound

$$\begin{aligned} & \mathcal{O}\left(\frac{h}{T}\left(\frac{h(\|H_0\| + \|H_1\|)}{h^2\Delta_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{h^2\Delta_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{h^3\Delta_*^3}\right)\right) \\ & \leq \mathcal{O}\left(\frac{1}{T}\left(\frac{\|H_0\| + \|H_1\|}{\Delta_*^2} + \frac{h(\|H_0\| + \|H_1\|)^2}{\Delta_*^2} + \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3}\right)\right) \\ & \leq \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{T\Delta_*^3}\right). \end{aligned} \quad (\text{E6})$$

In order to further bound the error by ϵ , it suffices to choose

$$T = \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3\epsilon}\right). \quad (\text{E7})$$

Since the error bound is independent of the time step h , we directly choose the largest possible time-step size

$$h = \frac{1}{\|H_0\| + \|H_1\|}, \quad (\text{E8})$$

which ensures the fixed-time gap condition of $W(s)$. Finally, the condition $T/h > 2\tilde{c}(\|H_0\| + \|H_1\|)/\Delta_*$ is naturally satisfied, since $\Delta_* \leq 2\|H(s)\| \leq 2(\|H_0\| + \|H_1\|)$ and

$$\begin{aligned} T_d & \sim \frac{(\|H_0\| + \|H_1\|)^3}{\Delta_*^3\epsilon} \\ & = \frac{1}{\epsilon} \left(\frac{(\|H_0\| + \|H_1\|)}{\Delta_*}\right)^2 \frac{\|H_0\| + \|H_1\|}{\Delta_*}, \end{aligned} \quad (\text{E9})$$

from which we can also infer that $T_d \gtrsim \frac{\|H_0\| + \|H_1\|}{\Delta_*}$ and thus satisfies the condition for T/h . ■

2. Product formulas

Proof of Theorem 2. For $s \in [0, 1 - h/T]$ and any $0 \leq j \leq T_d - 1$, the walk operator $W(j/T_d)$ is $U_{\text{pf},p}((j+1)h, jh)$ or $U_{\text{spf},p}((j+1)h, jh)$. We show in Lemmas C3 and C4 that, for the walk operator $W(s)$ in either case, we can choose $c_1(s)$ and $c_2(s)$ [defined in Eq. (11)] as

$$\begin{aligned} c_1(s) &= \mathcal{O}(h(\|H_0\| + \|H_1\|)), \\ c_2(s) &= \mathcal{O}(h(\|H_0\| + \|H_1\|) + h^2(\|H_0\| + \|H_1\|)^2). \end{aligned} \quad (\text{E10})$$

Then, we can apply Lemma 1 to obtain the desired error bound. ■

Proof of Lemma 3. According to Lemma 2, it suffices to consider only the second-order formula.

Notice that the spectral gaps of $e^{-ihH(s)}$ and $hH(s)$, though defined in slightly different ways, are of the same value for all $h \leq 1/(\|H_0\| + \|H_1\|)$. So, it suffices to investigate the spectral gaps of $U_{\text{spf},2}(sT + h, sT)$ and $e^{-ihH(s)}$. For every fixed s , we may bound the difference between $U_{\text{spf},2}(sT + h, sT)$ and $e^{-ihH(s)}$ by using the error bound for the second-order time-independent Trotter method because the discrete time points are fixed in different exponentials. For example, by

Proposition 16 of Ref. [6],

$$\begin{aligned} & \|U_{\text{spf},2}(sT + h, sT) - e^{-ihH(s)}\| \\ & \leq \frac{h^3}{12} \| [f(s)H_1, [f(s)H_1, (1-f(s))H_0]] \| \\ & \quad + \frac{h^3}{24} \| [(1-f(s))H_0, [(1-f(s))H_0, f(s)H_1]] \| \\ & \leq \frac{h^3}{192} (2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|). \end{aligned} \quad (\text{E11})$$

Equation (E11) implies that the difference between $U_{\text{spf},2}(sT + h, sT)$ and $e^{-ihH(s)}$ is small if we reduce the time-step size h , and further implies that the eigenvalues of $U_{\text{spf},2}(sT + h, sT)$ and $e^{-ihH(s)}$ are close according to Refs. [52,54]. Specifically, according to the eigenvalue perturbation theorem of Refs. [52,54], there exists an ordering $\lambda_j(s)$ and $\tilde{\lambda}_j(s)$ of the eigenvalues of $U_{\text{spf},2}(sT + h, sT)$ and $e^{-ihH(s)}$, respectively, such that

$$\begin{aligned} & \max_j |\lambda_j(s) - \tilde{\lambda}_j(s)| \\ & \leq \|U_{\text{spf},2}(sT + h, sT) - e^{-ihH(s)}\| \\ & \leq \frac{h^3}{192} (2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|) \\ & \leq \frac{h^3}{192} (8\|H_0\|\|H_1\|^2 + 4\|H_0\|^2\|H_1\|) \\ & \leq \frac{h^3}{192} \left(\frac{8}{3\sqrt{3}}(\|H_0\| + \|H_1\|)^3\right) \\ & \leq \frac{1}{72\sqrt{3}}. \end{aligned} \quad (\text{E12})$$

Now, let $\mathbb{S}^1$ denote the unit circle and $|z_1 - z_2|_{\mathbb{S}^1}$ denote the angular distance between $z_1, z_2 \in \mathbb{S}^1$. Then, we have

$$|\lambda_j(s) - \tilde{\lambda}_j(s)|_{\mathbb{S}^1} = 2 \arcsin\left(\frac{1}{2}|\lambda_j(s) - \tilde{\lambda}_j(s)|\right). \quad (\text{E13})$$

Because the arcsine has a monotonically increasing first derivative, the inequality in Eq. (E12) implies

$$\begin{aligned} |\lambda_j(s) - \tilde{\lambda}_j(s)|_{\mathbb{S}^1} & \leq 144\sqrt{3} \arcsin\left(\frac{1}{144\sqrt{3}}|\lambda_j(s) - \tilde{\lambda}_j(s)|\right) \\ & \leq \frac{96}{95} |\lambda_j(s) - \tilde{\lambda}_j(s)|. \end{aligned} \quad (\text{E14})$$

Let $\lambda_0(s)$ and $\lambda_1(s)$ denote the two eigenvalues that determine the gap. Then, the gap $U_{\text{spf},2}(sT + h, sT)$ can be bounded by

$$\begin{aligned} |\lambda_1(s) - \lambda_0(s)|_{\mathbb{S}^1} & \geq |\tilde{\lambda}_1(s) - \tilde{\lambda}_0(s)|_{\mathbb{S}^1} - |\tilde{\lambda}_1(s) - \lambda_1(s)|_{\mathbb{S}^1} \\ & \quad - |\tilde{\lambda}_0(s) - \lambda_0(s)|_{\mathbb{S}^1} \\ & \geq h\Delta_H(s) - \frac{96}{95} |\tilde{\lambda}_1(s) - \lambda_1(s)| \\ & \quad - \frac{96}{95} |\tilde{\lambda}_0(s) - \lambda_0(s)| \\ & \geq h\Delta_H(s) - \frac{h^3}{95} (2\|[H_1, [H_1, H_0]]\| \\ & \quad + \|[H_0, [H_0, H_1]]\|) \end{aligned} \quad (\text{E15})$$

and

$$\begin{aligned}
|\lambda_1(s) - \lambda_0(s)|_{\mathbb{S}^1} &\leq |\tilde{\lambda}_1(s) - \tilde{\lambda}_0(s)|_{\mathbb{S}^1} + |\tilde{\lambda}_1(s) - \lambda_1(s)|_{\mathbb{S}^1} \\
&\quad + |\tilde{\lambda}_0(s) - \lambda_0(s)|_{\mathbb{S}^1} \\
&\leq h\Delta_H(s) + \frac{96}{95}|\tilde{\lambda}_1(s) - \lambda_1(s)| \\
&\quad + \frac{96}{95}|\tilde{\lambda}_0(s) - \lambda_0(s)| \\
&\leq h\Delta_H(s) + \frac{h^3}{95}(2\|[H_1, [H_1, H_0]]\| \\
&\quad + \|[H_0, [H_0, H_1]]\|), \tag{E16}
\end{aligned}$$

where we use the fact again that the gaps of the Hamiltonian and the walk operator are the same. ■

Proof of Corollary 2. Let $T_d = T/h$, and we assume T_d is an integer. Define the walk operator

$$W(s) = e^{-ih(1-f(s))H_0/2} e^{-ihf(s)H_1} e^{-ih(1-f(s))H_0/2}. \tag{E17}$$

We first bound the fixed-time gap of $W(s)$. According to the choice of h , we always have

$$\frac{h^3}{95}(2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|) \leq \frac{1}{2}h\Delta_*. \tag{E18}$$

Using Lemma 3, the gap of $W(s)$ is bounded from below by $\frac{1}{2}h\Delta(s)$, which has a further lower bound $\frac{1}{2}h\Delta_*$.

For the multistep gap, we can use Lemma B1, and we need to verify that T_d is sufficiently large. Specifically, suppose that our choice of T is

$$T = C \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon} \tag{E19}$$

for a constant $C > 0$. Then, we have

$$T_d = T/h = C \frac{(\|H_0\| + \|H_1\|)^2}{h\Delta_*^3 \epsilon} \geq C \frac{(\|H_0\| + \|H_1\|)^2}{h\Delta_*^3}. \tag{E20}$$

Notice that $\Delta_* \leq 2\|H(s)\| \leq 2(\|H_0\| + \|H_1\|)$, so we have

$$T_d \geq \frac{C}{4} \frac{1}{h\Delta_*}. \tag{E21}$$

According to Lemma C4, we have $c_1(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|)) = \mathcal{O}(1)$, so we can choose a sufficiently large constant C such that $T_d \geq \frac{2\pi}{h\Delta_*/2} \sup c_1(s)$. Then, Lemma B1 ensures that the multistep gap of $W(s)$ is bounded from below by $h\Delta_*/4$.

Therefore, the error bound in Theorem 2 becomes

$$\begin{aligned}
&\mathcal{O}\left(\frac{h}{T}\left(\frac{h(\|H_0\| + \|H_1\|)}{h^2\Delta_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{h^2\Delta_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{h^3\Delta_*^3}\right)\right) \\
&\leq \mathcal{O}\left(\frac{1}{T}\left(\frac{(\|H_0\| + \|H_1\|)}{\Delta_*^2} + \frac{h(\|H_0\| + \|H_1\|)^2}{\Delta_*^2} + \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3}\right)\right) \\
&\leq \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{T\Delta_*^3}\right), \tag{E22}
\end{aligned}$$

and the desired choices of T and h directly follow from this error bound and the conditions for the multistep gap. ■

Proof of Lemma 4. Notice that the spectral gaps of $e^{-ihH(s)}$ and $hH(s)$ are of the same value for all $h \leq 1/(\|H_0\| + \|H_1\|)$. So, it suffices to investigate the spectral gaps of $U_{\text{spf},p}(sT + h, sT)$ and $e^{-ihH(s)}$. For every fixed s , we may bound the difference between $U_{\text{spf},p}(sT + h, sT)$ and $e^{-ihH(s)}$ by using the error bound of the time-independent product formula in Theorem 11 of Ref. [6], which gives

$$\|U_{\text{spf},p}(sT + h, sT) - e^{-ihH(s)}\| \leq \tilde{c}_p h^{p+1} \left(\sum_{\gamma_0, \dots, \gamma_p \in \{0,1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\| \right) \tag{E23}$$

for a p -dependent constant $\tilde{c}_p$.

According to the eigenvalue perturbation theorem of Refs. [52,54], there exists an ordering $\lambda_j(s)$ and $\tilde{\lambda}_j(s)$ of the eigenvalues of $U_{\text{spf},p}(sT + h, sT)$ and $e^{-ihH(s)}$, respectively, such that

$$\max_j |\lambda_j(s) - \tilde{\lambda}_j(s)| \leq \|U_{\text{spf},p}(sT + h, sT) - e^{-ihH(s)}\|. \tag{E24}$$

Let $\lambda_0(s)$ and $\lambda_1(s)$ denote the two eigenvalues that determine the gap, then the gap of $U_{\text{spf},p}(sT + h, sT)$ can be bounded by

$$\begin{aligned}
|\lambda_1(s) - \lambda_0(s)|_{\mathbb{S}^1} &\geq |\tilde{\lambda}_1(s) - \tilde{\lambda}_0(s)|_{\mathbb{S}^1} - |\tilde{\lambda}_1(s) - \lambda_1(s)|_{\mathbb{S}^1} - |\tilde{\lambda}_0(s) - \lambda_0(s)|_{\mathbb{S}^1} \\
&\geq h\Delta_H(s) - \frac{\pi}{2}|\tilde{\lambda}_1(s) - \lambda_1(s)| - \frac{\pi}{2}|\tilde{\lambda}_0(s) - \lambda_0(s)| \\
&\geq h\Delta_H(s) - \pi\tilde{c}_p h^{p+1} \left(\sum_{\gamma_0, \dots, \gamma_p \in \{0,1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\| \right) \tag{E25}
\end{aligned}$$

and

$$\begin{aligned}
& |\lambda_1(s) - \lambda_0(s)|_{\mathbb{S}^1} \\
& \leq |\tilde{\lambda}_1(s) - \tilde{\lambda}_0(s)|_{\mathbb{S}^1} + |\tilde{\lambda}_1(s) - \lambda_1(s)|_{\mathbb{S}^1} \\
& \quad + |\tilde{\lambda}_0(s) - \lambda_0(s)|_{\mathbb{S}^1} \\
& \leq h\Delta_H(s) + \frac{\pi}{2}|\tilde{\lambda}_1(s) - \lambda_1(s)| + \frac{\pi}{2}|\tilde{\lambda}_0(s) - \lambda_0(s)| \\
& \leq h\Delta_H(s) + \pi\tilde{c}_p h^{p+1} \\
& \quad \times \left(\sum_{\gamma_0, \dots, \gamma_p \in \{0,1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\| \right). \quad (\text{E26})
\end{aligned}$$

In the second line of both estimates, we use $\theta \leq \frac{\pi}{2} \sin \theta$ for all $\theta \in [0, \pi/2]$. The proof is completed by choosing $c_p = \pi\tilde{c}_p$. ■

Proof of Corollary 3. The sketch of the proof is as follows. We will first give a lower bound for the fixed-time spectral gap of the walk operator $W(s)$, then give a lower bound for the multistep gap by verifying the conditions in Lemma B1, and apply the discrete adiabatic theorem to bound the overall error between the actual and ideal evolution, from which we can infer the choices of T and h .

Let $T_d = T/h$, and we assume T_d is an integer. We first bound the fixed-time gap of $W(s)$ defined by Eq. (9). According to the choice of h with proper constant factor, we can make

$$c_p h^{p+1} \sum_{\gamma_0, \dots, \gamma_p \in \{0,1\}} \|[H_{\gamma_p}, \dots, [H_{\gamma_1}, H_{\gamma_0}]]\| \leq \frac{1}{2} h \Delta_*, \quad (\text{E27})$$

$$\begin{aligned}
& \mathcal{O}\left(\frac{h}{T} \left(\frac{h(\|H_0\| + \|H_1\|)}{h^2 \Delta_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{h^2 \Delta_*^2} + \frac{h^2(\|H_0\| + \|H_1\|)^2}{h^3 \Delta_*^3} \right)\right) \\
& \leq \mathcal{O}\left(\frac{1}{T} \left(\frac{(\|H_0\| + \|H_1\|)}{\Delta_*^2} + \frac{h(\|H_0\| + \|H_1\|)^2}{\Delta_*^2} + \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3} \right)\right) \\
& \leq \mathcal{O}\left(\frac{(\|H_0\| + \|H_1\|)^2}{T \Delta_*^3}\right), \quad (\text{E31})
\end{aligned}$$

and the desired choices of T and h directly follow from this error bound and the conditions for the multistep gap. ■

APPENDIX F: HIGH-ORDER DISCRETE ADIABATIC THEOREM

Here, we provide more discussion on the high-order discrete adiabatic theorem, which is claimed in Ref. [30] and we state as Conjecture 1 in the main text. First, in the statement of Conjecture 1, we adapt a slightly different statement compared to the original version in Ref. [30] for the purpose of clearer presentation. We will explain how to get Conjecture 1 from there. More importantly, we will then point out the missing steps in the analysis of Ref. [30] and explain why these missing steps imply that the proof in Ref. [30] is not valid. Meanwhile, we also show a numerical result verifying that, despite the flawed proof, the claim of the high-order discrete adiabatic theorem is very likely to be correct.

where c_p is the constant factor in Lemma 4. Then, using Lemma 4, the gap of $W(s)$ is bounded from below by $\frac{1}{2}h\Delta_*$, which has a further lower bound $\frac{1}{2}h\Delta_*$.

For the multistep gap, we can use Lemma B1, and we need to verify that T_d is sufficiently large. Specifically, suppose that our choice of T is

$$T \geq C \frac{(\|H_0\| + \|H_1\|)^2}{\Delta_*^3 \epsilon} \quad (\text{E28})$$

for a constant $C > 0$. Then, we have

$$T_d = T/h \geq C \frac{(\|H_0\| + \|H_1\|)^2}{h \Delta_*^3 \epsilon} \geq C \frac{(\|H_0\| + \|H_1\|)^2}{h \Delta_*^3}. \quad (\text{E29})$$

Notice that $\Delta_* \leq 2\|H(s)\| \leq 2(\|H_0\| + \|H_1\|)$, so we have

$$T_d \geq \frac{C}{4} \frac{1}{h \Delta_*}. \quad (\text{E30})$$

According to Lemma C4, we have $c_1(s) = \mathcal{O}(h(\|H_0\| + \|H_1\|)) = \mathcal{O}(1)$, so we can choose a sufficiently large constant C such that $T_d \geq \frac{2\pi}{h\Delta_*/2} \sup c_1(s)$. Then, Lemma B1 ensures that the multistep gap of $W(s)$ is bounded from below by $h\Delta_*/4$.

Therefore, the error bound in Theorem 2 becomes

1. A slight variant

We show how to derive Conjecture 1 from the original result in Ref. [30]. We need to introduce some operators before proceeding. Let $P(s)$ and $Q(s)$ denote the spectral projections onto $\sigma_P(s)$ and $\sigma_Q(s)$, respectively. Define

$$S(s) = P(s + 1/T_d)P(s) + Q(s + 1/T_d)Q(s), \quad (\text{F1})$$

$$v(s) = \sqrt{S(s)S(s)^\dagger}, \quad (\text{F2})$$

$$V(s) = v(s)^{-1}S(s). \quad (\text{F3})$$

The following is the original result from Ref. [30].

Lemma F1 (Higher-order discrete adiabatic theorem. Theorem 3 of Ref. [30]). Suppose that $V(s) - I$ is supported in $(0, s_*)$. Then, for any integer n such that $n/T_d \notin (0, s_*)$ and for any positive integer k , we have

$$\|Q(0)U_A^\dagger(n/T_d)U(n/T_d)P(0)\| \leq \frac{C_k}{T_d^k}, \quad (\text{F4})$$

where C_k is a constant independent of n and T_d .

Notice that Lemma F1 introduces a new parameter s_* , which could be larger than 1. Such an extension allows us to bound the discrete adiabatic error when the number of the walk operators is larger than T . Now, we prove Conjecture 1 from Lemma F1.

Proof of Conjecture 1. The idea is to smoothly extend $W(s)$ to a longer time interval $[0, 3]$ to make it satisfy the condition in Lemma F1. Specifically, we consider a walk operator on the time interval $[0, 3]$ and make it constant on $[0, 1]$ and $[2, 3]$ to make sure that it satisfies the boundary cancellation condition in the discrete sense as well. On the time interval $[0, 3]$, we define

$$\tilde{W}(s) = \begin{cases} W(0), & s \in [0, 1), \\ W(s-1), & s \in [1, 2], \\ W(1), & s \in (2, 3]. \end{cases} \quad (\text{F5})$$

The operators associated with $\tilde{W}(s)$ are denoted using the same letter with an upper tilde (e.g., $\tilde{P}(s)$ and $\tilde{Q}(s)$ denote the spectral projections of $\tilde{W}(s)$). Since $\tilde{W}^{(k)}(1) = W^{(k)}(0) = 0$ and $\tilde{W}^{(k)}(2) = W^{(k)}(1) = 0$ for all $k \geq 1$, the operator $\tilde{W}(s)$ is a smooth extension of $W(s)$.

Notice that $\tilde{W}(s)$ and thus $\tilde{P}(s)$ and $\tilde{Q}(s)$ remain unchanged on $[0, 1] \cup [2, 3]$. Then, for any $s \in [0, 1 - 1/T_d] \cup [2, 3 - 1/T_d]$, we must have

$$\begin{aligned} \tilde{S}(s) &= \tilde{P}(s + 1/T_d)\tilde{P}(s) + \tilde{Q}(s + 1/T_d)\tilde{Q}(s) \\ &= \tilde{P}(s)^2 + \tilde{Q}(s)^2 = I, \end{aligned} \quad (\text{F6})$$

so $\tilde{v}(s) = \sqrt{\tilde{S}(s)\tilde{S}(s)^\dagger} = I$ and $\tilde{V}(s) = \tilde{v}(s)^{-1}\tilde{S}(s) = I$. This means that $\tilde{V}(s) - I$ is supported in $(0, 2)$ and satisfies the

assumption of Lemma F1. As a result, we have

$$\|\tilde{Q}(0)\tilde{U}_A^\dagger(2)\tilde{U}(2)\tilde{P}(0)\| \leq \frac{C_k}{T_d^k}, \quad (\text{F7})$$

where C_k is a constant independent of T_d .

We now show how we may obtain a bound for the desired quantity from Eq. (F7). First, we have

$$\begin{aligned} &\|\tilde{Q}(0)\tilde{U}_A^\dagger(2)\tilde{U}(2)\tilde{P}(0)\| \\ &= \|\tilde{U}_A^\dagger(2)\tilde{U}(2)\tilde{P}(0) - \tilde{P}(0)\tilde{U}_A^\dagger(2)\tilde{U}(2)\tilde{P}(0)\| \\ &= \|\tilde{U}_A^\dagger(2)\tilde{U}(2)\tilde{P}(0) - \tilde{U}_A^\dagger(2)\tilde{P}(2)\tilde{U}(2)\tilde{P}(0)\| \\ &= \|\tilde{U}(2)\tilde{P}(0) - \tilde{P}(2)\tilde{U}(2)\tilde{P}(0)\|, \end{aligned} \quad (\text{F8})$$

where we use Eq. (14) in the second equality. Then, since $|\psi\rangle$ is within the eigenspace corresponding to $\sigma_{\tilde{P}}(0)$, we have

$$\begin{aligned} &\|\tilde{U}(2)|\psi\rangle - \tilde{P}(2)\tilde{U}(2)|\psi\rangle\| \\ &= \|\tilde{U}(2)\tilde{P}(0)|\psi\rangle - \tilde{P}(2)\tilde{U}(2)\tilde{P}(0)|\psi\rangle\| \\ &\leq \|\tilde{U}(2)\tilde{P}(0) - \tilde{P}(2)\tilde{U}(2)\tilde{P}(0)\| \\ &= \|\tilde{Q}(0)\tilde{U}_A^\dagger(2)\tilde{U}(2)\tilde{P}(0)\| \\ &\leq \frac{C_k}{T_d^k}, \end{aligned} \quad (\text{F9})$$

where C_k is the constant in Lemma F1. Finally, notice that, by definition, $\tilde{P}(2) = P(1)$, and $|\psi\rangle$ is an eigenstate of $\tilde{W}(s)$ for all $s \in [0, 1]$. Suppose the corresponding eigenvalue is $e^{i\theta}$ for a real number θ , then

$$\begin{aligned} \|\tilde{U}(2)|\psi\rangle - \tilde{P}(2)\tilde{U}(2)|\psi\rangle\| &= \left\| \left(\prod_{j=T_d}^{2T_d-1} \tilde{W}(j/T_d) \right) \left(\prod_{j=0}^{T_d-1} \tilde{W}(j/T_d) \right) |\psi\rangle - P(1) \left(\prod_{j=T_d}^{2T_d-1} \tilde{W}(j/T_d) \right) \left(\prod_{j=0}^{T_d-1} \tilde{W}(j/T_d) \right) |\psi\rangle \right\| \\ &= \left\| \left(\prod_{j=0}^{T_d-1} W(j/T_d) \right) W(0)^{T_d} |\psi\rangle - P(1) \left(\prod_{j=0}^{T_d-1} W(j/T_d) \right) W(0)^{T_d} |\psi\rangle \right\| \\ &= \|e^{iT_d\theta} U(1)|\psi\rangle - e^{iT_d\theta} P(1)U(1)|\psi\rangle\| \\ &= \|U(1)|\psi\rangle - P(1)U(1)|\psi\rangle\|. \end{aligned} \quad (\text{F10})$$

Therefore, we have

$$\begin{aligned} \|U(1)|\psi\rangle - P(1)U(1)|\psi\rangle\| &= \|\tilde{U}(2)|\psi\rangle - \tilde{P}(2)\tilde{U}(2)|\psi\rangle\| \\ &\leq \frac{C_k}{T_d^k}. \end{aligned} \quad (\text{F11})$$

■

2. Missing steps in the proof of the high-order discrete adiabatic theorem and a numerical validation

We first follow the notations in Ref. [30] to define several operators. Let $P(s)$ and $Q(s)$ be the spectral projections as before, and let $V(s)$ be defined through Eq. (F3). Let

$$\Omega(s) = U_A^\dagger(s)U(s), \quad (\text{F12})$$

$$\Theta(s) = U_A^\dagger(s + 1/T_d)V^\dagger(s)U_A(s + 1/T_d), \quad (\text{F13})$$

$$K(s) = T_d(1 - \Theta(s)). \quad (\text{F14})$$

It can be shown that the Volterra equation holds as

$$\Omega(n/T_d) = 1 - \frac{1}{T_d} \sum_{k=0}^{n-1} K(k/T_d)\Omega(k/T_d). \quad (\text{F15})$$

In Ref. [30], another set of operators $\{\Omega_j(s)\}$ is defined in a fixed-point-iteration fashion—let $\Omega_0(s) = 1$ for all s , and

$$\Omega_j(n/T_d) = -\frac{1}{T_d} \sum_{k=0}^{n-1} K(k/T_d)\Omega_{j-1}(k/T_d). \quad (\text{F16})$$

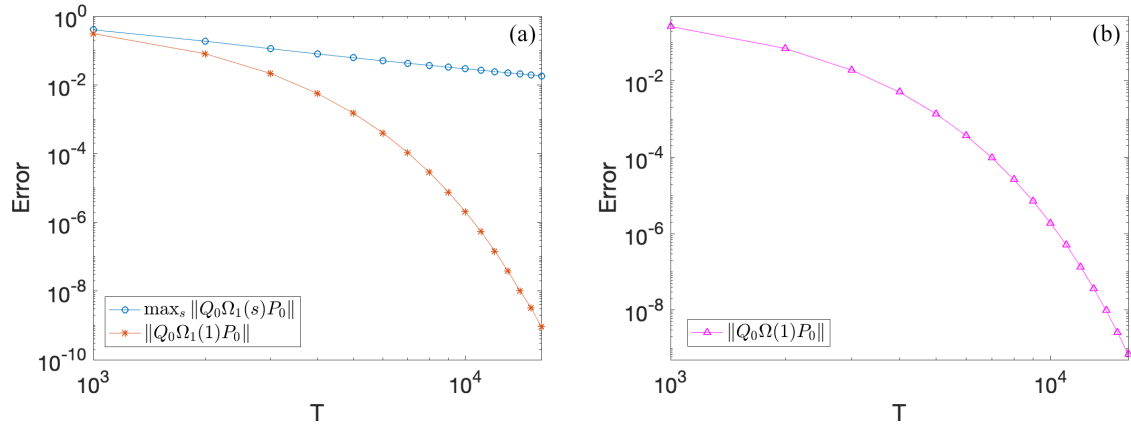


FIG. 5. Numerical tests of the high-order discrete adiabatic theorem and its intermediate step. (a) Numerical scaling of $\|Q_0 \Omega_1(s) P_0\|$ inside the interval and at the boundary. (b) Numerical scaling of $\|Q_0 \Omega_1(1) P_0\|$ at the boundary $s = 1$.

By taking the summation over j , we can see that $\sum_{j=0}^{\infty} \Omega_j(s)$ is expected to converge to $\Omega(s)$.

Lemma 1 in Ref. [30] attempts to show that $Q_0 \Omega_1(1) P_0$ is of order $\mathcal{O}(T_d^{-k})$ for arbitrary positive integer k under the boundary cancellation condition, and the high-order discrete adiabatic theorem becomes a consequence of this lemma. This was proven using mathematical induction over j . However, in the proof of Lemma 1 of Ref. [30], the induction assumption [Eq. (40) in Ref. [30]] was taken to be $Q_0 \Omega_j(n/T_d) P_0 = \mathcal{O}(T_d^{-k})$ for all $0 \leq n \leq T_d$, which is much stronger than the original claim that only holds when $n = 0$ and T_d . Furthermore, intuitively, the operator $Q_0 \Omega_j(n/T_d) P_0$ should not scale $\mathcal{O}(T_d^{-k})$ inside the time interval since the boundary cancellation condition is expected to accelerate the convergence only near the boundary.

We verify our statements numerically using a four-level model. We consider the walk operator to be the first-order exponential integrator with time-step size 1, i.e., $W(s) = e^{-iH(s)}$, where $H(s) = (1 - f(s))H_0 + f(s)H_1$. We choose the Hamiltonians $H_j = Q_j^\dagger D_j Q_j$ for $j = 0, 1$, where $D_0 = \text{diag}(0.5, 0.8, 1.2, 1.4)$ and $D_1 = \text{diag}(0.3, 1.0, 1.5, 1.9)$ are two diagonal matrices, Q_0 is the orthonormal basis of the matrix

$$\begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \end{pmatrix}, \quad (\text{F17})$$

and Q_1 is the orthonormal basis of

$$\begin{pmatrix} 3 & -0.5 & 0 & -2 \\ -0.5 & 3 & 1 & 0 \\ 0 & 1 & 3 & -1 \\ -2 & 0 & -1 & 3 \end{pmatrix}. \quad (\text{F18})$$

The scheduling function is the glue function $f(s) = c^{-1} \int_0^s \exp(-\frac{1}{s'(1-s')}) ds'$, where c is the normalization constant such that $f(1) = 1$. Notice that such a scheduling function satisfies the boundary cancellation condition.

Figure 5(a) shows the numerical scaling of $\max_s \|Q_0 \Omega_1(s) P_0\|$ and $\|Q_0 \Omega_1(1) P_0\|$ under different choices of T_d . Here, we test the scaling for Ω_1 instead of Ω_0

because Ω_0 is always the identity matrix, so the orthogonal projection is always 0. Our numerical results suggest that $\max_s \|Q_0 \Omega_1(s) P_0\|$ is of order $\mathcal{O}(1/T_d)$ while $\|Q_0 \Omega_1(1) P_0\|$ decays superpolynomially, which verifies that the induction assumption used in Ref. [30] is questionable.

Although the proof presented in Ref. [30] seems flawed, we believe that the conclusion of the high-order discrete adiabatic theorem still holds true. We verify this using the same example, and our numerical results shown in Fig. 5(b) support the claim that the adiabatic error $\|Q_0 \Omega_1(1) P_0\|$ at the boundary indeed converges superpolynomially in $1/T_d$.

APPENDIX G: TECHNICAL DETAILS OF THE COMPLEXITY ANALYSIS WITH BOUNDARY CANCELLATION CONDITION

Proof of Proposition 1. Let $W(s) = e^{-iH(s)}$, where $H(s) = (1 - f(s))H_0 + f(s)H_1$. We only need to verify that the walk operator $W(s)$ satisfies all the conditions of Conjecture 1. Since the function $f(s)$ is smooth over $[0, 1]$, the operator $W(s)$ is also smooth. The walk operator $W(s)$ also satisfies the gap condition since $H(s)$ is assumed to satisfy the gap condition and $\|H(s)\| \leq 1$. Finally, the boundary cancellation condition of $f(s)$ implies the boundary cancellation of $W(s)$. Therefore, our claim directly follows from Conjecture 1. ■

Proof of Proposition 2. Define the walk operator

$$W(s) = \prod_{k=0}^K \exp(-i\beta_{p,k} h f(s) H_1) \exp(-i\alpha_{p,k} h (1 - f(s)) H_0). \quad (\text{G1})$$

Since the function $f(s)$ is smooth over $[0, 1]$, the operator $W(s)$ is also smooth. Using Lemma 4, the walk operator $W(s)$ also satisfies the gap condition as $H(s)$ does by choosing a sufficiently small (but independent of ϵ) time-step size h . Finally, according to the chain rule, each term in the derivatives of $W(s)$ contains the derivatives of $f(s)$ as a multiplicative factor, which implies that $W(s)$ also satisfies the boundary cancellation condition. Therefore, our claim directly follows from Conjecture 1. ■

Proof of Corollary 4. First, according to the continuous high-order adiabatic theorem, which we detail in Lemma A2

in Appendix A, there exists an eigenstate $|u\rangle$ of H_1 corresponding to the eigenvalue of interest such that for any k ,

$$\| |\psi(T)\rangle - |u\rangle \| \leq \mathcal{O}(\exp(-cT^{\frac{1}{1+\alpha}})) \leq \mathcal{O}\left(\frac{1}{T^k}\right). \quad (\text{G2})$$

Similarly, for the numerical solution, according to Proposition 2, there exists an eigenstate $|v\rangle$ of e^{-ihH_1} corresponding to the eigenvalue of interest such that for any k ,

$$\| |\tilde{\phi}\rangle - |v\rangle \| \leq \mathcal{O}\left(\frac{1}{T^k}\right). \quad (\text{G3})$$

Notice that $|u\rangle$ and $|v\rangle$, if not exactly the same, only differ by a phase factor, since we assume that $\|H_1\| \leq 1$ and the spectrum of interest only consists of one simple eigenvalue. Therefore, the triangle inequality gives

$$\begin{aligned} & \| |\tilde{\phi}\rangle \langle \tilde{\phi}| - |\psi(T)\rangle \langle \psi(T)| \| \\ & \leq \| |\tilde{\phi}\rangle \langle \tilde{\phi}| - |v\rangle \langle v| \| + \| |\psi(T)\rangle \langle \psi(T)| - |u\rangle \langle u| \| \\ & \leq 2\| |\tilde{\phi}\rangle - |v\rangle \| + 2\| |\psi(T)\rangle - |u\rangle \| \\ & \leq \mathcal{O}\left(\frac{1}{T^k}\right). \end{aligned} \quad (\text{G4})$$

■

APPENDIX H: SPECTRAL GAP OF THE WALK OPERATOR IN ADIABATIC GROVER SEARCH

1. Direct computations

Here, we determine the spectral gap of the walk operator $W(s)$ for a step of Trotter as applied to a search problem in Sec. VI. First, we diagonalize H_0 using Eq. (46) as

$$H_0 = \begin{pmatrix} \sqrt{M/N} & \sqrt{(N-M)/N} \\ \sqrt{(N-M)/N} & -\sqrt{M/N} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{M/N} & \sqrt{(N-M)/N} \\ \sqrt{(N-M)/N} & -\sqrt{M/N} \end{pmatrix}. \quad (\text{H1})$$

That gives the walk operator $W(s)$ as

$$\begin{aligned} W(s) &= e^{-if(s)H_1} e^{-i(1-f(s))H_0} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & e^{-if(s)} \end{pmatrix} \begin{pmatrix} \sqrt{M/N} & \sqrt{(N-M)/N} \\ \sqrt{(N-M)/N} & -\sqrt{M/N} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{-i(1-f(s))} \end{pmatrix} \begin{pmatrix} \sqrt{M/N} & \sqrt{(N-M)/N} \\ \sqrt{(N-M)/N} & -\sqrt{M/N} \end{pmatrix} \\ &= \begin{pmatrix} \frac{M}{N} + e^{-i(1-f(s))} \frac{N-M}{N} & \frac{\sqrt{M(N-M)}}{N} (1 - e^{-i(1-f(s))}) \\ \frac{\sqrt{M(N-M)}}{N} (e^{-if(s)} - e^{-i}) & e^{-if(s)} \frac{N-M}{N} + e^{-i} \frac{M}{N} \end{pmatrix}. \end{aligned} \quad (\text{H2})$$

The eigenvalues of $W(s)$ satisfy the following quadratic equation:

$$\lambda^2 - \left[(1 + e^{-i}) \frac{M}{N} + (e^{-i(1-f(s))} + e^{-if(s)}) \frac{N-M}{N} \right] \lambda + e^{-i} = 0. \quad (\text{H3})$$

So, the eigenvalues can be represented as $\lambda = e^{-\frac{i}{2}} \mu$, where μ satisfies

$$\mu^2 - 2 \left(\frac{M}{N} \cos\left(\frac{1}{2}\right) + \frac{N-M}{N} \cos\left(\frac{1}{2} - f(s)\right) \right) \mu + 1 = 0. \quad (\text{H4})$$

Solving this quadratic equation yields the eigenvalues

$$\lambda_{\pm} = e^{-\frac{i}{2}} (\xi \pm i\sqrt{1-\xi^2}), \quad (\text{H5})$$

$$\xi = \frac{M}{N} \cos\left(\frac{1}{2}\right) + \frac{N-M}{N} \cos\left(\frac{1}{2} - f(s)\right). \quad (\text{H6})$$

The spectral gap of $W(s)$ is

$$\begin{aligned} \Delta_{0,W}(s) &= 2 \arccos \left(\frac{M}{N} \cos\left(\frac{1}{2}\right) + \frac{N-M}{N} \cos\left(\frac{1}{2} - f(s)\right) \right) \\ &= 2 \arccos \left(\cos\left(\frac{1}{2} - f(s)\right) - \frac{M}{N} \left[\cos\left(\frac{1}{2} - f(s)\right) - \cos\left(\frac{1}{2}\right) \right] \right). \end{aligned} \quad (\text{H7})$$

2. Proof of Lemma 5

This lemma lower bounds the gap of the walk operator $W(s)$ for a step of Trotter in terms of the spectral gap of the Hamiltonian. To bound this spectral gap, we may use Lemma 3 with $h = 1$ to give

$$\Delta_W(s; N, M, f) \geq \Delta_H(s; N, M, f) - \frac{\pi}{144\sqrt{3}} (2\|[H_1, [H_1, H_0]]\| + \|[H_0, [H_0, H_1]]\|) \geq \Delta_H(s; N, M, f) - \frac{\pi}{24\sqrt{3}} \|[H_0, H_1]\|. \quad (\text{H8})$$

The commutator in the basis $\{|e_0\rangle, |e_1\rangle\}$ can be computed as

$$[H_0, H_1] = \begin{pmatrix} 0 & -\sqrt{M(N-M)}/N \\ \sqrt{M(N-M)}/N & 0 \end{pmatrix} \quad (\text{H9})$$

and

$$\|[H_0, H_1]\| = \sqrt{M(N-M)}/N. \quad (\text{H10})$$

Then, Eq. (H8) becomes

$$\begin{aligned} \Delta_W(s; N, M, f) &\geq \sqrt{(1-2f(s))^2 + \frac{4M}{N}f(s)(1-f(s))} \\ &\quad - \frac{\pi}{24\sqrt{3}} \frac{\sqrt{M(N-M)}}{N} \\ &> \sqrt{(1-2f(s))^2 + \frac{4M}{N}f(s)(1-f(s))} \\ &\quad - \frac{\pi}{24\sqrt{3}} \sqrt{\frac{M}{N}} \\ &> \frac{2}{3} \sqrt{(1-2f(s))^2 + \frac{4M}{N}f(s)(1-f(s))} \\ &= \frac{2}{3} \Delta_H(s; N, M, f). \end{aligned} \quad (\text{H11})$$

APPENDIX I: PROOF OF THEOREM 3

This theorem bounds the error in using the Trotter formula to solve a search problem. The majority of the proof uses the general form of the discrete adiabatic theorem in Lemma 1 to bound the diabatic errors. To use Lemma 1, we first need to bound c_1 and c_2 . This can be done by straightforward calculations similar to the proof of Lemma C3 and we can choose

$$c_1(s) = 2|f'(s)|, \quad c_2(s) = 2|f''(s)| + 4|f'(s)|^2. \quad (\text{I1})$$

For general p , by the definition of $f(s)$, we have

$$f'(s) = d_{N,p} \Delta_H(s; N, 1, f(s))^p \quad (\text{I2})$$

and

$$\begin{aligned} f''(s) &= d_{N,p} \frac{\partial(\Delta^p)}{\partial f} f'(s) \\ &= d_{N,p} p \Delta_H(s; N, 1, f)^{p-1} \frac{\partial \Delta}{\partial f} d_{N,p} \Delta_H(s; N, 1, f(s))^p \\ &= p d_{N,p}^2 \Delta_H(s; N, 1, f)^{2p-1} \frac{\partial \Delta}{\partial f}, \end{aligned} \quad (\text{I3})$$

where

$$\begin{aligned} \left| \frac{\partial \Delta}{\partial f} \right| &= \left| \frac{(-2 + \frac{2}{N})(1-2f(s))}{\sqrt{(1-2f(s))^2 + \frac{4}{N}f(s)(1-f(s))}} \right| \\ &\leq \frac{(2-2/N)|1-2f(s)|}{\sqrt{(1-2f(s))^2}} \\ &\leq 2. \end{aligned} \quad (\text{I4})$$

Therefore, we can choose

$$\begin{aligned} c_1(s) &= 2d_{N,p} \Delta_H(s; N, 1, f)^p, \\ c_2(s) &= (4p+4)d_{N,p}^2 \Delta_H(s; N, 1, f)^{2p-1}. \end{aligned} \quad (\text{I5})$$

Here,

$$d_{N,p} = \int_0^1 \Delta_H(s; N, 1, f)^{-p} df. \quad (\text{I6})$$

The error bound in Lemma 1 involves the multistep gap and the maximum/minimum over several subsequent steps. Here, we show that, when T is sufficiently large (which can be ensured by the choice of T in Theorem 3), we can ignore the maximum and minimum and consider the single-step gap condition at sacrifice of extra multiplicative constant factors. We first focus on the minimum of the multistep gap of W . Since the two relevant eigenvalues determining the gap have different rotational directions on the circle for any time s , the multistep gap of W is exactly the minimum single step gap over two subsequent steps, so

$$\begin{aligned} \check{\Delta}_{2,W}(s; M) &= \min_{s'=s+k/T, -1 \leq k \leq 3} \Delta_W(s'; M) \\ &\geq \frac{2}{3} \min_{s'=s+\tau, |\tau| \leq 3/T} \Delta_H(s'; M). \end{aligned} \quad (\text{I7})$$

We bound the ratio of gaps at steps s and s' as

$$\begin{aligned} \frac{\Delta_H(s; M)}{\Delta_H(s'; M)} &= 1 + \frac{\Delta_H(s; M) - \Delta_H(s'; M)}{\Delta_H(s'; M)} \\ &\leq 1 + \frac{|s-s'|}{\Delta_H(s'; M)} \max_{\xi} \left| \frac{\partial \Delta(\xi; M)}{\partial f} \right| |f'(\xi)| \\ &\leq 1 + \frac{6d_{N,p}}{T} \max_{s: |s-s'| \leq 3/T} \frac{\Delta_H(s; M)}{\Delta_H(s'; M)}. \end{aligned} \quad (\text{I8})$$

Suppose that $T \geq 12d_{N,p}$, then for any $|s-s'| \leq 3/T$, we have

$$\frac{\Delta_H(s; M)}{\Delta_H(s'; M)} \leq 2. \quad (\text{I9})$$

This implies that

$$\check{\Delta}_{2,W}(s; M) \geq \frac{2}{3} \min_{s'=s+\tau, |\tau| \leq 3/T} \Delta_H(s'; M) \geq \frac{1}{3} \Delta_H(s; M). \quad (\text{I10})$$

Therefore, we can directly replace the minimum of the multistep gap by the single-step gap at fixed time s up to some constant factors. According to Eqs. (I5) and (I9), the functions $\hat{c}_1(s)$ and $\hat{c}_2(s)$ can also be replaced, up to constant factors, by $c_1(s)$ and $c_2(s)$.

We now compute each term in Lemma 1. For simplicity of notation, we omit the dependence on H , f , and N in the gap and use $\Delta(s; M)$ to denote $\Delta_H(s; N, M, f)$, and we ignore all constant factors in the computations. The boundary terms can be bounded as

$$\frac{c_1(0)}{\Delta(0; M)^2} = 2d_{N,p}, \quad (\text{I11})$$

$$\frac{c_1(1)}{\Delta(1; M)^2} = 2d_{N,p}. \quad (\text{I12})$$

For the summations, we first bound them as

$$\begin{aligned} \sum_{j=0}^{T-1} \frac{c_1(j/T)^2}{T \Delta(j/T; M)^3} &= \sum_{j=0}^{T-1} \frac{4d_{N,p}^2 \Delta(j/T; 1)^{2p}}{T \Delta(j/T; M)^3} \\ &\leq 4d_{N,p}^2 \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2} \end{aligned} \quad (\text{I13})$$

and

$$\begin{aligned} \sum_{j=0}^{T-1} \frac{c_2(j/T)}{T \Delta(j/T; M)^2} &= \sum_{j=0}^{T-1} \frac{(4p+4)d_{N,p}^2 \Delta(j/T; 1)^{2p-1}}{T \Delta(j/T; M)^2} \\ &= 4(p+1)d_{N,p}^2 \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2}. \end{aligned} \quad (\text{I14})$$

So, the overall error is bounded by

$$\mathcal{O}\left(\frac{d_{N,p}}{T} + \frac{d_{N,p}^2}{T} \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2}\right). \quad (\text{I15})$$

It remains to estimate $d_{N,p}$ and $\sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2}$.

Before we proceed, it is useful to preliminarily calculate $d_{N,p}$ for general $1 \leq p < 2$. By Eq. (16) and the change of variables $f = \frac{1}{2} + \frac{1}{2\sqrt{N-1}} \tan \theta$, we have

$$\begin{aligned} d_{N,p} &= \int_0^1 \frac{df}{((1-2f)^2 + \frac{4}{N}f(1-f))^{p/2}} \\ &= \int_0^1 \frac{df}{(4(1-1/N)(f-1/2)^2 + 1/N)^{p/2}} \\ &= \int_{-\arctan \sqrt{N-1}}^{\arctan \sqrt{N-1}} \frac{d\theta}{2\sqrt{N-1} \cos^2 \theta \left(\frac{1}{N} \tan^2 \theta + \frac{1}{N}\right)^{p/2}} \\ &= \frac{N^{p/2}}{\sqrt{N-1}} \int_0^{\arctan \sqrt{N-1}} \cos^{p-2} \theta d\theta. \end{aligned} \quad (\text{I16})$$

Here, the integral in the first line comes from Eq. (12) and the condition $f(1) = 1$.

1. $p = 1$

We first consider the limit case when $p = 1$. The error bound Eq. (115) becomes

$$\text{Error} \leq \mathcal{O}\left(\frac{d_{N,1}}{T} + \frac{d_{N,1}^2}{T} \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2}\right). \quad (\text{I17})$$

For $d_{N,1}$, using Eq. (116) we have

$$\begin{aligned} d_{N,1} &= \sqrt{\frac{N}{N-1}} \int_0^{\arctan \sqrt{N-1}} \frac{1}{\cos \theta} d\theta \\ &= \sqrt{\frac{N}{N-1}} \ln \left(\frac{1 + \sin \theta}{\cos \theta} \right) \Big|_0^{\arctan \sqrt{N-1}} \\ &= \sqrt{\frac{N}{N-1}} \ln(\sqrt{N} + \sqrt{N-1}) \\ &\leq 2 \ln(N). \end{aligned} \quad (\text{I18})$$

For the summation, we first use the fact that $\Delta(s; M)$ is symmetric with respect to $1/2$ and monotonically decreases on $[0, 1/2]$, and we can obtain

$$\begin{aligned} \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} &\leq 2 \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} \\ &= 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} + \frac{2}{T} \frac{\Delta(0; 1)}{\Delta(0; M)^2} \\ &\quad + \frac{2}{T} \frac{\Delta(\lfloor T/2 \rfloor / T; 1)}{\Delta(\lfloor T/2 \rfloor / T; M)^2} \\ &\leq 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} \\ &\quad + \frac{2}{T} \frac{\Delta(0; 1)}{\Delta(0; M)^2} + \frac{2}{T} \frac{1}{\Delta(\lfloor T/2 \rfloor / T; M)} \\ &\leq 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} \\ &\quad + \frac{2}{T} \left(1 + \sqrt{\frac{N}{M}}\right). \end{aligned} \quad (\text{I19})$$

Now, we focus on the dominant summation. Using monotonicity of $\Delta(s; 1)$, we have

$$2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} \leq 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \int_{(j-1)/T}^{j/T} \frac{\Delta(s; 1)}{\Delta(j/T; M)^2} ds. \quad (\text{I20})$$

We change the denominator of the integrand from $\Delta(j/T; M)^2$ to $\Delta(s; M)^2$ at the cost of an extra multiplicative factor. Specifically, for any $s \in [(j-1)/T, j/T]$, using

$$\begin{aligned} \left| \frac{d(\Delta(s; M)^2)}{ds} \right| &= \left| \left(-4 + \frac{4M}{N} \right) (1 - 2f(s)) d_{N,1} \Delta(s; 1) \right| \\ &\leq \left(4 - \frac{4M}{N} \right) (1 - 2f((j-1)/T)) d_{N,1} \\ &\quad \times \Delta((j-1)/T; 1) \\ &\leq 8 \ln(N) \Delta((j-1)/T; 1)^2, \end{aligned} \quad (\text{I21})$$

we have

$$\begin{aligned} &\frac{\Delta((j-1)/T; M)^2}{\Delta(j/T; M)^2} \\ &= 1 + \frac{\Delta((j-1)/T; M)^2 - \Delta(j/T; M)^2}{\Delta(j/T; M)^2} \\ &\leq 1 + \frac{1}{\Delta(j/T; M)^2} \frac{1}{T} \max_{s \in [(j-1)/T, j/T]} \left| \frac{d(\Delta(s; M)^2)}{ds} \right| \\ &\leq 1 + \frac{8 \ln(N)}{T} \frac{\Delta((j-1)/T; 1)^2}{\Delta(j/T; M)^2}. \end{aligned} \quad (\text{I22})$$

Suppose that $T \geq 16 \ln(N)$; we can conclude that

$$\frac{\Delta(s; M)^2}{\Delta(j/T; M)^2} \leq \frac{\Delta((j-1)/T; M)^2}{\Delta(j/T; M)^2} \leq 2. \quad (\text{I23})$$

Therefore, Eq. (I19) becomes

$$\begin{aligned} 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} &\leq 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \int_{(j-1)/T}^{j/T} \frac{\Delta(s; 1)}{\Delta(j/T; M)^2} ds \\ &\leq 4 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \int_{(j-1)/T}^{j/T} \frac{\Delta(s; 1)}{\Delta(s; M)^2} ds \\ &\leq 4 \int_0^{1/2} \frac{\Delta(s; 1)}{\Delta(s; M)^2} ds \\ &= 2 \int_0^1 \frac{\Delta(s; 1)}{\Delta(s; M)^2} ds. \end{aligned} \quad (\text{I24})$$

By changing the variable from s to f and using $df = d_{N,1} \Delta(s; 1) ds$, we have

$$\begin{aligned} 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} &\leq \frac{2}{d_{N,1}} \int_0^1 \frac{df}{\Delta(s; M)^2} \\ &= \frac{2}{d_{N,1}} \frac{N/M}{\sqrt{N/M - 1}} \\ &\quad \times \arctan \sqrt{N/M - 1} \\ &\leq \frac{\sqrt{2}\pi}{d_{N,1}} \sqrt{\frac{N}{M}}. \end{aligned} \quad (\text{I25})$$

Therefore, Eq. (I19) becomes

$$\sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} \leq \frac{\sqrt{2}\pi}{d_{N,1}} \sqrt{\frac{N}{M}} + \frac{2}{T} \left(1 + \sqrt{\frac{N}{M}} \right). \quad (\text{I26})$$

Plugging Eq. (I18) and Eq. (I26) back to Eq. (I17), we can bound the total error as

$$\begin{aligned} \text{Error} &\leq \mathcal{O} \left(\frac{d_{N,1}}{T} + \frac{d_{N,1}^2}{T} \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)}{\Delta(j/T; M)^2} \right) \\ &\leq \mathcal{O} \left(\frac{d_{N,1}}{T} + \frac{d_{N,1}}{T} \sqrt{2\pi} \sqrt{\frac{N}{M}} + \frac{2d_{N,1}^2}{T^2} \left(1 + \sqrt{\frac{N}{M}} \right) \right) \\ &\leq \mathcal{O} \left(\frac{\ln(N)}{T} + \frac{\ln(N)}{T} \sqrt{\frac{N}{M}} + \frac{\ln^2(N)}{T^2} \sqrt{\frac{N}{M}} \right) \\ &\leq \mathcal{O} \left(\frac{\ln(N)}{T} \sqrt{\frac{N}{M}} \right). \end{aligned} \quad (\text{I27})$$

2. $1 < p < 2$

Now, we consider $1 < p < 2$. Continuing with Eq. (I16) and using integration by parts, we may obtain

$$\begin{aligned} \int_0^{\arctan \sqrt{N-1}} \cos^{p-2} \theta d\theta &= -\frac{1}{p-1} \cos^{p-1} \theta \sin \theta \Big|_0^{\arctan \sqrt{N-1}} \\ &\quad + \frac{p}{p-1} \int_0^{\arctan \sqrt{N-1}} \cos^p \theta d\theta. \end{aligned} \quad (\text{I28})$$

Both terms on the right-hand side of Eq. (I28) are bounded independent of N , so $\int_0^{\arctan \sqrt{N-1}} \cos^{p-2} \theta d\theta = \mathcal{O}(1)$ and thus, by Eq. (I16),

$$d_{N,p} = \mathcal{O}(N^{\frac{p-1}{2}}). \quad (\text{I29})$$

For the summation, with the same reasoning of Eqs. (I19) and (I24), we have

$$\begin{aligned} \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2} &\leq 2 \sum_{j=1}^{\lfloor T/2 \rfloor - 1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2} + \frac{2}{T} \left(1 + \max \left\{ 1, \frac{N^{3/2-p}}{M^{3/2-p}} \right\} \right) \\ &\leq 2 \int_0^1 \frac{\Delta(s; 1)^{2p-1}}{\Delta(s; M)^2} ds + \frac{4}{T} \max \left\{ 1, \frac{N^{3/2-p}}{M^{3/2-p}} \right\}. \end{aligned} \quad (\text{I30})$$

We focus on the integral. By changing the variable from s to f and using $df = d_{N,p} \Delta(s; 1)^p ds$, we have

$$\begin{aligned} \int_0^1 \frac{\Delta(s; 1)^{2p-1}}{\Delta(s; M)^2} ds &= \frac{1}{d_{N,p}} \int_0^1 \frac{\Delta(s; 1)^{p-1}}{\Delta(s; M)^2} df \\ &= \frac{1}{d_{N,p}} \int_0^1 \frac{\left((1-2f)^2 + \frac{4}{N} f(1-f) \right)^{(p-1)/2}}{\left((1-2f)^2 + \frac{4M}{N} f(1-f) \right)} df \\ &= \frac{1}{d_{N,p}} \int_0^1 \frac{\left(4 \frac{N-1}{N} (f-1/2)^2 + \frac{1}{N} \right)^{(p-1)/2}}{4 \frac{N-M}{N} (f-1/2)^2 + \frac{M}{N}} df. \end{aligned} \quad (\text{I31})$$

By the change of variable $f = \frac{1}{2} + \frac{\sqrt{M}}{2\sqrt{N-M}} \tan \theta$, we have

$$\begin{aligned} \int_0^1 \frac{\Delta(s; 1)^{2p-1}}{\Delta(s; M)^2} ds &= \frac{1}{d_{N,p}} \int_{-\arctan \frac{\sqrt{N-M}}{\sqrt{M}}}^{\arctan \frac{\sqrt{N-M}}{\sqrt{M}}} \frac{\left(\frac{N-1}{N} \frac{M}{N-M} \tan^2 \theta + \frac{1}{N} \right)^{(p-1)/2}}{\frac{M}{N} (\tan^2 \theta + 1)} \frac{\sqrt{M}}{\sqrt{N-M}} \frac{1}{\cos^2 \theta} d\theta \\ &= \frac{2}{d_{N,p}} \frac{N}{\sqrt{M(N-M)}} \int_0^{\arctan \frac{\sqrt{N-M}}{\sqrt{M}}} \left(\frac{N-1}{N} \frac{M}{N-M} \tan^2 \theta + \frac{1}{N} \right)^{(p-1)/2} d\theta. \end{aligned} \quad (\text{I32})$$

Notice that, for $\theta \in [0, \pi/2)$, the function $\tan^2 \theta$ monotonically increases. So, we can separate the integral into two parts as

$$\begin{aligned} \int_0^1 \frac{\Delta(s; 1)^{2p-1}}{\Delta(s; M)^2} ds &= \frac{2}{d_{N,p}} \frac{N}{\sqrt{M(N-M)}} \left(\int_0^{\arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}}} + \int_{\arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}}}^{\arctan \frac{\sqrt{N-M}}{\sqrt{M}}} \right) \left(\frac{N-1}{N} \frac{M}{N-M} \tan^2 \theta + \frac{1}{N} \right)^{\frac{p-1}{2}} d\theta \\ &\leq \frac{2}{d_{N,p}} \frac{N}{\sqrt{M(N-M)}} \left(\int_0^{\arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}}} \left(\frac{2}{N} \right)^{\frac{p-1}{2}} d\theta + \int_{\arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}}}^{\arctan \frac{\sqrt{N-M}}{\sqrt{M}}} \left(2 \frac{N-1}{N} \frac{M}{N-M} \tan^2 \theta \right)^{\frac{p-1}{2}} d\theta \right) \\ &= \frac{2}{d_{N,p}} \frac{N}{\sqrt{M(N-M)}} \left(\frac{2^{\frac{p-1}{2}}}{N^{\frac{p-1}{2}}} \arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}} + 2^{\frac{p-1}{2}} \left(\frac{N-1}{N} \right)^{\frac{p-1}{2}} \frac{M^{\frac{p-1}{2}}}{(N-M)^{\frac{p-1}{2}}} \int_{\arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}}}^{\arctan \frac{\sqrt{N-M}}{\sqrt{M}}} \tan^{p-1} \theta d\theta \right). \end{aligned} \quad (\text{I33})$$

Using $1 < p < 2$ and thus

$$\int_{\arctan \frac{\sqrt{N-M}}{\sqrt{M(N-1)}}}^{\arctan \frac{\sqrt{N-M}}{\sqrt{M}}} \tan^{p-1} \theta d\theta \leq \int_0^{\pi/2} \tan^{p-1} \theta d\theta = \frac{\pi}{2} \sec\left(\frac{(p-1)\pi}{2}\right) = \mathcal{O}(1), \quad (\text{I34})$$

we have

$$\begin{aligned} \int_0^1 \frac{\Delta(s; 1)^{2p-1}}{\Delta(s; M)^2} ds &\leq \mathcal{O}\left(\frac{1}{d_{N,p}} \frac{N}{\sqrt{M(N-M)}} \left(\frac{1}{N^{\frac{p-1}{2}}} \frac{\sqrt{N-M}}{\sqrt{M(N-1)}} + \frac{M^{\frac{p-1}{2}}}{(N-M)^{\frac{p-1}{2}}} \right) \right) \\ &\leq \mathcal{O}\left(\frac{1}{d_{N,p}} \frac{\sqrt{N}}{\sqrt{M}} \left(\frac{1}{N^{\frac{p-1}{2}} \sqrt{M}} + \frac{M^{\frac{p-1}{2}}}{N^{\frac{p-1}{2}}} \right) \right) \\ &\leq \mathcal{O}\left(\frac{1}{d_{N,p}} \frac{N^{1-\frac{p}{2}}}{M^{1-\frac{p}{2}}} \right). \end{aligned} \quad (\text{I35})$$

Plugging this back into Eq. (I30), we have

$$\sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2} \leq \mathcal{O}\left(\frac{1}{d_{N,p}} \frac{N^{1-\frac{p}{2}}}{M^{1-\frac{p}{2}}} + \frac{1}{T} \max\left\{1, \frac{N^{3/2-p}}{M^{3/2-p}}\right\} \right). \quad (\text{I36})$$

Plugging Eqs. (I29) and (I36) back into Eq. (I15), we can bound the total error by

$$\begin{aligned} \mathcal{O}\left(\frac{d_{N,p}}{T} + \frac{d_{N,p}^2}{T} \sum_{j=0}^{T-1} \frac{1}{T} \frac{\Delta(j/T; 1)^{2p-1}}{\Delta(j/T; M)^2} \right) &\leq \mathcal{O}\left(\frac{N^{\frac{p-1}{2}}}{T} + \frac{d_{N,p}^2}{T} \left(\frac{1}{d_{N,p}} \frac{N^{1-\frac{p}{2}}}{M^{1-\frac{p}{2}}} + \frac{1}{T} \max\left\{1, \frac{N^{3/2-p}}{M^{3/2-p}}\right\} \right) \right) \\ &\leq \mathcal{O}\left(\frac{N^{\frac{p-1}{2}}}{T} + \frac{1}{T} \frac{\sqrt{N}}{M^{1-\frac{p}{2}}} + \frac{N^{p-1}}{T^2} \max\left\{1, \frac{N^{3/2-p}}{M^{3/2-p}}\right\} \right) \\ &\leq \mathcal{O}\left(\frac{1}{T} \frac{\sqrt{N}}{M^{1-\frac{p}{2}}} + \frac{N^{p-1}}{T^2} \max\left\{1, \frac{N^{3/2-p}}{M^{3/2-p}}\right\} \right). \end{aligned} \quad (\text{I37})$$

APPENDIX J: PROOF OF THEOREM 4

In this Appendix, we give the complete proof of Theorem 4. We start with summarizing the properties of the function $f(s)$ in the following lemma.

Lemma J1. Let $f(s)$ be the function defined in Eq. (57). Then,

- (1) $f(s) \in C^\infty[0, 1]$;
- (2) $f(0) = 0$, $f(1) = 1$, and $f^{(k)}(0) = f^{(k)}(1) = 0$ for all $k \geq 1$;
- (3) for all $s \in [0, 1/2]$ and $k \geq 1$, $f(s) + f(1-s) = 1$ and $f^{(k)}(s) = (-1)^{k+1} f^{(k)}(1-s)$.

To prove Theorem 4, we will frequently use the following lemma.

Lemma J2. Let $\Delta_H(s)$ be the gap defined in Eq. (49). Then, for any $s \in [0, 1/2]$ and any integer $l \geq 0$, we have

$$\frac{\exp\left(-\frac{1}{2s(1-2s)}\right)}{\Delta_H(s)(2s(1-2s))^l} \leq 2^{l+3} c_e^{-l/2} (l+1)^{l+2} (\ln(N/M))^{l+2}, \quad (\text{J1})$$

where c_e is the normalization factor defined in Eq. (56).

Proof. We start with

$$\begin{aligned} \Delta_H(s) &= \sqrt{(1-2f(s))^2 + \frac{4M}{N} f(s)(1-f(s))} \\ &= \sqrt{(1-M/N)(1-2f(s))^2 + \frac{M}{N}} \end{aligned}$$

$$\begin{aligned}
&= \sqrt{(1 - M/N)(1 - g(2s))^2 + \frac{M}{N}} \\
&\geq \frac{1}{\sqrt{2}} \sqrt{(1 - g(2s))^2 + \frac{M}{N}} \\
&\geq \frac{1}{2} \left(1 - g(2s) + \sqrt{\frac{M}{N}} \right). \tag{J2}
\end{aligned}$$

Let $t = 2s \in [0, 1]$, then

$$\frac{\exp\left(-\frac{1}{2s(1-2s)}\right)}{\Delta_H(s)(2s(1-2s))^l} \leq \frac{2 \exp\left(-\frac{1}{t(1-t)}\right)}{(1 - g(t) + \sqrt{\frac{M}{N}})(t(1-t))^l} = 2F(t), \tag{J3}$$

where we define

$$F(t) := \frac{\exp\left(-\frac{1}{t(1-t)}\right)}{(1 - g(t) + \sqrt{\frac{M}{N}})(t(1-t))^l}. \tag{J4}$$

It suffices to bound $F(t)$. This can be done with nuanced modifications of the proof of Lemma 14 of Ref. [33], but for completeness we provide the details again. Since $F(0) = F(1) = 0$ and $F(t) > 0$ for $t \in (0, 1)$, there exists a $t_* \in (0, 1)$ such that $F(t_*)$ reaches its maximum. At this point, $F'(t_*) = 0$, where $F'(t)$ can be computed as

$$\begin{aligned}
&\left(1 - g(t) + \sqrt{\frac{M}{N}}\right)^2 (t(1-t))^{2l} F'(t) \\
&= \left(1 - g(t) + \sqrt{\frac{M}{N}}\right) (t(1-t))^l \\
&\quad \times \exp\left(-\frac{1}{t(1-t)}\right) \frac{1-2t}{(t(1-t))^2} \\
&\quad - \exp\left(-\frac{1}{t(1-t)}\right) \left(-c_e^{-1} \exp\left(-\frac{1}{t(1-t)}\right) (t(1-t))^l\right. \\
&\quad \left.+ \left(1 - g(t) + \sqrt{\frac{M}{N}}\right) l(t(1-t))^{l-1} (1-2t)\right) \\
&= \exp\left(-\frac{1}{t(1-t)}\right) (t(1-t))^{l-2} G(t), \tag{J5}
\end{aligned}$$

where

$$\begin{aligned}
G(t) &= \left(1 - g(t) + \sqrt{\frac{M}{N}}\right) (1-2t)(1-lt(1-t)) \\
&\quad + c_e^{-1} \exp\left(-\frac{1}{t(1-t)}\right) (t(1-t))^2. \tag{J6}
\end{aligned}$$

For $t \in [1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}, 1]$ where $\sqrt{c_e} \approx 0.08$, we have

$$1 - g(t) + \sqrt{\frac{M}{N}} \geq \sqrt{\frac{M}{N}}, \tag{J7}$$

$$1 - 2t \leq \frac{2\sqrt{c_e}}{(l+1)\ln(N/M)} - 1 \leq \frac{2\sqrt{c_e}}{\ln 2} - 1, \tag{J8}$$

and

$$\begin{aligned}
1 - lt(1-t) &\geq 1 - l(1-t) \geq 1 - \frac{\sqrt{c_e}l}{(l+1)\ln(N/M)} \\
&\geq 1 - \frac{\sqrt{c_e}}{\ln(2)}. \tag{J9}
\end{aligned}$$

Then,

$$\begin{aligned}
&\left(1 - g(t) + \sqrt{\frac{M}{N}}\right) (1-2t)(1-lt(1-t)) \\
&\leq -\left(1 - \frac{2\sqrt{c_e}}{\ln 2}\right) \left(1 - \frac{\sqrt{c_e}}{\ln 2}\right) \sqrt{\frac{M}{N}} \leq -\frac{3}{5} \sqrt{\frac{M}{N}}. \tag{J10}
\end{aligned}$$

Meanwhile, for the same range of t ,

$$\begin{aligned}
&c_e^{-1} \exp\left(-\frac{1}{t(1-t)}\right) (t(1-t))^2 \\
&\leq c_e^{-1} \exp\left(-\frac{1}{t(1-t)}\right) (1-t)^2 \\
&\leq \frac{1}{c_e} \exp\left(-\left(1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}\right)^{-1}\right. \\
&\quad \left.\times \frac{(l+1)\ln(N/M)}{\sqrt{c_e}}\right) \left(\frac{\sqrt{c_e}}{(l+1)\ln(N/M)}\right)^2 \\
&\leq \frac{1}{(\ln 2)^2} \exp\left(-\left(1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}\right)^{-1}\right. \\
&\quad \left.\times \frac{(l+1)\ln(N/M)}{\sqrt{c_e}}\right) \\
&= \frac{1}{(\ln 2)^2} \left(\frac{N}{M}\right)^{-\left(1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}\right)^{-1} \frac{l+1}{\sqrt{c_e}}} \\
&\leq \frac{1}{(\ln 2)^2} \left(\frac{N}{M}\right)^{-\frac{l+1}{\sqrt{c_e}}} \\
&\leq \frac{1}{(\ln 2)^2} \left(\frac{N}{M}\right)^{-10} \\
&\leq \frac{1}{2^7} \sqrt{\frac{M}{N}}. \tag{J11}
\end{aligned}$$

Therefore, for $t \in [1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}, 1]$, we always have

$$G(t) \leq -\frac{3}{5} \sqrt{\frac{M}{N}} + \frac{1}{2^7} \sqrt{\frac{M}{N}} < 0. \tag{J12}$$

Since $F'(t_*) = 0$, we must have $G(t_*) = 0$, so Eq. (J12) implies that $t_* \leq 1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}$. Meanwhile, notice that for $t \in [0, 1/2]$, we have $F(t) < F(1-t)$, so $t_* \geq 1/2$. Therefore, we obtain the range of t_* that

$$t_* \in \left[\frac{1}{2}, 1 - \frac{\sqrt{c_e}}{(l+1)\ln(N/M)}\right]. \tag{J13}$$

We now bound $F(t)$. Using $G(t_*) = 0$ again, we have

$$\frac{\exp\left(-\frac{1}{t_*(1-t_*)}\right)}{1 - g(t_*) + \sqrt{\frac{M}{N}}} = \frac{c_e(2t_* - 1)(1 - lt_*(1 - t_*))}{(t_*(1 - t_*))^2}. \quad (\text{J14})$$

Therefore,

$$\begin{aligned} F(t) &\leq F(t_*) \\ &= \frac{\exp\left(-\frac{1}{t_*(1-t_*)}\right)}{(1 - g(t_*) + \sqrt{\frac{M}{N}})(t_*(1 - t_*))^l} \\ &= \frac{c_e(2t_* - 1)(1 - lt_*(1 - t_*))}{(t_*(1 - t_*))^{l+2}} \\ &\leq \frac{c_e}{(t_*(1 - t_*))^{l+2}} \\ &\leq \frac{2^{l+2}c_e}{(1 - t_*)^{l+2}} \\ &\leq 2^{l+2}c_e \left(\frac{(l+1)\ln(N/M)}{\sqrt{c_e}}\right)^{l+2} \\ &= 2^{l+2}c_e^{-l/2}(l+1)^{l+2}(\ln(N/M))^{l+2}. \end{aligned} \quad (\text{J15})$$

We are ready to present the main proof of Theorem 4. The idea is separately using Lemma 1 and Conjecture 1 to obtain two independent error bounds, so the overall error is bounded by the minimum of the two.

Proof of Theorem 4. By differentiating the product walk operator, we may choose

$$c_1(s) = 2f'(s), \quad c_2(s) = 2|f''(s)| + 4f'(s)^2. \quad (\text{J16})$$

We use the similar trick as in Appendix I to get rid of the hat and check notations and the multistep gap in Lemma 1. Specifically, for $|s - s'| \leq 3/T$, we have

$$\begin{aligned} \frac{\Delta_H(s; M)}{\Delta_H(s'; M)} &= 1 + \frac{\Delta_H(s; M) - \Delta_H(s'; M)}{\Delta_H(s'; M)} \\ &\leq 1 + \frac{|s - s'|}{\Delta_H(s'; M)} \max_{\xi} \left| \frac{\partial \Delta(\xi; M)}{\partial f} \right| |f'(\xi)| \\ &\leq 1 + \frac{6}{T \Delta_H(s'; M)} \max |f'| \\ &\leq 1 + \frac{6 \max |f'|}{T \sqrt{M/N}}. \end{aligned} \quad (\text{J17})$$

Here, $\max |f'|$ is an absolute constant, which is independent of N and M , so we may choose $T \geq 6\sqrt{N/M} \max |f'|$ and thus

$$\frac{\Delta_H(s; M)}{\Delta_H(s'; M)} \leq 2. \quad (\text{J18})$$

So, we can bound $\check{\Delta}_{2,W}(s; M)$ from below by $\frac{1}{3} \Delta_H(s; M)$ and drop the hat notations in c_1 and c_2 in the same way as in Appendix I.

Now, we bound each term in the upper bound of Lemma 1. The two boundary terms are 0 due to the boundary cancellation. For the summations, we use symmetry of $f(s)$ and

Lemma J2 and obtain

$$\begin{aligned} \sum_{j=0}^{T-1} \frac{c_1(j/T)^2}{T \Delta_W(j/T; M)^3} &\leq \frac{27}{2} \sum_{j=0}^{T-1} \frac{f'(j/T)^2}{T \Delta_H(j/T; M)^3} \\ &= 27 \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{g'(2j/T)^2}{T \Delta_H(j/T; M)^3} \\ &= \frac{27}{c_e^2} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T \Delta_H(j/T; M)} \\ &\quad \times \left(\frac{\exp\left(-\frac{1}{2j/T(1-2j/T)}\right)}{\Delta_H(j/T; M)} \right)^2 \\ &\leq \frac{27}{c_e^2} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T \sqrt{M/N}} 2^6 (\ln(N/M))^4 \\ &= \mathcal{O}\left(\sqrt{\frac{N}{M}} \left(\ln \frac{N}{M}\right)^4\right) \end{aligned} \quad (\text{J19})$$

and

$$\begin{aligned} \sum_{j=0}^{T-1} \frac{c_2(j/T)}{T \Delta_W(j/T; M)^2} &\leq \frac{9}{2} \sum_{j=0}^{T-1} \frac{|f''(j/T)|}{T \Delta_H(j/T; M)^2} + 9 \sum_{j=0}^{T-1} \frac{f'(j/T)^2}{T \Delta_H(j/T; M)^2} \\ &= 18 \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{|g''(2j/T)|}{T \Delta_H(j/T; M)^2} + 18 \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{g'(2j/T)^2}{T \Delta_H(j/T; M)^2} \\ &= \frac{18}{c_e} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{\exp\left(-\frac{1}{2j/T(1-2j/T)}\right) |1 - 4j/T|}{T \Delta_H(j/T; M)^2 (2j/T(1 - 2j/T))^2} \\ &\quad + \frac{18}{c_e^2} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{\left(\exp\left(-\frac{1}{2j/T(1-2j/T)}\right)\right)^2}{T \Delta_H(j/T; M)^2} \\ &\leq \frac{18}{c_e} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T \Delta_H(j/T; M)} \\ &\quad \times \frac{\exp\left(-\frac{1}{2j/T(1-2j/T)}\right)}{\Delta_H(j/T; M) (2j/T(1 - 2j/T))^2} \\ &\quad + \frac{18}{c_e^2} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T} \left(\frac{\exp\left(-\frac{1}{2j/T(1-2j/T)}\right)}{\Delta_H(j/T; M)} \right)^2 \\ &\leq \frac{18}{c_e} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T \sqrt{M/N}} 2^5 c_e^{-1} 3^4 (\ln(N/M))^4 \\ &\quad + \frac{18}{c_e^2} \sum_{j=0}^{\lfloor T/2 \rfloor} \frac{1}{T} 2^6 (\ln(N/M))^4 \\ &= \mathcal{O}\left(\sqrt{\frac{N}{M}} \left(\ln \frac{N}{M}\right)^4\right). \end{aligned} \quad (\text{J20})$$

Therefore, Lemma 1 implies an error bound

$$\mathcal{O}\left(\frac{1}{T}\sqrt{\frac{N}{M}}\left(\ln\frac{N}{M}\right)^4\right). \quad (\text{J21})$$

Meanwhile, since the scheduling function $f(s)$ satisfies the boundary cancellation condition, Conjecture 1 implies

another error bound

$$\frac{C_k(N, M)}{T^k} \quad (\text{J22})$$

for any integer $k \geq 1$. Here, the constant $C_k(N, M)$ is independent of T but may depend on k, N, M . Therefore, the overall error can be bounded by the minimum of Eqs. (J21) and (J22). ■

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