Lower bounds for adiabatic quantum algorithms by quantum speed limits

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We introduce a simple framework for estimating lower bounds on the runtime of a broad class of adiabatic quantum algorithms. The central formula consists of calculating the variance of the final Hamiltonian with respect to the initial state. After examining adiabatic versions of certain keystone circuit-based quantum algorithms, this technique is applied to adiabatic quantum algorithms with undetermined speedup. In particular, we analytically obtain lower bounds on adiabatic algorithms for finding $k$-clique in random graphs. Additionally, for a particular class of Hamiltonian, it is straightforward to prove the equivalence between our framework and the conventional approach based on spectral gap analysis.

I. INTRODUCTION

Adiabatic approximation in quantum mechanics has found applications in many fields since it was initially developed in the 1920s [1, 2]. Nonetheless, the idea that adiabatic approximation may serve as a basis for quantum computing did not emerge until the last two decades [3, 4]. It has been proved [5, 6] that adiabatic quantum computation is computationally equivalent to the standard circuit-based quantum computation [7, 8].

An adiabatic quantum algorithm (AQA) consists of three components [9, 10]: (i) a problem (or final) Hamiltonian $H_1$ whose ground state encodes solutions to the problem; (ii) a driver (or initial) Hamiltonian $H_0$ who does not commute with the final Hamiltonian $H_1$ and whose ground state is known; and (iii) a timing schedule $\lambda(t) \in [0, 1]$, a time-dependent strictly increasing function that interpolates between the initial Hamiltonian and the final Hamiltonian. The full time-dependent Hamiltonian $H_{\lambda(t)}$ of an AQA is then defined as

$$H_{\lambda(t)} := (1 - \lambda(t))H_0 + \lambda(t)H_1 \quad (1)$$

with boundary conditions $\lambda(0) = 0$ and $\lambda(T) = 1$, where $T$ is the runtime of the algorithm.

An AQA is executed by preparing a quantum system at the ground state of the initial Hamiltonian $H_0$ and then letting it evolve. The adiabatic theorem [1, 2, 11, 12] guarantees that the final state of time evolution remains close to the instantaneous ground state of the problem Hamiltonian $H_1$, provided that the system evolves slowly enough, or, equivalently, the runtime must be long enough. A typical sufficient condition for the runtime $T$ is that it must scale polynomially with an inverse of the minimum spectral gap (the difference between the two smallest energy eigenvalues) of the full Hamiltonian $H_{\lambda}$ [10, 12, 13]. Nevertheless, analytical calculation of spectral gap is possible only for relatively simple Hamiltonians, whereas performing numerical calculations is limited to small system size.

The main contribution of this work is to present a more elementary, alternative method to the conventional spectral gap analysis for estimating the runtime of adiabatic quantum algorithms. In contrast to the well-known gap conditions [10, 12, 13], which provide sufficient conditions for runtime, our formula provides a lower bound (or necessary condition). More significantly, our technique can be exploited to analytically obtain a lower bound on runtime for an adiabatic quantum algorithm with undetermined speedup, i.e., the adiabatic algorithm of Childs et al. [14] for finding $k$-clique in random graphs, where the conventional method based on spectral gap is unable to do so.

This paper is organized as follows. In Sec. II, we derive the main formula for estimating a necessary runtime using the quantum uncertainty of the final Hamiltonian with respect to the initial state. We shall clarify the condition for which the obtained necessary runtime can be interpreted as a lower bound (in the sense of computational complexity) on the runtime of AQA. After examining our formula with adiabatic versions [4, 15-18] of certain keystone quantum algorithms [19-23] in Sec. III and Sec. IV, our technique is applied in Sec. V to analytically obtain lower bounds for adiabatic algorithms of finding $k$-clique in random graphs. Section VI compares our approach to conventional spectral gap analysis and relevant prior works. Finally, conclusions are presented in Sec. VII.

II. FORMALISM

Consider a quantum system characterized by a time-dependent Hamiltonian $H_{\lambda}$ with $\lambda = \lambda(t)$ being a function of time $t$. For each $\lambda$, the instantaneous ground state $|\Phi_{\lambda}\rangle$ is the solution to the eigenvalue problem $H_{\lambda}|\Phi_{\lambda}\rangle = E_{\text{GS},\lambda}|\Phi_{\lambda}\rangle$, where $E_{\text{GS},\lambda}$ is the ground state energy. On the other hand, the actual dynamics of the quantum system is described by the physical (or time-evolved) state $|\Psi_{\lambda}\rangle$, which is the solution to the time-dependent Schrödinger equation $i\hbar \partial_{\lambda}|\Psi_{\lambda}\rangle = H_{\lambda}|\Psi_{\lambda}\rangle$ with initial condition $|\Psi_{0}\rangle = |\Phi_{0}\rangle$, where $i\hbar := \partial_{\lambda}$ is the driving rate. Mathematically, adiabaticity can be quantified...
by the fidelity between the physical state $|\Psi_\lambda\rangle$ and the instantaneous ground state $|\Phi_\lambda\rangle$, namely, the adiabatic fidelity $F(\lambda):=|\langle \Phi_\lambda | \Psi_\lambda \rangle|^2$. In essence, the quantum adiabatic theorem [1, 2, 11, 12] ensures the following condition
\[ 1 - F(\lambda) \leq \epsilon, \tag{2} \]
provided that the driving rate $\Gamma$ is small enough for any given allowance $\epsilon \in [0, 1]$.

Building upon the seminal work of Ref. [24], one of the main results of Ref. [25] is the following inequality that ties the adiabatic fidelity $F(\lambda)$, the overlap of instantaneous ground states $C(\lambda):=|\langle \Phi_\lambda | \Phi_\lambda \rangle|^2$, and the Bures angle for physical states $\theta(\lambda):=\arccos(|\langle \Psi_\lambda | \Psi_\lambda \rangle|)$ through
\[ |F(\lambda) - C(\lambda)| \leq \sin \theta(\lambda) \leq \sin \overline{R}(\lambda), \tag{3} \]
where $\overline{R}(\lambda):=\min (R(\lambda), \frac{\pi}{2})$.

\[ R(\lambda) := \int_0^\lambda d\lambda' \delta E_0(\lambda'), \tag{4a} \]
\[ \delta E_0(\lambda) := \sqrt{\langle H_\lambda^2 \rangle_0 - \langle H_\lambda \rangle_0^2}. \tag{4b} \]

Here, $\langle \cdot \cdot \cdot \rangle_0 := \langle \Psi_0 | \cdot \cdot \cdot | \Psi_0 \rangle$. The second inequality in Eq. (3), i.e., $\theta(\lambda) \leq \overline{R}(\lambda)$, sets an upper bound on the Bures angle of physical states and is dubbed as quantum speed limit [26-32]. This name is suggested by the fact that since the Bures angle $\theta(\lambda) \in [0, \pi/2]$ is a measure of distance, the quantum uncertainty $\delta E_0(\lambda)$ signifies speed.

In this work, we explore a union of the adiabatic condition [Eq. (2)] and the inequality of adiabatic fidelity [Eq. (3)] at the end of the time evolution of AQAs, $t = T$ [i.e., when $\lambda(t = T) = 1$]. Combining Eq. (2) with Eq. (3) leads to the following inequality that must be satisfied by the runtime $T$:
\[ T \geq \arcsin \left( \frac{\max (1 - \epsilon - C(1), 0)}{R(1)/T} \right). \tag{5} \]

This inequality may be interpreted as a necessary condition obeyed by the runtime $T$ of adiabatic quantum evolution.

**Proof.** We begin with rewriting the inequality [Eq. (3)] into the following form:
\[ C(\lambda) - \sin \overline{R}(\lambda) \leq F(\lambda) \leq C(\lambda) + \sin \overline{R}(\lambda). \tag{6} \]

This together with Eq. (2) yields $1 - \epsilon \leq F(\lambda) \leq C(\lambda) + \sin \overline{R}(\lambda)$, which can be expressed as
\[ \max (1 - \epsilon - C(\lambda), 0) \leq \sin \overline{R}(\lambda), \tag{7} \]

since $\sin \overline{R}(\lambda) \geq 0$ by definition. Now, because $\sin x$ is a monotonically increasing function for $x \in [0, \pi/2]$, the inequality above can be inverted to obtain
\[ \arcsin \left( \frac{\max (1 - \epsilon - C(1), 0)}{R(1)/T} \right) \leq \overline{R}(\lambda) \leq R(\lambda), \tag{8} \]
where we have used $\overline{R}(\lambda) \leq R(\lambda)$ to obtain the last inequality. Upon taking $\lambda(t = T) = 1$, the proof of Eq. (5) is therefore complete.

Notice that inequality Eq. (5) is applicable to Hamiltonians of any given form. Next, we shall specifically utilize inequality Eq. (5) for AQAs having a full Hamiltonian $H_{\lambda}(t)$ defined in Eq. (1). If so, the function $R(\lambda(t))$ per Eqs. (4) and (1) reads
\[ R(\lambda(t)) = t \overline{\lambda(t)} \delta V_n, \tag{9a} \]
\[ \delta V_n := \sqrt{\langle H_1^2 \rangle_0 - \langle H_1 \rangle_0^2}. \tag{9b} \]

Here, $\delta V_n$ is the quantum uncertainty of the final Hamiltonian $H_1$ with respect to the initial ground state $|\Phi_0\rangle$, and $\overline{\lambda(t)} := t^{-1} \int_0^t d\lambda'(t')$ is the time average of the schedule function $\lambda(t)$. The subscript $n$ emphasizes that the quantum uncertainty $\delta V_n$ often varies with the problem size (or number of qubits) $n$. Hence, with the help of Eq. (9), inequality Eq. (5) can be written as
\[ T \geq \arcsin \left( \frac{\max (1 - \epsilon - C(1), 0)}{\overline{\lambda(T)} \delta V_n} \right). \tag{10} \]

Now, since the numerator $\arcsin \left( \max (1 - \epsilon - C(1), 0) \right)$ is $O(1)$, and because $0 < \overline{\lambda(T)} \leq 1$ (as a consequence of $\lambda(t) \in [0, 1]$ by definition), we shall just concentrate on the asymptotic behavior of $\delta V_n$. [Eq. (9b)] for the purpose of performing asymptotic analysis using Eq. (10):
\[ T \geq T_{inf}, \quad T_{inf} := O(1/\delta V_n). \tag{11} \]

Observe that estimating a necessary runtime $T_{inf}$ using Eq. (11) requires only two ingredients, i.e., the initial state $|\Phi_0\rangle$ and the final Hamiltonian $H_1$. Although the schedule function $\lambda(t)$ is one of the three ingredients for specifying an AQA, our formula [Eq. (11)] for determining a necessary runtime does not depend on any particular form of $\lambda(t)$. This is unlike the conventional approach of spectral gap analysis [13] where an explicit form of $\lambda(t)$ must be specified; given an initial Hamiltonian and a final Hamiltonian, different forms of $\lambda(t)$ could result in different estimations of asymptotic forms of runtime. However, it is not possible for those runtime estimates using spectral gap analysis to be smaller than the necessary runtime determined by Eq. (11). In other words, for an AQA specified by an initial state and a final Hamiltonian, one can use Eq. (11) to obtain a necessary runtime. This necessary runtime might be saturated by choosing a particular schedule function or a different initial Hamiltonian.

Although the inequality Eq. (11) is established as a universal necessary condition for the runtime of any AQA, interpreting the necessary runtime $T_{inf}$ [Eq. (11)]
as a lower bound on time complexity only applies to those AQAs whose quantum uncertainty $\delta V_n$ does not diverge when $n$ goes to infinity, namely, if
\[
\lim_{n \to \infty} 1/\delta V_n \neq 0.
\]

Otherwise, one would incorrectly deduce that the required runtime decreases as the input size $n$ increases. The asymptotic property [Eq. (12)] can be fulfilled by a wide class of final Hamiltonians $H_f$ that meets the following condition\(^2\) (up to a redefinition\(^3\) of $H_1$):
\[
\langle H_f^2 \rangle_0 = \langle H_1 \rangle_0.
\]

To see this, imposing the moments condition [Eq. (13)] on the definition of quantum uncertainty $\delta V_n$ [Eq. (9b)] yields $\delta V_n = \sqrt{\langle H_1 \rangle_0 (1 - \langle H_1 \rangle_0)}$. This quantum uncertainty satisfies the desired asymptotic property [Eq. (12)] since the expectation value $\langle H_1 \rangle_0$ is bounded, $0 \leq \langle H_1 \rangle_0 \leq 1$, which is a consequence of the moments condition [Eq. (13)] together with the Cauchy-Schwarz inequality. If the moments condition [Eq. (13)] holds, the corresponding lower bound on runtime [Eq. (11)] reads
\[
T_{\text{int}} = \mathcal{O}(1/\delta V_n), \quad \delta V_n = \sqrt{\langle H_1 \rangle_0 (1 - \langle H_1 \rangle_0)}.
\]

A stronger condition than the moments condition [Eq. (13)] is when the final Hamiltonian is a projector, namely, if $H_f^2 \doteq H_f$. As we shall see shortly, the adiabatic version of Deutsch-Jozsa algorithm [15, 16], Bernstein-Vazirani algorithm [17], and Grover search [4, 18] all can be implemented using a projector final Hamiltonian. A representative final Hamiltonian that does not satisfy the asymptotic property [Eq. (12)] is the one containing Ising terms, whose quantum uncertainty scales as $\delta V_n \propto \sqrt{n}$. (see Appendix A).

In what follows, we shall focus on AQAs that satisfy the moments condition [Eq. (13)], and apply formula Eq. (14) to obtain a lower bound on runtime. For this purpose, we need to specify what kind of initial state $|\Phi_0\rangle$ and final Hamiltonian $H_f$ we wish to use. For an AQA consisting of $n$ qubits, the initial state $|\Phi_0\rangle$ can often be chosen as the uniform superposition of all basis states of the $2^n$-dimensional Hilbert space in the computational basis,
\[
|\Phi_0\rangle = \frac{1}{\sqrt{2^n}} \sum_{z \in \{0,1\}^n} |z\rangle = |\cdots \rangle^\otimes n.
\]

Here, $|z\rangle = |z_0\rangle \otimes |z_1\rangle \otimes \cdots \otimes |z_{n-1}\rangle$ with each $z_i \in \{0,1\}$, $\{0,1\}^n$ is the set of $2^n$ possible $n$-bit binary strings, and
\[
|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}. \quad \text{As for the final Hamiltonian } H_1, \text{ the following two types of final Hamiltonian satisfying Eq. (13) will be discussed in detail:}
\]

(i) Final Hamiltonian with orthogonal projection.

(ii) A special class of optimization problems.

## III. FINAL HAMILTONIAN OF TYPE-I

Let $\Pi_{\Phi_1}$ be an projector that projects onto the eigenstate of the final state $|\Phi_1\rangle$. In certain AQAs, their final Hamiltonian $H_1$ can be implemented by a complementary projector of $\Pi_{\Phi_1}$,
\[
H_1 = I - \Pi_{\Phi_1},
\]

where $I$ is an identity operator. Adiabatic Deutsch-Jozsa algorithm [15, 16] and adiabatic Bernstein-Vazirani algorithm [17] are two examples of AQAs whose final Hamiltonian has the form shown in Eq. (16).

### A. Example: Adiabatic Deutsch-Jozsa algorithm

Recall that in the problem of Deutsch-Jozsa [19], we are given a Boolean function $f : \{0,1\}^n \to \{0,1\}$. The task is to determine whether $f$ is constant or balanced (i.e., equal number of output of 0’s and 1’s). In the AQA proposed by Ref. [15], the final state is chosen as (here, $N = 2^n$)
\[
|\Phi_1\rangle = |\mu_1 \rangle |0\rangle + \frac{1 - \mu_1}{\sqrt{N}} \sum_{i=1}^{N-1} |i\rangle,
\]

where $\mu_1 = N^{-1} \sum_{z \in \{0,1\}^n} (-1)^{f(z)}$. If $f$ is constant (respectively, balanced), then $\mu_1 = 1$ (respectively, $\mu_1 = 0$). The corresponding final Hamiltonian can be constructed as a projector shown in Eq. (16) with $\Pi_{\Phi_1} = |\Phi_1\rangle \langle \Phi_1|$. The initial state is chosen as an equal weight superposition of all basis states [Eq. (15)]. In Ref. [15], using conventional spectral gap analysis yields the scaling of runtime $T \sim \mathcal{O}(N)$ for $\lambda(t) = \frac{1}{t}$ and $T \sim \mathcal{O}(\sqrt{N})$ for a local adiabatic evolution. These results do not reach the well-known [19] optimal runtime, i.e., $\mathcal{O}(1)$. Nevertheless, we shall demonstrate that using the formula Eq. (14) enables us to obtain the lowest runtime found in Ref. [15]. We compute the overlap $|\langle \Phi_1 | \Phi_0 \rangle|^2$ using Eqs. (15) and (17) as
\[
|\langle \Phi_1 | \Phi_0 \rangle|^2 = \frac{1}{N} \left( \mu_1 + (1 - \mu_1)\sqrt{N-1} \right)^2,
\]

and apply it to Eq. (14) to obtain $T_{\text{int}} = \mathcal{O}(\sqrt{N})$, which is consistent with the result obtained by Ref. [15] as mentioned above.

\(^2\) Throughout this paper, the notation "$\doteq$" is used to indicate the case where both sides of an equation are posited to be equal.

\(^3\) For instance, if $H_1^2 = -H_1$, one can define a new Hamiltonian $H_1' = \frac{1}{2} + H_1$ so that $H_1'^2 = H_1'$ holds.
From the general expression of $T_{\text{inf}}$ [Eq. (14)], it is clear that in order to reproduce the correct optimal runtime of the Deutsch-Jozsa algorithm, the overlap $|\langle \Phi_1 | \Phi_0 \rangle|^2$ should be independent of $N$. In light of this, the final state [Eq. (17)] should be modified. Exactly this modification has been carried out in Ref. [16] by replacing the final state of Eq. (17) with the one which is more symmetric in amplitudes:

$$|\Phi_1\rangle = \frac{\mu_{i}}{\sqrt{N/2}} \sum_{i=0}^{N/2-1} |2i\rangle + \frac{1-\mu_{i}}{\sqrt{N/2}} \sum_{i=0}^{N/2-1} |2i+1\rangle.$$  \hfill (19)

Upon using Eqs. (15) and (19), the overlap $|\langle \Phi_1 | \Phi_0 \rangle|^2$ reads

$$|\langle \Phi_1 | \Phi_0 \rangle|^2 = \frac{1}{N} \left( \frac{\mu_{i} N}{2} + \left(1 - \mu_{i}\right) \frac{N}{2} \right)^2 = \frac{1}{2}.$$  \hfill (20)

This result should be compared with that of Eq. (18). Bringing Eq. (20) to Eq. (14) yields $T_{\text{inf}} = \mathcal{O}(1)$. Therefore, the optimal runtime for the Deutsch-Jozsa problem is attained. In contrast to the usual approach of estimating runtime via spectral gap as done in Refs. [15, 16], our formalism clearly illustrates why the algorithm of Ref. [16] is superior to that of Ref. [15].

B. Example: Adiabatic Bernstein-Vazirani algorithm

As the second example for the final Hamiltonian of Type-I [Eq. (16)], we consider an adiabatic algorithm solving the Bernstein-Vazirani problem. Recall that in the Bernstein-Vazirani problem [20, 21], one is given an oracle that evaluates the function $f_z : \{0,1\}^n \rightarrow \{0,1\}$ with $f_z(s) = \sum_{i=0}^{n-1} s_i z_i \pmod{2}$. The task is to find the unknown $n$-bit binary string $s \in \{0,1\}^n$ using as few queries of the function $f_z$ as possible. The adiabatic algorithm proposed by Ref. [17] is the following. First, notice that the oracle function $f_z$ can be encoded in a projector final Hamiltonian as shown in Eq. (16) and acting on two subsystems, A and B, comprising $n$ qubits and 1 qubit, respectively,

$$H_1 = \mathbb{I}_A \otimes \mathbb{I}_B - \Pi_{\Phi_1},$$

$$\Pi_{\Phi_1} = \sum_{z \in \{0,1\}^n} |z\rangle_A |\Phi(z)\rangle_B \langle f_z(z)\rangle_B.$$  \hfill (21)

The ground state of $H_1$ is $|\Phi_1\rangle = \frac{1}{\sqrt{2^n}} \sum_{z \in \{0,1\}^n} |z\rangle_A \otimes |f_z(z)\rangle_B$, with eigenvalue 0. The initial state is again the uniform superposition state [Eq. (15)] $|\Phi_0\rangle = |+\rangle_A^\otimes \otimes |+\rangle_B$. We refer to Refs. [10, 17] for further details on the mechanism behind this adiabatic algorithm. For our purpose, we proceed to use the formula Eq. (14) to obtain a lower bound on the runtime. We first note that $H_1$ defined in Eq. (21) is apparently a projector, $H_1^2 = H_1$. The remaining task is to compute $\langle \Phi_0 | H_1 | \Phi_0 \rangle$:

$$\langle \Phi_0 | H_1 | \Phi_0 \rangle = 1 - \frac{1}{2^n} \sum_{z \in \{0,1\}^n} |\langle f_z(z)\rangle|^2 \equiv 1 - \frac{1}{2} \sum_{z \in \{0,1\}^n} \left( \frac{1}{\sqrt{2}} \right)^2 = \frac{1}{2}.$$  \hfill (22)

where in ($\ast$) we have used the following identity $|f_z(z)\rangle_B = \frac{1}{\sqrt{2}} (|+\rangle_B + (-1)^{f_z(z)} |-\rangle_B)$. Finally, it follows from Eq. (14) that $T_{\text{inf}} = \mathcal{O}(1)$ as expected.

IV. FINAL HAMILTONIAN OF TYPE-II

For optimization problems with a cost function $h : \{0,1\}^n \rightarrow \mathbb{R}$, we seek a minimum of $h$. In the framework of adiabatic quantum computation [3, 4], a final Hamiltonian can be defined to be diagonal in the computational basis, with cost function $h$ being the diagonal element

$$H_1 = \sum_{z \in \{0,1\}^n} h(z) |z\rangle \langle z|.$$  \hfill (23)

If the uniform superposition of all basis states [Eq. (15)] is chosen as the initial state, the quantum uncertainty [Eq. (9b)] reads $\delta V_n = (\hbar^2 - \bar{n})^{1/2}$, with the arithmetic average $\bar{n} = 2^{-n} \sum z h(z)$ and $\bar{n}^2 = 2^{-n} \sum z h^2(z)$. Furthermore, if we impose the moments condition [Eq. (13)], which amounts to requiring

$$\bar{n} \overset{!}{=} \mathbb{E} h,$$  \hfill (24)

then the lower bound $T_{\text{inf}}$ [Eq. (14)]

$$T_{\text{inf}} = \mathcal{O}(1/\delta V_n) \quad \text{with} \quad \delta V_n = \sqrt{\bar{n} (1 - \bar{n})},$$  \hfill (25)

is completely determined by the arithmetic average of the cost function, i.e., $\bar{n}$. Note that $0 \le \bar{n} \le 1$ as a result of Cauchy-Schwarz together with the moments condition [Eq. (24)]. Note also that the moments condition Eq. (24) can be expressed using matrix analysis terminology [33, 34] as $\|H_1\|_F^2 = \text{tr} H_1$, where $\| \cdot \|_F$ denotes the Frobenius norm (or Hilbert-Schmidt norm). If it is further assumed that the cost function $h$ is non-negative, the moments condition [Eq. (24)] can alternatively be written as $\|H_1\|_F^2 = \|H_1\|_{1r}$, where $\| \cdot \|_{1r}$ represents the trace norm (or nuclear norm).

Example: Adiabatic Grover search

Taking the unstructured search problem of Grover [22, 23] as an example, it can be formulated as a combinatorial optimization problem with the following cost
function [4, 35]: \( h(z) = 0 \) for \( M \) marked items and \( h(z) = 1 \) otherwise. For this case, one immediately finds 
\( \tilde{h}^2 = \tilde{T} = 1 - M/N \) (here, \( N = 2^n \)). It then follows from Eq. (25) that a lower bound \( T_{\inf} = O(\sqrt{N/M}) \), as expected [18, 36, 37]. We note that the final Hamiltonian of adiabatic Grover search can be equivalently written as 
\( H_f = \mathbb{I} - \sum_{z \in \mathcal{M}} |z\rangle\langle z| \), where \( \mathcal{M} \) is the space of solution (of size \( M \)). Hence, this final Hamiltonian also belongs to the type-I final Hamiltonian [see Eq. (16)]. It is with this expression of projector final Hamiltonian that Ref. [38] used a formula similar to Eq. (10) to obtain the optimal runtime for adiabatic Grover search. For completeness, we present a similar calculation using our formula in Appendix B.

Thus far, three adiabatic versions of keystone quantum algorithms have been examined. We shall now apply our technique to the adiabatic algorithm proposed by Childs et al. [14] for finding \( k \)-clique in random graphs.

V. ADIABATIC ALGORITHM FOR FINDING \( k \)-CLIQUE

Consider a random graph \( G \) where every pair of vertices is connected or disconnected with a probability of \( 1/2 \). A clique is a subgraph of \( G \) in which every pair of vertices is connected by an edge. The problem of finding cliques of \( k \) vertices (called \( k \)-clique) in a random graph is an NP-complete problem if both \( n \) and \( k \) are treated as inputs [39, 40].

In the algorithm proposed by Ref. [14], each vertex is associated with a qubit. Hence, there are \( n \) qubits for a graph of \( n \) vertices. As before, each qubit state is represented by \( |z_i\rangle \) with \( z_i \in \{0, 1\} \) for \( i \in \{0, \ldots, n-1\} \). A vertex \( i \) is included into a subgraph of \( k \) vertices only if \( z_i = 1 \).

Although the full Hilbert space is \( 2^n \)-dimensional, we can focus only on the subspace spanned by quantum states with Hamming weight \( k \) since we are only interested in those quantum states that represent cliques of \( k \) vertices. For notational convenience, we denote the set of \( n \)-bit binary strings of Hamming weight \( k \) as \( \mathcal{S}_k := \{ z \in \{0, 1\}^n : |z| = k \} \}, \) where \( |z| = \sum_{i=0}^{n-1} z_i \) is the Hamming weight of the \( n \)-bit binary string \( z \). The size of \( \mathcal{S}_k \) is \( \binom{n}{k} = C(n,k) \). In the subspace generated by binary strings from \( \mathcal{S}_k \), the initial state can be chosen as a Dicke state [41–43]

\[ |\Phi_0\rangle := \frac{1}{\sqrt{C(n,k)}} \sum_{z \in \mathcal{S}_k} |z\rangle. \]  

In Ref. [14], the final Hamiltonian is of the form shown in Eq. (23) with the cost function

\[ h_C(z) := \sum_{i,j=0,i>j}^{n-1} (1 - G_{ij}) z_i z_j, \]  

where \( G_{ij} \) with \( i, j \in \{0, \ldots, n-1\} \) is the matrix element of the adjacency matrix for a graph \( G \). As usual, \( G_{ij} = 1 \) if the vertices \( i \) and \( j \) are connected by an edge; otherwise, \( G_{ij} = 0 \). Observe that the cost function \( h_C(z) \) takes values in \( \{0, 1, \ldots, L_k\} \), where \( L_k = C(k,2) \) is the total number of edges for a graph of \( k \) vertices.

We proceed to obtain a lower bound on runtime using Eq. (11) for the algorithm defined above. Since each \( G_{ij} \in \{0, 1\} \) is a random variable, an exact computation for the arithmetic average \( h_C(z) \) and \( \tilde{h}^2_C \) is not possible without knowing an explicit instance of \( G_{ij} \). We attempt to consider a “mean-field” (or “randomized”) approach by replacing \( G_{ij} \) with its (classical) expectation value \( E[G_{ij}] = 1/2 \), and obtain (see Appendix C) \( E[\tilde{h}_C] = L_k/2 \) and \( E[\tilde{h}^2_C] = (L_k + 1)L_k/4 \). It follows from Eq. (11) that a lower bound on runtime \( T_{\inf rand} \) reads 
\[ T_{\inf rand} = O(\sqrt{1/L_k}), \]  

which is independent of \( n \). It is likely that this \( n \)-independent lower bound is considerably lower than the sufficient runtime obtained using the spectral gap analysis (though it is not available). We also notice that the moments condition [Eq. (24)] is not met for the cost function defined in Eq. (27). Nevertheless, we note that the \( k \) dependence in \( T_{\inf rand} \) seems consistent with the numerical data found in Ref. [14], saying that the median runtime for finding cliques of \( k = 5 \) is longer than that for finding cliques of \( k = 6 \). Specifically, \( T_{\inf rand}(k=5)/T_{\inf rand}(k=6) = 30.87/18.56 \approx 1.66 \) found in Ref. [14], whereas our result indicates \( T_{\inf rand}(k=5)/T_{\inf rand}(k=6) = \sqrt{15}/10 \approx 1.22 \).

To make better use of our formula Eq. (25), we propose the following deformed cost function

\[ h(z) := \frac{1}{2} \left( 1 + h_C(z) - |1 - h_C(z)| \right). \]  

This amounts to introduce \( h(z) = \min(h_C(z), 1) \), where \( h_C(z) \) is defined in Eq. (27). In other words, those \( h_C(z) > 1 \) are mapped to \( h(z) = 1 \). Therefore, the deformed cost function is Boolean-valued \( h(z) \in \{0, 1\} \). This deformed cost function is similar to that of adiabatic Grover search discussed previously. One finds that the cost function defined in Eq. (28) along with the initial state defined in Eq. (26) satisfies the moments condition [Eq. (24)]. Explicitly, \( h = \tilde{h}^2 = (1 - M/C(n,k)) \), which renders a lower bound from Eq. (25)

\[ T_{\inf} = O\left( \sqrt{C(n,k)/M} \right), \]  

where \( M \) is the number of cliques of \( k \) vertices. The result [Eq. (29)] is consistent with that of a circuit-based algorithm of Ref. [44] in which the time complexity is related to the number of Grover iterations. For the special case of \( n \gg k \), Eq. (29) simplifies \( T_{\inf} = O\left(n^{k/2}\right) \) for \( n \gg k \). A well-studied case is \( k = 3 \), i.e., the so-called \( 3 \)-clique problem (or triangle-finding problem); the resulting lower bound is \( T_{\inf} = O\left(n^{3/2}\right) \). The exponent, \( 3/2 \), agrees with that found in a quantum algorithm [45] for the triangle-finding problem using a plain Grover search.
VI. DISCUSSIONS

A. Connection to spectral gap analysis

We shall now attempt to connect our approach with conventional spectral gap analysis. An equivalence between the two approaches can be directly shown for a particular class of Hamiltonians where both the initial and final Hamiltonians are of the projector form $H_0 = I - |\Phi_0\rangle\langle\Phi_0|$ and $H_1 = I - |\Phi_1\rangle\langle\Phi_1|$. It was then proved in Ref. [46] that the spectral gap of the full Hamiltonian $H_\lambda$ [Eq. (1)], denoted as $g(H_\lambda)$, is bounded from below: $g(H_\lambda) \geq |\langle\Phi_1|\Phi_0\rangle| = g_{\min}$, where $g_{\min} = \min_{\lambda \in [0,1]} g(H_\lambda)$ is the minimal spectral gap. If the schedule function $\lambda(t)$ is chosen simply as $\lambda(t) = t/T$, spectral gap analysis [13, 18] yields the scaling of runtime $T_{\text{gap}} \sim O(1/g^2_{\min})$. Furthermore, it is possible to improve [13, 18] the error dependence on the minimal gap by adopting a nonlinear schedule function; if so, one obtains $T_{\text{gap}} \sim O(1/g_{\min})$. On the other hand, using our formalism, we directly obtain $(H_\lambda)_{t=0} = (H_\lambda)_{t=T} = 1 - |\langle\Phi_1|\Phi_0\rangle|^2 = 1 - g_{\min}^2$. Consequently, a lower bound on runtime follows from Eq. (14): $T_{\text{inf}} \sim O(1/g_{\min})$.

If the minimal gap $g_{\min} = |\langle\Phi_1|\Phi_0\rangle|$ is independent of $n$, then the two estimates $T_{\text{gap}}$ and $T_{\text{inf}}$ are equal: $T_{\text{gap}} = T_{\text{inf}} = O(1)$. This is the case for the adiabatic Deutsch-Jozsa algorithm and the adiabatic Bernstein-Vazirani algorithm discussed previously. For the case of adiabatic Grover search, the optimal runtime obtained from the spectral gap analysis along with a nonlinear schedule function yields [18] $T_{\text{gap}} = O(1/g_{\min})$, which again agrees with our lower bound $T_{\text{inf}} = O(1/g_{\min})$.

B. Comparison with prior works

The performance of adiabatic quantum algorithms has been extensively investigated in a variety of settings. Among the existing research on this topic, three groups of studies that utilize quantum speed limits are particularly relevant to our current work. (i) A new class of quantum speed limits is presented in Refs. [47, 48] and applied to adiabatic searches. A lower bound on runtime is defined there as the minimum time it takes for the physical state to be orthogonal to the initial state. This definition is, however, too restrictive. Additionally, it is unclear whether the results obtained in Refs. [47, 48] are applicable adiabatic searches.

(ii) While the main result of Ref. [38] is an inequality similar to Eq. (10), the present work makes several significant advances. Our method for estimating lower bounds is more systematic and rigorous, and we carefully clarified the applicability of Eq. (10). In particular, we highlighted the importance of the asymptotic property [Eq. (12)] and the irrelevance of the schedule function $\lambda(t)$ in asymptotic analysis. Furthermore, we explored a wider range of adiabatic quantum algorithms, including the adiabatic Grover algorithm examined in Ref. [38] as well as several additional adiabatic algorithms. Notably, we obtained an analytical result on lower bounds for the adiabatic algorithm of Childs et al. [14] for finding $k$-clique in random graphs, which is an algorithm with undetermined quantum speedup.

(iii) It is also worth noting that quantum speed limits and the formalism of shortcuts to adiabaticity [49–56] are combined in Ref. [57] to investigate the performance of adiabatic quantum computation. However, the purpose and scope of Ref. [57] is significantly different from ours.

VII. CONCLUDING REMARKS

We have shown that for a wide class of adiabatic quantum algorithms (AQAs) in which the asymptotic property presented in Eq. (12) holds, nontrivial lower bounds on the runtime of adiabatic algorithms can be estimated by calculating the quantum uncertainty of the final Hamiltonian with respect to the initial state [see Eq. (11)]. A runtime estimation obtained by conventional spectral gap analysis is by no means smaller than the necessary runtime derived using our method. The reason is that our formula provides a necessary condition that must be obeyed by the runtime of adiabatic quantum evolution. Choosing a specific schedule function or initial Hamiltonian may cause the necessary runtime to be saturated.

Our findings may shed new light on the design of new adiabatic quantum algorithms. For instance, if a potential quantum speedup of an adiabatic quantum algorithm is undetermined, one may attempt a deformation of the original adiabatic algorithm to fulfill the moments condition [Eq. (13)] and then apply Eq. (14) to obtain a lower bound on runtime. The runtime of the deformed algorithm thus obtained may be utilized to estimate the spectral gap (and hence, a sufficient runtime) of the original algorithm by means of matrix inequalities such as Weyl’s inequalities [33, 34]. For optimization problems, it is important to emphasize that the lower bound formula [Eq. (25)] is not valid for every optimization problem but only for those in which the cost function meets the moments condition [Eq. (24)]. Therefore, it would be interesting to investigate further the implications of the moments condition on general Boolean functions using techniques from Boolean function analysis [58]. Another future direction would be to derive bounds on the runtime of adiabatic quantum algorithms in open quantum systems.

\footnote{Indeed, the final state of most adiabatic quantum algorithms is never orthogonal to the initial state, even though the overlap between the two is typically very small.}
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We then obtain

\[ |\tilde{\Phi}\rangle := H_1|\Phi_0\rangle = -\sum_{i=0}^{n-1} Z_i Z_{i+1} |+\rangle^\otimes n = -\sum_{i=0}^{n-1} (|\rangle_i \otimes |\rangle_{i+1} \otimes |+\rangle^\otimes n-2). \]  

We then find

\[ \langle \Phi_0 | H_1 | \Phi_0 \rangle = \langle \Phi_0 | \tilde{\Phi} \rangle = \langle + |^\otimes n \left( -\sum_{i=0}^{n-1} (|\rangle_i \otimes |\rangle_{i+1} \otimes |+\rangle^\otimes n-2) \right) = 0, \]  

\[ \langle \Phi_0 | H_1^2 | \Phi_0 \rangle = \langle \tilde{\Phi} | \tilde{\Phi} \rangle = \sum_{i,j=0}^{n-1} (|\rangle_i \otimes (-i+1) \otimes (+|)^\otimes n-2) (|\rangle_j \otimes (-|_{j+1} \otimes +|)^\otimes n-2) = \sum_{i,j=0}^{n-1} \delta_{ij} = n. \]  

It then follows from Eq. (9b) that the quantum uncertainty reads \( \delta V_n = \sqrt{n} \).

Appendix B: Detail calculation for adiabatic Grover search

Consider a set of \( N \) items among which \( M < N \) items are marked, the goal being to find marked items in minimum time. We use \( n \) qubits to encode the \( N \) items. Hence, the Hilbert space is of dimension \( N = 2^n \). In this space, the basis states can be written as \( |i\rangle \) with \( i \in \{0, \ldots, N-1\} \). The desired final state is \( |\Phi_1\rangle = \frac{1}{\sqrt{M}} \sum_{m \in \mathcal{M}} |m\rangle \), and the corresponding final Hamiltonian can be chosen as a projector \( H_f = \mathbb{I} - \sum_{m \in \mathcal{M}} |m\rangle \langle m| \), where \( \mathcal{M} \) is the space of solution (of size \( M \)). One can easily see that the ground state of \( H_f \) is \( |\Phi_1\rangle \) with eigenenergy zero.

The remaining task is to calculate the quantum uncertainty \( \delta V_n \) [Eq. (9b)] with \( |\Phi_0\rangle \) given by the uniform superposition state [Eq. (15)]. First, we calculate the overlap \( \langle \Phi_1 | \Phi_0 \rangle^2 \),

\[ \langle \Phi_1 | \Phi_0 \rangle^2 = \left( \frac{1}{\sqrt{M}} \sum_{m \in \mathcal{M}} \langle m | \right) \left( \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i| \right)^2 = \frac{1}{MN} \sum_{m \in \mathcal{M}} \sum_{i=0}^{N-1} \langle m | i \rangle^2 = \frac{M}{N}. \]  

We then obtain \( \langle \Phi_0 | H_1 | \Phi_0 \rangle = 1 - \langle \Phi_1 | \Phi_0 \rangle^2 = 1 - \frac{M}{N}. \) Bringing this result to Eq. (14) yields \( T_{\inf} = O(\sqrt{N/M}) \).

Appendix A: Quantum uncertainty of Ising terms

Consider a final Hamiltonian \( H_f \) that consists of Ising terms \( H_f = -\sum_{i=0}^{n-1} Z_i Z_{i+1} \), where \( Z_i \) is the third Pauli matrix acting on the \( i \)th qubit. Recall that \( Z|\rangle = |\rangle \) and \( Z|-\rangle = |-\rangle \). Choosing the initial state \( |\Phi_0 \rangle \) as the uniform superposition state [Eq. (15)]. We first compute

\[ \frac{\hbar^2}{C(n, k)} \sum_{z \in \{0, 1\}^n : |z| = k} h_C(z), \]  

\[ \frac{\hbar^2}{C(n, k)} \sum_{z \in \{0, 1\}^n : |z| = k} h_C^2(z), \]  

with the cost function \( h_C(z) = \sum_{i > j} (1 - G_{ij}) z_i z_j \) as defined in Eq. (27). To conduct the calculation, one encounters terms like \( \sum_{i > j} G_{ij} \), which cannot be done generically without knowing the explicit form of \( G_{ij} \). We attempt a “mean-field” approach by considering the “average property” of \( G_{ij} \) since each pair of vertices has probability \( p \) to be connected and probability \( (1 - p) \) otherwise. Note that the value of \( p \) is 1/2 in the main text.

1. Mean-field approach

We shall approximate \( G_{ij} \) by its expected value, \( E[G_{ij}] \). Specifically, since each \( G_{ij} = 1 \) with probability \( p \) and \( G_{ij} = 0 \) with probability \( 1 - p \), we obtain

\[ E[G_{ij}] = p. \]  

Appendix C: Detail calculation for adiabatic algorithm of finding k-clique in random graphs

We want to calculate \( \langle \Phi_0 | H_1 | \Phi_0 \rangle = \frac{\hbar^2}{C(n, k)} \sum_{z \in \{0, 1\}^n : |z| = k} h_C(z), \) and

\[ \langle \Phi_0 | H_1^2 | \Phi_0 \rangle = \frac{\hbar^2}{C(n, k)} \sum_{z \in \{0, 1\}^n : |z| = k} h_C^2(z), \]  

where

\[ h_C(z) = \sum_{i > j} (1 - G_{ij}) z_i z_j \]  

as defined in Eq. (27). To conduct the calculation, one encounters terms like \( \sum_{i > j} G_{ij} \), which cannot be done generically without knowing the explicit form of \( G_{ij} \). We attempt a “mean-field” approach by considering the “average property” of \( G_{ij} \) since each pair of vertices has probability \( p \) to be connected and probability \( (1 - p) \) otherwise. Note that the value of \( p \) is 1/2 in the main text.
We now compute $\overline{h_C}$ (C1):

$$\overline{h_C} = \frac{1}{C(n,k)} \sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i > j} (1 - G_{ij}) z_i z_j$$

$$\approx \mathbb{E}[h_C]$$

$$= \frac{1}{C(n,k)} \sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i > j} (1 - \mathbb{E}[G_{ij}]) z_i z_j. \quad (C3)$$

There are $C(n,k)$ states $|z|$ satisfy $|z| = k$ that we have to consider. For each such state, there are $k$'s $z_i$ for which $z_i = 1$. Therefore, the first term in the parenthesis of Eq. (C3) is simply

$$\sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i > j} z_i z_j = \sum_{z \in \{0,1\}^n \mid |z| = k} C(k,2) = C(n,k) C(k,2) = C(n,k) L_k. \quad (C4)$$

Here, for notational convenience, we define $L_k \equiv C(k,2)$. The second term in the parenthesis of Eq. (C3) can be calculated with the help of Eq. (C2)

$$\sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i > j} \mathbb{E}[G_{ij}] z_i z_j = p C(n,k) L_k. \quad (C5)$$

Bringing Eqs. (C4) and (C5) back to Eq. (C3) yields

$$\mathbb{E}[h_C] = (1 - p) L_k. \quad (C6)$$

Next, we compute $\overline{h_C}$ (C1):

$$\overline{h_C} = \frac{1}{C(n,k)} \sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i' > j', i' > j} (1 - 2G_{ij} + G_{i'j'}G_{ij}) z_{i'} z_j' z_i z_j$$

$$= \frac{1}{C(n,k)} \sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i' > j'} \sum_{i > j} (1 - 2\mathbb{E}[G_{ij}] + \mathbb{E}[G_{i'j'}G_{ij}]) z_{i'} z_j' z_i z_j. \quad (C7)$$

There are three terms in the parenthesis of Eq. (C7). The first term is deterministic,

$$\sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i' > j', i' > j} z_{i'} z_j' z_i z_j = \sum_{z \in \{0,1\}^n \mid |z| = k} \left( \sum_{i' > j'} z_{i'} z_j' \right) \left( \sum_{i > j} z_i z_j \right) = \sum_{z \in \{0,1\}^n \mid |z| = k} L_k L_k = C(n,k) L_k^2. \quad (C8)$$

The second term in the parenthesis of Eq. (C7) reads

$$\sum_{z \in \{0,1\}^n \mid |z| = k} \sum_{i' > j'} \sum_{i > j} (-2\mathbb{E}[G_{ij}]) z_{i'} z_j' z_i z_j = -2 \sum_{z \in \{0,1\}^n \mid |z| = k} \left( \sum_{i' > j'} z_{i'} z_j' \right) \left( \sum_{i > j} \mathbb{E}[G_{ij}] z_i z_j \right)$$

$$(C9)$$

Before proceeding to calculate the third term in the parenthesis of Eq. (C7), we notice the following decomposition property

$$\sum_{i' > j', i' > j} \mathbb{E}[G_{i'j'}G_{ij}] = \sum_{i > j} \mathbb{E}[G_{ij} G_{ij}] + \sum_{i' > j, i > j'} \mathbb{E}[G_{i'j'} G_{ij}]$$

$$= \sum_{i > j} \mathbb{E}[G_{ij}^2] + \sum_{i' > j, i > j'} \mathbb{E}[G_{i'j'}] \mathbb{E}[G_{ij}]$$

$$= \sum_{i > j} p + \sum_{i' > j, i > j'} p^2 = L_k p + (L_k^2 - L_k) p^2. \quad (C10)$$

Finally, the third term in the parenthesis of Eq. (C7) is

$$\sum_{z \in \{0,1\}^n \mid |z| = k} \left( \sum_{i' > j', i' > j} \mathbb{E}[G_{i'j'}G_{ij}] z_{i'} z_j' z_i z_j \right) \equiv p C(n,k) L_k^2 \left( p + \frac{(1 - p)}{L_k} \right). \quad (C11)$$
Upon using the above results, Eq. (C7) reads
\[
E[hC] = \left( 1 - 2p + p \left( p + \frac{1-p}{L_k} \right) \right) L_k^2 \\
= (1-p)^2 L_k^2 + p(1-p) L_k.
\]  (C12)
Hence, the quantum uncertainty reads \( \delta V_n = \sqrt{p(1-p)L_k} \). It then follows from Eq. (11) a lower bound on runtime
\[ T_{\text{inf}} = O \left( \sqrt{\frac{1}{L_k}} \right), \]  (C13)
which is independent of \( n \). Note that if the cost function \( h_C(z) \) is rescaled as \( h_C(z) \rightarrow h_C(z)/L_k \), one should find \( T_{\text{inf}} = O \left( \sqrt{L_k} \right) \).

2. Combinatorial approach

In this section, we use an explicit combinatorial method to reproduce the same result as we found in Eq. (C13). The following observation is crucial: If a binary string \( z \) of Hamming weight \( k \) represents a graph that is a \( k \)-clique after adding \( \alpha \) connected edges, then \( h_C(z) = \alpha \), where \( \alpha \in \{0, 1, \cdots, C(k, 2)\} \).

To simplify the notation, let us define \( L_k \equiv C(k, 2) \) for convenience. Now the question is what is the multiplicity \( m_\alpha \) for each possible value of cost function \( h_C(z) = \alpha \). Since each of the \( L_k \) edges has probability \( p \) to be present when random graphs are generated uniformly, we expect
\[
m_\alpha = p^{L_k - \alpha} (1-p)^\alpha C(L_k, \alpha) C(n, k),
\]  (C14)
for \( \alpha \in \{0, 1, \cdots, L_k\} \). One verifies that the sum of all multiplicity equals \( C(n, k) \), i.e., the number of binary strings of Hamming weight \( k \)
\[
\sum_{\alpha=0}^{L_k} m_\alpha = C(n, k) \sum_{\alpha=0}^{L_k} p^{L_k - \alpha} (1-p)^\alpha C(L_k, \alpha) \\
= (1-p)^L_k, \]  (C16)
which is the same as Eq. (C6). We then compute \( E[hC] \):
\[
E[hC] = \frac{1}{C(n, k)} \sum_{\alpha=0}^{L_k} m_\alpha \alpha = \frac{L_k}{C(n, k)} \sum_{\alpha=0}^{L_k} p^{L_k - \alpha} (1-p)^\alpha C(L_k, \alpha) \alpha \\
= (1-p)^2 L_k^2 + p(1-p)L_k, \]  (C17)
which is identical to Eq. (C12).

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