On the gap of Hamiltonians for the adiabatic simulation of quantum circuits

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The time or cost of simulating a quantum circuit by adiabatic evolution is determined by the spectral gap of the Hamiltonians involved in the simulation. In “standard” constructions based on Feynman’s Hamiltonian, such a gap decreases polynomially with the number of gates in the circuit, $L$. Because a larger gap implies a smaller cost, we study the limits of spectral gap amplification in this context. We show that, under some assumptions on the ground states and the cost of evolving with the Hamiltonians (which apply to the standard constructions), an upper bound on the gap of order $1/L^2$ follows. In addition, if the Hamiltonians satisfy a frustration-free property, the upper bound is of order $1/L^3$. Our proofs use recent results on adiabatic state transformations, spectral gap amplification, and the simulation of continuous-time quantum query algorithms. They also consider a reduction from the unstructured search problem, whose lower bound in the oracle cost translates into the upper bounds in the gaps. The impact of our results is that improving the gap beyond that of standard constructions (i.e., $1/L^2$), if possible, is challenging.

I. INTRODUCTION

Adiabatic quantum computing (AQC) is an alternative to the standard circuit model of quantum computation. In AQC, the input is a (qubit) Hamiltonian $H(1)$ and the goal is to prepare the ground state of $H(1)$ by means of slow or adiabatic evolutions. One then sets an initial Hamiltonian $H(0)$ and builds a Hamiltonian path $H(g), 0 \leq g \leq 1$, that interpolates between $H(0)$ and $H(1)$. If the ground states of $H(g)$ are continuously related and remain at a spectral gap of order $\Delta$ with any other eigenstate during the evolution, the quantum adiabatic approximation implies that, for

$$\dot{g}(t) \leq \epsilon \frac{\Delta}{\hbar},$$

the ground state of $H(1)$ can be adiabatically prepared with fidelity $1 - \epsilon$. $0 < q \leq 3$ and $\hbar$ depends on $\|\partial^n H(g)/\partial g^n\|^{q+1}$, $n = 1, 2$, for differentiable paths [1–5].

A key feature of AQC is that it constitutes a “natural” model for problems that efficiently reduce to the computation of ground-state properties. Some of these are problems in combinatorial optimization [6–12], and problems in many-body physics, e.g., the computation of a quantum phase diagram [13]. Whether AQC is robust to decoherence or not is unclear and a complete fault-tolerant implementation of AQC remains unknown [14–15]. Nevertheless, the role of the spectral gap is imperative in a noisy implementation of AQC: a bigger $\Delta$ could imply a smaller running time [Eq. (1)] and a reduction of the (unwanted) population of excited states due to thermal effects. Our goal is then to study the limits and possibilities of amplifying the gap in AQC. Roughly stated, we are addressing the following question: Given $H(g)$ with gap $\Delta(g)$ and ground state $|\psi(g)\rangle$, can we find $\tilde{H}(g)$ with gap $\tilde{\Delta}(g) \gg \Delta(g)$ and ground state satisfying $|\tilde{\psi}(g)\rangle \approx |\psi(g)\rangle$? Our motivation is the same as that of Ref. [16]. We are particularly interested in amplifying the gap of those Hamiltonians that arise in the adiabatic simulation of general quantum circuits—see below.

The power of AQC and the standard quantum circuit model are equivalent. That is, any algorithm in the AQC model with a running time $T$, that prepares a quantum state $|\psi(1)\rangle$, can be simulated with a quantum circuit of $L \in \text{poly}(T)$ unitary gates that prepares a sufficiently close state to $|\psi(1)\rangle$ when acting on some trivial initial state $|\tilde{\phi}\rangle$. The converse also holds: Any quantum circuit of $L$ unitary gates that prepares a quantum state $|\phi\rangle$, when acting on some trivial initial state, can be simulated within the AQC model by evolving adiabatically with suitable Hamiltonians $H(g)$ for time $T \in \text{poly}(L)$. The ground state of the final Hamiltonian, $|\psi(1)\rangle$, has a large probability of being in $|\phi\rangle$ after a simple measurement [21–23]. $H(g)$ depends on the unitaries that specify the quantum circuit.

To describe our results in detail, we review the first “standard” construction in Ref. [21], which is based on Feynman’s Hamiltonian [24]. $U$ is a quantum circuit.
acting on $n$ qubits that prepares the “system” state $|\phi_L^c\rangle = U_L \ldots U_1 |\phi^0\rangle$, after the action of $L$ unitary gates $U_1, \ldots, U_L$. There is also an ancillary system, denoted by “clock”, whose basis states are $\{|0\rangle_c, |1\rangle_c, \ldots, |L\rangle_c\}$. The (final) Hamiltonian $H^U$ is mainly a sum of two terms. The first term is the so-called Feynman Hamiltonian:

$$H_{\text{Feynman}}^U = \sum_{l=1}^{L} h_{l}^{m},$$

$$h_{l}^{m} = \frac{1}{2} (|l\rangle \langle l| + |l-1\rangle \langle l-1|) - U^i \otimes |l\rangle \langle l-1| - U^j \otimes |l\rangle \langle l-1|,$$  \hspace{1cm} (2)

$\mathbb{I}$ is the trivial operation on the system’s state. $H_{\text{Feynman}}^U$ can be easily diagonalized by using the Fourier transform. The eigenvalues are $1 - \cos k$, with $k = 2\pi m/(L+1)$ and $m \in \mathbb{Z}$. Then, the lowest eigenvalue is zero ($k = 0$) and the gap is of order $1/L^2$ for the smallest nonzero eigenvalue. Each eigenvalue appears with multiplicity $2^n$, corresponding to each state $|\sigma\rangle$ of the system. The eigenstates of $H_{\text{Feynman}}^U$ are

$$\frac{1}{\sqrt{L+1}} \sum_{l=0}^{L} e^{ikl} U^l \ldots U^0 |\sigma\rangle \otimes |l\rangle,$$  \hspace{1cm} (3)

where $U^0 = \mathbb{I}$. If $|\sigma\rangle = |\phi^0\rangle$, the eigenstate in Eq. (3) has probability $1/(L+1)$ of being in the state output by the circuit. That is, we can prepare $|\phi^0\rangle$ with such a probability by a projective measurement of the clock register on the state of Eq. (3). We can remove the multiplicity of the lowest eigenvalue if we add a second term, $H_{\text{input}}$, whose expected value vanishes when $|\sigma\rangle = |\phi^0\rangle$ and is strictly positive otherwise. For example, if $|\phi^0\rangle = |+\rangle^{\otimes n}$, where $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, $H_{\text{input}}$ in Ref. [21] corresponds to

$$H_{\text{input}} = \sum_{j=1}^{n} |\sim\rangle \langle \sim| \otimes |0\rangle \langle 0|,$$

with $|\sim\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$. In this case, $H_{\text{input}}$ sets a “penalty” if the system-clock initial state is different from $|+\rangle^{\otimes n} \otimes |0\rangle_c$. The lowest eigenvalue of $H_{\text{input}}$ is zero and the gap is a constant independent of $L$ (i.e., $\Delta_{\text{input}} = 1$).

Then, the Hamiltonian

$$H^U = H_{\text{Feynman}}^U + H_{\text{input}}$$

has

$$|\psi^U\rangle = \frac{1}{\sqrt{L+1}} \sum_{l=0}^{L} |\phi_l^c\rangle \otimes |l\rangle_c$$  \hspace{1cm} (5)

as unique ground state $|k = 0\rangle$ in Eq. (3), where $|\phi_l^c\rangle = U_l \ldots U_0 |\phi^0\rangle$. We will refer to $|\psi^U\rangle$ as the “history state”. The lowest eigenvalue of $H^U$ is also zero and the spectral gap satisfies $\Delta^U \in \Theta(1/L^2)$ [25]. It is simple to construct an interpolating path $H^U(g)$ that has a spectral gap $\Delta^U(g) = \Delta^U \in \Theta(1/polyL)$ for all $g$ and $H^U(1) = H^U$. This is done by, for example, parametrizing the unitaries in the circuit so that $U^1 \rightarrow U^1(g)$ in Eq. (1), and $U^1(0) = \mathbb{I}$, $U^1(1) = U^1$. Then, the ground state $|\psi^U(1)\rangle = |\psi^U\rangle$ can be prepared from $|\psi^U(0)\rangle = |\phi^0\rangle \otimes \sum_l |l\rangle_c / \sqrt{L+1}$ by evolving adiabatically with $H(g)$ for time $T \in poly[L]$ [see Eq. (3)].

$H^U$ is often regarded as “unphysical” as the system-clock interactions may represent non-local interactions of actual quantum subsystems (qubits). Then, a number of steps that include modifications of the gates in the circuit and techniques from perturbation theory (e.g., perturbation gadgets) [26], allow us to reduce $H^U$ to a physical, local Hamiltonian $H_{\text{local}}^U$. Such steps preserve the two main ingredients for showing the equivalence between DQC and the circuit model: i) that the spectral gap of the local Hamiltonian, $\Delta^U_{\text{local}}$, is bounded from below by $1/poly(L)$ and ii) that the ground state has sufficiently large probability of being in $|\phi^0\rangle$ after a simple quantum operation (e.g., a simple projective measurement). It is important to remark that $\Delta^U_{\text{local}}$ is smaller than $\Delta^U$ in standard constructions [21][23]. For this reason, some attempts to improve the running time of the adiabatic simulation of a quantum circuit consider first the amplification of $\Delta^U$ by making simple modifications to $H^U$ (see Ref. [27] for an example); Our results concern the amplification of $\Delta^U$.

In this report we show that, under some assumptions on the ground states and the time or cost of evolving with the Hamiltonians, an upper bound on the gap of order $1/L$ follows. Furthermore, if the Hamiltonians additionally satisfy a so-called frustration-free property, then the upper bound is $1/L^2$. An implication of our results is that simple modifications to $H^U$ in Eq. (1) are not sufficient to amplify its gap. While such modifications could be useful to prepare the desired state via a constant-Hamiltonian evolution [28], they may not be useful to prepare the state adiabatically. Our proofs are constructive, i.e., we find a reduction from the unstructured search problem [29] (Sec. [31]), whose lower bound on the oracle cost [30] (i.e., the number of queries to the oracle needed) can be transformed into the upper bounds on the gaps (Sec. [33]). Clearly, the only way to obtain a bigger gap, if gap amplification is indeed possible, is by avoiding one or more assumptions needed for our proofs. This suggests a migration from those constructions that are based on Feynman’s Hamiltonian.

II. SEARCH BY A GENERALIZED MEASUREMENT-BASED METHOD

The proof of an upper bound on $\Delta^U$ uses a reduction from the unstructured search problem or SEARCH. In this section, we show a quantum method that solves SEARCH using measurements.

For a system of $n$ qubits, we let $N = 2^n$ be the dimension of the associated state (Hilbert) space $H$. Given an
or the measurement-based method is described in Table I. A generalization of \(|\psi_X\rangle\) and \(|\zeta_X\rangle\) which are the probabilities of projecting \(|\phi_X^L\rangle\) and \(|\phi_X^R\rangle\) into \(|\phi_X^M\rangle\) and \(|\phi_X^N\rangle\), respectively, after a measurement. A generalization of the measurement-based method is described in Table I. The probability of success is \(p_s \geq p_{\nu,\zeta_X} \cdot p_{X,\zeta_X}\).

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### Table I. Generalized measurement-based method

| Measure | Description |
|---------|-------------|
| i-      | Prepare \(|\nu\rangle\) |
| ii-     | Measure \(|\zeta_X\rangle\) |
| iii-    | Measure \(|X\rangle\) |

We now obtain the time \(T\) of solving SEARCH (with probability \(p_s\)) with the generalized measurement-based method. We let \(G_X\) be the Hamiltonian that has \(|\zeta_X\rangle\) as unique ground state and the corresponding spectral gap of \(G_X\) is \(\Delta^{\mu_X}\). \(G_X\) acts on the Hilbert space \(H'\) and depends on \(O_X\). \(T\) is determined by the total time of evolution with \(G_X\) needed to simulate the measurement of \(|\zeta_X\rangle\) in step ii. Using the phase estimation algorithm \([32]\) or evolution randomization \([33]\), this time is

\[
T = \frac{c}{\Delta^{\mu_X}},
\]

for some constant \(c \geq \pi\). The lower bound in the oracle cost of SEARCH can then be used to set a lower bound on \(T\) or, equivalently, an upper bound in \(\Delta^{\mu_X}\). This results from noting that the evolution under \(G_X\) can be well approximated with a discrete sequence of unitaries that contains \(O_X\). Nevertheless, to make a rigorous statement on \(\Delta^{\mu_X}\), some assumptions on \(G_X\) and the ground state are needed. We provide such assumptions and our main results in the next section.

### III. GAP BOUNDS

We list three assumptions on \(G_X\) and its ground state, \(|\zeta_X\rangle\).

**Assumption 1:**

\[p_{\nu,\zeta_X} \in \Theta(1) \forall X.\]

That is, there exists an \(X\)-independent state \(|\nu\rangle\) that can be projected into \(|\zeta_X\rangle\), with high probability, after a measurement.

**Assumption 2:**

\[p_{X,\zeta_X} \in \Theta(1) \forall X.\]

That is, \(|\zeta_X\rangle\) can be projected into \(|X\rangle\), with high probability, after a measurement. Assumptions 1 and 2 result in a probability of success \(p_s \in \Theta(1)\) when solving SEARCH with the generalized measurement-based method of Table I.

Assumptions 1 and 2 may be combined into one as described in Appendix A. Also, a generalization of Assumption 2 to any circuit \(\mathcal{U}\) is a requirement of having a ground state with large probability of being in the state output by the circuit after measurement. This property is desired for Hamiltonians involved in the adiabatic simulation of quantum circuits.
Assumption 3: For all \( t \in \mathbb{R} \) and fixed \( \epsilon, 0 \leq \epsilon < 1 \), there exists a unitary operation \( W_X = (S, O_X)^r \), where \( S \) is also a unitary operation that does not depend on \( X \), \( O_X = O_X \otimes I \) is the oracle for searching on the larger Hilbert space \( \mathcal{H} \), \( r \leq |c't|^\gamma \), and
\[
||e^{igXt} - W_X|| \leq \epsilon.
\]
\( c' > 0 \) and \( \gamma \geq 0 \) are constants.

Assumption 3 implies that the evolution operator determined by \( G_X \) can be approximated, at precision \( \epsilon \), by a sequence of unitary operations that uses the oracle order \( |c't|^\gamma \) times. For some specific \( G_X \), such an approximation may follow from the results in Refs. [17–19] on Hamiltonian simulation (see Sec. [IV]).

Theorem. If \( G_X \) and \( |\zeta_X\rangle \) satisfy Assumptions 1, 2, and 3,
\[
\Delta U_X \in \mathcal{O}(1/L^{1/\gamma}).
\]
In addition, if \( G_X \) satisfies a frustration-free property [34, 35],
\[
\Delta U_X \in \mathcal{O}(1/L^{2/\gamma}).
\]

The definition of a frustration-free Hamiltonian is included in the proof. The second bound applies under an additional requirement on \( G_X \). This requirement together with the constants for the upper bounds are also discussed in the proof.

We note that the gap in the second upper bound may not be the “relevant” gap for the adiabatic simulation. In certain cases, for example, the adiabatic simulation may not allow for transitions from the ground state to the first-excited state due to symmetry reasons. Nevertheless, the first bound still holds for the relevant gap in these cases.

Proof. Simulating the measurement in step ii of the generalized measurement-based method requires an evolution time \( T = c/\Delta U_X \) [Eq. (7)]. From Assumption 3, the evolution can be approximated by a quantum circuit that uses the oracle \( r \) times, with \( r \leq (c'T)^\gamma \). The lower bound on the cost of solving SEARCH [30] implies
\[
\left(\frac{c'}{\Delta U_X}\right)^\gamma \geq r \geq \alpha \sqrt{N} \geq \alpha 2L,
\]
where \( \alpha > 0 \) is a constant because \( p_s \in \mathcal{O}(1) \). Then,
\[
\Delta U_X \leq c'/\alpha 2L^{1/\gamma}.
\]

\( G_X \) is a frustration-free Hamiltonian if it is a sum of positive semidefinite terms and the ground state \( |\zeta_X\rangle \) is a ground state of every term [34, 35]. In this case, it is possible to preprocess \( G_X \) and build a Hamiltonian \( \tilde{G}_X \) that has
\[
|\tilde{\zeta}_X\rangle = |\zeta_X\rangle \otimes |0\rangle_a
\]
as (unique) eigenstate of eigenvalue zero, where \( |0\rangle_a \) denotes some simple, \( X \)-independent state of an ancillary system \( a \). The corresponding spectral gap of \( \tilde{G}_X \) for this state is \( \tilde{\Delta U_X} \geq \sqrt{\Delta U_X} \) — see Ref. [35] for details on spectral gap amplification. Then, SEARCH can be solved with probability \( p_s \in \mathcal{O}(1) \), using the generalized measurement-based method, by evolving with \( \tilde{G}_X \) for time \( T = c/\sqrt{\Delta U_X} \). If Assumption 3 also applies for approximating the evolution operator \( e^{-igXt} \), then \( \sqrt{\Delta U_X} \leq c'(2\alpha L)^{1/\gamma} \). This completes the proof.

Corollary. If \( \gamma = 1 \), then \( \Delta U_X \in \mathcal{O}(1/L) \). In addition, if \( G_X \) is frustration free as explained above, \( \Delta U_X \in \mathcal{O}(1/L^2) \).

It is possible to achieve \( \gamma \rightarrow 1 \) for some \( G_X \) (see Sec. [IV]).

Corollary. If the eigenvalues of \( H^i \) do not depend on \( U \), the upper bounds on \( \Delta U_X \) are upper bounds on \( \Delta U \).

IV. DISCUSSION: VALIDITY OF THE ASSUMPTIONS AND IMPPLICATIONS

We review the validity of the assumptions and implications for some constructions found in the literature. The first is the standard construction in Ref. [21], also discussed in Sec. [I]. In this case, we consider a modification of Grover’s algorithm so that \( \mathcal{U}_X = I^{L/4}(RO_X)^{L/4}I^{L/4} \), with \( L \in \Theta(\sqrt{N}) \) and \( I \) the trivial (identity) operation. Such a modification is unnecessary but it simplifies the analysis below. The state output by the modified circuit is unchanged; the only change is in the Hamiltonians. As before, we let \( G_X = H^iU_X \) be the Hamiltonian associated with \( \mathcal{U}_X \) and \( |\zeta_X\rangle = |\psi^iU_X\rangle \) be its ground state [i.e., the history state of Eq. (4) with \( U = U_X \)]. For the modified circuit, the ground state has large overlap with the \( X \)-independent state
\[
|\nu\rangle = |\phi^0\rangle \otimes \frac{1}{\sqrt{L/4 + 1}} \sum_{l=0}^{L/4} |l\rangle_c.
\]
Similarly, \( |\zeta_X\rangle \) has large overlap with the state
\[
|X\rangle \otimes \sum_{l=3L/4}^{L} |l\rangle_c,
\]
because \( |X\rangle \approx |\phi^i_{X\rangle} \) [see Eq. (10)]. These Eqs. imply \( p_{\nu,\zeta_X} \approx 1/4 \) and \( p_{X,\zeta_X} \approx 1/4 \), so that Assumptions 1 and 2 are readily satisfied. To study Assumption 3, we write
\[
G_X = -OX \sum_{l:U=OX} \sum_{l=0}^{L} |l\rangle \langle l-1|_c + |l-1\rangle \langle l|_c + \ldots
\]
\[
= O_X \otimes P_c + H_{s-c}.
\]
(9)

\( P_c \) is a Hamiltonian acting on the clock register that is a sum of commuting terms like \( |l\rangle \langle l-1|_c + |l-1\rangle \langle l|_c \); the operators \( O_X \) are interleaved with the operations \( R \) in
Grover’s algorithm. Then, the eigenvalues of $P_c$ are $\pm 1$ and $\|P_c\| \leq 1$, where $\|\cdot\|$ is the operator norm. $H_{s-c}$ is a system-clock-Hamiltonian that does not depend on $X$; $H_{s-c}$ is a sum of $H_{\text{input}}$ and those terms in $H_{\text{Feymman}}^{\text{triv}}$ that do not depend on $O_X$. Using the results in Ref. [19], the operator $\exp(iG_Xt)$ can be well approximated using $O(\|t\| \log ||t||)$ oracles $O_X$ (see Appendix [C]). Thus, Assumption 3 is satisfied for the construction of Ref. [21] and $\gamma \to 1$ asymptotically.

To prove that $G_X$ is frustration free, we note that

$$G_X = W(U_X) H^1 W(U_X)^\dagger,$$

where $H^1$ is the Hamiltonian of Eq. (1) for the trivial circuit and

$$W(U_X) = \sum_{l=0}^{L} U_l \otimes |l\rangle \langle l_c|$$

is a unitary operation. For the modified Grover’s algorithm, $U_l \in \{I, R, O_X\}$. It is simple to verify that $|\psi^+\rangle \propto |\phi^0\rangle \sum_l |l\rangle_c$, $H^1 |\psi^+\rangle = 0$, $h^{\text{t},l} \geq 0$, $H_{\text{input}} |\psi^+\rangle = 0$, $H_{\text{input}} \geq 0$. This implies that $H^1$ is frustration free and so are $G_X$ and $H^{\text{t}}$ for any $\mathcal{U}$. Then, there exists

$$\tilde{G}_X = W(U_X) H^1 W(U_X)^\dagger$$

whose ground state is $|\tilde{\chi} \rangle = |\chi \rangle \otimes |0\rangle_a$ and whose gap is $\sqrt{N}$. $\phi_a$ is an ancillary system of dimension $L+n$. The operators $h^{\text{t},l}$ have eigenvalues $0, 1$ and $\sqrt{h^{\text{t},l}} = h^{\text{t},l}$. Then, from the results in Ref. [35], Sec. IV, we obtain

$$\tilde{G}_X = \tilde{H}_F^{\text{t},X} + \tilde{H}_{\text{input}},$$

with

$$\tilde{H}_F^{\text{t},X} = \sum_{l=1}^{L} h^{\text{t},l} \otimes |l\rangle \langle l_a| + |0\rangle \langle l_c|,$$

$$\tilde{H}_{\text{input}} = \sum_{j=1}^{n} |\rangle \langle -j| \otimes |0\rangle \langle 0_c| \otimes$$

$$\otimes |L+j\rangle \langle l_a| + |0\rangle \langle L+j| \rangle \langle a|.$$ 

When $U_l = O_X$ in the modified Grover’s algorithm,

$$h^{\text{t},l} = \frac{1}{2} [I \otimes |l\rangle \langle l_c| + |l-1\rangle \langle l-1|_c] +$$

$$+ O_X \otimes |l\rangle \langle l-1|_c + |l-1\rangle \langle l-1|_c].$$

Thus, another representation for $G_X$ is

$$\tilde{G}_X = O_X \otimes \tilde{P}_{c-a} + \tilde{H}_{s-c-a},$$

with $\|\tilde{P}_{c-a}\| \leq 1$ because $\|\tilde{H}_F^{\text{t},X}\| \leq 1$ (see Appendix [C]). The system-clock-ancilla Hamiltonian $\tilde{H}_{s-c-a}$ is independent of $X$. Then, the evolution operator $e^{iG_Xt}$ can be approximated from the results in Ref. [19] using the oracle $O(\|t\| \log ||t||)$ times and the gadget in Appendix [B]. It follows that $\gamma \to 1$ asymptotically for this case as well, and the gap satisfies $\Delta^{\text{t}} \leq \tilde{O}(1/L^2)$. (The $\tilde{O}$ notation accounts for the additional logarithmic factor.) This upper bound is also valid for any $\Delta^{\text{t}}$, because the eigenvalues of $H^{\text{t}}$ do not depend on $\mathcal{U}$ (Eq. (10)). Our result is compatible with the lower bound on $\Delta^{\text{t}}$ obtained in Ref. [21] (see Sec. [I]). It proves that our technique to establish limits in the gap is effective. Nevertheless, as we show below, our technique is powerful when analyzing the gaps of Hamiltonians that are simple modifications to the $G_X$ above, where obtaining the spectrum directly can be challenging. We note again that, since the local Hamiltonian constructed in Ref. [21] has a smaller gap than that of $H^{\text{t}}$ or $G_X$, the bound on the gap of $G_X$ translates into a bound on the gap of the local Hamiltonian.

We use the previous analysis to show a more general result. Consider a general Hamiltonian $H^{\text{t}} = W(\mathcal{U}) H^1 W(\mathcal{U})^\dagger$ for the adiabatic simulation of a quantum circuit, which uses a clock register, and whose ground state is of the form

$$|\psi^{\text{t}}\rangle = W(\mathcal{U}) |\psi^{\text{t}}\rangle$$

and $|\psi^{\text{t}}\rangle = |\phi^0\rangle \sum_l |l\rangle_c$. With no loss of generality, we can assume that there exists $\ell_0$ such that

$$\sum_{l=\ell_0}^{L} |\alpha_l|^2 \in \Theta(1).$$

If this condition is not satisfied, we can always apply an operation that permutes the clock states or we can add trivial operations to the circuit so that Eq. (15) is satisfied (the spectrum of $H^{\text{t}}$ is unchanged). We let $\ell_0$ be the largest $l$ to satisfy Eq. (15). Then, we consider a modification of Grover’s algorithm so that

$$U_X = |0\rangle \langle 0_b| \otimes I + |1\rangle \langle 1_b| \otimes \left( I^{l_0} \otimes (R_0 X)^{L-l_0} \right),$$

where $b$ is an ancillary qubit (see Appendix [A]), $L \in \Theta(\sqrt{N})$. Basically, the modified Grover’s algorithm acts trivially, if the state of an ancillary qubit is $|0\rangle_b$, or implements the original Grover’s algorithm, if the state of the ancilla is $|1\rangle_b$. The initial state is $|\psi^{\text{t}}\rangle \otimes |\phi^0\rangle$, and $|\phi^0\rangle$ is the equal superposition state as required in Grover’s algorithm. Assumptions 1 and 2 then follow from Eq. (15), for those ground states that can be described by Eq. (14). Additionally, if the Hamiltonian associated with $U_X$ can be represented as in Eq. (9), with $\|P_c\| \leq 1$, the evolution under $G_X$ can be well approximated using $O(\log \ell)$ oracles and the upper bound on $\Delta^{\text{t}}$ is of $\tilde{O}(1/L)$. Such Hamiltonians include those $H^{\text{t}}$ arising from modified Feynman Hamiltonians, where $H^{\text{t}} = \sum_l |\beta_l|^2 |\phi^l\rangle \langle \phi^l|$ and $|\beta_l|^2 \leq 1$, and those Hamiltonians that have an additional term

$$H_{\text{pointer}} = \sum_l E_l \otimes |l\rangle \langle l_c|.$$
that acts solely in the clock space.

For those $H^{\text{f}}$, the spectrum is independent of $\mathcal{U}$ (i.e., $\Delta^{\mathcal{U}_X} = \Delta^{\mathcal{U}}$) and in particular,

$$G_X = W(\mathcal{U}_X) H^{\mathcal{U}} W(\mathcal{U}_X)^\dagger$$

[see Eqs. (11) and (11)]. The unitaries $\mathcal{U}^j$ involved in the definition of $W(\mathcal{U}_X)$ are $\mathcal{U}^j \in \{ I, |0\rangle \langle 0| \otimes I + |1\rangle \langle 1| \otimes O_X, |0\rangle \langle 0| \otimes I + |1\rangle \langle 1| \otimes R \}$, for the current $\mathcal{U}_X$. $H^{\mathcal{U}}$ acts trivially in the system and has tridiagonal form in the basis $\{ |0\rangle_e, \ldots, |L_e\rangle_e \}$. Then, with no loss of generality, we can assume that $H^{\mathcal{U}}$ is frustration free \footnote{Assumption 3 is work in progress. Finally, Assumptions 1 and 2 do not apply to the construction in A. Mizel, e-print: arXiv:1002.0836 (2010).}. It follows that $G_X$ is also frustration free and we can build

$$\tilde{G}_X = W(\mathcal{U}_X) \tilde{H}^{\mathcal{U}} W(\mathcal{U}_X)^\dagger,$$

by using the results of Ref. \footnote{Assumption 2 is mostly an statement about the ground state of the Hamiltonian $H^{\mathcal{U}}$ that simulates a quantum circuit, $|\psi^{\mathcal{U}}\rangle$. Ideally, such state has large probability of being in the state output by the circuit, $|\phi^L\rangle$; that is,

$$\Pr(|\phi^L\rangle | \psi^{\mathcal{U}}\rangle = \text{Tr}[|\phi^L\rangle \langle \phi^L| | \psi^{\mathcal{U}}\rangle \langle \psi^{\mathcal{U}}|] \in \Theta(1).$$

In general, Assumption 2 is mostly an statement about the ground state of the Hamiltonian $H^{\mathcal{U}}$ that simulates a quantum circuit, $|\psi^{\mathcal{U}}\rangle$. Ideally, such state has large probability of being in the state output by the circuit, $|\phi^L\rangle$; that is,

$$\Pr(|\phi^L\rangle | \psi^{\mathcal{U}}\rangle = \text{Tr}[|\phi^L\rangle \langle \phi^L| | \psi^{\mathcal{U}}\rangle \langle \psi^{\mathcal{U}}|] \in \Theta(1).$$

We can then consider a modified quantum circuit that uses an additional ancilla $b$ prepared in $|+\rangle_b$ so that it applies the unitary $\mathcal{U}$ (original circuit) controlled on the state $|1\rangle$ of the ancilla, or does nothing otherwise. If we denote the modified circuit by $\bar{\mathcal{U}}$, the output state is

$$|\tilde{\phi^L}\rangle = \bar{\mathcal{U}} (|+\rangle \otimes |\phi^0\rangle) \in \Theta(1).$$

In this way, if the ground state of $H^{\mathcal{U}}$ is a superposition of system-clock states of the form $|\phi^L\rangle \otimes |0\rangle_c$, the ground state of $H^{\mathcal{U}}$ will be a superposition of states of the form $|\phi^L\rangle \otimes |1\rangle_c$, with $|\phi^L\rangle = \mathcal{U}^1 \cdots \mathcal{U}^0 (|+\rangle_b \otimes |\phi^0\rangle)$. When $\mathcal{U} = \mathcal{U}_X$ corresponds to Grover’s algorithm, if $|\psi^{\mathcal{U}}\rangle$ has large probability of being in $|\phi^L\rangle$ after measurement, then it has large probability of being in both, $|\phi^0\rangle$ and $|\phi^L\rangle$, after respective measurements. Since $|\phi^0\rangle$ is independent of $X$, $|\phi^L\rangle$ satisfies Assumption 1 and 2 simultaneously. Thus, in Grover’s algorithm, Assumptions 1 and 2 can be combined into a single one for Hamiltonians whose ground states are superpositions of $|\phi^L\rangle \otimes |0\rangle_c$. The gap bounds will apply to $H^{\mathcal{U}_X}$ in this case.

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Appendix A: More on Assumptions 1 and 2

In general, Assumption 2 is mostly an statement about the ground state of the Hamiltonian $H^{\mathcal{U}}$ that simulates a quantum circuit, $|\psi^{\mathcal{U}}\rangle$. Ideally, such state has large probability of being in the state output by the circuit, $|\phi^L\rangle$; that is,

$$\Pr(|\phi^L\rangle | \psi^{\mathcal{U}}\rangle = \text{Tr}[|\phi^L\rangle \langle \phi^L| | \psi^{\mathcal{U}}\rangle \langle \psi^{\mathcal{U}}|] \in \Theta(1).$$

We can then consider a modified quantum circuit that uses an additional ancilla $b$ prepared in $|+\rangle_b$ so that it applies the unitary $\mathcal{U}$ (original circuit) controlled on the state $|1\rangle$ of the ancilla, or does nothing otherwise. If we denote the modified circuit by $\bar{\mathcal{U}}$, the output state is

$$|\tilde{\phi^L}\rangle = \bar{\mathcal{U}} (|+\rangle \otimes |\phi^0\rangle) \in \Theta(1).$$

In this way, if the ground state of $H^{\mathcal{U}}$ is a superposition of system-clock states of the form $|\phi^L\rangle \otimes |0\rangle_c$, the ground state of $H^{\mathcal{U}}$ will be a superposition of states of the form $|\phi^L\rangle \otimes |1\rangle_c$, with $|\phi^L\rangle = \mathcal{U}^1 \cdots \mathcal{U}^0 (|+\rangle_b \otimes |\phi^0\rangle)$. When $\mathcal{U} = \mathcal{U}_X$ corresponds to Grover’s algorithm, if $|\psi^{\mathcal{U}}\rangle$ has large probability of being in $|\phi^L\rangle$ after measurement, then it has large probability of being in both, $|\phi^0\rangle$ and $|\phi^L\rangle$, after respective measurements. Since $|\phi^0\rangle$ is independent of $X$, $|\phi^L\rangle$ satisfies Assumption 1 and 2 simultaneously. Thus, in Grover’s algorithm, Assumptions 1 and 2 can be combined into a single one for Hamiltonians whose ground states are superpositions of $|\phi^L\rangle \otimes |0\rangle_c$. The gap bounds will apply to $H^{\mathcal{U}_X}$ in this case.

Appendix B: Oracle simulation of the Feynman Hamiltonian associated with Grover’s algorithm

Following Ref. \footnote{Following Ref. \cite{Boixo:10}, the first step is to use the Trotter-Suzuki approximation that, in the case of the evolution under $G_X = O_X \otimes P_c + H_{s,c}$, it yields terms of the form $e^{-isO_X \otimes P_c}$ (B1) for some small $s \in \mathbb{R}$. The goal in this section is to present gadget that implements Eq. (B1) (i.e., a fractional oracle) using $O_X$. Then, the problem is reduced to the one analyzed in Ref. \cite{Boixo:10}, for which the oracle cost is known.}, the first step is to use the Trotter-Suzuki approximation that, in the case of the evolution under $G_X = O_X \otimes P_c + H_{s,c}$, it yields terms of the form

$$e^{-isO_X \otimes P_c} \text{ (B1)}$$

for some small $s \in \mathbb{R}$. The goal in this section is to present gadget that implements Eq. (B1) (i.e., a fractional oracle) using $O_X$. Then, the problem is reduced to the one analyzed in Ref. \cite{Boixo:10}, for which the oracle cost is known.
First, we note that there exists a unitary operation $V_c$ such that

$$V_c e^{-isO_X \otimes D_c} = e^{-isO_X \otimes D_c},$$

(B2)

where $D_c$ is a diagonal operator acting on the clock register, i.e.,

$$D_c = \sum_k \lambda_k |k\rangle \langle k|_c,$$

and $|\lambda_k| \leq 1$ because $\|P_c\| \leq 1$. $V_c$ commutes with $O_X$ and it does not depend on $X$. The "gadget" of Fig. 1 uses this observation to implement the operation of the rhs of Eq. (B2). Then, the desired operator of Eq. (B1) can be implemented by conjugating the circuit of Fig. 1 with $O_X$. This has to be compared with Fig. 3 of Ref. [19].

| $k\rangle_c$ | $|0\rangle_b$ | $R_1$ | $R_2$ | $|k\rangle_c$ |

FIG. 1: Simulation of $\exp\{-isO_X \otimes D_c\}$ [Eq. (B2)]. $b$ is an ancilla qubit. The controlled operations are: $R_1 |0\rangle_b \propto \sqrt{\cos(s\lambda_k/2)} |0\rangle_b - i \sqrt{\sin(s\lambda_k/2)} |1\rangle_b$ and $R_2 |0\rangle_b \propto \sqrt{\cos(s\lambda_k/2)} |0\rangle_b + \sqrt{\sin(s\lambda_k/2)} |1\rangle_b$ (see Fig. 3 in Ref. [19]). The ancilla is measured at the end and the simulation of $e^{-is\lambda k O_X \otimes |k\rangle \langle k|_c}$ succeeds if the outcome is $|0\rangle_b$. The oracle is controlled in the state $|1\rangle_b$.

If we use the simulation of Fig. 1 in the scheme shown in Fig. 4 of Ref. [19], the total number of oracles needed for approximating the evolution operator $e^{-iO_X t}$ is of order $O(|t| \log |t|)$. This requires implementing other simulation "tricks" to reduce the oracle cost, such as reducing the Hamming weight of the state of the ancillas for each simulation of $e^{-isO_X \otimes D_c}$, coming from the Trotter-Suzuki approximation (see Ref. [19] for more details).

Appendix C: The modified Hamiltonians $\tilde{G}_X$

The first modified Hamiltonian we analyze is the one in Eq. (12) for Grover’s algorithm, and write $G_X = \tilde{H}^{d_X}$. Then,

$$\tilde{G}_X =$$

$$= -O_X \otimes \sum_{l: U^l = O_X} [\langle l | (l - 1) |_{c} + |l - 1\rangle \langle l|_c] \otimes [\langle l | 0\rangle_a + |0\rangle \langle l|_a] + \ldots$$

$$= O_X \otimes P_{c-a} + \tilde{H}_{s-c-a}.$$
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[37] To be rigorous, the state $|\nu\rangle$ has to be redefined as $|\nu\rangle \otimes |0\rangle$ for this case.

[38] While the subspace of eigenvalue zero of $\tilde{G}_X$ is highly degenerate, the degeneracy is irrelevant and can be easily removed by adding other $X$-independent terms [35].

[39] The frustration free property can be obtained by adding, for example, a constant to $H^X$ so that its lowest eigenvalue is zero.