

From quantum circuits to adiabatic algorithms

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This paper explores several aspects of the adiabatic quantum-computation model. We first show a way that directly maps any arbitrary circuit in the standard quantum-computing model to an adiabatic algorithm of the same depth. Specifically, we look for a smooth time-dependent Hamiltonian whose unique ground state slowly changes from the initial state of the circuit to its final state. Since this construction requires in general an n -local Hamiltonian, we will study whether approximation is possible using previous results on ground-state entanglement and perturbation theory. Finally we will point out how the adiabatic model can be relaxed in various ways to allow for 2-local partially adiabatic algorithms as well as 2-local holonomic quantum algorithms.

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I. INTRODUCTION

Adiabatic evolution as a quantum computation model has attracted much attention since its introduction by Farhi *et al.* [1]. The basic idea is the following. Start with a Hamiltonian whose ground state is easily reachable and prepare our state in the ground state. Change it slowly to a new Hamiltonian that encodes the solution of the problem and maintain a large energy gap between the ground state and the excited state that the evolving state couples to. The adiabatic theorem [2] then guarantees that the resulted state will be very close to the ground state of the new Hamiltonian. The original form of the Hamiltonian considered in [1] is a straight-line interpolation: $H(s) = (1-s)H_{initial} + sH_{final}$. Recently, it was proved that any standard quantum circuit, specified by a sequence of unitary operators, can be implemented as an adiabatic evolution of this form [3,4]. The authors use computational complexity techniques developed for proving the QMA-completeness of the k -local Hamiltonian problem (Kempe *et al.* [4] achieved the case for $k=2$); the evolving state encodes the entire computational history. Roughly speaking, they construct a Hamiltonian whose ground state is the superposition of all the stages in a given circuit. If the circuit has depth L , the time required to obtain this ground state is $O(1/L^6)$ for the 3-local Hamiltonian and there is an $O(1/L)$ probability of obtaining the final state of the circuit given this superposition. On a seemingly unrelated note, Farhi *et al.* [5] showed after [1] that if we do not restrict adiabatic evolution to the straight-line path and add terms that vanish at the end points, we may be able to turn an inefficient computation into an efficient one. A general method for finding an efficient path is, however, not known. In light of these two developments, we may ask—can we always find an efficient adiabatic evolution path, not necessarily of the straight-line form, for problems efficiently solvable by quantum circuits such that we directly obtain the desired final state? Starting with this question, we will present several variations on how to implement the standard circuit model by adiabatic evolution.

The first result we show is that once we specify (a) the unitary transformation that takes the eigenstates at the beginning to those at the end of the evolution, and (b) how we want the eigenvalues to evolve, we can immediately derive the form of time-dependent Hamiltonian required without the use of any ancilla qubits. Conceptually the simplest example is a time-dependent similarity transform $U(t)H_{initial}U(t)^\dagger$. This observation should allow us to engineer Hamiltonians according to computational needs. However, a Hamiltonian of the type $\dots U_2 U_1 H_{initial} U_1^\dagger U_2^\dagger \dots$ can be highly nonlocal even if U_1, U_2, \dots and $H_{initial}$ have simple local forms. Since we are interested in the ground state, we should ask whether it is possible to find a local approximation.

It turns out that while approximations are possible to a certain extent, there is much constraint. We will demonstrate this point in two steps. First we will make use of the results by Haselgrove *et al.* [6], which show how the entanglement of the eigenstates of a Hamiltonian is related to what bodies in the system each term in the Hamiltonian acts on nontrivially. Intuitively speaking, if an eigenstate shows strong correlation between bodies which the Hamiltonian does not directly couple, i.e., act nontrivially on all as a tensor product, the Hamiltonian cannot distinguish very well between such a state and other similarly entangled states that are orthogonal to it. This results in a small energy gap. Since a quantum circuit can generate highly correlated states, when we want to make them ground states of a Hamiltonian in an adiabatic algorithm, they will be difficult to approximate. Then, as an explicit example, we will use the approximation method developed in [4], derived from perturbation theory, and apply it on our construction. We will see that we could indeed make a local approximation under the constraint implied by [6], but the resulting evolution can be inefficient.

Next we look at how this approach of transforming the Hamiltonian adiabatically is related to the manipulation of geometric phase. We start by asking, given that local approximation is difficult, why the adiabatic model is more demanding than the basic circuit model, for which 2-local Hamiltonians easily suffice with $U = \exp(iH_{2-local}t)$ for each gate. There are at least two crucial differences between the two models.

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(I) The adiabatic model keeps track of exactly where the state is at every moment throughout the evolution and penalizes any deviation, while the circuit model keeps no information about the state at all. This makes the former more resistant to error.

(II) The adiabatic model allows time variability in the application of the Hamiltonian, while the basic circuit model requires precise pulse timing.

The word “adiabatic” itself only suggests property II above, so if we are willing to relax property I, we will have much more freedom to design our Hamiltonian. The main issue we need to deal with, as we will show, is the geometric phase. Suppose we implement the Hamiltonian $U(s)H_{\text{initial}}U(s)^\dagger$ without making sure that we start with the ground state or any eigenstate of the initial Hamiltonian. Instead of having $U(s)$ applied on our initial state, there will be further transformation due to the relative phases accumulated between different eigenstates. The dynamical component of the phase is straightforward to cancel out, but the geometric component is more subtle to calculate. To avoid having to cancel the geometric component, we may either make sure we always start with an eigenstate of the Hamiltonian, or take advantage of the geometric phase to implement the desired transformation. This would naturally lead us to the holonomic quantum computing model developed by Zanardi *et al.* [7], which in fact precedes the adiabatic algorithm of [5].

Let us give a lightning review of the idea of holonomic quantum computing (HQC). Wilzcek and Zee introduced in [8] the observation that if a Hamiltonian with degenerate eigenstates goes through a cycle adiabatically without changing the degeneracy of each level, the degenerate subspace can be viewed as a gauge group on the manifold corresponding to the parameter space of the Hamiltonian. After each cyclic evolution, an arbitrary state in the degenerate space will undergo a unitary transformation depending on the path taken; the set of all possible such unitary transformations given a parameter space that specifies the Hamiltonian is called the holonomy group, and the parameter space is often called the control manifold. Elements of the group generally do not commute, so the transformation is called the non-Abelian geometric phase. Zanardi *et al.* [7] applied this idea on quantum computing by choosing initial Hamiltonians for which the computational states are completely degenerate. Transformations are then applied by holonomy. In addition to time variability, the geometric nature (such as dependency on the area of the loop) also gives HQC some resistance to errors.

Seeing HQC as a generalized adiabatic model brings us many additional insights. First, we can apply the local approximation techniques of [4] to show that 2-local Hamiltonians are sufficient to implement HQC. Furthermore, we show that the construction of [3], etc., originally developed for computational complexity proofs, has a hidden gauge freedom and can be viewed as half a holonomic cycle. This view allows us to improve the adiabatic implementation so that we obtain only the desired final state instead of the computational history.

This paper is organized as follows. In Sec. II, we give the direct way to construct an adiabatic equivalent of any circuit without encoding the computational history. It makes use of

only the same number of qubits as in the circuit and a running time of the same order as the depth of the circuit, as shown in Sec. III. This in general involves n -local Hamiltonians, and Sec. IV discusses why this can be difficult to approximate by studying entanglement properties of the ground state of Hamiltonians. In Sec. V we show one way to construct a 2-local Hamiltonian whose worst-case run time scales exponentially with n , illustrating a tradeoff between resource requirement and running time. In Sec. VI, we look at how 2-local constructions can be useful for generalized adiabatic algorithms and how computation models that use Abelian and non-Abelian geometric phases [7,9] fall into this category. Finally, we return in Sec. VII to the computational history approach of [3] and note its interesting connection to holonomic quantum computing.

II. A DIRECT MAPPING

We adopt a general definition of adiabatic computation and look for a time-dependent, differentiable Hamiltonian $H(s)$, where $0 < s < 1$ is the time parameter, such that $H(0)$ is an initial Hamiltonian with a unique, easily reachable ground state and $H(1)$ is a Hamiltonian with a unique ground state encoding the solution of our problem. A quantum circuit can be given in the form $|\psi\rangle = U_l U_{l-1} \dots U_1 |0\rangle$, where U_i are unitary operators representing one or two qubit gates. To map this transformation into adiabatic evolution, we start with a Hamiltonian $H(0)$, whose ground state is $|0\rangle$, and we would like to have $H(s)$ such that $|\psi\rangle$ is the ground state of $H(1)$. The most common problem in constructing such an $H(s)$ is that the energy gap between the ground state and the first excited state varies during the evolution. A small gap implies a larger probability for the ground state to be excited, and in turn a longer evolution time if we want to compensate for it.

Our main observation is that it is possible to maintain a constant gap size as long as we keep the Hamiltonian $H(s)$ to be of the form $U(s)H(0)U^\dagger(s)$. Let us be more specific. Suppose the circuit requires us to perform unitary gate U on state $|0\rangle$. Let $K = -i \log U$ and $\tilde{U}(s) = \exp(isK)$, such that $\tilde{U}(0) = 1$ and $\tilde{U}(1) = U$. We start with a Hamiltonian H with $|0\rangle$ as its ground state:

$$H|n\rangle = E_n|n\rangle. \quad (1)$$

We can add $V(s)$ such that the following is true:

$$[H + V(s)]\tilde{U}(s)|n\rangle = f(n,s)\tilde{U}(s)|n\rangle \quad (2)$$

if

$$V(s)\tilde{U}(s)|n\rangle = [\tilde{U}(s), H]|n\rangle + [f(n,s) - E_n]\tilde{U}(s)|n\rangle. \quad (3)$$

This completely specifies $V(s)$, and if $f(n,s) = E_n$, $V(s)$ is just, in the original (computational) basis, $\tilde{U}(s)H\tilde{U}(s)^\dagger - H$. It is clear that as s goes to 1 slowly, we obtain $U|0\rangle$ as our ground state without worrying about a shrinking gap. Note that $f(n,s)$ allows us to manipulate the gap size.

Using the idea above, we can now spell out the explicit mapping. Given U_1, \dots, U_l , we first replace the overall time

tively speaking, if an eigenstate shows strong correlation between bodies that the Hamiltonian does not directly couple (i.e., act nontrivially on all of them as a tensor product), the Hamiltonian cannot distinguish very well between such a state and other similarly entangled states that are orthogonal to it. This results in a small energy gap. The following theorem from [6] makes this idea concrete and suffices for our purpose.

Theorem 1. Consider a state $|\psi\rangle$ and a Hamiltonian H whose eigenvalues and eigenstates are E_j and $|E_j\rangle$, respectively, with $j=0, \dots, d-1$; d is the dimension of the Hilbert space and $|E_0\rangle$ is the ground state of H . Let F be the overlap of $|\psi\rangle$ with $|E_0\rangle$ and E_{tot} be the difference between the maximum and minimum eigenvalues. Then for all density matrices ρ with eigenvalues $\rho_1 \leq \rho_2 \leq \rho_3 \dots$, such that $\text{tr}(\rho H) = \langle \psi | H | \psi \rangle$, the following inequality holds:

$$\sum_{j=1}^{d-1} (E_j - E_0) \rho_{j+1} \leq (1 - F^2) E_{\text{tot}}. \quad (10)$$

The proof is elementary and we will refer the readers to the lucid explanation in [6]. Now we may apply this theorem on the construction in Sec. (2).

Claim 1. Let H_0 be a 1-local Hamiltonian with unique ground state $|0\rangle$. There does not exist a general k -local approximation for the n -local Hamiltonian UH_0U^\dagger , where $k \leq n-1$ and U is a polynomial-sized circuit, such that the approximation produces exactly the same ground state and first excited state. Specifically, one cannot always construct a k -local Hamiltonian which has $U|0\rangle$ as a nondegenerate eigenstate.

Proof. We will start with the case without ancilla qubits. Consider the state $|\psi\rangle = (1/\sqrt{2})(|000\dots\rangle + |111\dots\rangle)$, the n -qubit Greenberger-Horne-Zeilinger (GHZ) state. Consider also a k -local Hamiltonian H whose ground state $|E_0\rangle = |\psi\rangle$, so $F=1$. If we choose

$$\rho = \frac{1}{2}(|000\dots\rangle\langle 000\dots| + |111\dots\rangle\langle 111\dots|) \quad (11)$$

where “...” again indicates n zeros or ones, it is easy to see that $\text{tr}_{n-k}\rho = \text{tr}_{n-k}|\psi\rangle\langle\psi|$ for $k \leq n-1$, where tr_{n-k} means tracing over any $n-k$ qubits. It then follows that for $k \leq n-1$, $\text{tr}(\rho H) = \langle \psi | H | \psi \rangle$ for a k -local Hamiltonian H . Putting this into the inequality in Theorem 1, we obtain $E_1 - E_0 = 0$, meaning that the ground state corresponding to E_0 is degenerate.

Now suppose a k -local exact approximation exists. Choose the n -qubit polynomial-sized circuit $U = (\text{Hadamard})_1 \Pi_{i=1}^{n-1} (\text{CNOT})_{i,i+1}$, i.e., a Hadamard gate acts on the first qubit, followed by a series of CNOT gates on the first and second, the second and third, and so on. Clearly, this circuit acting on the initial state $|000\dots\rangle$ produces $|\psi\rangle$. Suppose we start with a simple 1-local Hamiltonian H_0 (e.g., set $H_0 = \sum_{i=1}^n \sigma_z^i$) which has $|000\dots\rangle$ as a nondegenerate ground state. If there exists a procedure that exactly approximates UH_0U^\dagger with a k -local Hamiltonian, $k \leq n-1$, this implies there exists a k -local Hamiltonian which has $|\psi\rangle$ as a nondegenerate ground state. Hence we have arrived at a contradiction.

To generalize this to the case with ancilla qubits, a slight extension of Theorem 1 is needed. Let the ground states of the k -local approximation be $|\psi\rangle|a_j\rangle$, where $|a_j\rangle$, $j=1, \dots, m$, enumerates the degeneracies due to the ancilla qubits. This product form is necessary if we want the computational qubits to remain as $|\psi\rangle$. Let $\rho' = \sum_{j=1}^m \rho \otimes |a_j\rangle\langle a_j|/m$. Setting $E_0 = 0$; it is easy to check that $\text{tr}(\rho' H) = \sum_{j=1}^m \text{tr}(\rho \otimes |a_j\rangle\langle a_j|/m) = 0$, which would force the ground-state degeneracy to be $2m$. This in turn implies that there must be degenerate ground states due to states orthogonal to $|\psi\rangle$, contradicting the assumption that there is a k -local Hamiltonian with $|\psi\rangle|a_j\rangle$ as the only ground states. ■

So far we have seen that a local Hamiltonian cannot have certain states as its ground state, as shown by [6,10]. This is rather expected as it is well known [11] that there are quantum states not determined by any reduced density matrices. The more interesting connection we would like to point out here, however, is the trade-off between proximity to a non-local state and the energy gap, as apparent in Theorem 1. Since the energy gap condition is essential to adiabatic algorithms (while some forms of adiabatic theorem without the gap condition exist, they cannot guarantee the final state to arbitrary accuracy [12]), this places another direct trade-off between accuracy and running time. Now that an exact approximation is not possible, we will look at how close we can get.

In [4], a 2-local approximation for 3-local Hamiltonians is constructed (see Sec. V). Normalizing the total energy to unity, the ground-state energy gap for the 2-local Hamiltonian scales as δ^3 for a ground state $O(\delta)$ close to the original ground state. In fact we can use Theorem 1 to make this more precise: If the energy gap scales as δ^3 , the ground state for the 2-local Hamiltonian has to be at least $O(\delta^3)$ away from an original GHZ-type ground state. This proves that there does not exist an approximation scheme better than [4] in such a way that the energy gap scales, say, logarithmically [i.e., $O(1/\log\delta^{-1})$] instead of polynomially with the accuracy $O(\delta)$ of the ground state.

Following this idea, we can place some bounds on how good the approximation for an n -local Hamiltonian can be. For simplicity we will consider a 2-local approximation, should one exist, that has a unique ground state, ancilla qubits included. Consider the state $|\phi\rangle$:

$$|\phi\rangle = \frac{1}{2}(|000\rangle + |111\rangle) \otimes \frac{1}{2}(|000\rangle + |111\rangle) \otimes \dots, \quad (12)$$

which is a tensor product of mostly three-qubit GHZ states. It is not difficult to see that there are $\approx 2^{n/3}$ orthogonal states to it that are not distinguishable by 2-local terms. Thus we can form a density operator of rank $\approx 2^{n/3}$ and substitute it into the inequality (10). This tells us that the average energy of these $\approx 2^{n/3}$ states has a gap with the ground state that is at most $(1-F^2) \sim O(\delta)$. We can tighten this bound a little by considering the distribution of states. If we start with the 1-local Hamiltonian $H_0 = \sum_{i=1}^n \sigma_z^i$ (the minimal form required for a unique ground state), UH_0U^\dagger has n eigenvalues $E_j = j/n$ with degeneracy $n!/[(j!(n-j)!)]$. Simple counting shows that for the lowest $\approx 2^{n/3}$ states, the average energy is at least

$\approx nE_1/6$. Thus we can tighten the bound to $E_1 - E_0 < O(\delta/n)$.

Before we conclude this section, we should briefly note another line of attack due to [10]. Generalizing beyond the GHZ-type states, states corresponding to nondegenerate quantum error correction codes (QECCs) also turn out to be interesting for the study of local Hamiltonians. These are states with the property that, for some constant t usually much smaller than n , any Pauli matrix operators acting non-trivially on up to t qubits will take the state to a set of orthogonal states. Therefore, for a QECC state $|x\rangle$, if the operator $H - EI$ is t -local, $(H - EI)|x\rangle$ will be a sum of orthogonal states, implying that $\|(H - EI)|x\rangle\|$ cannot be close to zero. This prevents any QECC states from being even close to any eigenstate of a t -local Hamiltonian. Recasting this result in our language, we see that there does not exist a k -local approximation to arbitrary n -local Hamiltonians UH_0U^\dagger for sufficiently large n without ancilla qubits, because QECC states can also be generated efficiently by quantum circuits (see references in [10]). With ancilla qubits, however, cancellation can occur for $(H - EI)|x\rangle|a\rangle$ if $|a\rangle$ is not a QECC state. We obtain instead a set of constraint equations that the approximation Hamiltonian has to satisfy in order to produce QECC states as an eigenstate.

We hope that the discussion above would be useful for further research on not only the possibility of local approximation, but also the connection between local properties of Hamiltonians and polynomial-sized quantum circuits.

V. A LOCAL APPROXIMATION USING THE THREE-QUBIT GADGET

After an abstract discussion of possible local approximations, we will now look explicitly at how an approximation scheme can be used in an adiabatic algorithm. We will use as an example the 3- to 2-local reduction introduced by [4], referred to as the three-qubit gadget from now on.

Let us begin with some general considerations. In order to directly map a quantum circuit to an adiabatic algorithm gate by gate with some approximation every time, we would need L approximations where L is the depth of the circuit. To achieve an error within $O(\epsilon)$ for the final state, including the error due to adiabatic approximation discussed in Sec. III, we can estimate the required accuracy at each step as the following. Consider the worst-case scenario, when all the errors accumulated are in the same direction. We first express the angle between the correct final state and the approximate final state as $\theta = O(\sqrt{\epsilon})$ for small θ . The average angle accumulated at each step is θ/L because the unitary gates preserve angles. The allowed error at each step is therefore $1 - \cos^2(\theta/L) = O(\epsilon/L^2)$. Hence as long as the energy gap size scales polynomially with this allowed error, the adiabatic algorithm is efficient. We will see one such example in Sec. VI.

At every step, however, if we repeatedly apply the same approximation procedure on the approximate Hamiltonian from the previous step, the energy gap size would generally not scale polynomially with the allowed error. This is because, as observed in Sec. IV, the energy gap will have to be

scaled down by at least a factor of $O(\delta)$ for an allowed error of $O(\delta)$. Repeatedly approximating approximate Hamiltonians thus results in an energy gap of at most $O(\delta^L)$. This would hold true for any schemes.

We may now look at the specific scheme based on [4]. The authors develop a framework of perturbation theory that gives sufficient conditions for how one Hamiltonian can approximate another. The basic idea they consider is as follows. A 3-local Hamiltonian H_3 can be represented as a 2-local Hamiltonian restricted to a certain subspace, the intuition being that when the interaction involves more bodies, we have finer restrictions on the eigenspaces. Let this 2-local Hamiltonian be V_2 and the subspace be S . If we add another 2-local Hamiltonian H_2 , such that H_2 is zero on S and large everywhere else, it is not difficult to see that the lower spectrum of $\tilde{H}_2 = H_2 + V_2$ is close to that of H_3 , as H_2 gives penalty to states outside of S and restricts V_2 to S .

With this intuition, the next tool we need is a good measure of the lower spectrum of \tilde{H}_2 . This is provided by the self-energy $\Sigma_-(z)$ (analogous to the sum of one-particle-irreducible diagrams in field theory) defined as follows. First we define the Green's function $\tilde{G}(z)$ of \tilde{H}_2 as

$$\tilde{G}(z) = (zI - \tilde{H}_2)^{-1}. \tag{13}$$

Now we define $\Sigma_-(z)$ by

$$\tilde{G}_-(z) = [zI_- - \Sigma_-(z)]^{-1}, \tag{14}$$

where $\tilde{G}_-(z)$ is $\tilde{G}(z)$ restricted to the lower spectrum of H_2 (not \tilde{H}_2). With this definition, [4] proved that (Theorem 4, Lemma 9) if

$$\|\Sigma_-(z) - H_{eff}\| \leq \delta \tag{15}$$

for some operator H_{eff} , then both the lower eigenvalues and the ground states of \tilde{H}_2 will be $O(\delta)$ close to H_{eff} . From this result, we would have a good approximation for H_3 if there is an H_{eff} that is manifestly the same as H_3 on the computational qubits in the energy range we are interested in.

For any 3-local term H_3 , Kempe *et al.* propose an H_2 on ancilla qubits and a V_2 coupling the computational qubits with ancilla qubits, such that when we calculate Σ_- , the above equation is satisfied. This construction is called a three-qubit gadget. To apply this to our adiabatic algorithm, we note from Sec. II that for each 2-qubit quantum gate we add to the Hamiltonian, an m -local Hamiltonian can become at most $(m+1)$ -local. This means if we start with a 1- or 2-local Hamiltonian and apply the three-qubit gadget at every step, we should arrive at a 2-local Hamiltonian at the end. Let us write out the terms explicitly.

To begin with, the following Hamiltonian on the ancilla qubits (playing the role of H_2 above) is added:

$$H_{anc} = -\frac{\delta^{-3}}{4} \sum_{i=1}^l \sum_m I \otimes (\sigma_{im1}^z \sigma_{im2}^z + \sigma_{im1}^z \sigma_{im3}^z + \sigma_{im2}^z \sigma_{im3}^z - 3I). \tag{16}$$

Terms like σ_{im1}^z are Pauli matrices on ancilla qubits identified by three indices: i corresponds to the time step which runs from 1 to l ; the meaning of the second and third indices will become clear shortly. δ would become the error of the 2-local approximation; a smaller δ would correspond to a better approximated spectrum and ground state. Next we give a stepwise approximation, such that given a 2-local Hamiltonian $H^{(i-1)}$ at the beginning of each time step (see Sec. II), we find a 2-local perturbation $V'(s_i)$ to approximate the possibly 3-local $V(s_i) (= U_i H^{(i-1)} U_i^\dagger - H^{(i-1)})$ when U_i is applied. To do this, we first write Eq. (5) in the following form:

$$\begin{aligned} V(s_i) &= \tilde{U}_i(s_i) \left(\sum_i h_j^{(i)} \right) \tilde{U}_i^\dagger(s_i) - \sum_i h_j^{(i)} \\ &= Y_i - 6 \sum_m B_{im1} B_{im2} B_{im3} \end{aligned} \quad (17)$$

where Y_i is 2-local and the B 's are positive semidefinite commuting operators acting on three different qubits. This decomposition is always possible because the Pauli matrix product $\sigma^\alpha \otimes \sigma^\beta \otimes \sigma^\gamma$ forms a basis for 3-local matrices. If the coefficient of a term is positive, we can rewrite the basis term as $(1 + \sigma^\alpha) \otimes (1 + \sigma^\beta) \otimes (1 + \sigma^\gamma) + 2$ -local terms; if it is negative, we can rewrite it as $-(1 - \sigma^\alpha) \otimes (1 + \sigma^\beta) \otimes (1 + \sigma^\gamma) + 2$ -local terms. This way we arrive at the form of Eq. (17), and we can see that m is the number of such product terms in the decomposition. Note that while this decomposition may not be obvious in practice, it is a constructive procedure that can be done with a classical computer program. Now we can construct $V'(s_i)$:

$$\begin{aligned} V'(s_i) &= Y_i + \sum_m \{ \delta^{-1} (B_{m1}^2 + B_{m2}^2 + B_{m3}^2) \\ &\quad - \delta^{-2} (B_{im1} \otimes \sigma_{im1}^x + B_{im2} \otimes \sigma_{im2}^x + B_{im3} \otimes \sigma_{im3}^x) \} \end{aligned} \quad (18)$$

where the Pauli matrices in the last sum act on the ancilla qubits. Each term in the sum involving three ancillae is a three-qubit gadget. In summary, our total Hamiltonian is $H_{anc} + H(0) + \sum_i V'(s_i)$, and the error introduced in this 2-local approximation at each time step is $O(\delta)$.

To check that Σ_- satisfies Eq. (15), put $H_2 = H_{anc}$, $V_2 = V'(s_i)$, and expand Σ_- as

$$\begin{aligned} \Sigma_-(z) &= V_{--} + (z - \Delta)^{-1} V_{-+} V_{+-} + (z - \Delta)^{-2} V_{-+} V_{++} V_{+-} \\ &\quad + (z - \Delta)^{-3} V_{-+} V_{++} V_{+-} + \dots \end{aligned}$$

where Δ is the gap of H_2 and V_{+-} denotes the part of V_2 that couples the lower spectrum to the upper spectrum, etc. We can obtain, after some algebra,

$$\begin{aligned} \Sigma_-(z) &= Y_i \otimes I_{anc} - 6 \sum_{m=1}^M B_{im1} B_{im2} B_{im3} \otimes (\sigma_{im1}^x \otimes \sigma_{im2}^x \otimes \sigma_{im3}^x) \\ &\quad + O(\delta). \end{aligned} \quad (19) \quad \text{where}$$

Since the B 's are semipositive definite, the lowest eigenvalue is achieved when $\sigma_{im1}^x \otimes \sigma_{im2}^x \otimes \sigma_{im3}^x$ is replaced by 1 [i.e., the ancilla qubits are in $(|000\rangle + |111\rangle)/\sqrt{2}$; H_{anc} has restricted the ancilla qubits to be in the subspace spanned by $|000\rangle$ and $|111\rangle$], and we effectively recover $V(s_i)$. We can see that the purpose of those $\sigma_{im1\dots}$ terms is to enforce the product relation among the $\{B_{im1}, B_{im2}, B_{im3}\}$. Notice that the first excited state is also the same as in $V(s_i)$ because the B terms are positive definite, so if the ancilla qubits are in $(|000\rangle - |111\rangle)/\sqrt{2}$, the increase in energy will be more than that of the excited states due to the computational qubits.

Under what condition will this procedure be inefficient? Note that in Eq. (18), the original B_{im1} terms are multiplied by δ^{-2} . The local reduction requires the approximating terms to be very large compared to other terms in the Hamiltonian. If reduction is later applied repeatedly to terms coupling to ancilla qubits from the previous steps, the energy level required for the reduction scales exponentially. When we normalize the total energy to unity, this equivalently means the gap between the ground state and the first excited state shrinks exponentially. Such repeated approximation could be useful when we need to implement a shallow circuit with the noise-resistant properties of the adiabatic computation model and the restriction of 2-local interaction. For example, in conjunction with teleportation circuits, the repeated approximation may not be necessary as we can teleport many independently and adiabatically prepared unitary operations. For a generally efficient mapping, we would need either a procedure that directly reduces an n -local Hamiltonian to a 2-local approximation, subjected to the constraints described in Sec. IV, or some kind of adaptive mapping that exploit structures of specific circuits.

In the next section, we will see how similar repeated use of the three-qubit gadget can give rise to an efficient adiabatic algorithm once we relax the model.

VI. GENERALIZED ADIABATIC ALGORITHMS AND HOLONOMIC QUANTUM COMPUTING

As mentioned in the Introduction, if we are willing to relax the property that the Hamiltonian keeps track exactly what the correct state is, we will have more freedom to design the Hamiltonian. Going back to the construction in Sec. I, it is clear that we need different Hamiltonians for the *same* quantum gate at different stages of the computation. Yet we know that the unitary transformation due to the application of a time-dependent Hamiltonian over a period of time, $U = \mathcal{T} \exp[i \int_0^T H(t) dt]$ is independent of the state, so why do we need different Hamiltonians for different stages? The reason is that we have so far ignored the phases of the transformation due to the adiabatic evolution. The phases include both dynamical and geometric components:

$$\phi_n(T) = \exp \left(-i \int_0^T E_n(t) dt + i \gamma_n(T) \right) \quad (20)$$

$$\gamma_n(T) = i \int_0^T \langle n, t | \frac{d}{dt} | n, t \rangle dt \quad (21)$$

is the geometric phase¹ and $E_n(t)$, $|n, t\rangle$ are the eigenvalues and eigenvectors of $H(t)$. Therefore, if we naively apply $U(t)H_0U^\dagger(t)$ to a state $|\psi\rangle$ without making sure that $|\psi\rangle$ is an eigenstate of H_0 , relative phases can develop between the eigenstates superposed to form $|\psi\rangle$. It is not difficult to cancel out the relative dynamical phases—all we need to do is to apply $-H_0$ for the same period of time (or modulo 2π). For the geometric phases, they are often ignored in an open-path evolution since they can be gauged away by choosing a different set of basis. However, the moment we decompose $|\psi\rangle$ into eigenstates of $H(0)$, the gauge is fixed; if we choose a different set of basis at some other time, we would not obtain $U|\psi\rangle$ at the end. Therefore the open-path geometric phase must be taken into account and cancelled accordingly. This gives rise to the following partially adiabatic algorithm.

- To apply two-qubit gate U from a circuit,
 - (1) pick a simple, 1-local Hamiltonian H_0 , $\|H_0\| \leq 1$;
 - (2) apply the $\frac{1}{2}[I + U(t)H_0U(t)^\dagger]$ at any rate from $t=0$ to T ; $U(0)=I$ and $U(T)=U$;
 - (3) calculate G such that $G|n\rangle = \gamma_n|n\rangle$;
 - (4) apply $\frac{1}{2}(I - H_0 + 2G/T)$ for time T .

This algorithm, of course, does not enjoy property II for all time because of step 4. But if we make good use of the transformation due to the geometric phase, such that, for example, $e^{iG}U(T) = U$ [which is nontrivial to solve since G depends on the path $U(t)$], the G term can be dropped from step 4, and the cancellation can be greatly simplified—in fact the cancellation would be the same whatever gate we want to implement.

This is also reminiscent of the geometric quantum computation model [9], which uses the Abelian geometric phase to implement each gate and requires the cancellation of dynamical phases. The difference is that our algorithm uses an open path and thus involves nongeometric components.

Next let us consider how we can avoid having to cancel the phases. This is only possible if any state we want to apply the quantum gate on is an eigenstate of H_0 . But Sec. IV tells us this state cannot be a unique eigenstate without H_0 becoming n -local in general, so we will have to deal with degenerate states. Without any knowledge about the state, we would have to make all 2^n n -qubit states degenerate—but this means that H_0 acts trivially on all qubits. The dilemma is solved by adding ancilla qubits—we can arrive at a nontrivial $U(t)H_0U(t)^\dagger$ if $U(t)$ couples between the computational qubits and the ancilla qubits. Notice that $U(0)H_0U(0)^\dagger = U(T)H_0U(T)$ since both are trivial on computational qubits, so the Hamiltonian goes through a cycle. All the relative phases are accumulated between states corresponding to the ancilla qubits and do not affect our calcula-

tion. We have thus arrived at the holonomic quantum computation model [7].

In order to have a nontrivial control manifold, we can use qubits with states $|0\rangle$ and $|1\rangle$ as the usual qubit states and $|2\rangle$ for control, or we can add ancilla qubits. In general, identifying the manifold that has the right holonomy group and finding the path for each two-qubit transformation in the circuit model is very difficult. Recently, Tanimura *et al.* [14] settled the mathematical question of finding a shortest path given an arbitrary holonomy group element in a homogeneous bundle, which implies that with the addition of just one ancilla qubit, we can implement any two-qubit transformation in the space of computational states. Let us consider the implementation of a CNOT gate as an example of this result. Take the Hamiltonian on the ancilla qubit to be

$$H_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}.$$

We can write the time-dependent Hamiltonian, including the two qubits to be transformed, as

$$H(t) = E_1 e^{tX} V_1 V_1^\dagger e^{-tX} + E_0 e^{tX} V_0 V_0^\dagger e^{-tX}, \quad t \in [0, 1], \quad (22)$$

where V_0, V_1 are 8×4 matrices:

$$V_0 = \begin{pmatrix} I_4 & \\ & \end{pmatrix}, \quad V_1 = \begin{pmatrix} 0 & \\ & I_4 \end{pmatrix}.$$

I_4 denotes the 4×4 identity matrix. We start by preparing the ancilla qubit in the ground state E_0 . To implement a CNOT gate optimally, [14] found X to be:

$$X = \begin{pmatrix} A & B \\ -B^\dagger & 0 \end{pmatrix}$$

where A and B are

$$A = i\pi \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad B = \frac{i\pi}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We can see that the Hamiltonian only acts on the two computational qubits and the one ancilla qubit, so other computational qubits are not affected at all. To do the same computation using 2-local Hamiltonians, we can now apply the three-qubit gadgets of [4] described earlier. At the end of each cycle, unlike the case in Sec. V, the ancilla qubits for the reduction can be discarded and reused in the next step. The total number of ancilla qubits required is three times the number of terms in $\sum_m B_{im1} B_{im2} B_{im3}$ of Eq. (17), which is a constant. Following the same analysis, if we want the final state to be accurate up to $O(\epsilon)$, the allowed error at each step should be $O(\epsilon/L^2)$ where L is the depth of the circuit. The energy gap required is thus $O(\epsilon^3/L^6)$ and the running time is $O(L^{12}/\epsilon^6)$. Note that this bound may be far from tight, and it is quite possible that most circuits can be implemented in far shorter time. In any case, we have arrived at a fully adiabatic evolution that computes efficiently any problem solvable by

¹This is not a closed path and thus is not gauge invariant, as pointed out in [13]. We will nonetheless keep the terminology. To readers unfamiliar with Berry's phase, the word "gauge" here refers to the $U(1)$ degree of freedom associated with a normalized eigenvector in the Hilbert space.

quantum circuit using only 2-local Hamiltonians and a constant number of ancilla qubits.

VII. CONNECTION TO THE HISTORY APPROACH

Comparing the above running time estimate to the results in [3,4], which we will refer to as the history approach, it appears that the latter still seems superior even though it produces the entire history of the computation instead of only the final output. [This just means one has to repeat the process $O(L)$ times to get the final output or put in identity gates.] It is natural to ask what is special about this approach and how it is related to the models we have studied. For a circuit of n qubits and L gates, the history approach has the following final state:

$$|\psi_{final}\rangle = \frac{1}{\sqrt{L+1}} \sum_{l=0}^L U_l U_{l-1} \cdots |0\rangle \otimes |1^{l0^{L-l}}\rangle^c \quad (23)$$

where $|1^{l0^{L-l}}\rangle^c$ denotes the state of L ancilla qubits serving as a clock. We refer the readers to [3] for the general form of the 3-local Hamiltonian which has the above state as its unique ground state. Let us just look at the simplest example—a circuit with one two-qubit gate U and n computational qubits. The initial and final states are

$$|\psi_{ini}\rangle = |0\rangle \otimes |0\rangle^c, \quad (24)$$

$$|\psi_{final}\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |0\rangle^c + U|0\rangle \otimes |1\rangle^c), \quad (25)$$

where one ancilla qubit suffices for the clock. The corresponding Hamiltonians are

$$H_{ini} = |1\rangle\langle 1|^c, \quad (26)$$

$$H_{out} = \frac{1}{2}(I \otimes |0\rangle\langle 0|^c + I \otimes |1\rangle\langle 1|^c - U \otimes |1\rangle\langle 0|^c - U^\dagger \otimes |0\rangle\langle 1|^c). \quad (27)$$

Actually we have deliberately omitted a term

$$\sum_n |1\rangle\langle 1| \otimes |0\rangle\langle 0|^c$$

that would make $|\psi_{ini}\rangle$ the unique ground state of H_{ini} . This does not change our analysis as long as we prepare the state in $|\psi_{ini}\rangle$ at the beginning. In [3] this is the H_{input} term, which does not affect the evolution equation because it remains zero for all time. Aharonov *et al.* show—for this case, trivially—that slowly interpolating from H_{ini} to H_{final} takes $|\psi_{ini}\rangle$ to $|\psi_{final}\rangle$. Notice that the Hamiltonians are highly degenerate in the sense that if we replace $|\psi_{ini}\rangle$ and $|\psi_{final}\rangle$ by

$$|\psi'_{ini}\rangle = V|0\rangle \otimes |0\rangle^c, \quad (28)$$

$$|\psi'_{final}\rangle = \frac{1}{\sqrt{2}}(V|0\rangle \otimes |0\rangle^c + UV|0\rangle \otimes |1\rangle^c) \quad (29)$$

for some $U(n)$ unitary operator V , the same analysis will go through. This gauge freedom is already reminiscent of HQC;

let us make the connection more explicit. Define the time-dependent Hamiltonian

$$H(t) = \frac{1}{2}[P(t)I \otimes |0\rangle\langle 0|^c + Q(t)I \otimes |1\rangle\langle 1|^c - R(t)U \otimes |1\rangle\langle 0|^c - R(t)U^\dagger \otimes |0\rangle\langle 1|^c] \quad (30)$$

such that $P=R=0$, $Q=2$ gives H_{ini} and $P=Q=R=1$ gives H_{final} . It is easy to see that

$$|\psi(t)\rangle = \{\text{normalization}\}[\alpha(t)|0\rangle \otimes |0\rangle^c + \beta(t)U|0\rangle \otimes |1\rangle^c] \quad (31)$$

is a ground state as long as $PQ=R^2$ and $P\alpha=R\beta$. Suppose we have completed the original evolution and obtained $|\psi_{final}\rangle$ ($\alpha, \beta=1$), but decided to keep going. We can slowly change from $P=Q=R=1$ to $P=2$, $Q=R=0$ while maintaining $PQ=R^2$ (this helps to keep a large gap), and we would arrive at $U|0\rangle \otimes |1\rangle^c$ ($\alpha=0, \beta=1$). This is essentially a holonomic cycle if we adiabatically rotate the clock qubit back to $|0\rangle^c$. In practice we can just relabel the clock qubit if we want to do this repeatedly.

This gives rise to the interpretation that the history approach is in fact half of a holonomic cycle. The cycle we have just shown is very similar to the CNOT example in Sec. VI, as it requires a 3-local Hamiltonian, which too can be reduced by the three-qubit gadget, and one ancilla qubit; it is merely a different path in the control manifold. Repeated application of the gadget allows efficient universal quantum computing, as described in Sec. VI.

We can take this further and interpret the history approach for L quantum gates as part of a holonomic cycle with a control manifold augmented with the space of L ancilla qubits. For the 3-local Hamiltonian case, this is not difficult to see. Suppose we have starting Hamiltonian H_i and final Hamiltonian H_f , such that linear adiabatic evolution takes the starting state

$$\psi_i = |0\rangle \otimes |0\rangle^c \quad (32)$$

to

$$\psi_f = \frac{1}{\sqrt{L+1}} \sum_{i=0, \dots, L} U_i \cdots U_0 |0\rangle \otimes |i\rangle^c \quad (33)$$

where $U_0=1$ and we have simplified the notation for the clock. These Hamiltonians can be constructed according to [3], except we omit the term $H_{input} = \sum_i |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|^c$ so that we preserve the gauge freedom mentioned above. This does not affect the adiabatic evolution because the Hamiltonian does not couple between the degenerate spaces. Now we can similarly construct another pair of Hamiltonians H'_i and H'_f corresponding to a reverse circuit $U_L^\dagger, U_{L-1}^\dagger, \dots$ such that it takes

$$\psi'_i = U_L \cdots U_0 |0\rangle \otimes |0\rangle^c \quad (34)$$

to

$$\psi'_f = \frac{1}{\sqrt{L+1}} \sum_{i=0, \dots, L} U_{L-i} \cdots U_0 |0\rangle \otimes |i\rangle^c. \quad (35)$$

Simple inspection shows that ψ_f and ψ'_f are the same up to relabeling of clock qubits. Therefore, if we implement the evolution $H_i \rightarrow H_f(H'_i) \rightarrow H'_i$ up to relabeled clocks, we can take

$$\psi_i = |0\rangle \otimes |0\rangle^c \quad (36)$$

to

$$\psi'_i = U_L \cdots U_0 |0\rangle \otimes |0\rangle^c \quad (37)$$

and thus complete a holonomic implementation of the L gates. This opens up the possibility of further optimizing the path; a more complete analysis is left for the future.

VIII. DISCUSSION

We have looked at various forms of adiabatic quantum computation and studied their resource requirements as well as possible approximations. One issue we have not addressed at all is what noise-resistant properties different models can have. It would appear that the direct, nonholonomic approach in Sec. II places stronger conditions on the states, as any deviation requires higher energy, whereas the degenerate states in the holonomic approach have no protection against transition within the degenerate level. This generalization may, however, be simplistic; a better analysis should be with respect to particular experimental implementations. We simply hope that this paper has provided a more unifying picture of adiabatic algorithms that will eventually lead to a toolbox experimentalists can refer to for different specific applications.

There are at least a few directions for further studies. (1) In Sec. II we constructed an adiabatic equivalent of any arbitrary circuit. What remain unclear are the general proper-

ties of such Hamiltonians, namely, those of the form UH_0U^\dagger where H_0 is a simple Hamiltonian and U is a polynomial-sized circuit. If it is n -local, in what sense is it simpler than the most general Hamiltonian? Are there things about a circuit that we can learn through this corresponding Hamiltonian? (2) We discussed in Sec. IV various constraints on approximating UH_0U^\dagger with k -local terms. The general picture is still unclear; it would be useful to understand precisely under what condition an n -local Hamiltonian can be approximated by a 2-local one. (3) We have proposed one partially adiabatic algorithm in Sec. VI and we have suggested that the adiabatic construction in Sec. V could be useful as a small section of a larger algorithm. It is interesting to investigate what merits, if any, these partially adiabatic algorithms possess. (4) For HQC, there should be room for improvement. If we implement one two-qubit gate at a time, it is important to see how the use of three-qubit gadget can be optimized and how a tighter bound on the evolution time can be obtained. At the same time, the history approach discussed in Sec. VII may lead to a further class of HQC methods that implement many gates together efficiently. (5) In order to build an efficient computation model using only 2-local Hamiltonian and adiabatic evolution, we have been naturally led to the use of non-Abelian geometric phase. The use of holonomy, however, may not be the only option. For example, open-path non-Abelian geometric phase [15] can be nontrivial as well and may lead to further ways of implementing multiple qubit gates. These questions are beyond the scope of this paper, and we believe that adiabatic quantum computing remains an exciting area to explore.

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