Quantum Speedup by Quantum Annealing

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We study the glued-trees problem of Childs, et. al. [1] in the adiabatic model of quantum computing and provide an annealing schedule to solve an oracular problem exponentially faster than classically possible. The Hamiltonians involved in the quantum annealing do not suffer from the so-called sign problem. Unlike the typical scenario, our schedule is efficient even though the minimum energy gap of the Hamiltonians is exponentially small in the problem size. We discuss generalizations based on initial-state randomization to avoid some slowdowns in adiabatic quantum computing due to small gaps.

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Quantum annealing is a powerful heuristic to solve problems in optimization [2, 3]. In quantum computing, the method consists of preparing a low-energy or ground state $|\psi\rangle$ of a quantum system such that, after a simple measurement, the optimal solution is obtained with large probability. $|\psi\rangle$ is prepared by following a particular annealing schedule, with a parametrized Hamiltonian path subject to initial and final conditions. A ground state of the initial Hamiltonian is then transformed to $|\psi\rangle$ by varying the parameter slowly. In contrast to more general quantum adiabatic state transformations, the Hamiltonians along the path in quantum annealing are termed *stoquastic* and do not suffer from the so-called *numerical sign problem* [4]: for a specified basis, the off-diagonal Hamiltonian-matrix entries are nonpositive [5]. This property is useful for classical simulations [3].

A sufficient condition for convergence of the quantum method is given by the quantum adiabatic approximation. It asserts that, if the rate of change of the Hamiltonian scales with the energy gap Δ between their two lowest-energy states, $|\psi\rangle$ can be prepared with controlled accuracy [6, 7]. Such an approximation may also be necessary [8]. However, it could result in undesired overheads if Δ is small but transitions between the lowest-energy states are forbidden due to selection rules, or if transitions between lowest-energy states can be exploited to prepare $|\psi\rangle$. The latter case corresponds to the annealing schedule in this Letter. It turns out that the *relevant* energy gap for the adiabatic approximation in these cases is not Δ and can be much bigger.

Because of the properties of the Hamiltonians, the annealing can also be simulated using probabilistic classical methods such as quantum Monte-Carlo (QMC) [9]. The goal in QMC is to sample according to the distribution of the ground state, i.e. with probabilities coming from amplitudes squared. While we lack of necessary conditions that guarantee convergence, the power of QMC is widely recognized [3, 9, 10]. In fact, if the Hamiltonians satisfy an additional frustration-free property, efficient QMC simulations for quantum annealing exist [11, 12]. An important open question is whether a quantum-computer simulation of general quantum annealing processes can ever be done using substantially less resources than QMC or other classical simulation.

In this Letter, we answer this question in the affirmative: We provide an oracular problem and give a simple and *natural* quantum-annealing schedule that, on a quantum computer, prepares a quantum state $|\psi\rangle$ encoding the solution. The time required to prepare $|\psi\rangle$ is polynomial in the problem size, herein $\mathrm{poly}(n)$. The oracular problem was first introduced in Ref. [1] in the context of quantum walks, where it was also shown that no classical method can give the solution using $\mathrm{poly}(n)$ number of oracle calls. Thus, our result places a limit on the power of classical methods that simulate quantum evolutions.

We do not answer the general question of existence of efficient classical simulations when Δ is $1/\mathrm{poly}(n)$. The annealing schedule we provide is not intended to follow the ground state in the path; diabatic transitions to the closest (first-excited) eigenstate are allowed. Nevertheless, the system (almost) remains in the subspace spanned by these two states at all times. There are regions in the path where $\Delta \propto \exp(-n)$. We induce transitions in that subspace by choosing an annealing rate that is much larger than Δ, i.e. at $1/\mathrm{poly}(n)$ rates. Contrary to the typical case, such transitions are useful here. They guarantee the preparation of $|\psi\rangle$ due to a symmetry argument: The same type of transition that transforms the ground into the first-excited state, later transforms the first-excited into the final ground state $|\psi\rangle$. The extent of this argument goes beyond the problem considered in this Letter and may be used as an alternative for those problems in which the quantum adiabatic algorithm fails due to small gaps.

In more detail, the oracular problem from Ref. [1] is as follows. We are given an oracle that consists of the adjacency matrix A of two binary trees that are randomly *glued* (by a random cycle) as in Fig 1. There are $N \in \mathcal{O}(2^n)$ vertices named with randomly chosen $2n$-bit strings. The oracle outputs the names of the adjacent vertices on any given input vertex name. There are two special vertices, ENTRANCE and EXIT – the roots of the binary trees. They can be identified because they are the only vertices of degree two in the graph. The *Glued-Trees* problem is: Given an oracle A for the graph and the name of the ENTRANCE, find the name of the EXIT.

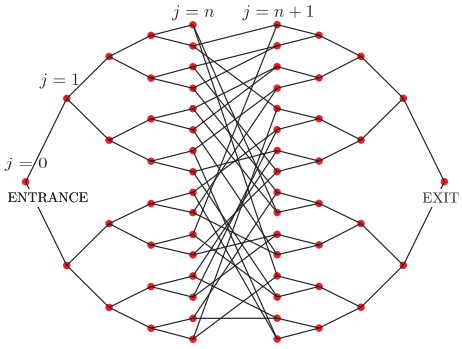

FIG. 1: Two binary trees of depth $n = 4$ glued randomly. The number of vertices is $N = 2^{n+2} - 2$. Each vertex is labeled with a randomly chosen $2n$-bit string. j is the column number.

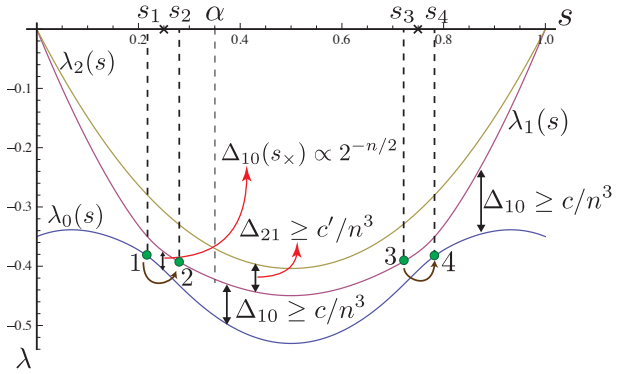

FIG. 2: The three lowest eigenvalues of $H(s)$ in the subspace $\{|\mathrm{col}\rangle_j\}_j$, for $\alpha = 1/\sqrt{8}$ and $n = 10$. $\Delta_{jk} = \lambda_j - \lambda_k$ is the gap between the j-th and k-th eigenstates, respectively. We divide the evolution in five stages according to s_1, s_2, s_3, and s_4 [see text after Eq. (5)], with $s_1 < s_\times = \alpha/\sqrt{2} = 0.25 < s_2$ and $s_3 = 1 - s_2 < 1 - s_\times < s_4 = 1 - s_1$. Inside $[s_1, s_2]$ and $[s_3, s_4]$, the gap Δ_{10} becomes exponentially small in n. Elsewhere, Δ_{10} is only polynomially small in n. Brown arrows $1 \to 2$ and $3 \to 4$ depict level transitions for an annealing rate in which $\dot{s}(t) \propto 1/\mathrm{poly}(n)$.

An efficient method based on quantum walks can solve this problem with constant probability, while no classical algorithm that uses less than a subexponential (in n) number of oracles exists [1]. Still, a quantum annealing method that uses simple and stoquastic Hamiltonians remained unknown. We will then present a quantum annealing approach that efficiently outputs the name of the EXIT with arbitrarily high probability, c.f. [7, 13].

We assume a Hamiltonian version of the oracle so that evolutions under A can be implemented. We also allow for evolutions under H_0 and H_1, these being the diagonal Hamiltonians that distinguish the ENTRANCE and EXIT, respectively. Such evolutions can be realized efficiently [14], i.e. using $\mathcal{O}(T)$ oracles for evolution time $T > 0$. We let $a(V) \in \{0,1\}^{2n}$ be the name of vertex V. Then, $H_0 |a'\rangle = -\delta_{a(\mathrm{ENTRANCE}),a'} |a'\rangle$ and $H_1 |a'\rangle = -\delta_{a(\mathrm{EXIT}),a'} |a'\rangle$, so that their ground states encode $a(\mathrm{ENTRANCE})$ and $a(\mathrm{EXIT})$, respectively. The Hamiltonian path for the annealing will consist of a specific interpolation involving H_0, A, and H_1.

The (orthonormal) states

$$|\mathrm{col}_j\rangle = \frac{1}{\sqrt{N_j}} \sum_{i \in j\mathrm{th\ column}} |a(i)\rangle \ . \tag{1}$$

will be useful [1]. These are uniform-superposition states over all states labeled by the names of vertices at the $j-$th column. $N_j = 2^j$ for $0 \le j \le n$ and $N_j = 2^{2n+1-j}$ for $n+1 \le j \le 2n+1$; see Fig. 1. In particular, $|\mathrm{col}_0\rangle = |a(\mathrm{ENTRANCE})\rangle$ and $|\mathrm{col}_{2n+1}\rangle = |a(\mathrm{EXIT})\rangle$. The subspace spanned by $\{|\mathrm{col}_j\rangle\}_{0 \le j \le 2n+1}$ is then invariant under the action of A, H_0, and H_1. In the basis determined by Eqs. (1), A has non-zero matrix elements in its first off-diagonals only. For simplicity, we redefine $A \leftarrow \sqrt{2}A$ so that the matrix elements are

$$\langle \mathrm{col}_j | A | \mathrm{col}_{j+1} \rangle = \begin{cases} \sqrt{2} & j = n \\ 1 & \text{otherwise.} \end{cases} \tag{2}$$

Also, $\langle \mathrm{col}_j | H_0 | \mathrm{col}_j \rangle = -\delta_{j,0}$ and $\langle \mathrm{col}_j | H_1 | \mathrm{col}_j \rangle = -\delta_{j,2n+1}$.

We choose the Hamiltonian path

$$H(s) = (1-s)\alpha H_0 - s(1-s)A + s\alpha H_1 \tag{3}$$

that interpolates between H_0 and H_1 for $0 \le s \le 1$. The parameter α is independent of n and satisfies $0 < \alpha < 1/2$. $H(s)$ corresponds to a perturbed tight-binding model in physics. We will show that annealing at a rate $\dot{s}(t) \propto 1/\mathrm{poly}(n)$, the resulting evolution transforms $|a(\mathrm{ENTRANCE})\rangle$ to a state that has arbitrarily high overlap with $|a(\mathrm{EXIT})\rangle$.

Spectral properties— We use the spectral properties of $H(s)$ to prove the efficiency of the quantum method; particularly relevant are the spectral gaps. The following analysis is valid if we restrict to the invariant subspace spanned by $\{|\mathrm{col}_j\rangle\}_j$. Figure 2 shows the three lowest eigenvalues of $H(s)$, obtained numerically, in this subspace. This suggests a particular eigenvalue behavior. We can analytically study the Hamiltonians by proposing the *ansatz* $|\phi\rangle = \sum_j \gamma_j |\mathrm{col}_j\rangle$, with

$$\begin{aligned} \gamma_j &= a e^{ipj} + b e^{-ipj} \ , \ 0 \le j \le n \ , \\ \gamma_j &= c e^{ip(2n+1-j)} + d e^{-ip(2n+1-j)} \ , \ n+1 \le j \le 2n+1 \ , \end{aligned} \tag{4}$$

and $p \in \mathbb{C}$. The eigenvalue condition $H|\phi\rangle = \lambda |\phi\rangle$ and $\langle\phi|\,\phi\rangle = 1$ allow us to find expressions for a, b, c, d, and λ. The resulting eigenvalues are $\lambda = -2s(1-s)\cos p$. We provide a detailed analysis of the spectrum in Supp. Mat. and present only the relevant results here. Because of the $s \leftrightarrow (1-s)$ symmetry, it suffices to analyze the parameter region $s \in [0, 1/2]$.

In the following, $x \approx_\theta y$ if $|x - y| \le \theta$ and $\theta \ge 0$. When $n \to \infty$, the two lowest eigenvalues cross, or become equal, at $s = s_\times = \alpha/\sqrt{2}$. Different eigenvalue

behavior is obtained at both sides of $s_\times$. For $n < \infty$ and $0 \le s \le s_\times$, the spectral gap between the two lowest eigenvalues is

$$\begin{aligned}\Delta_{10}(s) &= \lambda_1(s) - \lambda_0(s) \\ &\approx_\epsilon -(1-s)\left(\frac{3s}{\sqrt{2}} - \frac{\alpha^2+s^2}{\alpha}\right) , \end{aligned} \tag{5}$$

with $\epsilon \in \mathcal{O}(2^{-n/2})$. The eigenvalue crossing is avoided for $n < \infty$ and $\Delta_{10}(s)$ is exponentially small in n near $s_\times$. This finite-size gap behavior is typical for *avoided crossings* in which eigenstates rapidly change as a function of s. In addition, Eq. (5) gives $\Delta_{10}(s) \ge c/n^3$ for $0 \le s \le s_1 = s_\times - \delta$ and $s_2 = s_\times + \delta \le s \le 1/2$, with $\delta \in \Omega(1/n^3)$.

The second excited state has an eigenvalue that corresponds to $p \approx_\nu \pi/(n+1)$, with $\nu \in \mathcal{O}(1/(n+1)^2)$. These eigenvalues reflect the relationship between $H(s)$ an the tight-binding model. The spectral gap between the first and second excited state for $0 \le s \le \alpha$ is then

$$\begin{aligned}\Delta_{21}(s) &= \lambda_2(s) - \lambda_1(s) \\ &\approx_{\epsilon/2+\nu} -s(1-s)\left(\cos\left(\frac{\pi}{n+1}\right) - \frac{3}{\sqrt{2}}\right) . \end{aligned} \tag{6}$$

In particular, $\Delta_{21}(s) \in \Omega(1)$ in the region $s_1 \le s \le \alpha$.

For $\alpha \le s \le 1/2$, the second eigenvalue also corresponds to $p \approx_\nu \pi/(n+1)$. To bound the gap with the third eigenvalue, a more detailed analysis that approximates p at order $1/(n+1)^2$ is carried in the Supp. Mat.. It results in $\Delta_{21}(s) \ge c'/n^3$, for some $c' > 0$ (see Fig. 2).

Annealing schedules— We use the following adiabatic approximation from Refs. [6]: Let the initial state be an eigenstate of $H(s_0)$ and $\Delta(s)$ the spectral gap to the nearest (non-degenerate) eigenstate in some region $s_0 \le s \le s_f$. Then, an annealing rate of $\dot{s}(t) \propto \varepsilon\Delta^2(s)$ or smaller suffices to prepare the eigenstate of $H(s_f)$ at error amplitude smaller than $\sqrt{\varepsilon(s_f - s_0)}$; i.e. the overlap between the evolved state and the eigenstate is at least $\sqrt{1-\varepsilon(s_f-s_0)}$. (Better error scaling is possible [7, 13].) We assume that $0 < \varepsilon \ll 1$, and that ε is an arbitrary and small constant independent of n.

To prove that $\dot{s}(t) \propto \varepsilon/n^6$ suffices to solve the Glued-Trees problem with low error, we split the evolution according to $[0,1] = \bigcup_{i=1}^5 V_i$, with $V_1 = [0, s_1)$, $V_2 = [s_1, s_2)$, $V_3 = [s_2, s_3)$, $V_4 = [s_3, s_4)$, and $V_5 = [s_4, 1]$. The values of s_i were determined previously; see Fig. 2. We denote $|\phi_0(s)\rangle$ and $|\phi_1(s)\rangle$ the *instantaneous* ground and first-excited states, respectively. $|\phi_0(0)\rangle = |a(\text{ENTRANCE})\rangle$ and $|\phi_0(1)\rangle = |a(\text{EXIT})\rangle$ encodes the solution. $|\phi_0(s)\rangle$ is different for different values of s. Then, due to the gap bounds and the adiabatic approximation, the following transformations occur:

$$\begin{aligned} |\phi_0(0)\rangle &\to_{\sqrt{\varepsilon s_1}} |\phi_0(s_1)\rangle , \\ |\phi_1(s_2)\rangle &\to_{\sqrt{\varepsilon(s_3-s_2)}} |\phi_1(s_3)\rangle , \\ |\phi_0(s_4)\rangle &\to_{\sqrt{\varepsilon(1-s_4)}} |\phi_0(1)\rangle , \end{aligned} \tag{7}$$

where $\to_x$ indicates that the transformation occurred at error amplitude of order x.

Because $\Delta_{21}(s) \in \Omega(1)$ for $s \in V_2$, transformations between the ground or first-excited state and the second excited state occur with amplitude smaller than $\sqrt{\varepsilon}$. Thus, all relevant transitions in V_2 occur in the manifold spanned by $\{|\phi_0(s)\rangle, |\phi_1(s)\rangle\}$. For our annealing rate, the following *diabatic* transformations occur with low error amplitude (see below):

$$\begin{aligned} |\phi_0(s_1)\rangle &\to |\phi_1(s_2)\rangle , \\ |\phi_1(s_3)\rangle &\to |\phi_0(s_4)\rangle . \end{aligned} \tag{8}$$

To show that the approximation errors for Eqs. (8) are small, we introduce the state $|u\rangle$ – the uniform superposition over all vertex names:

$$|u\rangle = \frac{1}{\sqrt{N}} \sum_{i \in \text{graph}} |a(i)\rangle = \sum_{j=0}^{2n+1} \sqrt{\frac{N_j}{N}} |\text{col}_j\rangle . \tag{9}$$

Here, $N_j = 2^j$ for $0 \le j \le n$ and $N_j = 2^{2n+1-j}$ for $n+1 \le j \le 2n+1$. Interestingly, $|u\rangle$ is *almost* an eigenstate for all s: $H(s)|u\rangle \approx_{\epsilon/2} -(s(1-s)3/\sqrt{2})|u\rangle$ and $\epsilon \in \mathcal{O}(2^{-n/2})$ – see Supp. Mat.. We define $f(t) = |\langle u|U(t)|u\rangle|^2$, where $U(t)$ is the evolution operator and $f(0) = 1$. Schrödinger's equation yields $\dot{f}(t) = -i\langle u|H(s(t))U(t)|u\rangle\langle u|U^\dagger(t)|u\rangle + c.c. \approx_\epsilon 0$. If $T \in \mathcal{O}(n^3/\varepsilon)$ is the time needed to change s from s_1 to s_2 with our annealing schedule (while $|s_2 - s_1| \in \Omega(1/n^3)$), we have $f(T) \approx_{\epsilon'} 1$ for $\epsilon' \in \mathcal{O}(2^{-n/2}n^3/\varepsilon)$. In addition, $|\langle u|\phi_1(s_1)\rangle| \approx_{\epsilon'} 1$ and $|\langle u|\phi_0(s_2)\rangle| \approx_{\epsilon'} 1$ – see Supp. Mat.. This results in $|\langle\phi_1(s_1)|U(T)|\phi_0(s_2)\rangle|^2 \approx_{5\epsilon'} 1$.

The transformation $|\phi_1(s_1)\rangle \to_{\sqrt{5\epsilon'}} |\phi_0(s_2)\rangle$ then occurs. Moreover, because $U(t)$ is unitary, we also have $|\phi_0(s_1)\rangle \to_{\sqrt{5\epsilon'}} |\phi_1(s_2)\rangle$ and, from symmetry arguments, $|\phi_1(s_3)\rangle \to_{\sqrt{5\epsilon'}} |\phi_0(s_4)\rangle$. These transitions of levels are shown in Fig. 2. Together with Eqs. (7), they prove the success of our quantum annealing method. When $2^{-n/2}n^3 \ll \varepsilon^2$, we have $\epsilon' \ll \varepsilon$ and the overall error amplitude is dominated by that of the adiabatic approximation in this case. This error is of order $\sqrt{\varepsilon} \ll 1$.

In Fig. 3 we show the overlaps between $U(t)|\phi_0(0)\rangle$ and the instantaneous ground and first-excited states, respectively, for our choice of $\dot{s}(t)$. It provides evidence for the diabatic transition among the two low energy levels.

Initial-state randomization: A generalization— In the Glued-Trees problem, all the interesting quantum dynamics occurred in the manifold given by the ground and first-excited states only. For more general problems, however, the relevant manifold may contain more eigenstates (e.g., due to initial ground state degeneracy). In this Sec. we build a randomization method that allow us to prepare the final ground state in these problems, with large probability, provided that some assumptions are met.

To this end, we consider again the Glued-Trees problem and the region $s \in [\chi, 1-\chi]$. Here, $\chi \in \mathcal{O}(1/n^3)$ and $\Delta_{21}(s) \ge c'/n^3$ for all s in the region – see Fig. 2. Then,

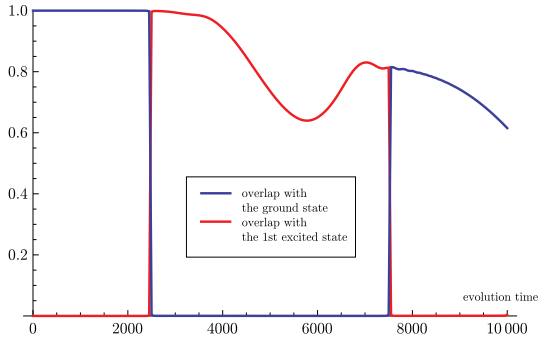

FIG. 3: Overlap of the evolved state $U(t)\,|a(\text{ENTRANCE})\rangle$ with the instantaneous ground (blue line) and first-excited (red line) states, $|\phi_0(s(t))\rangle$ and $|\phi_1(s(t))\rangle$, as a function of time. In this case, $n = 40$, $\alpha = 1/\sqrt{8}$, and $s(t) = t/10000$. We performed the simulation in the column subspace.

if we randomly prepare $|\phi_0(\chi)\rangle$ or $|\phi_1(\chi)\rangle$ and anneal using the schedule $\dot{s}(t) \propto \varepsilon/n^6$, the highly excited levels are effectively decoupled from the evolution. It implies that, when $s = 1-\chi$, the evolved state is (almost) the uniform combination of $|\phi_0(1-\chi)\rangle$ and $|\phi_1(1-\chi)\rangle$. Because χ is small for large n, and since $|\phi_1(\chi)\rangle \approx |u\rangle$, the method also works if the initial state is sampled randomly from $\{|a(\text{ENTRANCE})\rangle\,, |u\rangle\}$. Such state preparation can be done efficiently. An advantage is that a full analysis of the low-energy spectrum is not needed to prove the success of the randomization method (at the expense of reducing the error probability on the state preparation to 1/2).

The randomization method can be generalized as follows. It is well-known that efficient quantum adiabatic transport within $k \geq 2$ eigenstates is possible if these eigenstates are at gaps $1/\text{poly}(n)$ from the rest [6, 7]. Then, if uniform sampling from the k initial eigenstates can be done efficiently, any of the final k eigenstates can be prepared efficiently with probability of order $1/k$. If k is not too big, the method works regardless of whether the k lowest eigenvalues have small gaps or cross.

General Hamiltonians will not satisfy the requirements on the gaps, but some physical models do. An example is the one-dimensional spin-1/2 Ising model in a transverse field. As the Ising coupling J is changed from 0 to $J \gg 1$, the two lowest eigenvalues have a spectral gap that decreases exponentially with the system size n. However, the third eigenvalue is always at a distance $1/\text{poly}(n)$ from the two lowest ones. This property is common for systems that undergo through a critical point and break a discrete symmetry. At the critical point, the eigenvalues satisfy a dispersion relation $E(q) \propto q^z$, where z is the dynamical exponent and q is the momentum. The values of q differ by multiples of $2\pi/n$ so that the gaps are $1/\text{poly}(n)$ in that point. At the phase with broken symmetry, only a few low eigenvalues are separated at constant gaps from the rest – see [16] for more details.

Discussion— We provided an oracular problem that can be solved efficiently by quantum annealing whereas exponential time is required for any classical method. We described why our algorithm works even when the gaps are exponentially small and showed a generalization of the method based on initial-state randomization. While results on efficient adiabatic quantum simulations of quantum circuits could also be used to prove an exponential quantum speedup in this case [15], the resulting Hamiltonians are rather complex and *not* stoquastic. The construction in Ref. [15] assumes a polynomially small gap; whether this assumption is necessary or not in general needs to be analyzed on a case by case basis.

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