Size Dependence of the Minimum Excitation Gap in the Quantum Adiabatic Algorithm

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We study the typical (median) value of the minimum gap in the quantum version of the exact cover problem using quantum Monte Carlo simulations, in order to understand the complexity of the quantum adiabatic algorithm for much larger sizes than before. For a range of sizes $N \leq 128$, where the classical Davis-Putnam algorithm shows exponential median complexity, the quantum adiabatic algorithm shows polynomial median complexity. The bottleneck of the algorithm is an isolated avoided-crossing point of a Landau-Zener type (collision between the two lowest energy levels only).

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There is considerable interest in finding optimization problems which could be solved much more efficiently by an eventual quantum computer than by a classical computer. An important class of classically intractable problems is the NP-hard category [1]. Many optimization problems of current interest have parameters which are random, and so each problem corresponds to a large number (possibly infinite) of "instances." The term NP-hard actually refers to the behavior of the computationally *hardest* instance, but, from a practical point of view, it is also of great interest to know how the time to solve a *typical* instance [2,3], the typical complexity, scales with problem size. Numerical studies of NP-hard problems show that this scaling is exponential in a broad class of problem parameters [2,3]. It would be a very important breakthrough to show that a quantum computer can solve the same class of problem instances of an NP-hard problem in less than exponential time.

In this Letter, we study the typical complexity as a function of system size for a particular quantum algorithm, the quantum adiabatic algorithm (QAA) proposed by Farhi *et al.* [4]. The idea is that one adds to a "problem" Hamiltonian $\mathcal{H}_{\rm P}$, whose ground state represents a solution of a classical optimization problem, a noncommuting "driver" Hamiltonian $\mathcal{H}_{\rm D}$, so the total Hamiltonian is

$$\mathcal{H}(\lambda) = (1-\lambda)\mathcal{H}_{\rm D} + \lambda\mathcal{H}_{\rm P}, \tag{1}$$

where $\lambda \equiv \lambda(t)$ is a *time-dependent* control parameter. For $\mathcal{H}_{\rm P}$ we are interested in binary optimization problems expressed in terms of classical Ising spins taking values ± 1 or, equivalently, in terms of the z components of the Pauli matrices for each spin $\hat{\sigma}_i^z$. The driver Hamiltonian is then simply $\mathcal{H}_{\rm D} = -\sum_{i=1}^{N} \hat{\sigma}_i^x$, where $\hat{\sigma}_i^x$ is the x-component Pauli matrix.

The control parameter $\lambda(t)$ is 0 at $t = 0$, so $\mathcal{H} = \mathcal{H}_{\rm D}$, which has a trivial ground state in which all 2^N basis states (in the $\hat{\sigma}^z$ basis) have equal amplitude. It then increases with t, reaching 1 at $t = \mathcal{T}$ ($\mathcal{T}$ is the run time or complexity of the algorithm), at which point $\mathcal{H} = \mathcal{H}_{\rm P}$. If the time evolution of $\lambda(t)$ is sufficiently slow, the process will be adiabatic. Hence, starting the system in the ground state of $\mathcal{H}_{\rm D}$ (all spins aligned along x), the system will end up in the classical ground state, which is what we want, with only a small probability of failure. An upper bound for the complexity of the QAA can be given [5,6], in terms of the eigenstates and eigenvalues of the Hamiltonian $\mathcal{H}\Phi_n = E_n\Phi_m$, by

$$\mathcal{T} \gg \hbar|\max_{\lambda} V_{10}(\lambda)|/(\Delta E_{\rm min})^2, \tag{2}$$

where $\Delta E_{\rm min}$ corresponds to the minimum of the first excitation gap $\Delta E_{\rm min} = \min_\lambda \Delta E(\lambda)$, with $\Delta E = E_1 - E_0$, and $V_{n0}(\lambda) = \langle\Psi_0|d\mathcal{H}/d\lambda|\Psi_n\rangle$. Typically, matrix elements of $\mathcal{H}$ scale as a low polynomial of a number of spins N and the question of whether the complexity $\mathcal{T}$ depends polynomially or exponentially with N depends on how the minimum gap $\Delta E_{\rm min}$ scales with N. The size dependence of the minimum gap will therefore be the central focus of this Letter.

It is difficult to study the typical complexity of the QAA *analytically* since λ^*, the value of λ at the minimum of the gap $\Delta E(\lambda)$, is different for each instance with fluctuations being $\mathcal{O}(N^{-1/2})$, so the ensemble averaging over random instances can be performed only *after* λ^* has been found for each case. In the original work of Farhi *et al.* [4], the complexity of the adiabatic algorithm was studied *numerically* by direct integration in time of the system with Hamiltonian $\mathcal{H}$. Since the size of the Hilbert space increases exponentially (it is of order 2^N), they were limited to very small sizes $N \lesssim 20$. Subsequently, Hogg [7] considered sizes up to $N = 24$. These early papers [4,7] found that the complexity of the algorithm scales as a roughly as N^2. However, this power law complexity may be an artifact of the very small sizes studied, so it is of great interest to determine whether the complexity continues to be polynomial for much larger sizes or whether a "crossover" to exponential complexity is seen. To investigate this ques-

tion, it is not possible to include all terms in the Hilbert space (as was done in the early work) since this becomes much too large. Here we use quantum Monte Carlo (QMC) simulations, with which we can study much larger sizes because only a *sampling* of the states is performed.

There have also been QMC simulations (see, e.g., Ref. [8] for a discussion) in which t in Eq. (1) is the number of Monte Carlo sweeps, and one estimates how the final excess energy (i.e., the energy above the ground state) varies with the *total* number of sweeps $\mathcal{T}$. However, this is a "fake" dynamics, which is not necessarily representative [8] of the real time unitary evolution guided by the Schrödinger equation. Therefore the computational complexity of such a procedure does not necessarily correspond to that of the quantum adiabatic algorithm [4].

To make a comparison with the earlier work, we study (essentially) the same model of $\mathcal{H}_{\mathrm{P}}$ used by Farhi *et al.* [4]. It corresponds to an exact cover problem, which is a particular version of a constraint satisfaction, a commonly studied problem in the NP-hard category. In exact cover there are N Ising spins and M "clauses," each of which involves three spins (chosen at random). The energy of a clause is zero if one spin is -1 and the other two are 1; otherwise, the energy is 1. Thus $\mathcal{H}_{\mathrm{P}}$ equals

$$\mathcal{H}_{\mathrm{P}} = \frac{1}{8}\sum_{\alpha=1}^{M}(5 - \hat{\sigma}^z_{\alpha_1} - \hat{\sigma}^z_{\alpha_2} - \hat{\sigma}^z_{\alpha_3} + \hat{\sigma}^z_{\alpha_1}\hat{\sigma}^z_{\alpha_2} + \hat{\sigma}^z_{\alpha_2}\hat{\sigma}^z_{\alpha_3} + \hat{\sigma}^z_{\alpha_3}\hat{\sigma}^z_{\alpha_1} + 3\hat{\sigma}^z_{\alpha_1}\hat{\sigma}^z_{\alpha_2}\hat{\sigma}^z_{\alpha_3}), \qquad (3)$$

where α_1, α_2, and α_3 are the three spins in clause α and the $\{\hat{\sigma}^z_i\}_{i=0}^{i=N}$ are Pauli matrices. In the absence of the driver Hamiltonian, the Pauli matrices can be replaced by classical Ising spins taking values ± 1. An instance has a "satisfying assignment" if there is at least one choice for the spins where the total energy is zero. As the ratio M/N is increased, there is a phase transition where the number of satisfying assignments goes to zero. The version used by Farhi *et al.* considers only instances with a *unique* satisfying assignment (USA); i.e., there is only *one* state with energy 0. This has the advantage that the gap $\Delta E(\lambda)$ is greater than zero in both limiting cases $\mathcal{H} = \mathcal{H}_{\mathrm{D}}$ and $\mathcal{H} = \mathcal{H}_{\mathrm{P}}$ but will have a minimum at an intermediate value $\lambda = \lambda^*$; see Fig. 1. The aim is to determine the size N dependence of the typical value of ΔE_{min}, averaged over many instances.

We generate instances with a USA as follows. For each size N, we take M clauses and prune off (i) isolated sites and (ii) clauses (think of them as triangles) which are only connected to other clauses at one corner, since these give a trivial degeneracy without changing the complexity. This leaves N' sites and M' clauses. Using the standard Davis-Putnam-Logemann-Loveland (DPLL) [9] algorithm, we then see if the remaining N' sites with M' clauses have a USA. For each N, we choose M to maximize the probability of finding a USA. Although the probability of finding a USA decreases exponentially with N, we have easily been able to find instances for N up to 256, and the values of M are shown in Table I. For the sizes which we will study by QMC simulations ($N \leq 128$), the DPLL algorithm clearly shows exponential complexity; see Fig. 2.

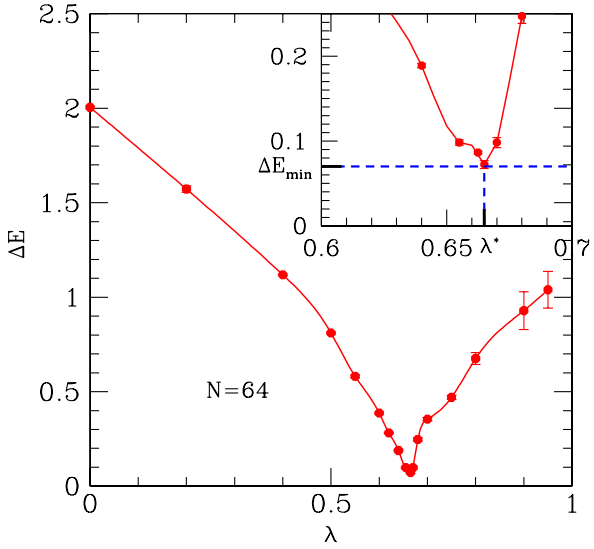

FIG. 1 (color online). QMC results for the gap between the ground state and the first excited state as a function of the control parameter λ for one instance with $N = 64$. The region around the minimum value of the gap ΔE_{min}, which occurs at $\lambda = \lambda^*$, is blown up in the inset.

For each instance, we use QMC calculations to simulate the quantum system in Eqs. (1) and (3) with N' spins and M' clauses. We simulate an effective classical model with Ising spins $\sigma^z_i(\tau) = \pm 1$ in which τ ($0 \leq \tau < \beta \equiv T^{-1}$) is imaginary time. In practice, imaginary time is discretized into L_τ "time slices" each representing $\Delta\tau = \beta/L_\tau$ of imaginary time. For a different model, the 1D Ising chain in a transverse field, we have verified numerically [11] that the scaling behavior of the energy gap [12] is the same for $\Delta\tau \to 0$ as for finite $\Delta\tau$, and hence it is plausible that a discrete $\Delta\tau$ will work here, too.

We calculate the time-dependent correlation function

$$C(\tau) = \frac{1}{N'L_\tau}\sum_{i=1}^{N'}\sum_{\tau_0=1}^{L_\tau}\langle\sigma^z_i(\tau_0+\tau)\sigma^z_i(\tau_0)\rangle, \qquad (4)$$

TABLE I. For sizes N up to 256, we show values of the number of clauses M for which the probability of a USA, constructed as described in the text, is maximized. The ratio M/N is denoted by α and is expected to approach the value at the quantum phase transition $\alpha_c \simeq 0.625$ [10] for $N \to \infty$. For the QMC simulations, we used only the sizes up to $N = 128$.

N	16	32	64	128	192	256
M	12	23	44	86	126	166
α	0.7500	0.7188	0.6875	0.6719	0.6563	0.6484

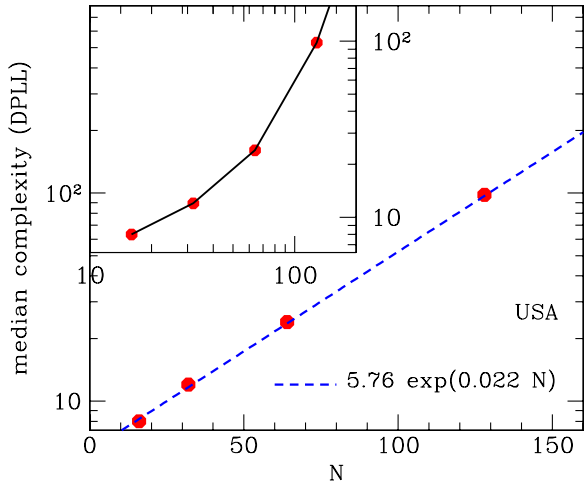

FIG. 2 (color online). A log-linear plot of the median complexity of the exact cover problem using the (classical) DPLL algorithm as a function of N. The straight line fit works well demonstrating that the complexity increases exponentially with N even for quite modest sizes. This figure is for samples with a USA, but the data for all samples (with the same number of clauses M) are very similar. The inset plots the same data on a log-log scale. The pronounced curvature shows that the data cannot be fitted to a power law.

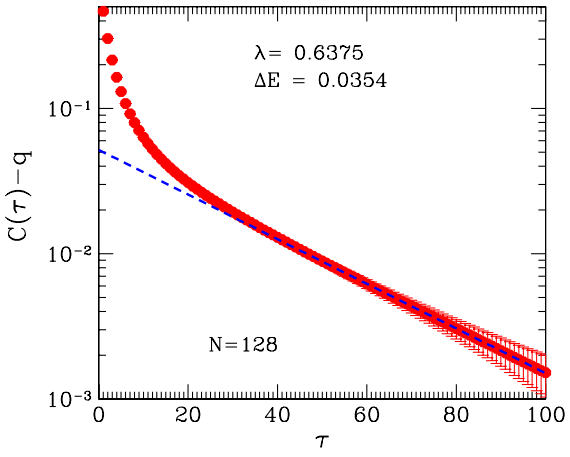

FIG. 3 (color online). A log-linear plot of the time-dependent correlation function for an instance with $N = 128$ near the minimum gap. The energy gap is the negative of the slope at large values of τ. The number of time slices was $L_\tau = 300$. The error bars were estimated by repeating the runs many (typically 100) times.

with $\Delta\tau = 1$ and L_τ large enough that $\beta\Delta E \gg 1$, so the system is in the ground state. For $\tau \ll \beta$, the correlation function $C(\tau)$ will be a sum of exponentials

$$C(\tau) = q + \sum_{n\geq 1} A_n \exp[-(E_n - E_0)\tau], \tag{5}$$

where the A_n are constants and q, the long time limit of the correlation function, is *determined* from

$$q = \frac{1}{N'}\sum_{i=1}^{N'}\left(\frac{1}{L_\tau}\sum_{\tau_0=1}^{L_\tau}\langle\sigma_i^z(\tau_0)\rangle\right)^2. \tag{6}$$

At large τ, the sum in Eq. (5) is dominated by the term corresponding to the first excited state ($n = 1$), and so ΔE can be obtained by fitting $\log[C(\tau) - q]$ against τ for large τ. Figure 3 shows such a fit for an instance with $N = 128$ near the minimum gap.

We determine $\Delta E_{\min}$, the *minimum* value of the gap (to the first excited state), as λ is varied. Figure 1 shows QMC results for the gap between the ground state and the first excited state as a function of the control parameter λ for one instance with $N = 64$. The inset shows more clearly the region of the minimum gap. The gap is greater than zero for both $\lambda = 0$ and 1 (a property of this model) and is much smaller at an intermediate value λ^* in the vicinity of the quantum phase transition. Each instance has to be carefully monitored to find the minimum gap, since λ^* is different for each instance.

For the largest size studied, $N = 128$, we found that for some instances it was difficult to determine q accurately for a range of λ, because the simulation was not fully equilibrated; the required number of sweeps increases rapidly with N. As a result, plots of $C(\tau) - q$ (see Fig. 3) were strongly curved. In a few cases, the error in the computed value of q was small, and the problem could be cured by allowing q to vary slightly away from the computed value when doing the fits. However, we did not trust this procedure if the correction to q was large. For the remaining 13 out of 50 instances, we were able to provide an upper bound for the minimum gap (from the range of λ where q was successfully computed), and this turned out to be less than our eventual estimate for the median gap. Hence, we were able to obtain reliable data for sizes up to $N = 128$. However, at present we are not able to study much larger sizes because of the difficulty in determining q.

Since we are interested in the *typical* minimum gap (among different instances) rather than the average (or smallest), we show in Fig. 4 the *median* of the minimum gap for $N \leq 128$. The main figure is a log-log plot, and the dashed line corresponds to the median $\Delta E_{\min}$ varying as $N^{-0.73}$. The pronounced curvature in the inset (log-linear plot) shows that the behavior is *not* exponential. The minimum gap therefore follows a power law for this range of sizes, implying polynomial complexity. This result is consistent with that found by Farhi *et al.* [4] and Hogg [7] for much smaller sizes ($N \lesssim 20$–24). Bañuls *et al.* [13] studied the QAA using matrix product states for sizes up to $N = 60$, but their result that the complexity becomes *independent* of size for $N \gtrsim 40$ is surprising and quite different from ours.

In addition to the energy gap $\Delta E(\lambda)$, we also investigated $-d^2E_0/d\lambda^2 = 2\sum_{m=1}^{2^N}|V_{0m}|^2/(E_m - E_0)$ since this

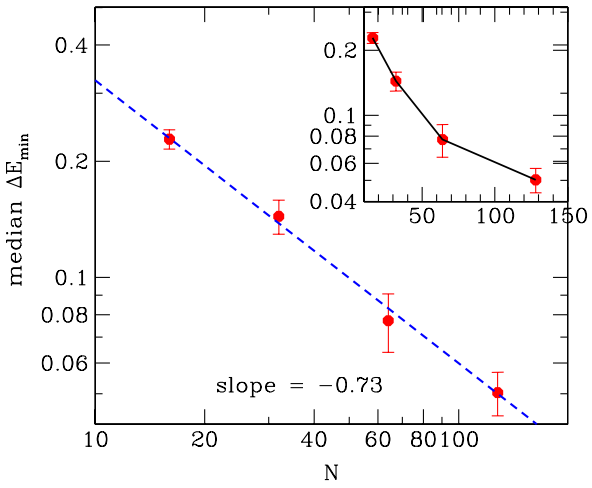

FIG. 4 (color online). A log-log plot of the median of the minimum gap as a function of the number of bits N up to $N = 128$. From the satisfactory straight line fit, it is seen that the median $\Delta E_{\min}$ decreases as a power law $N^{-\mu}$, with $\mu = 0.73 \pm 0.06$. The number of instances is 50 except for $N = 64$ for which it is 45. The inset shows a log-linear plot. The pronounced curvature shows that the behavior is not exponential for this range of sizes, in contrast to the classical DPLL algorithm, data for which are shown in Fig. 2.

gives additional information about matrix elements near the avoided-crossing point λ^*. We determined this from $\chi = \int_0^\beta \langle [\mathcal{H}_P(\tau)\mathcal{H}_P(0) - \langle \mathcal{H}_P \rangle^2] \rangle d\tau = -(1-\lambda)^2 d^2E_0/d\lambda^2$, finding that V_{0m} depends on N very weakly near $\lambda \simeq \lambda^*$. We also found that the location of the maximum of $-d^2E_0/d\lambda^2$ coincides to a good precision with λ^*; see Fig. 5. Hence the sum in the expression for $d^2E_0/d\lambda^2$ is dominated by its first term ($m = 1$) in the vicinity of the avoided crossing at λ^*, which is of the Landau-Zener

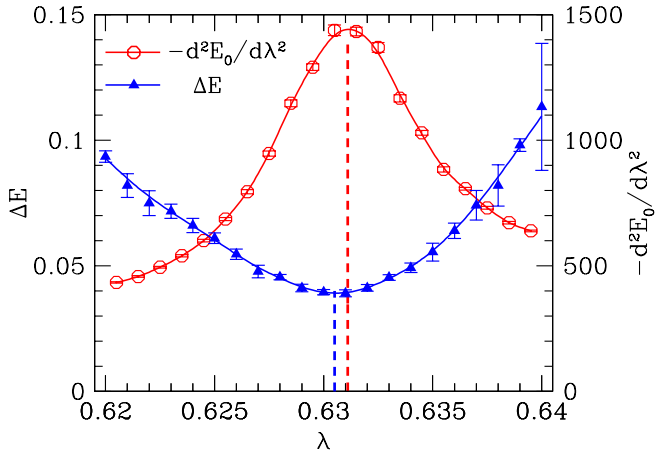

FIG. 5 (color online). The gap $\Delta E(\lambda)$ (blue) and $-d^2E_0/d\lambda^2$ (red) against λ for an instance with $N = 128$. Solid lines are cubic interpolations. The location of the minimum gap $\lambda^* = 0.6306$ is, within a margin of error, equal to the maximum of $-d^2E_0/d\lambda^2$ at $\lambda = 0.6311$ (both shown by vertical dashed lines).

type (collision of E_1 and E_0 levels only). This suggests that $\mathcal{T} = \hbar|V_{10}(\lambda^*)|/[\varepsilon(\Delta E_{\min})^2]$ is an accurate estimate for the algorithm complexity, where $\varepsilon \ll 1$ is an N-independent constant. As a result, $\mathcal{T} \sim N^{2\mu}$, where $\mu = 0.73 \pm 0.06$.

In conclusion, by using QMC simulations we have considerably extended the range of sizes over which the complexity of the QAA can be investigated. For sizes up to $N = 128$, where the benchmark classical algorithm for satisfiability problems (DPLL) shows exponential complexity, the QAA shows polynomial behavior of the *median* minimum gap and hence presumably polynomial behavior of the median complexity (contrast Fig. 4 with Fig. 2). However, our results for the median do not rule out the possibility that some instances have exponential complexity. We also found a Landau-Zener (pairwise) character of the avoided crossing at the minimum gap point.

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