First order phase transition in the Quantum Adiabatic Algorithm

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(Dated: January 19, 2010)

We simulate the quantum adiabatic algorithm (QAA) for the exact cover problem for sizes up to \( N = 256 \) using quantum Monte Carlo simulations incorporating parallel tempering. At large \( N \) we find that some instances have a discontinuous (first order) quantum phase transition during the evolution of the QAA. This fraction increases with increasing \( N \) and may tend to 1 for \( N \to \infty \).

PACS numbers: 03.67.Lx, 03.67.Ac, 64.70.Tg, 75.10.Nr

It is of great interest to know if an eventual quantum computer could solve a broad range of hard “optimization” problems more efficiently than a classical computer. An important class is the NP-hard category [1], for which it is believed that all classical algorithms take a time exponential in the problem size.

The most promising approach to solving optimization problems on a quantum computer seems to be the quantum adiabatic algorithm (QAA), proposed by Farhi et al. [2]. The idea, which is related to quantum annealing [3], is that one adds to a “problem” Hamiltonian, \( H_P \), whose ground state represents a solution of a classical optimization problem, a non-commuting “driver” Hamiltonian, \( H_D \), so the total Hamiltonian is

\[
H(s) = (1 - s)H_D + sH_P,
\]

(1)

where \( s(t) \) is a time dependent control parameter. \( H_P \) is expressed in terms of classical Ising spins taking values \( \pm 1 \), or equivalently in terms of the \( z \)-components of the Pauli matrices for each spin, \( \sigma^z \). The simplest driver Hamiltonian is then then \( H_D = -\sum_{i=1}^N \sigma^z_i \) where \( \sigma^z_i \) is the \( x \)-component Pauli matrix.

The control parameter \( s(t) \) is 0 at \( t = 0 \), so \( H = H_D \), which has a trivial ground state in which all \( 2^N \) basis states (in the \( \sigma^z \) basis) have equal amplitude. It then increases with \( t \), reaching 1 at \( t = T \), where \( T \) is the runtime of the algorithm, at which point \( H = H_P \). If the time evolution of \( s(t) \) is sufficiently slow, the process will be adiabatic. Hence, starting the system in the ground state of \( H_D \), the system will end up in the ground state of \( H_P \) and the problem is solved. The time \( T \) required to find the ground state with significant probability is called the complexity. The bottleneck of the QAA is likely to be at one or more places where the energy gap from the ground state to the first excited state becomes very small, possibly due to a quantum phase transition.

Early numerical work [2, 4] on very small systems, \( N \leq 24 \) (for a particular constraint satisfaction problem known as “exact cover 3”, also called 1-in-3 sat), found that the complexity scaled polynomially with size, roughly as \( N^2 \), which caused a good deal of excitement.

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.

In previous work [5] we have used quantum Monte Carlo (QMC) simulations to investigate much larger sizes of the exact cover problem, up to \( N = 128 \). We found evidence that, while the median complexity is still polynomial, an increasing fraction of instances became very hard to equilibrate for the larger sizes. We have now considerably improved the algorithm, borrowing techniques from the the spin glass field to speed up equilibration. We have therefore been able to understand much better these “troublesome” instances, and find that they have a first order quantum phase transition. Furthermore, we have increased the range of sizes still further, up to \( N = 256 \), finding that the fraction instances with a first order transition continues to increase with \( N \), plausibly tending 1 for \( N \to \infty \). The gap at a first order phase transition is likely to be exponentially small [6, 7], and hence lead to exponential complexity for the QAA.

We now describe the model and our results in more detail. To make a comparison with the earlier work we study (essentially) the same model for \( H_P \) used by Farhi et al. [2]. This problem, known as exact cover, is a random satisfiability problem, a class which is known to be NP-hard. 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 \(1\), and otherwise the energy is a positive integer. The simplest Hamiltonian with this property is

\[
H_P = \frac{1}{4} \sum_{\alpha=1}^M (\hat{\sigma}^z_{\alpha_1} + \hat{\sigma}^z_{\alpha_2} + \hat{\sigma}^z_{\alpha_3} - 1)^2,
\]

(2)

where \( \alpha_1, \alpha_2 \) and \( \alpha_3 \) are the three spins in clause \( \alpha \), and the \( \{\hat{\sigma}^z_i\}_{i=1,\ldots,N} \) are Pauli matrices. In the absence of the driver Hamiltonian, the Pauli matrices can be replaced by classical Ising spins \( S_i \) taking values \( \pm 1 \). 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 $\alpha \equiv M/N$ is increased, there is a phase transition at $\alpha_s$ 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 $\Delta E(s)$ between the ground state and first excited state is greater than zero in both limiting cases, $H = H_D$ and $H = H_P$, but will have a minimum at an intermediate value $s = s^*$. In addition, it ensures that we work close to the satisfiability transition where the problem is particularly hard \cite{5}. Hence here, and in the earlier work \cite{3}, we consider instances with a USA.

The method of generating instances with a USA is described in Ref. \cite{3}. For each size $N$ we choose the number of clauses $M$ which maximizes the probability of finding a USA, see Table I. The actual number of spins simulated $N'$, is somewhat less than $N$ due to isolated sites being omitted, and others that do not affect the complexity are also “pruned off” \cite{3}. The value of $\alpha \equiv M/N$ seems to be close to the critical value $\alpha_s \simeq 0.626$ \cite{10} for $N \to \infty$.

In QMC we simulate an effective classical model with Ising spins $S_i(\tau) = \pm 1$ in which $\tau$ (0 $\leq$ $\tau$ $< \beta$ $\equiv$ $T^{-1}$) is imaginary time. Following common practice, we discretize imaginary time into $L$ “time slices” each representing $\Delta \tau = \beta/L$, of imaginary time. We take $\Delta \tau = 1$.

As discussed previously \cite{3}, for $\beta \Delta E \gg 1$ (where $\Delta E \equiv E_1 - E_0$ is the energy gap), and $\tau \ll \beta$, the time-dependent correlation function

$$C(\tau) = \frac{1}{N' L^2} \sum_{i=1}^{N'} \sum_{\tau_0=1}^{L} \langle S_i(\tau_0 + \tau)S_i(\tau_0) \rangle,$$  \hspace{1cm} (3)

is a sum of exponentials, i.e.

$$C(\tau) = q + \sum_{n \geq 1} A_n \exp[-(E_n - E_0)\tau],$$  \hspace{1cm} (4)

where the $A_n$ are constants and $q$, the spin glass order parameter, is given by

$$q = \frac{1}{N'} \sum_{i=1}^{N'} \langle S_i \rangle^2.$$  \hspace{1cm} (5)

At large $\tau$, the sum in Eq. (4) is dominated by the term corresponding to the first excited state, ($n = 1$), and so $\Delta E \equiv E_1 - E_0$ can be obtained by fitting $\log[C(\tau) - q]$ against $\tau$ for large $\tau$.

We have considerably improved the algorithm relative to that in Ref. \cite{3} by incorporating “parallel tempering” \cite{11, 12}, which has been very successful in speeding up simulations of spin glass systems. Whereas in spin glasses, one simulates copies of the system at different, close-by temperatures, in the quantum case, the copies are at different values of the control parameter $s$.

As already mentioned, the focus of the present study is to determine which instances have a first order transition. Parallel tempering is very good at equilibrating the system on either side of the transition. However, it is still difficult (i) to determine exactly where the transition occurs, because both phases are metastable in the region where they are not the equilibrium state, and (ii) to accurately determine the minimum gap for first-order instances, because it is so small. We have performed runs starting the spins both from a random initial configuration, and from the solution of the problem Hamiltonian. If we start by “seeding” the spins with the exact solution, we are confident that the Monte Carlo is in the correct phase for $s$ close to 1. It is also in the correct phase for small $s$ because equilibration is easy in this region. Hence, if a long simulation starting the spins from the exact solution produces a sharp discontinuity, we feel that this is almost certainly the correct behavior.

In order to investigate whether or not a first order transition occurs we focus on the spin glass order parameter $q$ defined in Eq. (5). The expectation value of $q$ is always non-zero because of terms linear in the $\sigma^z$ (magnetic field terms) in the Hamiltonian, Eq. (2). To determine the square of the average without bias we simulated two copies of the spins at each value of $s$ and evaluate $\langle S_i \rangle^2$ as $\langle S_i(1) \rangle \langle S_i(2) \rangle$. A representative result for an instance with a first order transition is shown in Fig. 1. The dip before the jump clearly seen in Fig. 1 provides clear evidence for a two-phase coexistence, and hence a first order transition, for the following reason. If both copies are in the same phase, then the mean value of $\langle S_i \rangle$ is the same in both copies. However, right at the first order transition, one copy can be in one phase (the low-$q$ phase, say) and the other copy in the other (high-$q$ phase). The average value of $\langle S_i \rangle$ can have different signs in the two phases for some sites $i$. Hence, the typical Hamming distance between the spin configurations in the two copies can be even greater (and so $q$ even smaller) than when both copies are in the low-$q$ phase. In every instance where we observed a sharp jump, this was preceded by a dip. Hence we use the dip as a precise criterion for a first order transition.

Of course, even a first order transition is rounded out for a finite-size system. To estimate the size of the rounding we need to consider the two cases $\Delta E_{\text{min}} \gg T$ and $\Delta E_{\text{min}} \ll T$ separately, where $\Delta E_{\text{min}}$ is the minimum

| N  | 16 | 32 | 64 | 128 | 192 | 256 |
|----|----|----|----|-----|-----|-----|
| M  | 12 | 23 | 44 | 86  | 126 | 166 |
| $\alpha$ | 0.7500 | 0.7188 | 0.6875 | 0.6719 | 0.6563 | 0.6484 |

TABLE I: The sizes studied in the simulation.
value of the gap at the transition. If $\Delta E_{\text{min}} \gg T$, $\delta s$ is the range of $s$ over which $\Delta E$ changes by an amount $\Delta E_{\text{min}}$, whereas if $\Delta E_{\text{min}} \ll T$, $\delta s$ is the range of $s$ over which $\Delta E$ changes by an amount equal to $T$. Hence

$$\delta s = \begin{cases} \Delta E_{\text{min}} \left( \frac{\partial \Delta E}{\partial s} \right)^{-1}, & (\Delta E_{\text{min}} \gg T), \\ T \left( \frac{\partial \Delta E}{\partial s} \right)^{-1}, & (\Delta E_{\text{min}} \ll T). \end{cases} \quad (6)$$

Figure 2 shows the finite-size rounding for an instance with $N = 64$, small enough that we can equilibrate through the (first order) transition. For $\beta \lesssim 1024$ the width of the transition region increases as $\beta = 1/T$ decreases, but for $\beta \gtrsim 1024$ the width is independent of $\beta$. For this instance we find $\Delta E_{\text{min}} = 0.0021$ as shown in the inset, so the width of the rounding becomes independent of $T$ when $T \ll \Delta E$ as expected.

In Fig. 3 we plot the fraction of instances with a first order transition. For each size we have studied $N_{\text{inst}} = 50$ instances. If we denote the first-order fraction by $r$ then the error bar in $r$ is $\sqrt{r(1-r)/(N_{\text{inst}}-1)}$. The figure shows that $r$ increases rapidly with $N$ and, very plausibly, tends to 1 for $N \to \infty$. We see that the first order fraction is slightly greater than a half for $N = 128$. In our earlier work [5] we found that the median complexity continued to be polynomial up to $N = 128$ (the largest size studied). However, there is no contrast with the present work because, as already noted in Ref. [5], the models used are slightly different, and as a result the crossover to a first order transition occurs at a slightly lower value of $N$ in the present model. The crossover to first order would have been seen in the earlier model if somewhat
larger sizes had been studied.

Exponentially small gaps have been discussed before in the context of the QAA. Some time ago, one of us [13] pointed out for a different problem, number partitioning, that the minimum gap is exponentially small, because of a transition between the states that are "localized" and "extended" in the computational basis.

Altshuler et al. [5] predict an exponentially small gap at large N for exact cover. Performing perturbation theory away from s = 1 they argue that there will be a level crossing between two "localized" states for s close to 1 at which point the ground state configuration changes abruptly. In our numerics, there is a big variation in the location of the first order transition for a given size, but we do not detect a systematic shift towards s = 1 as the size increases. However, Altshuler et al. predict that 1 − s ∼ N−1/8, which is probably too slow to be visible in our data. It will be interesting to investigate in future work whether the first order transition found here is due to the mechanism they propose.

Farhi et al. [14] used a continuous imaginary time QMC method to study a very similar problem to ours, except that two solutions far away in Hamming space are "planted" into the Hamiltonian. This ensures that there is a finite probability of a first order transition where the equilibrium state changes from one planted solution to another. By contrast, our work does nothing explicit to impose a first order transition.

Jörg et al. [15] studied quantum annealing for the quantum random energy model (REM), the classical version of which [16] has a "1-step replica symmetry breaking" (also called a "random first order") transition. Following Goldschmidt [17], they find a discontinuous quantum transition and argue that this leads to an exponentially small gap. They also observed that an exponentially small gap is seen in quantum versions of several models with random first order transitions and suggested that this may be the general feature of all such models, including satisfiability [18]. However, the classical REM has zero spin glass order parameter q in the disordered phase [16] whereas classical random satisfiability models have lower symmetry because q is always non-zero due to the terms linear in σ2 in Eq. (2). Consequently, it is not obvious to us that the first order quantum transition observed here is due to the same mechanism as that found [16] for the quantum REM. Very recently, a first order transition has also been found in another model by Jörg et al. [19].

To conclude, we have a found a crossover to a first order quantum phase transition during the evolution of the QAA for instances of exact cover with a unique satisfying assignment when the size becomes greater than about 100. It is possible that the complexity for random instances of exact cover could be different. We are therefore studying instances of exact cover with the USA constraint removed, and will also study other models in addition to exact cover.

We thank Eddie Farhi, Florent Krzakala, Boris Altshuler and Mike Moore for helpful discussions and correspondence. The work of APY is supported in part by the National Security Agency (NSA) under Army Research Office (ARO) contract number W911NF-09-1-0391, and by a Special Research Grant from the Committee on Research at UCSC. The work of SK and VNS is supported by National Security Agency’s Laboratory of Physics Sciences and the NASA Ames NAS Supercomputing Center. We are grateful to Andre Petukhov for generously allowing us a to use the Gamow computer cluster at the South Dakota School of Mines and Technology.

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The random energy model is equivalent to a $p$-spin glass with both infinite range and infinite coordination (i.e. interactions among all sets of $p$ spins) in the limit of $p \to \infty$, see Ref. [20], $q$ vanishes in the paramagnetic phase because the interactions are scaled with $N$ due to the infinite coordination. Here we consider random satisfiability models which have infinite range but finite coordination number, for which $q$ is always non-zero.

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