Complexity of the quantum adiabatic algorithm

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Introduction

• What is the “Quantum Adiabiatic Algorithm”?
• Motivation for studying the complexity of the Quantum Adiabatic Algorithm for much larger sizes than has been studied before.
• The Monte Carlo method that will be used to do this.
• Results for the a particular problem (Exact Cover).
• Conclusions.
Problem Studied

What problems can be studied more efficiently on a quantum computer than a classical computer?
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The best known is Shor’s factoring algorithm which factors an integer of $n$ bits in a time which is polynomial in $n$, as opposed to the best classical algorithm which take a time of order $\exp(c n^{1/3})$. 
Problem Studied: II

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Could a quantum computer solve typical instances of NP-Hard problems with just polynomial complexity, i.e.

$$\text{complexity } \propto N^\sigma,$$

for some value of $\sigma$?
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Problem Hamiltonian $\mathcal{H}_P$ is a function of the bits, or equivalently the spins

$$\sigma_i^z = 1 - 2b_i = \pm 1.$$  

Add a “driver Hamiltonian”, which is simple and does not commute with $\mathcal{H}_P$. The simplest is a “transverse field” $\mathcal{H}_D = -\hbar \sum_i \sigma_i^x$.

The total Hamiltonian is

$$\mathcal{H} = [1 - \lambda(t)] \mathcal{H}_D + \lambda(t) \mathcal{H}_P,$$

where the “control parameter” $\lambda(t)$ varies from 0 at $t = 0$ to 1 at $t = T$, the running time, or complexity.
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At $t = T$, just have $\mathcal{H}_P$. If the evolution is adiabatic, the system is in the ground state of $\mathcal{H}_P$ and the problem is solved.
The **Quantum Adiabatic Algorithm** is less demanding on the hardware than algorithms like Shor’s.

The QAA **gradually** evolves the Hamiltonian, which is represented by the connections in the computer, whereas Shor’s algorithm proceeds by a series of **discrete** unitary transformations.

It is easier to avoid interference between the bits and to maintain quantum coherence if changes are made gradually, rather than in a series of discrete jumps.

Here there is **real interest in the quantum computing community** in building a quantum computer which uses the QAA.

Even if one can build one **will it be more efficient than a classical computer** for NP-hard problems?
Complexity of the QAA

How does $\tau$ vary with $N$ in order to maintain adiabatic evolution with high probability?
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The problem is severe at an “avoided level crossing” with a small “minimum gap” between the ground state and the first excited state.

The dashed lines show a crossing that the ground state and first excited would have in the absence of any coupling between them. However, there is actually “level repulsion” so the two levels, shown by the solid lines, do not cross but have a minimum gap $\Delta E_{\text{min}}$. 
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**Landau-Zener theory.** To stay in ground state, $\text{time } \propto (\Delta E_{\text{min}})^{-2}$. 
Quantum Phase Transition

As \( \lambda(t) \) is varied the system is likely to go through a Quantum Phase Transition where the gap will be particularly small.

Hence we are, effectively interested in:

The Size Dependence of the Energy Gap at a Quantum Phase Transition
Early Simulations

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Farhi et al. (2001), Hogg (2003): integrated the time dependent Schrödinger equation. Limited to very small sizes, $N \lesssim 20–24$, because the number of basis states $2^N$ grows exponentially.

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\[ \implies \text{“Monte Carlo” methods} \]
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Working through the details, one ends up with copies of the system at different values of imaginary time $\tau$ where $0 \leq \tau < \beta$. One discretizes imaginary time (Trotter decomposition) into $L_\tau$ “time slices” separated by the time-slice width $\Delta \tau$. We have

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The exact quantum mechanical Hamiltonian is reproduced in the limit $\Delta \tau \to 0$. However, we shall argue that this limit is not necessary for our purposes.
Trotter decomposition in QMC.

At each time slice 3 sites are shown. An independent spin $\sigma_i^z(\tau)$ lives at each site and each of the $L_\tau$ time slices. If spins $i$ and $j$ have an interaction in $\mathcal{H}_P$, then, each time slice, these spins interact with a coupling $K_{ij}$, the same for each slice. Spins on the same site but at neighboring time slices are coupled by an interaction $K_\tau$, again the same for all slices. (Details on next slide.)

The slice at time $\tau = \beta$ is identified with the slice at $\tau = 0$ (i.e. we have periodic boundary conditions in the imaginary time direction).
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1. couplings between different spins at the same time slice, arising from the problem Hamiltonian:

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\mathcal{H}_P(\{\sigma^z\}) \implies \sum_{m=0}^{L_\tau-1} \mathcal{H}_P(\{\sigma^z_i(\tau_m)\}) \Delta \tau
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2. couplings between different spins at the same site but neighboring time slices arising from the driver Hamiltonian

\[
\mathcal{H}_D = - \sum_i \sigma^x_i \implies - \sum_{m=0}^{L-1} K \sigma^z_i(\tau_m) \sigma^z_i(\tau_{m+1})
\]

where \( e^{-2K} = \tanh(\Delta \tau \hbar) \).
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In quantum mechanics, correlations between a spin at an initial (real) time $t_0$ and a later time $t_0 + t$ have the form

$$C(t) \equiv \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z(t_0) \sigma_i^z(t_0 + t) \rangle = \frac{1}{N} \sum_{i=1}^{N} \left[ \sum_n |\langle 0 | \sigma_i^z | n \rangle|^2 \right] e^{i(E_n - E_0)t}.$$
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In imaginary time, the complex exponentials are replaced by real, decaying exponentials:

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Hence, at large $\tau$, we have

$$C(\tau) = q + \frac{1}{N} \sum_{i=1}^{N} | \langle 0 | \sigma_i^z | 1 \rangle |^2 e^{-(E_1 - E_0) \tau},$$

where $q = N^{-1} \sum_i \langle \sigma_i^z \rangle^2$. (See next slide for some results.)
Results for the time dependent correlation function against $\tau$ for one instance of the Exact Cover problem with $N = 128$ near the location of the minimum gap. Note that the vertical axis is logarithmic. Fitting to the straight line region gives a slope (equal to the gap $\Delta E$) equal to 0.0354.

We took $L_\tau = 300$, $\Delta \tau = 1$, so $T^{-1} \equiv \beta = 300$. Hence the condition $T \ll \Delta E$ is well satisfied.
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We have $N$ bits and form randomly $M$ triples of bits (known as "clauses"). The energy of a clause is 0 if one bit is 1 and the other two are 0; otherwise the energy is 1. Writing in terms of spin variables, $\sigma^z_i = 1 - 2b_i$, the problem Hamiltonian $H_P$ is given by

$$H_P = \frac{1}{8} \sum_{\alpha=1}^{M} \left( 5 - \sigma^z_{\alpha_1} - \sigma^z_{\alpha_2} - \sigma^z_{\alpha_3} + \sigma^z_{\alpha_1} \sigma^z_{\alpha_2} \right. $$

$$\left. + \sigma^z_{\alpha_2} \sigma^z_{\alpha_3} + \sigma^z_{\alpha_3} \sigma^z_{\alpha_1} + 3 \sigma^z_{\alpha_1} \sigma^z_{\alpha_2} \sigma^z_{\alpha_3} \right),$$  

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Following Farhi et al. we take instances with a "**Unique Satisfying Assignment**" (USA). To find these with reasonable probability, we adjust the ratio $M/N$ for each size $N$. 
Results for the gap to the first excited state $\Delta E$ as a function of the control parameter $\lambda$ for one instance with $N = 64$. The gap has is finite for $\lambda = 0$ (this is due to the driver Hamiltonian, $\sum_i \sigma_i^x$). It is also finite for $\lambda = 1$ because we chose instances with this property (Unique Satisfying Assignment). There is a minimum of the gap at an intermediate value of $\lambda$, presumably close to a quantum phase transition.

We compute $\Delta E_{\text{min}}$ for many (50) instances for several different sizes, $N = 16, 32, 64, 128$. 
We take the median value of the minimum gap among different instances for a given size $N$ to be a measure of the “typical” minimum gap.
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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 $\Delta E_{\text{min}}$ decreases as a power law,

$$\text{median } \Delta E_{\text{min}} \propto N^{-\mu},$$

for these sizes, with

$$\mu = 0.73 \pm 0.06.$$ 

The inset shows a log-linear plot. The pronounced curvature shows that the behavior is \textit{not exponential} for this range of sizes.

Expect \textbf{complexity} $\propto N^{2\mu}$ (if matrix element effects are small).
Note: The discretization of imaginary time does not affect the way the complexity varies with $N$, though it does affect the precise value of the energy gap for given $N$ and $\lambda$. Once the relaxation time $(\Delta E)^{-1}$ is much larger than the “lattice spacing” $\Delta \tau$ the lattice discretization is unimportant. Hence, whether the minimum gap varies exponentially with $N$ or as a power law will not depend on the value of $\Delta \tau$. 
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In the theory of continuous phase transitions this concept of “universality” is well established. Universality means that some (universal) quantities like “critical exponents” don’t depend on microscopic details such as the lattice structure. Other (non-universal) quantities, such as the location of the critical point, do depend on details.
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Example: Exact solution of the Ising model in two dimensions. The magnetization tends to zero as \( T \to T_c^- \), like \( (T_c - T)^{\beta} \). With a lot of work, this can be calculated on different lattices, e.g. square and triangular. The value of \( T_c \) depends on the lattice (it is “non-universal”) but \( \beta = 1/8 \), the same for all lattice structures, i.e. it is “universal”.
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Note: One can simulate the \( \Delta \tau \to 0 \) limit, but this is more complicated.
A commonly used classical algorithm for satisfiability problems is the Davis Putnum algorithm. This is guaranteed to correctly say whether or not there is a satisfying assignment. The figure shows the complexity for the instances used in the QMC simulations. It is clearly exponential for the range of sizes studied.
A classical algorithm which is more analogous to QAA is WALKSAT, a local heuristic search algorithm. Like simulated annealing, it includes “up-hill” moves in a stochastic way. Using the default value of the “noise parameter" the complexity for the QAA instances with USA crosses over from power-law to (presumably) exponential for \( N \gtrsim 100 \). (But note the QMC is so far only for \( N \leq 128 \).)
Adjusting the noise parameter, the crossover to exponential behavior is pushed to larger sizes $N \gtrsim 200$. (Remember: the QMC is so far only for $N \leq 128$).
Conclusions

- Using Quantum Monte Carlo simulations (QMC) we have been able to study the complexity of the Quantum Adiabative Algorithm (QAA) for the Exact Cover problem with a Unique Satsifying Assignment (USA) for much larger sizes (up to 128) than in earlier work (20–24).
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