Complexity of the quantum adiabatic algorithm

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Introduction



- Can we use a quantum computer to solve hard optimization problems. Is the "Quantum Adiabatic Algorithm" useful?
- To answer this, need to know the **complexity** of the Quantum Adiabatic Algorithm for **large sizes**.
- Discuss the Monte Carlo method that will be used to do this.
- **Results** for a particular problem (Exact Cover).
- Conclusions.

Problem Studied I



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The best known is Shor's factoring algorithm which factors an integer of n bits in a time which is of order n^3 , i.e. polynomial in n, as opposed to the best classical algorithm which takes a time of order $\exp(c n^{1/3} \log^{2/3} n)$.

Relevant for encryption: \implies Important in commerce and for the military.

Problem Studied



Can a quantum computer solve a **general** class of hard problems: "optimization problems" in which we need to minimize a function of N binary variables, $z_i = 0, 1$, with constraints.

In particular, we are interested in an important subset of optimization problems called



Problem Studied: II



For NP-Complete problems we are interested in how the computer time, the complexity, depends on N. All known classical algorithms have **exponential complexity**,

complexity $\propto \exp(\text{const. }N)$.

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If so, the "quantum polynomial" complexity class (called **BQP**) would include not only all problems in P, and integer factoring, but also all problems in NP.

Would be an extremely exciting result for the quantum computing community.



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Problem Hamiltonian \mathcal{H}_P is a function of the bits, $z_i = 0, 1$, or equivalently the Ising spins $\sigma_i^z = 1 - 2z_i = \pm 1$.

Add a "driver Hamiltonian", which is simple and does not commute with

 \mathcal{H}_P . The simplest is a "transverse field" $\mathcal{H}_D = -h \sum \sigma_i^x$. The total Hamiltonian is

 $\mathcal{H} = \left[1 - \lambda(t)
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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.

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Landau-Zener theory. To stay in ground state, time $\propto (\Delta E_{\min})^{-2}$.

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



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 \implies "Monte Carlo" methods



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We choose the probabilities to satisfy the **detailed balance condition**:

$$P_l^{\mathrm{eq}} w_{l \to m} = P_m^{\mathrm{eq}} w_{m \to l}$$

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One can then determine $\langle A \rangle$ as a time average from states generated after equilibration is reached, i.e.

$$\langle A
angle \simeq rac{1}{N_{ ext{meas}}} \sum_{lpha=1}^{N_{ ext{meas}}} A_lpha \, .$$



A common way of implementing the detailed balance condition, is the **Metropolis** probability

$$w_{l \to m} = \left\{ egin{array}{cc} \exp[-eta(E_m-E_l)] & ext{if } E_m > E_l \ 1 & ext{otherwise} \end{array}
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How can we also simulate **quantum** fluctuations using Monte Carlo methods?



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Working through the details, one ends up with a Classical Action comprising copies of the system at different values of imaginary time τ where $0 \leq \tau < \beta$. One discretizes imaginary time (Trotter decomposition) into L_{τ} "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 $\Delta \tau \rightarrow 0$. However, this limit is not necessary for our purposes.



One simulates a classical action in space and imaginary time with Ising spins $S_i(\tau_m) = \pm 1$ where $\tau_m = m\Delta\tau$ and $m = 0, 1, \dots, L_{\tau} - 1$.



At each time slice 3 sites are shown. An independent Ising spin $S_i(\tau)$ lives at each site and each of the L_{τ} time slices. If spins *i* and *j* have an interaction in \mathcal{H}_P , then, each time slice, these spins interact with a coupling

 $K_{ij} = \Delta \tau J_{ij},$

the same for each slice. Spins on the same site but at neighboring time slices are coupled by an interaction K_{τ} , where

 $e^{-2K_{\tau}} = \tanh(\Delta \tau h),$ again the same for all slices.

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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$$C(t) \equiv rac{1}{N}\sum_{i=1}^N ig\langle \sigma_i^z(t_0)\sigma_i^z(t_0+t)
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Hence, at large τ , we have

$$C(au) = q + rac{1}{N} \sum_{i=1}^{N} ig| \langle 0 | \sigma_{i}^{z} | 1
angle ig|^{2} e^{-(E_{1}-E_{0}) au} \,,$$

where $q = N^{-1} \sum_{i} \langle \sigma_{i}^{z} \rangle^{2}$ is the (Edwards-Anderson) spin glass order parameter.

Sample results for $C(\tau)$





Results for the time dependent correlation function against τ for one instance of the Exact Cover problem with N = 128 near the location of the minimium gap. Note that the vertical axis is logarithmic. Fitting to the straight line region gives a slope (equal to the gap ΔE) 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.

Equilibration and error bars

The simulations are long to ensure the system comes to equilibrium. The simulation is run many times to reduce the noise and (from the variance between runs) to determine the error bars.





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$$\begin{aligned} \mathcal{H}_{\rm P} &= \frac{1}{4} \sum_{\alpha=1}^{2} \left(\sigma_{\alpha_1}^{z} + \sigma_{\alpha_2}^{z} + \sigma_{\alpha_3}^{z} - 1 \right) \\ &= \frac{1}{2} \sum_{\alpha=1}^{M} \left(2 - \sigma_{\alpha_1}^{z} - \sigma_{\alpha_2}^{z} - \sigma_{\alpha_3}^{z} + \sigma_{\alpha_1}^{z} \sigma_{\alpha_2}^{z} + \sigma_{\alpha_2}^{z} \sigma_{\alpha_3}^{z} + \sigma_{\alpha_3}^{z} \sigma_{\alpha_1}^{z} \right) \end{aligned}$$

where α_1, α_2 and α_3 are the three spins in clause α .

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Note that we have an Ising model on a **"random graph"** with a **magnetic field** on the spins which prefers them to line "up", and **antiferromagnetic interactions** between pairs of spins.

Exact Cover Problem: II



 $M/N \ll 1$: the number of clauses is small, it is easy to satisfy them all, and there are many satisfying assignments.

 $M/N \gg 1$: there are too many clauses to be satisfied and there will be no satisfying assignment.

 $N \rightarrow \infty$: there is a phase transition at some value of the ratio M/N where the number of satisfying assignments tends to zero.

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. This means that we are close to the phase transition, where the problem is expected to be particularly hard.

Dependence of gap on λ





Results for the gap to the first excited state ΔE as a function of the control parameter λ for one instance with N = 64. The gap has is finite for $\lambda = 0$ (this is due to the driver Hamiltonian, $-h \sum_i \sigma_i^x$, where we took h = 1). 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 λ , presumably close to a

quantum phase transition.

We compute ΔE_{\min} for many (50) instances for several different sizes, N = 16, 32, 64, 128, 192 and 256.

Size dependence



We take the **median** value of the minimum gap among different instances for a gives size N to be a measure of the "typical" minimum gap.

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But this behavior does NOT continue for larger sizes because ...

First order transition



 \cdots the transition becomes discontinuous (first order).

Compute the "spin glass order parameter"



Fraction First order



Instances with a first order transition presumably have an exponentially small gap.

The fraction which are first order appears to tend to 1 for $N \rightarrow \infty$.



Related work:

Krzakala et al. argue (using "replica methods") that a first order transition, between a disordered and an more ordered state, is expected for satisfiability problems. Altshuler, Krovi, Roland (2009), and Farhi et al. (2009) argue that there could be a first order transition bewteen two "ordered" states for λ close to 1 (i.e. close to the problem Hamiltonian.)

Classical Algorithm



Interesting to compare the QAA with a classical algorithm.



A classical algorithm which is more analgous to QAA is WALKSAT, a local **heuristic** search algorithm. Like simulated annealing, it includes "uphill" 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 $N \gtrsim 100$.

Note: similarity with QAA.

Stoquastic Hamiltonians



To do the QMC simulations we need to avoid the infamous "minus-sign problem" which plagues simulations of fermions and "frustrated" quantum spin systems (Kawashima's talk). Systems without a sign problem are now called "stoquastic" (Bravyi et al. (2006)). They are characterized by

- All off-diagonal matrix elements of *H* are negative (or can be made so by local unitary transformations).
- All elements of the density matrix $\rho \propto \exp(-\beta \mathcal{H})$ are non-negative.
- All eigenvector components of the ground state are positive.

Finding the ground state energy of stoquastic and general Hamiltonians (to within a small uncertainty ϵ) are probably in different (quantum) computational classes.

Stoquastic Hamiltonians are easier to simulate, and perhaps

less powerful for computation than general Hamiltonians.

Perhaps we could avoid the first order transition by making \mathcal{H}_D non-stoquastic (for $0 < \lambda < 1$). But we can't simulate this, so we

probably won't know unless a real quantum computer can be built.



 Using Quantum Monte Carlo simulations (QMC) we have been able to study the complexity of the Quantum Adiabatic Algorithm (QAA) for the (NP Complete) Exact Cover problem with a Unique Satisfying Assignment (USA) for much larger sizes (up to 256) than in earlier work (20–24).



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- We see a "crossover" to a first order quantum phase transition (with presumably exponential complexity) when $N \gtrsim 100$.



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