First order phase transition in the Quantum Adiabatic Algorithm

A.P. Young, S. Knysh, and V. Smelyanskiy

Work supported by

Talk at the Conference on Quantum Statistical Mechanics, Computation, and Information, ICTP, Trieste, June 14-18, 2010
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- Comparison with a classical algorithm (WALKSAT)
- Conclusions
Complexity Classes

- **NP**: set of problems which can be verified in polynomial time.
- **P**: set of problems which can be solved in polynomial time on a classical computer.
- **NP-complete**: a set of hard problems. All problems in NP can be mapped into an NP-complete one in polynomial time. Takes an exponentially large time on a classical computer, for worst (and typical?) case.
- **BQP**: set of problems that can be solved in polynomial time on a quantum computer. Integer factoring is in BQP (Shor’s algorithm) but (probably) not in P.
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- **NP-complete**: a set of hard problems. All problems in NP can be mapped into an NP-complete one in polynomial time. Takes an exponentially large time on a classical computer, for worst (and typical?) case.
- **BQP**: set of problems that can be solved in polynomial time on a quantum computer. Integer factoring is in BQP (Shor’s algorithm) but (probably) not in P.

Could a quantum computer solve NP-complete problems in polynomial time (i.e. does BQP contain NP-complete)? If so, would increase importance of building a quantum computer.
The Quantum Adiabatic Algorithm I

Proposed by Farhi et. al to solve hard optimization problems on a quantum computer.

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

\( \mathcal{H}_D \) (g.s.): adiabatic?

\( 0 \leq \lambda(t) \leq 1, \quad \lambda(0) = 0, \quad \lambda(T) = 1 \)

\( \mathcal{H}_P \) is the problem Hamiltonian, depends on the \( \sigma^z_i \)

\( \mathcal{H}_D \) is the driver Hamiltonian = \( -\hbar \sum \sigma^x_i \)

\( T \) is the running time
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The Quantum Adiabatic Algorithm II

System starts in ground state of driver Hamiltonian. If process is adiabatic (and $T \to 0$), it ends in g.s. of problem Hamiltonian, and problem is solved.

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Minimum $\mathcal{T}$ is the “complexity”.

Is $\mathcal{T}$ exponential or polynomial in the problem size $N$?
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Landau Zener Theory: To stay in the ground state, the time needed is proportional to $\Delta E_{\text{min}}^{-2}$.

Using QMC, compute $\Delta E$ for different $\lambda$: $\rightarrow \Delta E_{\text{min}}$
The Exact Cover Problem

Studied in early numerics and our recent Quantum Monte Carlo simulations. An NP-complete “constraint satisfaction problem”

N Ising spins, \( \pm 1 \), pick \( M \) triplets (“clauses”) at random. A clause is “satisfied” (has zero energy) if two of the spins are up and one is down. Otherwise is “unsatisfied” (has positive energy, “cost”).

Is there an assignment of the bits which satisfies all the clauses?

Small \( M/N \), (exponentially) many satisfying assignments,
Large \( M/N \), no satisfying assignments.
The Exact Cover Problem II

Satisfiability transition at (Smelyanskiy et al., Zdeborova et al.)

\[(M/N)_c \approx 0.626 \quad (N \rightarrow \infty)\]

For finite \(N\), work close to the “transition”, i.e. point where number of satisfying assignments (SA) drops to 0.

Reasons:

(i) Problem is hard near the transition (Kirkpatrick et al)

(ii) Convenient to study instances with a “unique satisfying assignment” (USA).

(For finite \(N\), the “transition”, and hence the greatest probability of a USA, occurs at \(M/N\) a little above the infinite-N critical value)

Example of a USA with \(N=7, M = 5\) (V. Choi)
Early Simulations

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\[ \mathcal{H}_P = \sum_{\alpha=1}^{M} \frac{1}{4} \left( \sigma_{\alpha,1}^{z} + \sigma_{\alpha,2}^{z} + \sigma_{\alpha,3}^{z} - 1 \right)^2 \]
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Early numerical work (enumerate all states) (Farhi et al.) found

$$\mathcal{T} \propto N^2$$

but only for $N \leq 20$
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\( 2^N \) basis states. So how can we do much larger sizes?

⇒ Quantum Monte Simulations (classical algorithm; do a sampling of the states)
Quantum Monte Carlo: I

In Quantum Monte Carlo (QMC) simulations we can only study equilibrium (possibly time-dependent) quantities.

**Reason:** QMC depends on the correspondence between the time evolution operator in quantum mechanics, $e^{-iHt}$, and the Boltzmann operator in (equilibrium) statistical mechanics, $e^{-\beta H}$. We see that $\beta \equiv 1/T$ is like imaginary time.

One ends up simulating an effective classical Hamiltonian (really an action) in space and imaginary time $\tau$, where $0 \leq \tau < \beta$.

**Simplest** is to discretize imaginary time into $L_\tau$ “time slices” each of width $\Delta \tau$ where $T^{-1} \equiv \beta = L_\tau / \Delta \tau$.

There are also continuous imaginary time algorithms (e.g. Farhi’s talk).
**Time Dependence**

We assume that $T$ is sufficiently low that the system is in its ground state, i.e. $T \ll \Delta E \equiv E_1 - E_0$.

In quantum mechanics, correlations between spins at an initial (real) time $t_0$ and a later time $t_0 + t$ have the form

$$C(t) \equiv \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z(t_0)\sigma_i^z(t_0 + t) \rangle = \frac{1}{N} \sum_{i=1}^{N} \left[ \sum_n |\langle 0|\sigma_i^z|n \rangle|^2 \right] e^{i(E_n - E_0)t}.$$

In imaginary time, complex exponentials are replaced by real, decaying exponentials

$$C(\tau) = \frac{1}{N} \sum_{i=1}^{N} \left[ \sum_n |\langle 0|\sigma_i^z|n \rangle|^2 e^{-(E_n - E_0)\tau} \right].$$

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 $q = \frac{1}{N} \sum_{i=1}^{N} \langle 0|\sigma_i^z|0 \rangle^2$. 

$$= \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z \rangle^2$$
Results for the time dependent correlation function for one instance of Exact Cover with $N = 128$, near the location of the minimum gap. (Vertical axis is logarithmic.) Fitting to the straight line region gives the slope $\Delta E = 0.0354$. We took $L_\tau = 300, \Delta \tau = 1$, so $T^{-1} = \beta = 300$ so $T \ll \Delta E$, as required.

Use “parallel tempering” to speed up equilibration. Simulation is run many times to reduce the noise and get error bars.
Dependence of gap on $\lambda$

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 value $2$ ($= 2 \times$ transverse field) for $\lambda = 0$, and value $1$ for $\lambda \to 1$ (lowest excited state has one clause not satisfied). Remember this has a USA so the ground state at $\lambda = 1$ is unique.

There is a minimum gap at an intermediate value of $\lambda$. Compute $\Delta E_{\text{min}}$ for 50 instances for $N = 16, 32, 64, 128, 192, 256$.
Size Dependence

We take the median value of the minimum gap among different instances of a given size \( N \) as a measure of the “typical” gap.

A log-log lot of the median minimum gap as a function of \( N \) up to \( N = 64 \), In this range we have a power law variation:

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

where \( \mu = 0.94 \pm 0.13 \).

Complexity \( \propto N^{2\mu} \) (neglect matrix element effects), so consistent with \( N^2 \) behavior found in early work.

But this behavior does NOT continue for larger sizes because ...
First order Quantum Phase Transition

... the transition becomes discontinuous (1st order).

e.g. the spin glass order parameter

$$q = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z \rangle^2$$

Figure shows one instance for $N = 128$.
Note: big jump in ordering, transition far from $\lambda = 1$.
We averaged over 50 instances at each size for sizes between 16 and 256.
$$q = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z \rangle^2$$

Detailed study of one instance for $N = 64$. We see the intrinsic rounding of the quantum first order transition when $\beta \Delta E_{\text{min}} >> 1$, where $\Delta E_{\text{min}} = 0.0021$ (see inset). (Note the expanded horizontal scale.)

Why the dip?
Some spins point in opposite directions in the “low-q” and “high-q” states. At the transition the system is in a superposition of both states, and so the amount of ordering is even less than in the low-q state.
Sometimes, multiple first order transitions
Fraction first order seems to tend to 1 as N tends to infinity. Still first order even when we make the costs and transverse fields random.

So far: 1 set of random interactions for each instance.

Now doing: many sets of random interactions for a few instances, to see if at least one set will avoid 1st order.
Gap?

Instances with a first order transition:
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Instances with a first order transition:

- have a very small minimum gap,
- for larger sizes with a strongly first order transition, it is too small to measure,
- expect the minimum gap is exponentially small in $N$ (Amin and Choi, Jörg et al, Altshuler et al).
Comparison with WALKSAT

A classical, heuristic, local-search algorithm is WALKSAT.

Using the default value of the “noise parameter” the complexity varies roughly like $N^{2.3}$ for small sizes but crosses over to presumably exponential complexity for $N \gtrsim 100$.

Note rough similarity with QAA
Are instances which are hard for QAA also hard for WALKSAT?

Up to $N = 128$ there is only a small correlation between difficulty of the instances for QAA and WALKSAT.

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Stoquastic Hamiltonians

To do QMC simulations one needs to avoid the infamous “minus-sign problem”, which plagues simulations of fermions and “frustrated” quantum systems. Systems without a sign problem are 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 $\rho \propto \exp(-\beta H)$ non-negative
- All eigenvector components of the ground state are positive

Finding ground state energy of stoquastic and general Hamiltonians are probably in different quantum computational classes.

Stoquastic Hamiltonians can be simulated but are perhaps less powerful for computation than general Hamiltonians.

Would QAA work better if we added $\lambda(1-\lambda) H_{\text{frust}}$ where $H_{\text{frust}}$ contains frustrating $\sigma^x \sigma^x$ terms? Need a quantum computer.
Conclusions

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Thank You