Complexity of the quantum adiabatic algorithm

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WHERE DISCOVERIES BEGIN

Introduction

- What is a **Quantum Computer**?
- Why all the fuss? **Shor's "killer app."**
- What else could we do with one? 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**.

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A traditional **quantum algorithm** manipulates the qubits by a sequence of **quantum logic gates.**
(Here we will discuss a rather different type of quantum algorithm.)

Quantum Computer II

Many proposed implementations:

- Superconductor-based (Josephson junctions)
- Trapped ions
- Quantum dots
- Topological quantum computer (anyons)
- . . .

And also many experimental difficulties:

- Need to be able to couple to the qubits in order to **manipulate** them.
- But otherwise need to prevent coupling of bits to outside world because this causes **decoherence**.
- Need **scalability** to large number of bits.

So far, quantum computing operations have only been successfully carried out on a **very small numbers of bits**.

Shor's "killer app."

There are algorithms for some **specific** problems which are much more efficient than the fastest classical algorithm.

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

For large $\mathbf{n}$ the quantum computer wins.

Relevant for **encryption** since the popular **RSA** encryption scheme (internet transactions) exploits the difficulty of factoring large integers.

$\Longrightarrow$ Important in commerce and for the military.

Also **Grover's algorithm** for searching an unstructured list,

($O(\sqrt{N})$ rather than $O(N)$).

Problem Studied

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

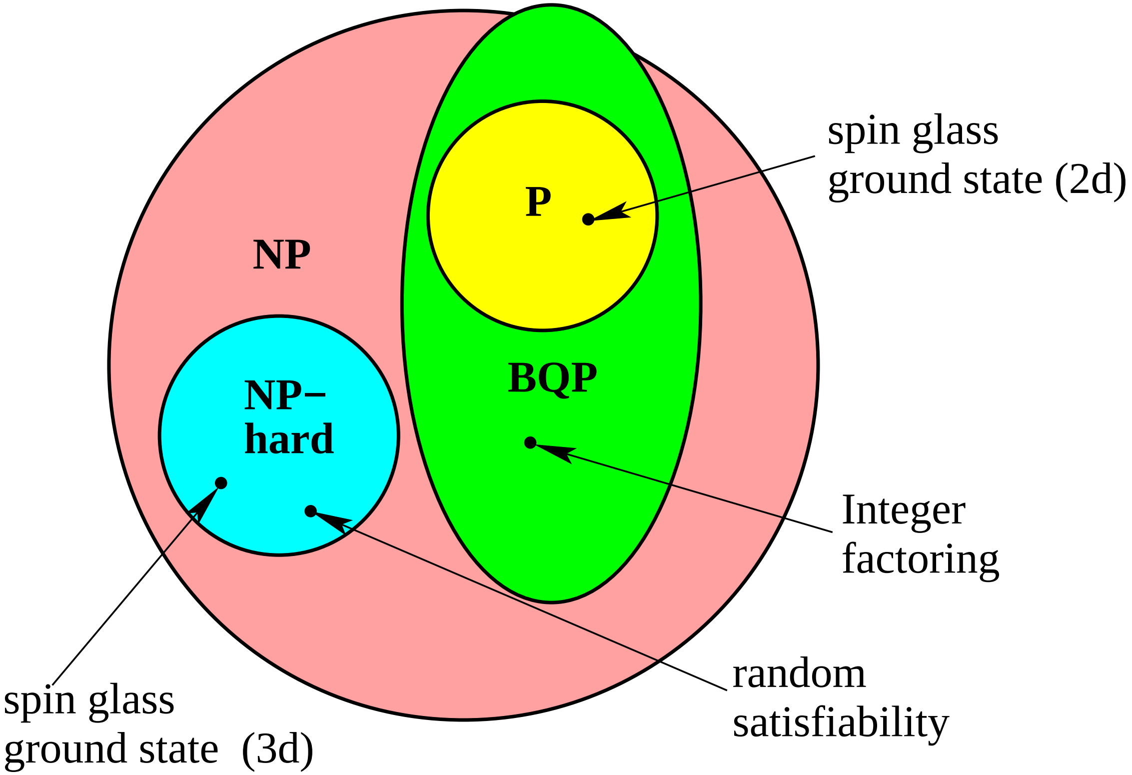
In particular, we are interested in an important subset of optimization problems called

NP-Hard.

Note: Integer factoring is believed to be not **NP-hard**.

It is in the quantum polynomial complexity class **BQP**.

Does **BQP** include **NP-hard**?



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For NP-hard problems we are interested in how the computer time, the complexity, depends on $\mathbf{N}$. All known classical algorithms have **exponential complexity**,

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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” $\mathcal{H}_D = -h \sum_i \sigma_i^x$.

The total Hamiltonian is

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

where the **“control parameter”** $\lambda(t)$ varies from **0** at $t = 0$ to **1** at $t = \mathcal{T}$, the **running time**, or **complexity**.

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At $t = \mathcal{T}$, 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**.

Quantum Adiabatic Algorithm

The **Quantum Adiabatic Algorithm** is less demanding on the hardware than algorithms like Shor’s.

The QAA **gradually** evolves the Hamiltonian, which is hardwired into the connections in the computer, e.g. by changing a magnetic field, 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.

However, even if one can build one **will it be more efficient than a classical computer** for NP-hard problems?

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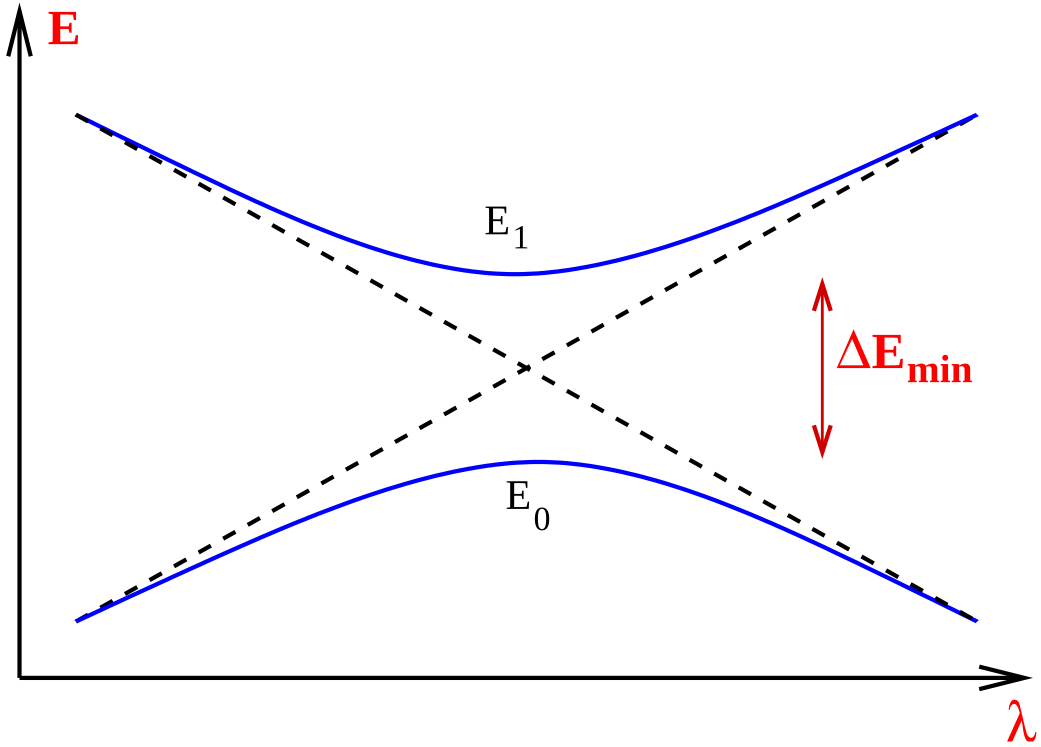

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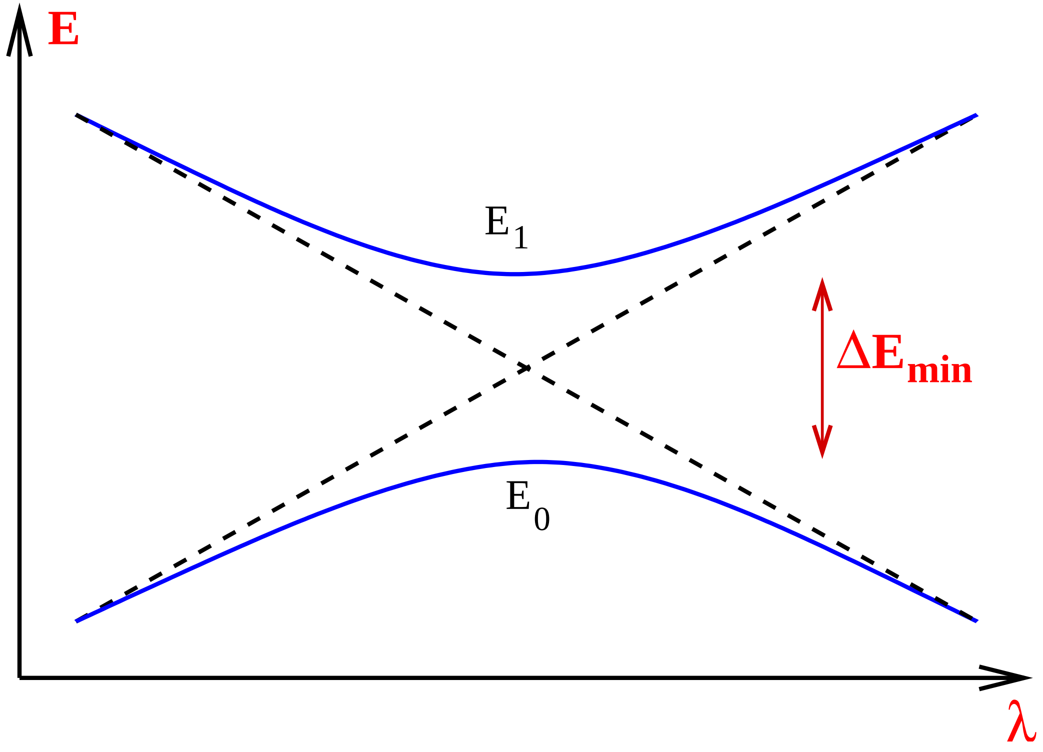

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Landau-Zener theory. To stay in ground state, time $\propto (\boldsymbol{\Delta E_{\mathrm{min}}})^{-2}$.

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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$\Longrightarrow$ **“Monte Carlo" methods**

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QMC depends on the correspondence between the time evolution operator in quantum mechanics $\boxed{e^{-i\mathcal{H}t}}$ and the Boltzmann operator in statistical mechanics $\boxed{e^{-\mathcal{H}\beta}}$. We see that $\beta \equiv T^{-1}$ is like **imaginary time**.

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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 $0 \le \tau < \beta$. 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 $\Delta\tau \to 0$. However, this limit is not necessary for our purposes.

Model simulated

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 $m = 0, 1, \cdots, L_\tau - 1$.

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$$\mathcal{H}_P(\{\sigma^z\}) \Longrightarrow \sum_{m=0}^{L_\tau - 1} \mathcal{H}_P(\{S_i(\tau_m)\})\Delta\tau.$$

For example, for a two-spin interaction,

$$J_{ij}\sigma_i^z\sigma_j^z \Longrightarrow K_{ij}\sum_{m=0}^{L_\tau - 1} S_i(\tau_m)S_j(\tau_m).$$

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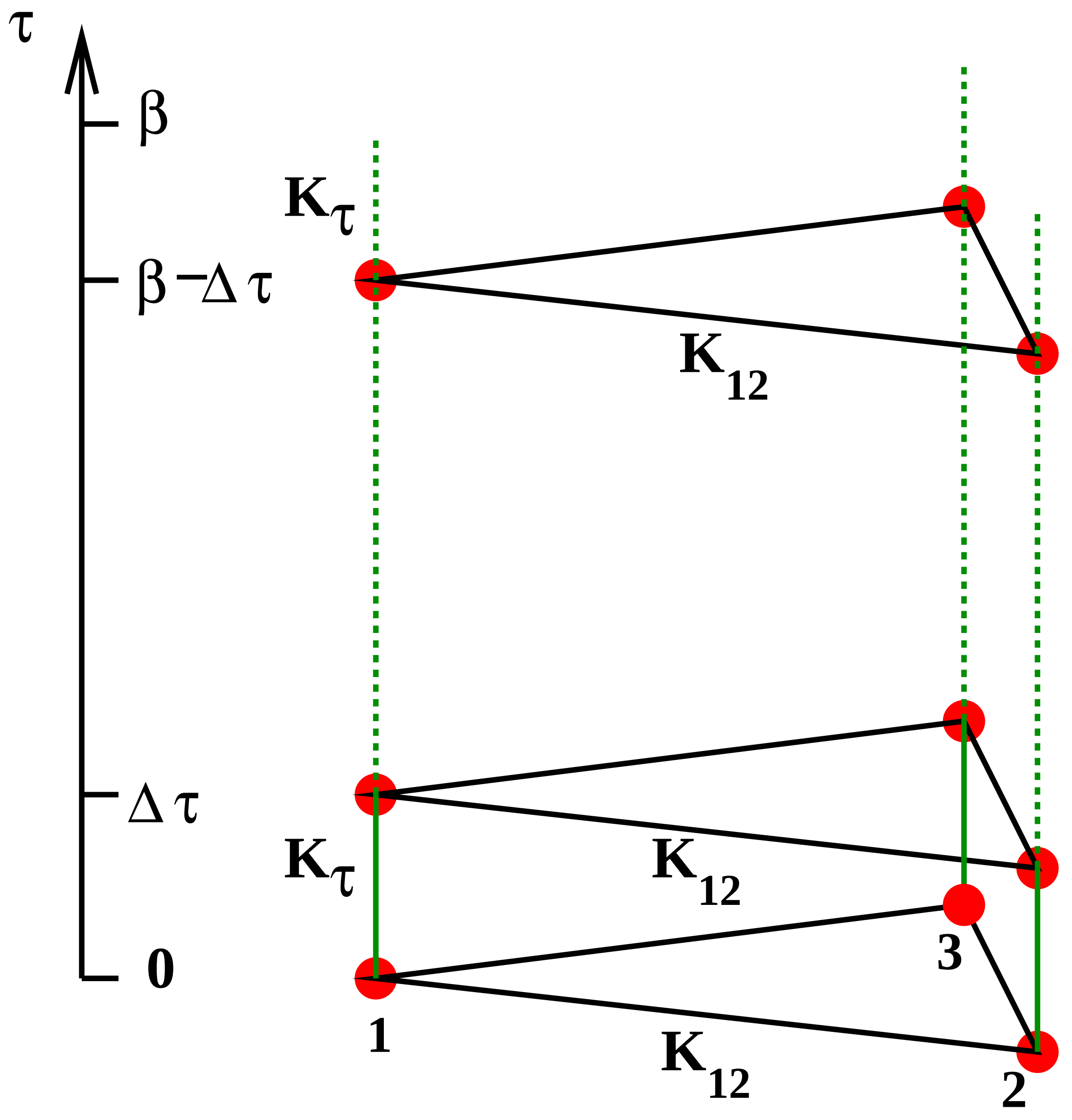
2. Ferromagnetic couplings between different spins at the same site but neighboring time slices arising from the driver Hamiltonian
$$-h\sigma_i^x \Longrightarrow -K_\tau \sum_{m=0}^{L_\tau - 1} S_i(\tau_m)S_i(\tau_{m+1})$$
where $e^{-2K_\tau} = \tanh(\Delta\tau\, h)$.

Quantum Monte Carlo: II



Trotter decomposition in QMC.

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}, the same for each slice. Spins on the same site but at neighboring time slices are coupled by an interaction K_τ, 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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In quantum mechanics, correlations between a spin at an initial (real) time t_0 and a later time $t_0 + t$ have the form

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

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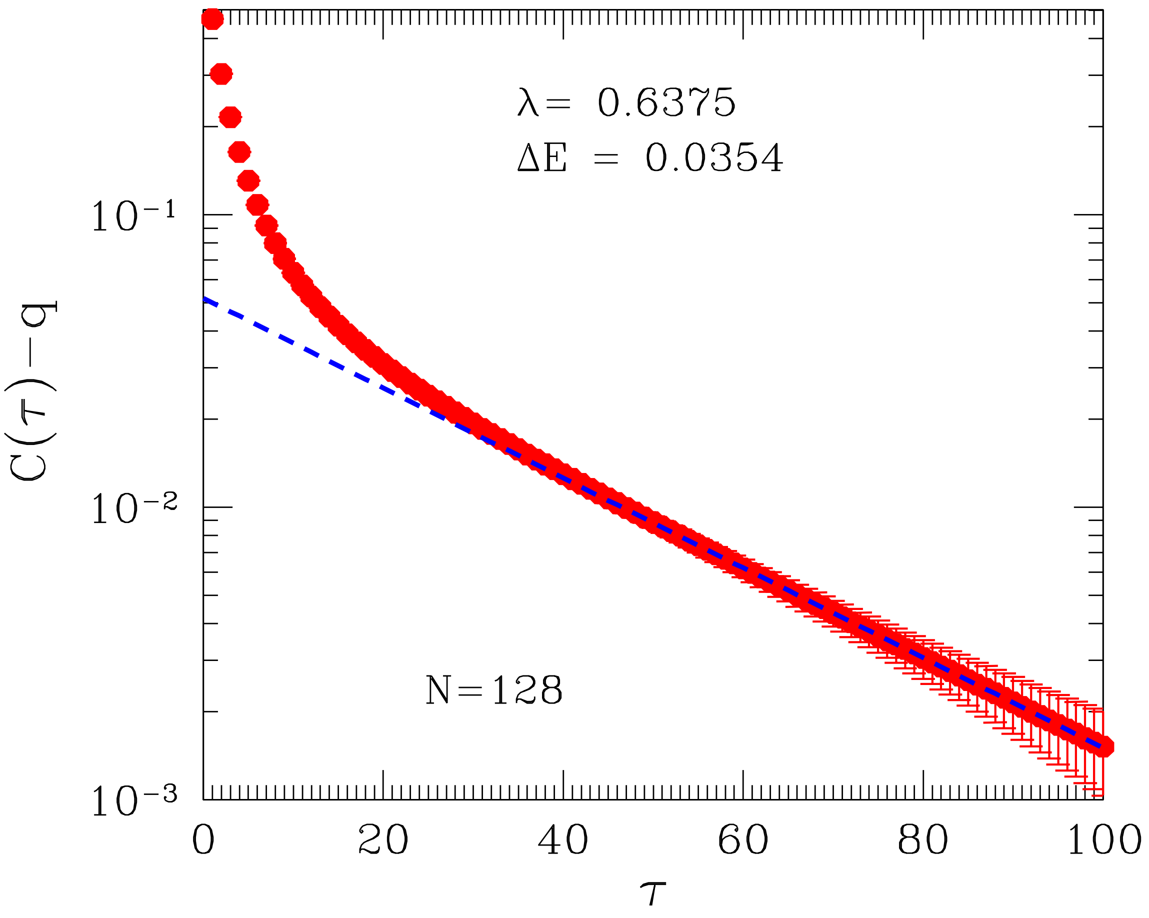
Hence, at large τ, we have

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

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 minimum 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.

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\begin{aligned}
\mathcal{H}_{\mathrm{P}} &= \frac{1}{4}\sum_{\alpha=1}^{M}\left(\sigma^z_{\alpha_1} + \sigma^z_{\alpha_2} + \sigma^z_{\alpha_3} - 1\right)^2 \\
&= \frac{1}{2}\sum_{\alpha=1}^{M}\left(2 - \sigma^z_{\alpha_1} - \sigma^z_{\alpha_2} - \sigma^z_{\alpha_3} + \sigma^z_{\alpha_1}\sigma^z_{\alpha_2} + \sigma^z_{\alpha_2}\sigma^z_{\alpha_3} + \sigma^z_{\alpha_3}\sigma^z_{\alpha_1}\right)
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If there is a **“satisfying assignment”** the energy is zero. Otherwise the energy is a positive integer.

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We simulated the same problem as Farhi et al., namely **Exact Cover**.

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 positive. Writing in terms of spin variables, $\sigma_i^z = 1 - 2b_i$, the simplest such Hamiltonian $\mathcal{H}_\mathrm{P}$ is given by

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

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

If there is a **"satisfying assignment"** the energy is zero. Otherwise the energy is a positive integer.

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

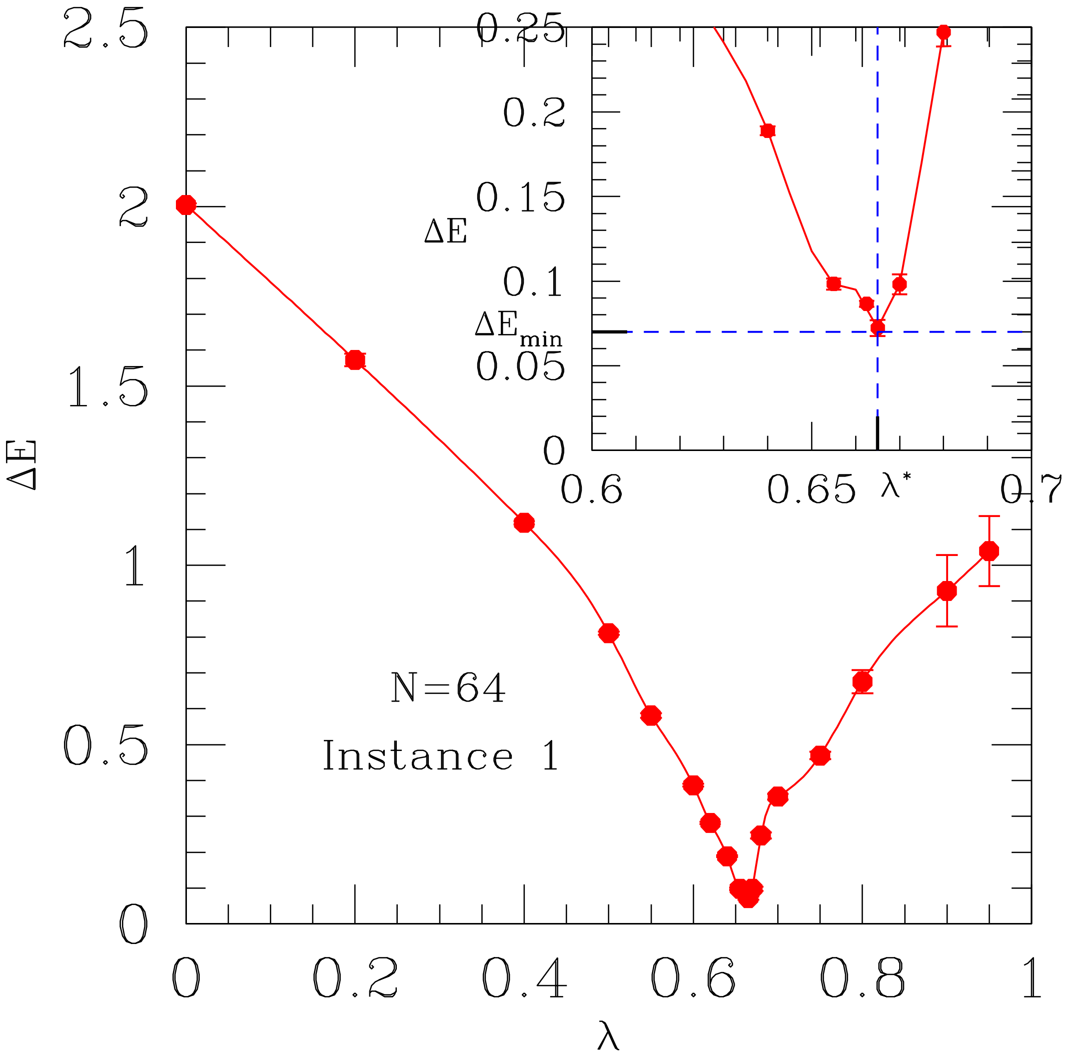
$M/N \ll 1$: the number of clauses is small, it is easy to satisfy them all, and there are **many satisfying assignments**.

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

$N \to \infty$: 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 $\Delta E_{\min}$ 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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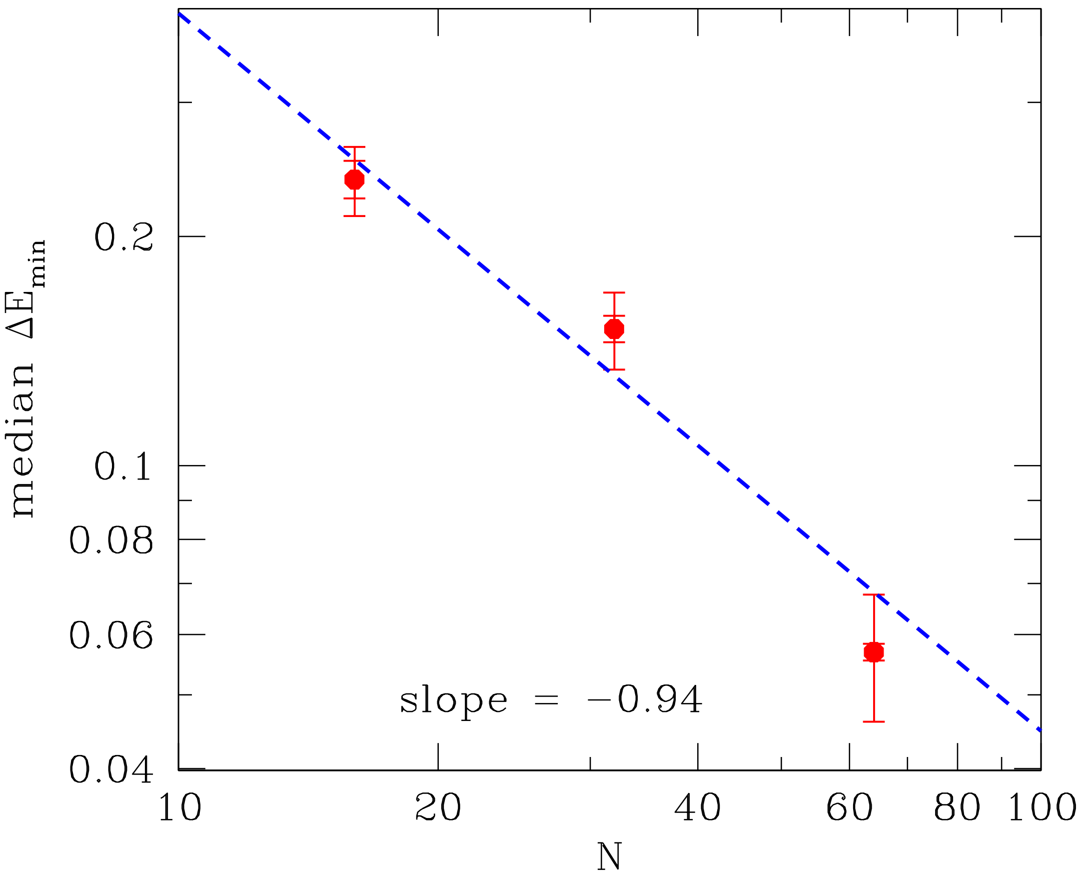


50 instances for each size.

A log-log plot of the **median** of the minimum gap as a function of the number of bits N up to $N = 64$. Up to this size the median $\Delta E_{\min}$ *decreases as a power law*,

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

for these sizes, with

$$\boxed{\mu = 0.94 \pm 0.13.}$$

$\boxed{\text{Complexity } \propto N^{2\mu}}$ (if matrix element effects are small) $\boxed{\text{consistent with } N^2 \text{ behavior}}$ found in early work.

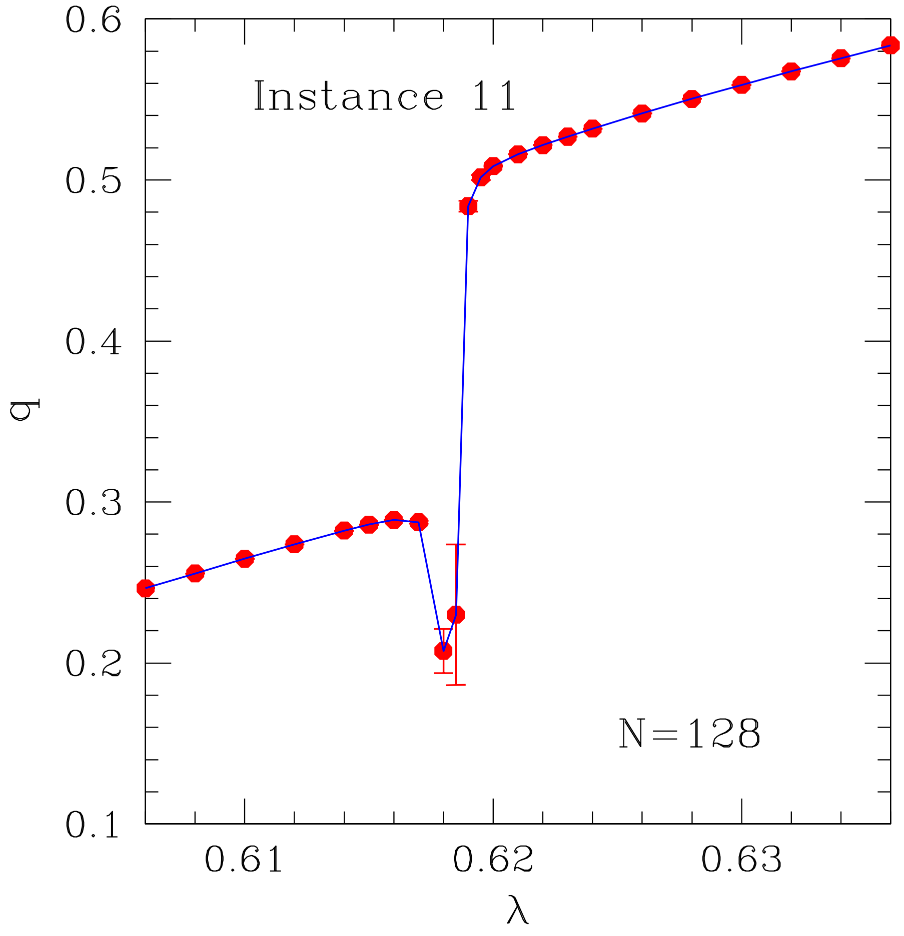
But this behavior does NOT continue for larger sizes because ...

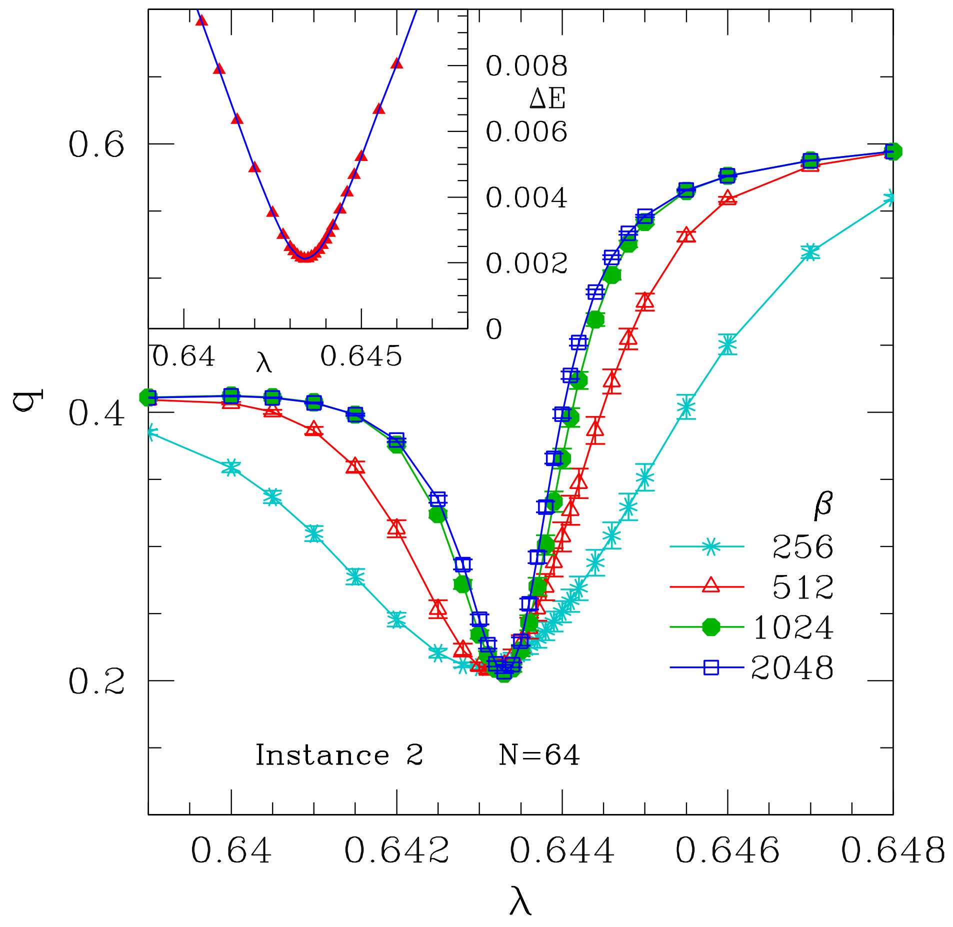
First order transition

$\cdots$ the transition becomes discontinuous (first order).

Compute the "spin glass order parameter"

$$q = \frac{1}{N}\sum_{i=1}^{N}\langle\, S_i^{(1)} S_i^{(2)}\,\rangle\,.$$

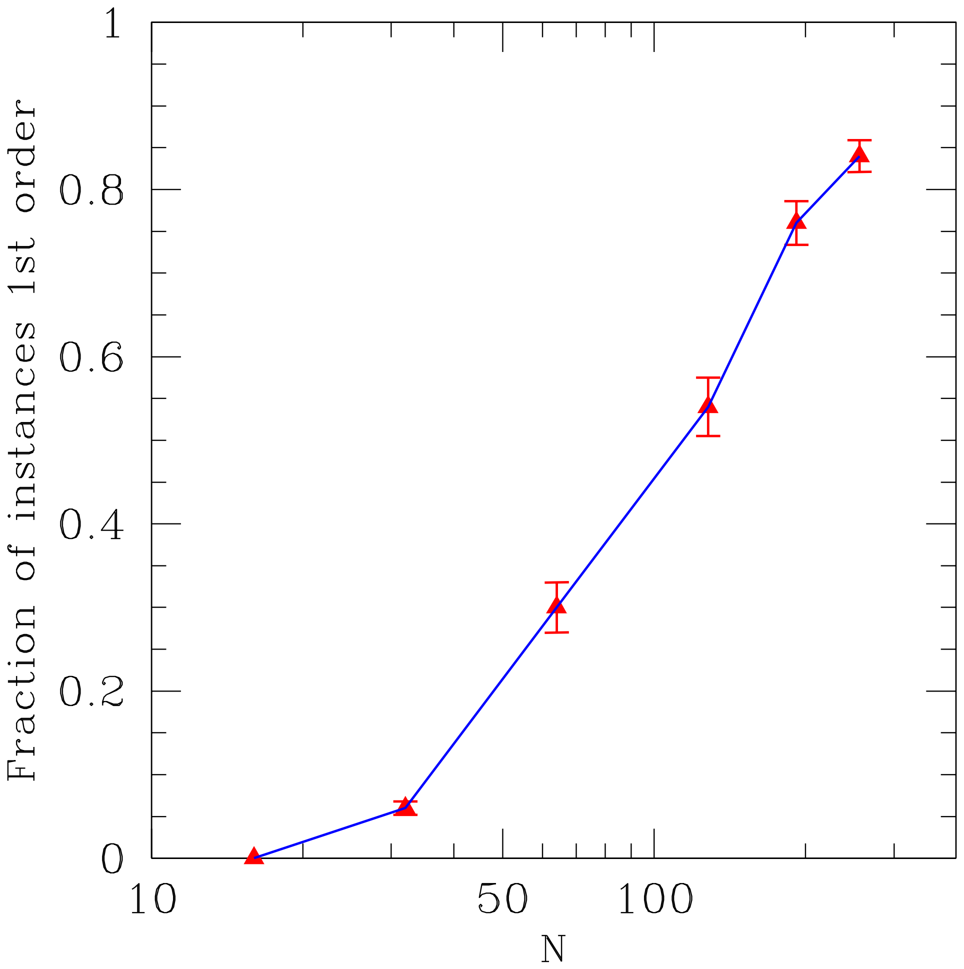




Fraction First order

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

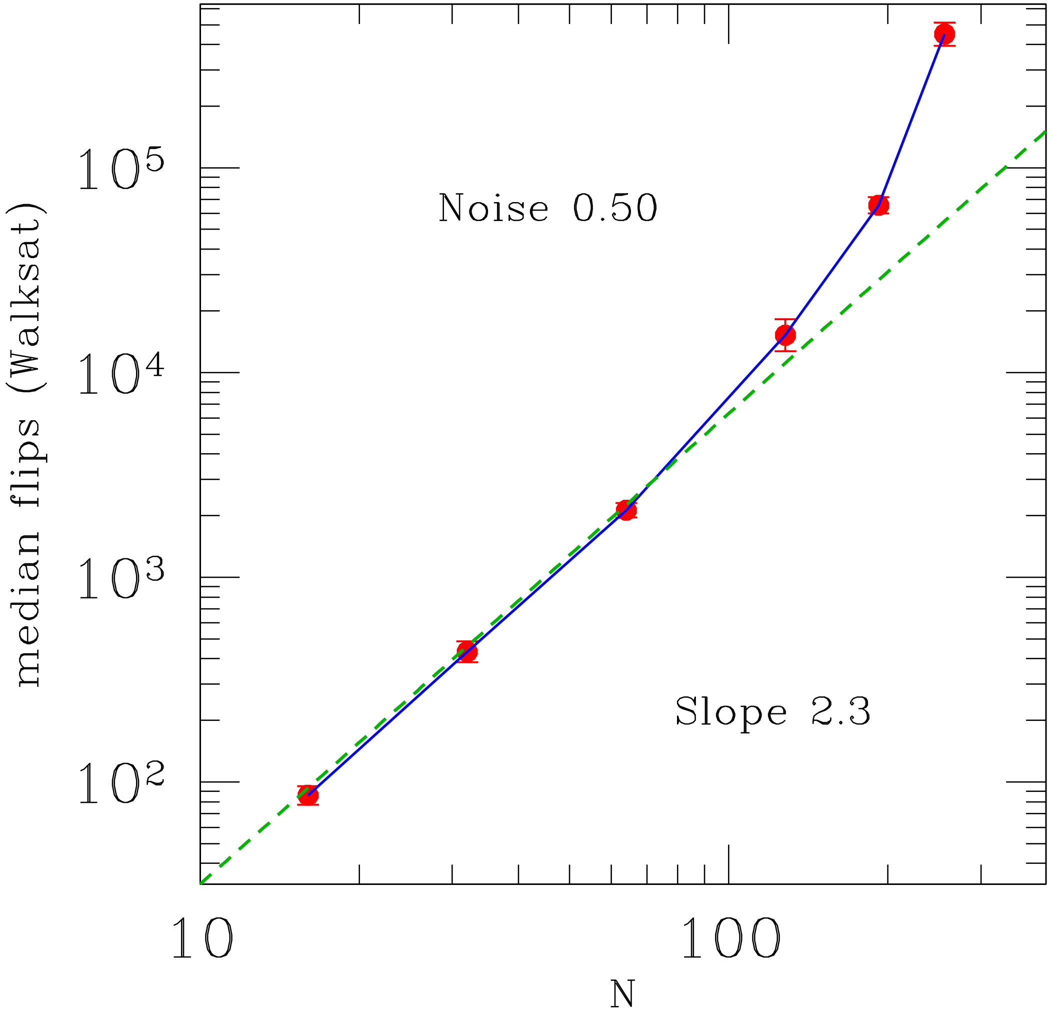
The fraction which are first order appears to tend to 1 for $N \to \infty$.



Recent work by Altshuler, Krovi, Roland (2009), perturbation theory away from $\lambda = 1$, the problem Hamiltonian (similar to Anderson's classic work on localization). For large N they argue there is a high probability of a level crossing with an exponentially small gap at $1 - \lambda \sim N^{-1/8}$.

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. Systems without a sign problem are now called “stoquastic” (Bravyi et al. (2006)). They are characterized by

- All off-diagonal matrix elements of $\mathcal{H}$ 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.

Conclusions

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Thank you