Spin glasses and quantum phase transitions

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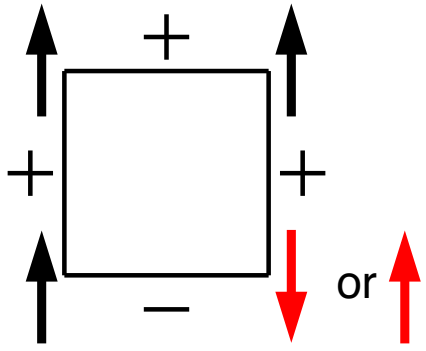
Use computer simulations to understand:

1. Spin glasses
2. Optimization Problems
3. Quantum phase transitions (with possible relevance to quantum computers)

What is a spin glass?

A system with disorder and frustration.



Most theory uses the simplest model with these ingredients:
the Edwards-Anderson Model:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i h_i S_i \,,$$

$$[J_{ij}]_{\rm av} = 0, \qquad [J_{ij}^2]_{\rm av} = J^2 \,.$$

Even determining the ground state is non-trivial.
Connection with optimization problems in computer science.

Phase transition

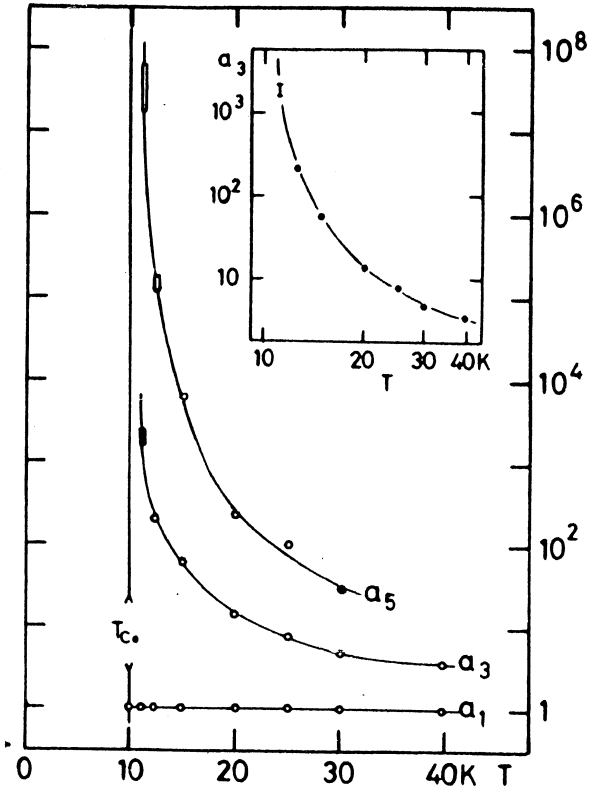
Non-linear susceptibility A phase transition occurs. Experimental signature is the divergence of the non-linear susceptibilty.

χ_{nl}, is defined by

$$m = \chi h - \chi_{nl} h^3 + \cdots$$

Find: $\chi_{nl} \sim (T - T_{SG})$, with γ generally in the range 2.5–3.5; i.e. there is a finite temperature spin glass transition.

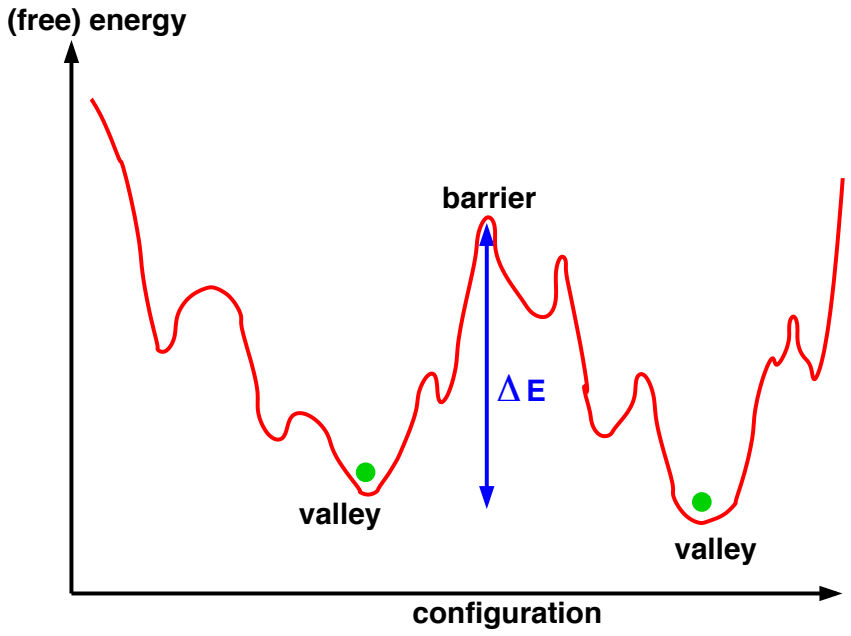
e.g. results of Omari et al, (1983) for $CuMn_{1\%}$.



Slow Dynamics

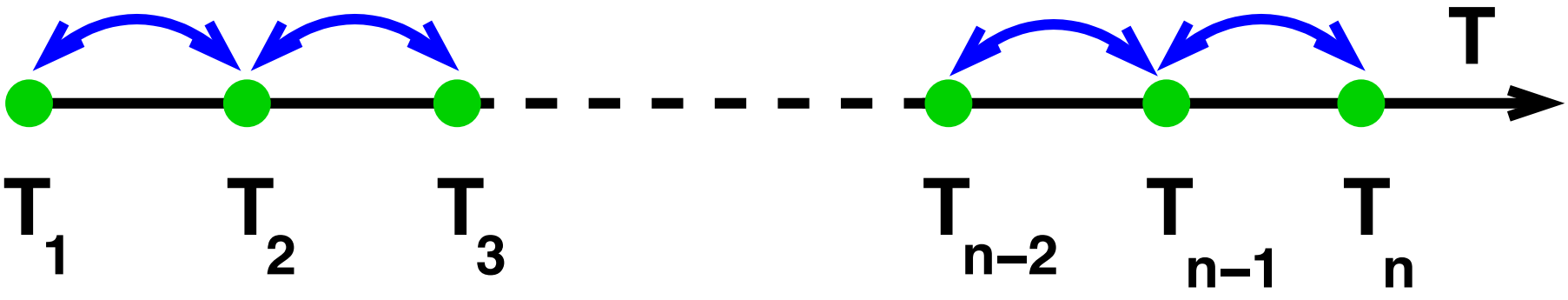
Slow dynamics

The dynamics is very slow at low T. System not in equilibrium due to complicated energy landscape: system trapped in one "valley" for long times.



Parallel Tempering

Problem: Very slow Monte Carlo dynamics at low-T; system trapped in a valley. Needs more energy to overcome barriers.
This is achieved by parallel tempering: simulate copies at many different temperatures:



Lowest T: system would be trapped:
Highest T: system has enough energy to fluctuate quickly over barriers.
Perform global moves in which spin configurations at neighboring temperatures are swapped.
Result: temperature of each copy performs a random walk between T_1 and T_n.
Advantages:

- satisfies detailed balance
- simple
- system can now visit many valleys at low-T (with correct relative weight)

Recent spin glass work

Is there a transition in a magnetic field (Almeida-Thouless line)?

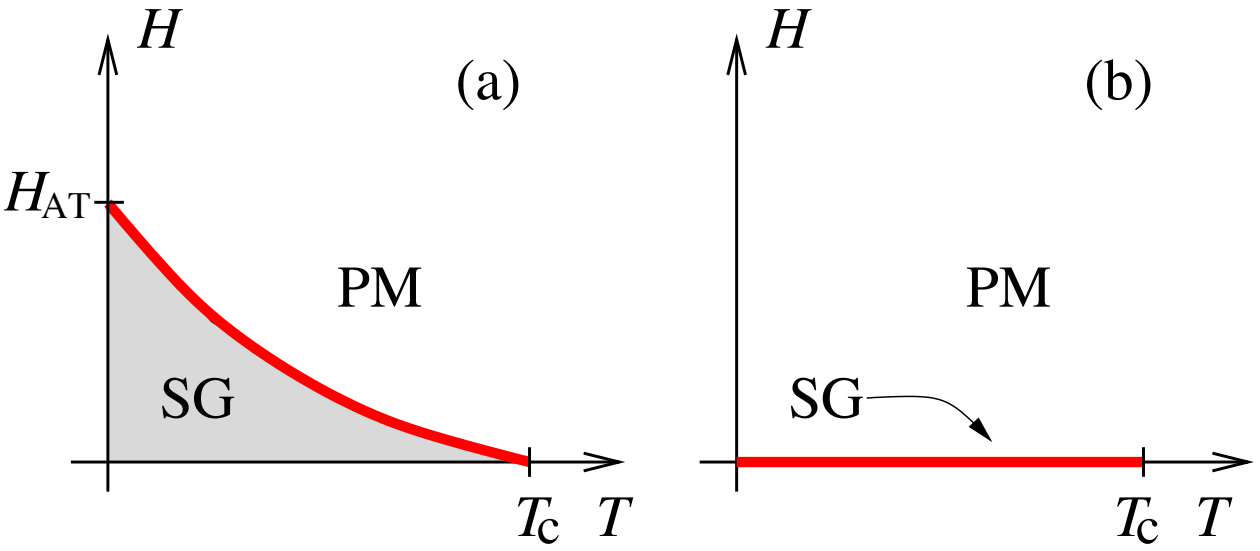


Fig. (a) is one of the most surprising predictions of the mean field theory of spin glasses. One normally expects that a field would break the symmetry so there would be no transition in a magnetic field. (This happens in a ferromagnet, for example.) However, in a spin glass, "mean-field theory" predicts a transition without symmetry breaking but in which the nature of the spin glass state changes, by the development of many "valleys" in the energy landscape.

Seems that this transition does not occur (we have Fig (b)) though a gradual "crossover" does happen. The simulations indicate that a real transition in a magnetic field would occur in high dimensions, though.

Recent spin glass work

Is the resistance of superconductors really zero in a magnetic field.

Have looked at related models which describe the behavior of a superconductor (with disorder) in a magnetic field. Is there a spin-glass like phase (called the "vortex glass")? This would have strictly zero resistance. The resistance is certainly very small, this is why superconducting magnets work, e.g. the LHC. Theoretically of interest to know if there is a phase transition which would lead to a state with strictly zero resistance because of collective effects.

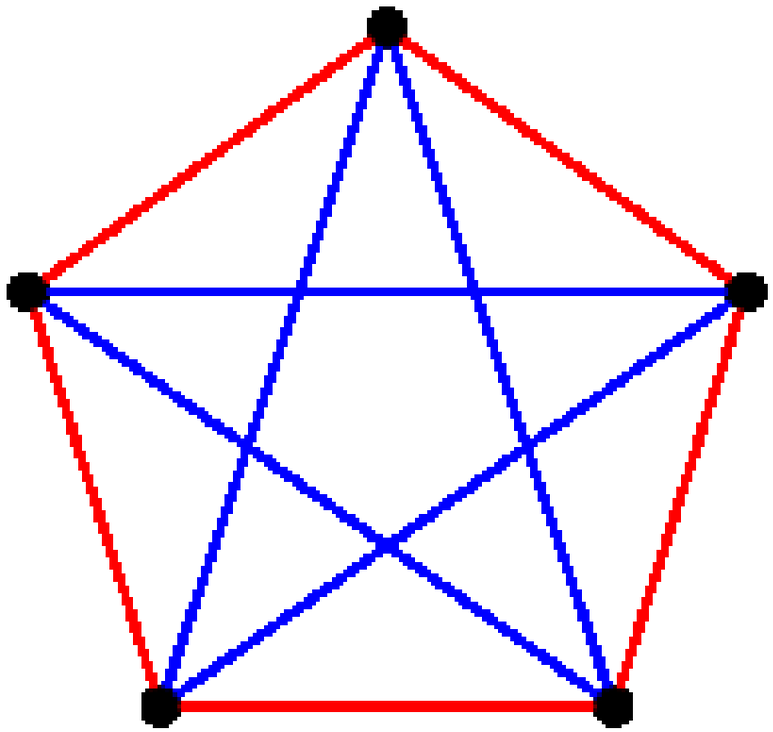
My own work, which is on models that have very different parameters from experimental systems (so effects which can be very hard to see experimentally can be easily visible in the simulations) indicates that the transition would be rounded out but only extremely close to the putative transition, due to "screening" effects between the vortices (probably not observable experimentally).

Optimization Problems

Finding the ground state of a spin glass is a non-trivial "optimization problem".

Can techniques used for spin glasses also be used in other fields?

We are considering the problem of **Ramsey Numbers** in graph theory. Consider a "complete" graph with n_v vertices and $N = n_v (n_v - 1)/2$ edges. Color each edge red or blue. The Ramsey numbers $R(l, m)$ are the smallest values of nv such that each graph has either a complete red subgraph of size l or a complete blue subgraph of size m.



Above figure shows that $R(3, 3) > 5$. Actual value is 6.

Optimization Problems

Values of Ramsey numbers are not known even for small values of l and m.

Ramsey Numbers $R(l,m)$						
$l \downarrow \quad m \rightarrow$	1	2	3	4	5	6
1	1	1	1	1	1	1
2	1	2	3	4	5	6
3	1	3	6	9	14	18
4	1	4	9	18	25	35–41
5	1	5	14	25	43–49	58–87
6	1	6	18	35–41	58–87	102–165

Trying to improve the bounds for R(4, 6) and R(5, 5).

What is a quantum computer?

Classical computer: bit is 0 **or** 1

Quantum computer: qubit: linear superposition of 0 **and** 1.

N qubits: linear superposition of 2^N basis states

Actions on the quantum state act on all 2^N basis states

⇒ Quantum Parallelism

But: to get the result, need to make a measurement

⇒ Don't get 2^N results. Rather there are 2^N probabilities and one gets **one result** according to these probabilities.

Seems that quantum mechanics is not useful for computing

Nonetheless, in some cases useful results can be obtained by doing clever processing **before** the measurement.

The most famous is Shor's algorithm for factoring integers

Optimization problems

Shor's algorithm (factoring large integers) is rather specialized.

Would a quantum computer also be useful for more general problems, such as optimization problems, i.e. minimizing a function of N variables with constraints?

Of interest in many fields in science and engineering.

Here we will take "Problem Hamiltonians" (i.e. the function to be minimized) which involve binary variables, 0 or 1, (or equivalently Ising spins $\sigma^z = \pm 1$).

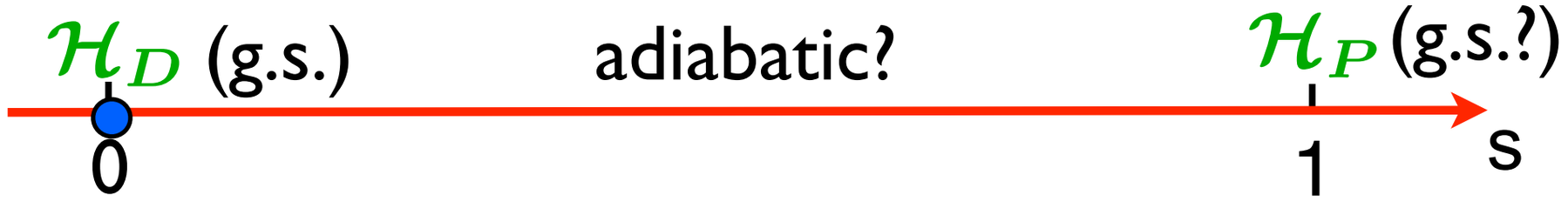
How could we try to solve such optimization problems on a quantum computer?

An idea from physics ....

Quantum Adiabatic Algorithm

Proposed by Farhi et. al (2001) to solve hard optimization problems on a quantum computer.

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



$\mathcal{H}_P$ **is the problem Hamiltonian, depends on the** σ_i^z

$\mathcal{H}_D$ **is the driver Hamiltonian** $= -h\sum(\sigma_i^x - 1)$

$0 \leq s(t) \leq 1, \qquad s(0) = 0, \qquad s(\mathcal{T}) = 1$

$\mathcal{T}$ **is the running time**

System starts in ground state of driver Hamiltonian. If process is adiabatic (and T → 0), it ends in g.s. of problem Hamiltonian, and problem is solved. Minimum $\mathcal{T}$ is the "complexity".

Is $\mathcal{T}$ exponential or polynomial in the problem size N?

Early Numerics

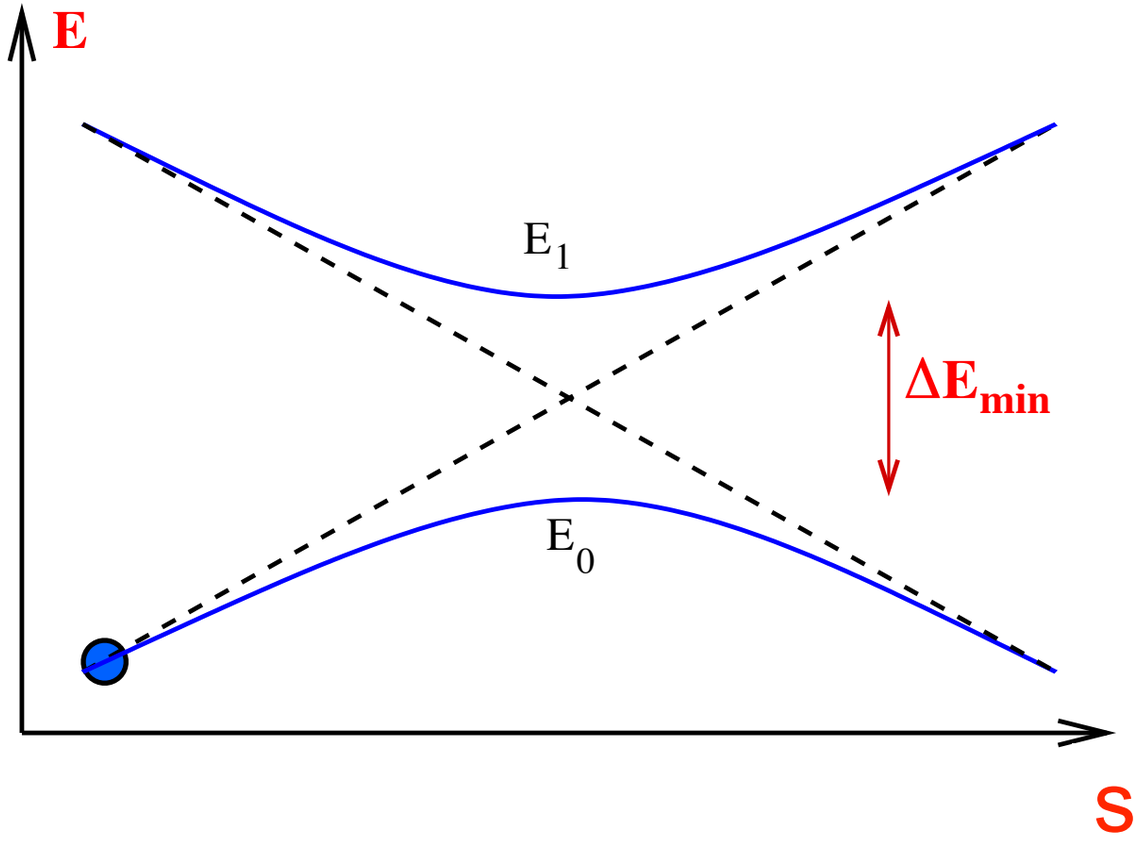
Early numerics, Farhi et al. for very small sizes $N \leq 20$, on a particular problem found the time varied only as N^2 , i.e. polynomial!

But possible “crossover” to exponential at larger sizes?

To explore large sizes, need techniques from statistical physics, Quantum Monte Carlo.

Quantum Phase Transition

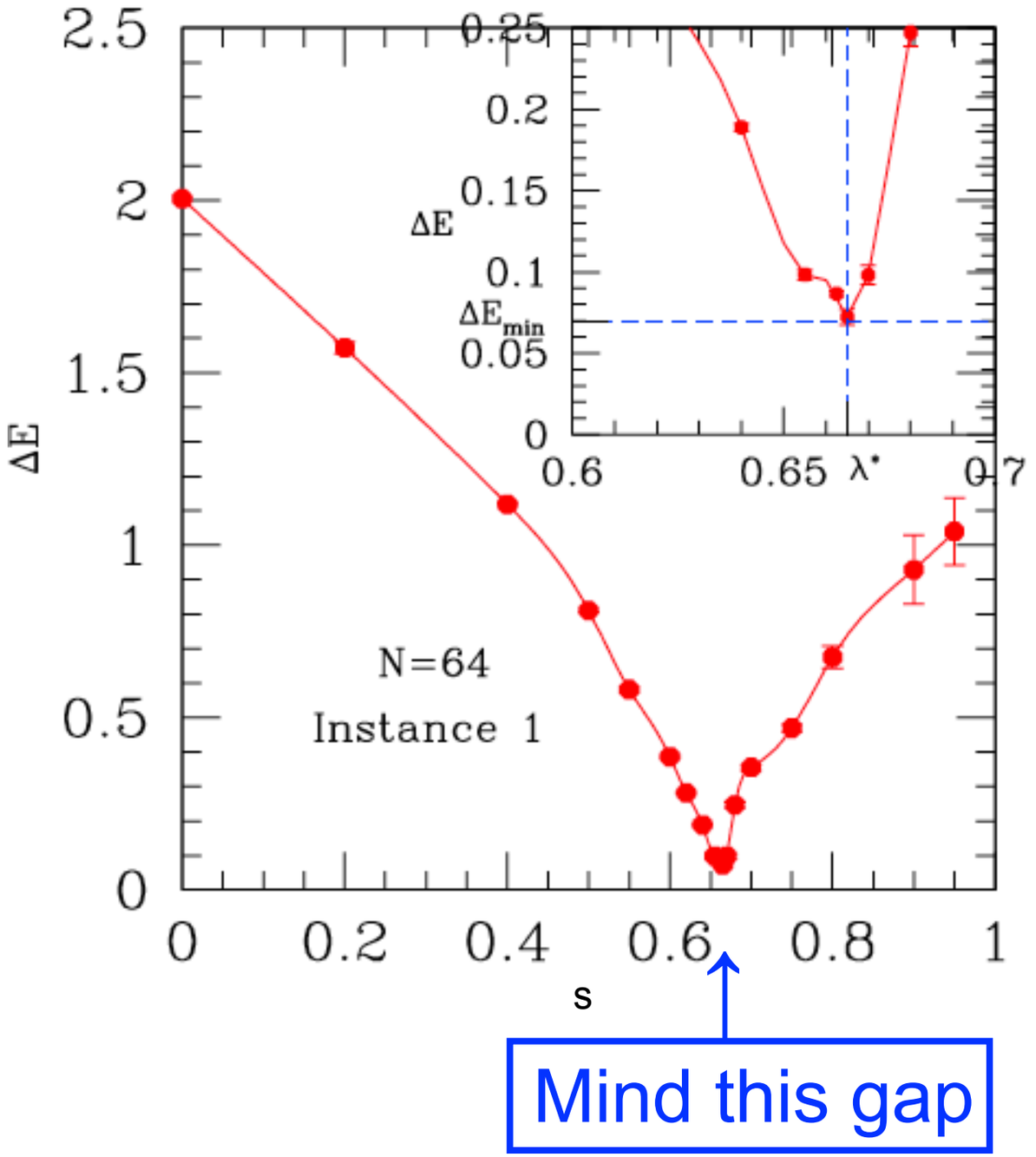
Bottleneck is likely to be a quantum phase transition (QPT) where the gap to the first excited state is very small



Landau Zener Theory:
To stay in the ground state the time needed is proportional to ΔE_{min}^{-2}

Using QMC, we compute ΔE for different s: → ΔE_{min}

Dependence of gap on s



Results for the dependence of the gap to the first excited state, ΔE, with s, for one instance of 1-in-3 SAT with N = 64.

The gap has a minimum for s about 0.66 which is the bottleneck for the QAA.

We compute the minimum gap for many (50) instances for each size N and look how the median minimum gap varies with size.

Satisfiability Problems I

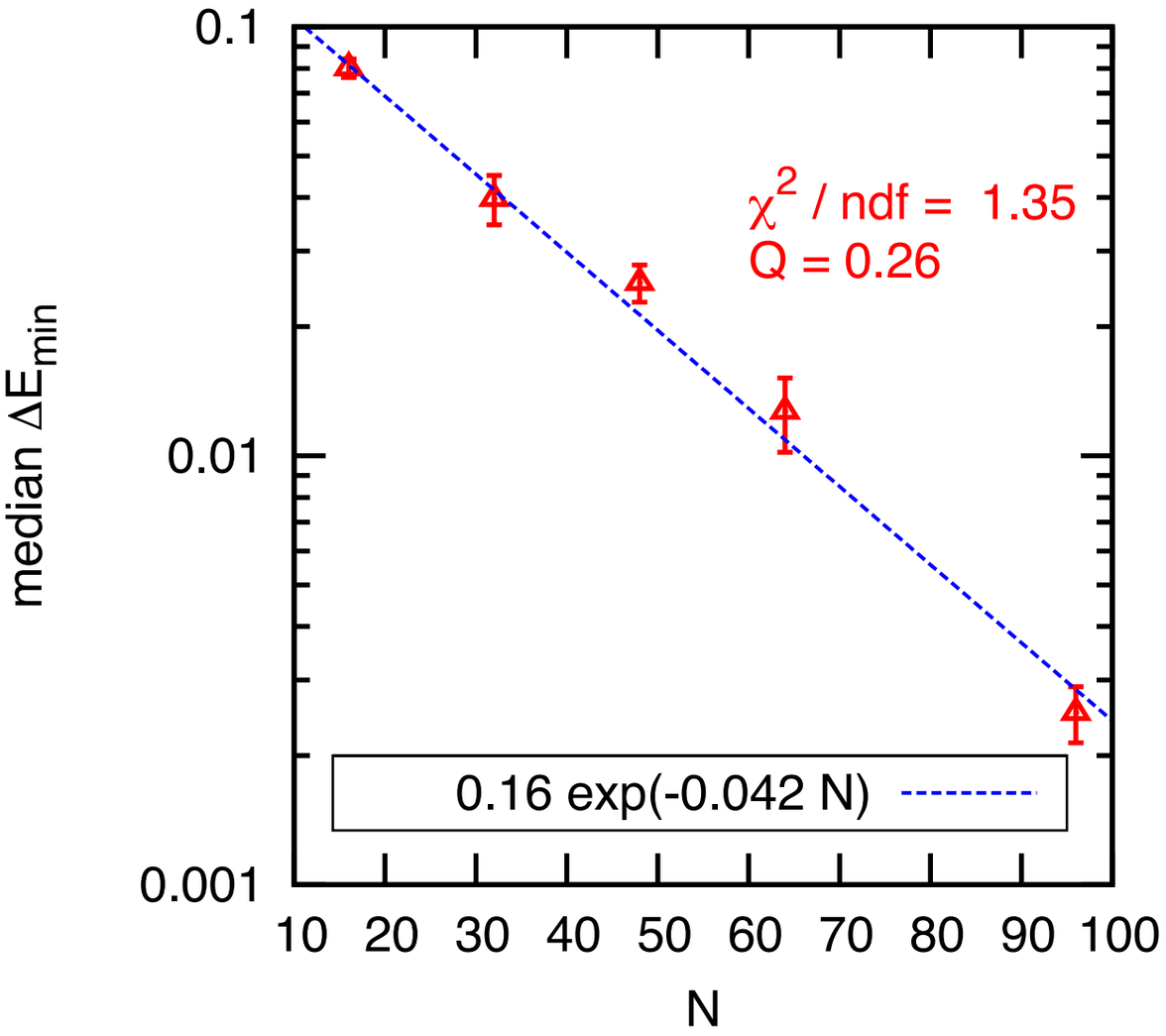
In satisfiability problems (SAT) we ask whether there is an assignment of N bits which satisfies all of M logical conditions ("clauses"). We assign an energy to each clause such that it is zero if the clause is satisfied and a positive value if not satisfied.

i.e. We need to determine if the ground state energy is 0.

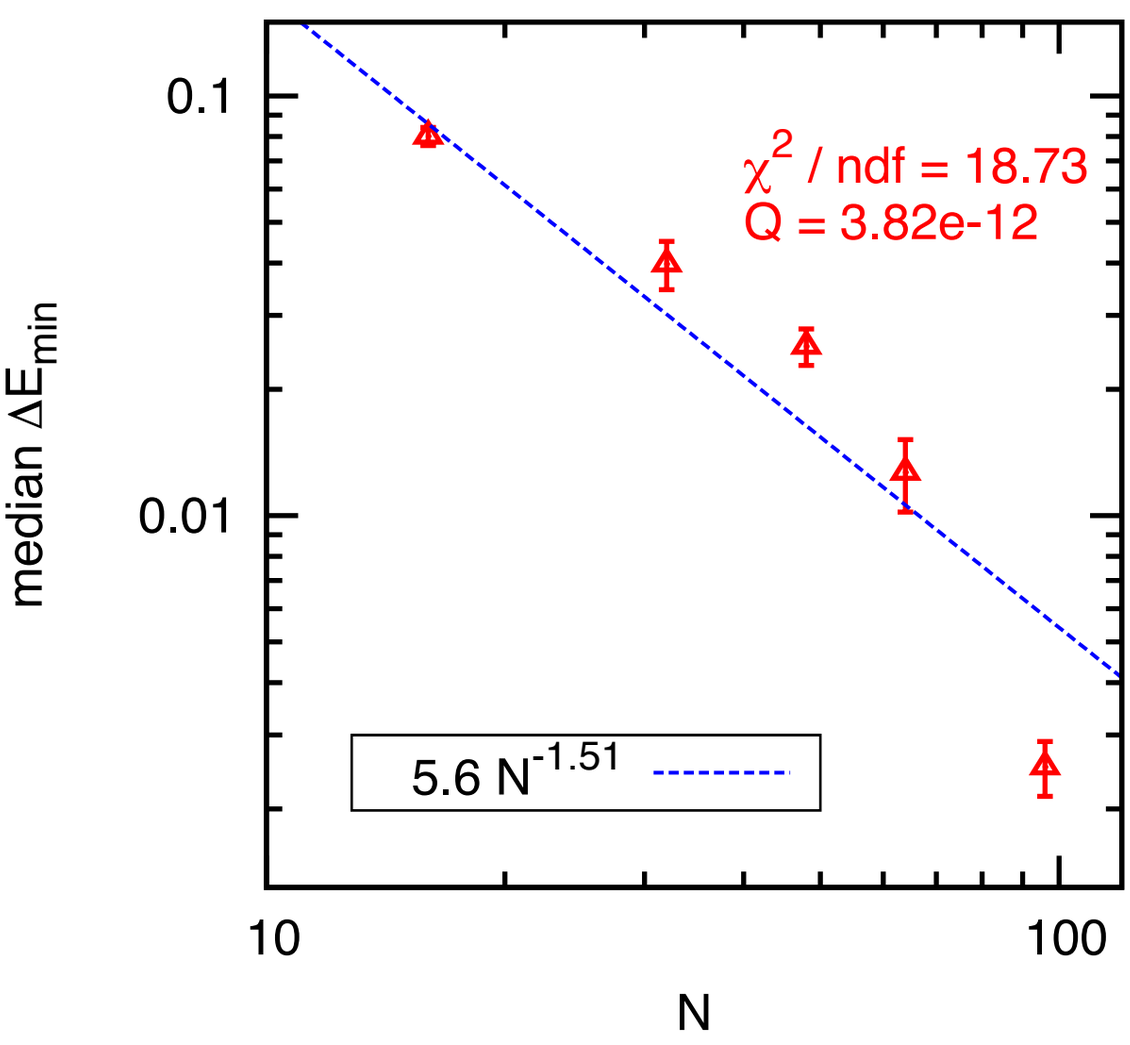
We take the ratio of M/N to be at the satisfiability threshold, and study instances with a "unique satisfying assignment" (USA).
(so gap to 1st excited state has a minimum whose value indicates the complexity.)

Locked 1-in-3

Plots of the median minimum gap (average over 50 instances)



Exponential fit



Power law fit

Clearly the behavior of the minimum gap is exponential

Comparison with a classical algorithm, WalkSAT: I

WalkSAT is a classical, heuristic, local search algorithm. It is a reasonable classical algorithm to compare with QAA.

We have compared the running time of the QAA for the three SAT problems studied with that of WalkSAT.

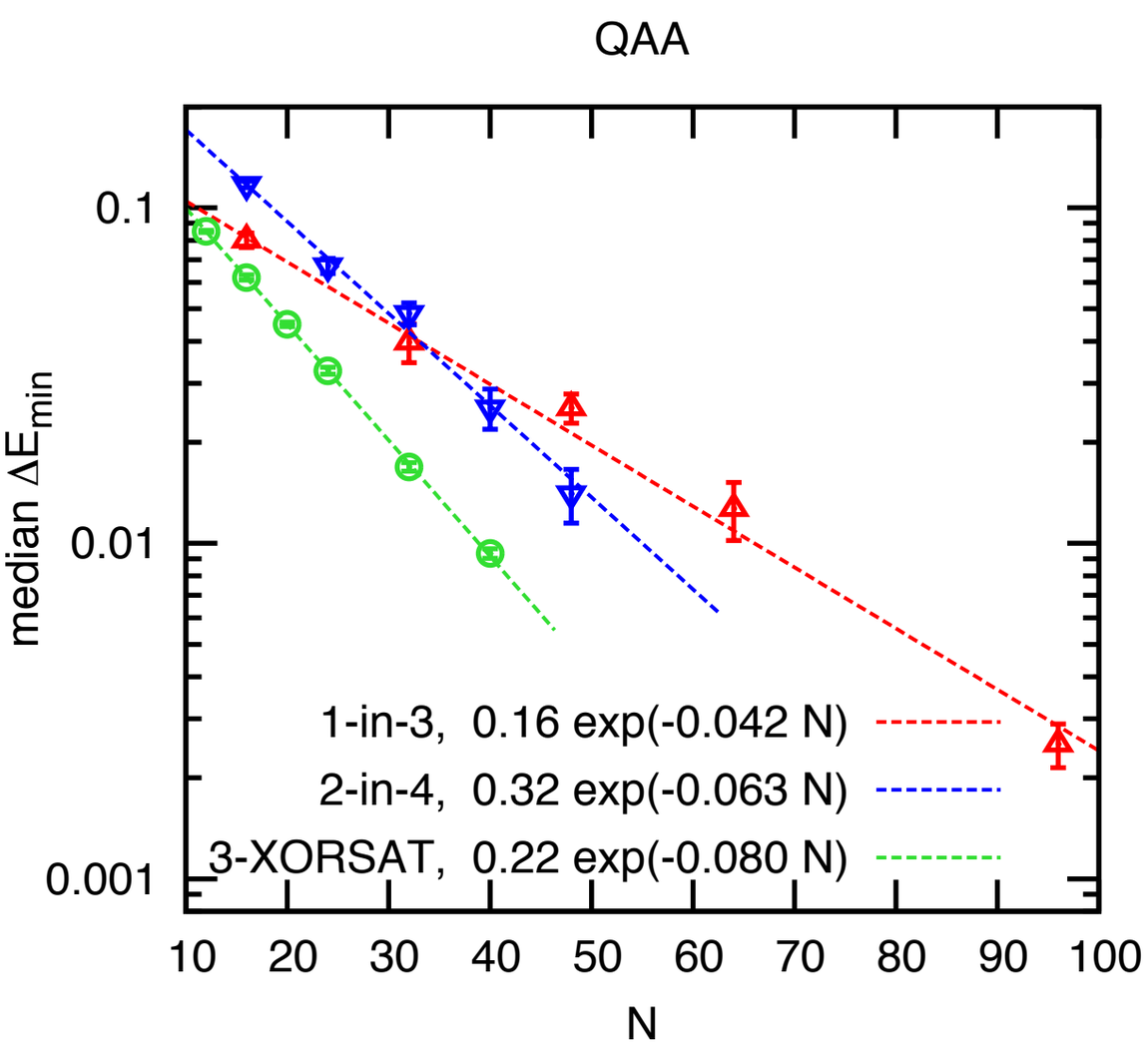
For QAA, Landau-Zener theory states that the time is proportional to $1/(\Delta E_{min})^2$ (neglecting N dependence of matrix elements).

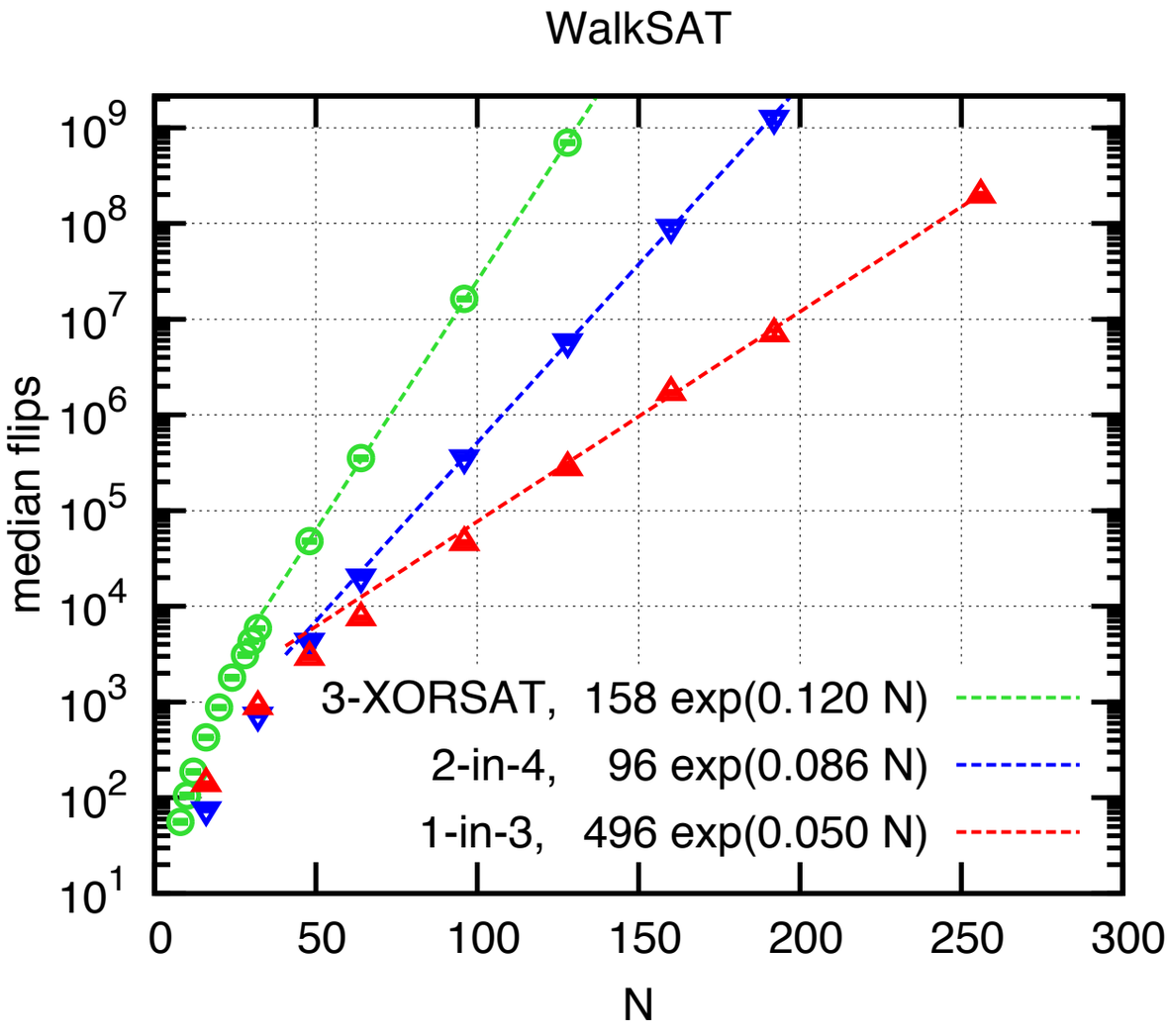
For WalkSAT the running time is proportional to number of "bit flips".

We write the running time as proportional to $\exp(\mu N)$.

We will compare the values of μ among the different models and between QAA and WalkSAT.

Comparison with a classical algorithm, WalkSAT: II





Exponential behavior for both QAA and WalkSAT

The trend is the same in both QAA and WalkSAT.
3-XORSAT is the hardest, and locked 1-in-3 SAT the easiest.

Comparison with a classical algorithm, WalkSAT: III

Model	QAA	WalkSAT	Ratio
1-in-3	0.084(3)	0.0505(5)	1.66
2-in-4	0.126(7)	0.0858(8)	1.47
3-XORSAT	0.159(2)	0.1198(4)	1.32

Exponential complexity in both cases. QAA not better than WalkSAT.

Values of μ (where time ~ exp[μ N]).

These results used the **simplest implementation** of the QAA **for instances with a USA**.
Interesting to also study **random instances** to see if they also have exponential complexity in QAA.
Also look for **better paths in Hamiltonian space**.

Conclusions for quantum computing

- Simple application of QAA gives **exponentially small gaps** for SAT problems with a USA. This implies that the time to solve the problem would grow exponentially with N (like classical algorithms).
- Need to see if the exponentially small gap is absent in other cases:
  - look at other problems
  - repeatedly run the algorithm with different random values for the transverse fields (and costs).
  - try to find a clever way to optimize the path in Hamiltonian space “on the fly” during the simulation to increase the minimum gap.