

Mind the gap: Solving optimization problems on a quantum computer.

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SANTA CRUZ



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WHERE DISCOVERIES BEGIN

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Why is quantum different?

- **Quantum Parallelism**

A quantum state is a linear combination of basis states. Acting with a discrete unitary transformation acts **in parallel** on all states. This is the basis of the **traditional paradigm of quantum computing**, e.g. **Shor's algorithm** for factoring integers:

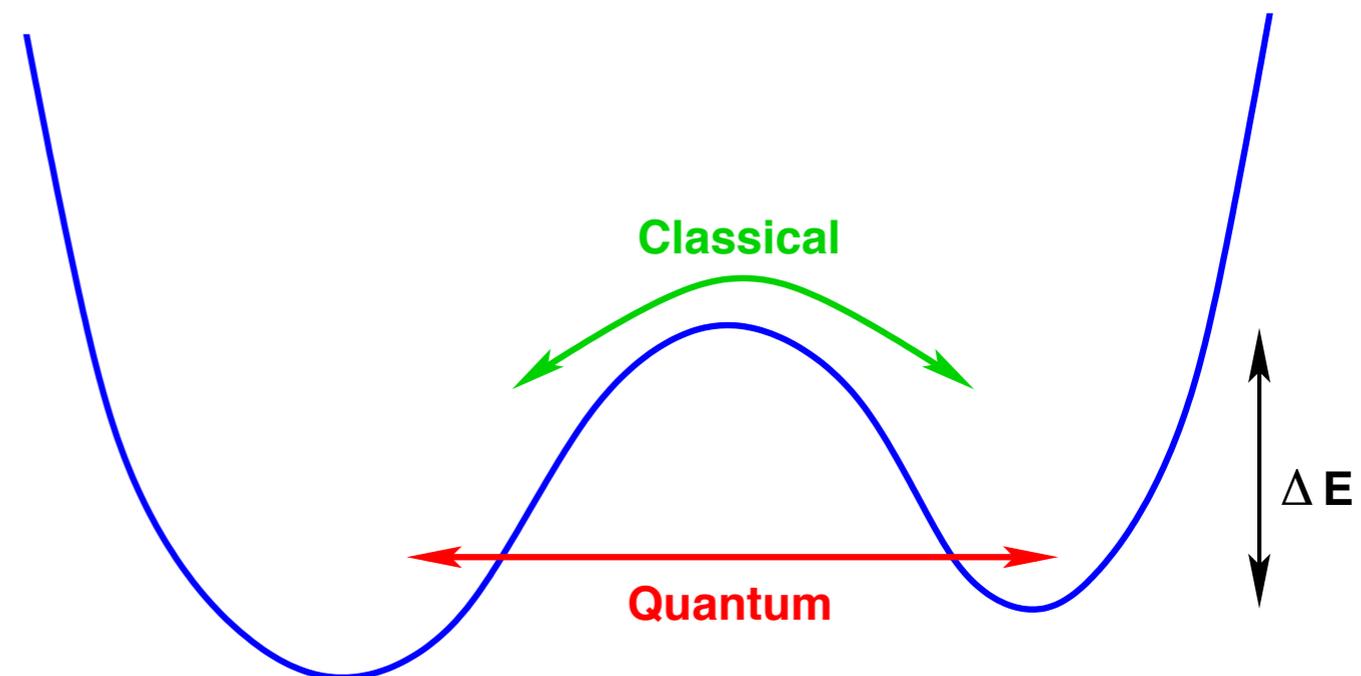
Exponential time (classical) → polynomial time (QM)

Exponential speedup!

- **Quantum Tunneling**

Classically, a particle has to be thermally activated over a barrier, in QM it can tunnel through it. This gives a 2nd paradigm for QC known as

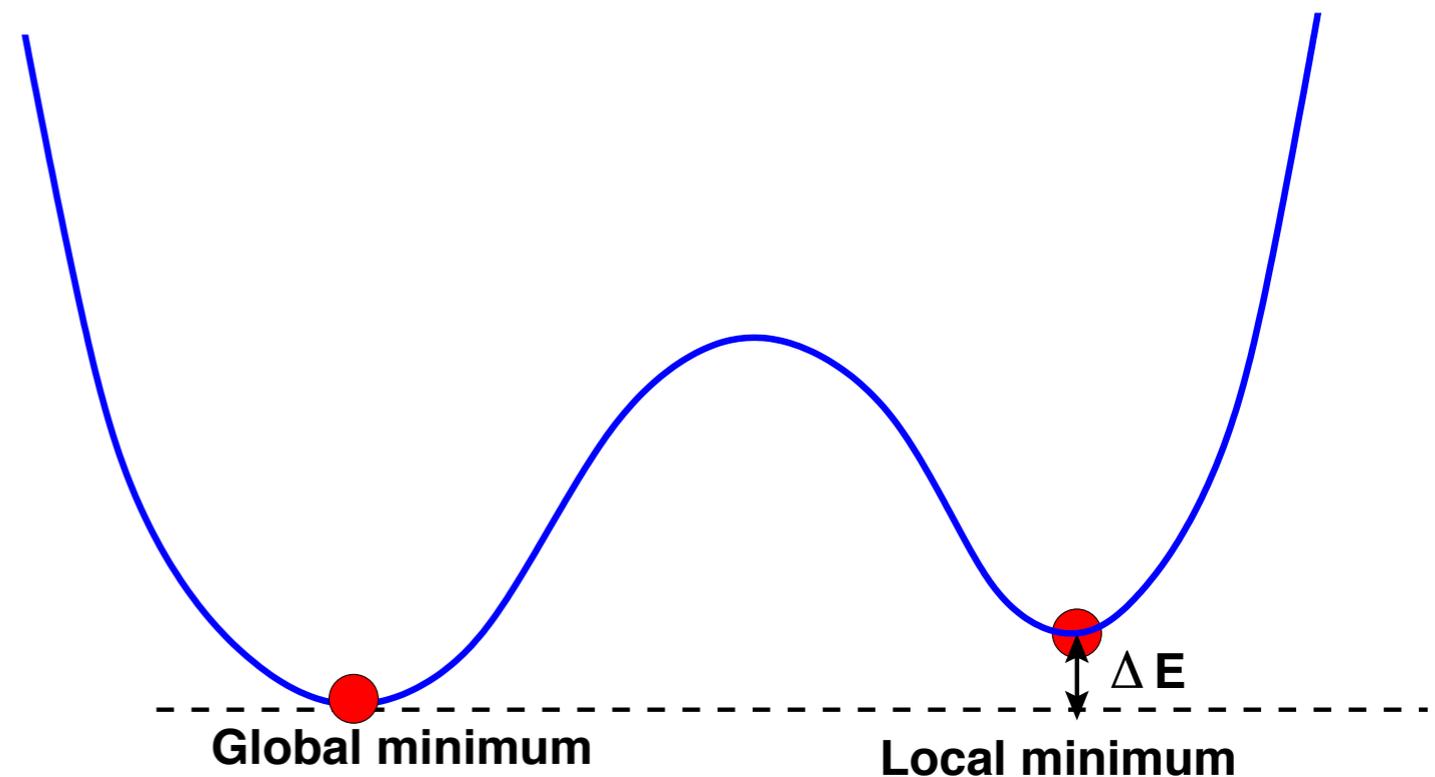
Quantum Annealing/Quantum Adiabatic Algorithm



Quantum Annealing / Quantum Adiabatic Algorithm (for solving Optimization Problems)

Suppose we have to find the minimum of a function (Hamiltonian) of many variables, an **optimization problem**. In problems of interest no set of variables simultaneously minimizes each term. This is called “**frustration**” in the spin glass language.

Optimization problems occur in physics, e.g. **spin glasses**, biology, e.g. **protein folding**, computer science, e.g. **SAT** problems, engineering, e.g. **pattern recognition** (interest of **Google**).



Minimizing w.r.t. each variable in turn (**greedy algorithm**) you get stuck in a **local minimum**. How can we get out of a local minimum to find the **global minimum**?

Physics inspired methods for Optimization Problems

- **Thermal (classical) annealing** (Kirkpatrick et al.)
also known as simulated annealing (**SA**). Put in a **non-zero temperature** and do (classical) Monte Carlo. Some probability to go “uphill” in energy, so can escape from local minima by **thermal activation OVER** the barriers. $T \rightarrow 0 \text{ as } t \rightarrow \infty$
- **Quantum Annealing (QA)** (Santoro et al, Kadawoki & Nishimori)
Same general idea as SA but induce **quantum** (rather than thermal) **fluctuations** by adding a simple but **non-commuting driver Hamiltonian H_D** . System then escape from local minima by **quantum tunneling THROUGH** barriers. $H_D \rightarrow 0 \text{ as } t \rightarrow \infty$
Often simulated on a classical computer using QMC. Then called **Simulated Quantum Annealing (SQA)** (Troyer et al.)
- **Quantum Adiabatic Algorithm (QAA)** (Farhi et al.)
Similar to QA but (a) always stay in the ground state of the Hamiltonian (**adiabatic theorem**) and (b) runs on a **quantum computer / quantum annealer**. (See rest of talk.)

Quantum Adiabatic Algorithm

Want to find the ground state of a **problem Hamiltonian** \mathcal{H}_P involving Ising spins, $\sigma_i^z = \pm 1$, or equivalently, bits $b_i = 0$ or 1 , e.g. a spin glass

$$\mathcal{H}_P = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^z$$

Make quantum by adding a **non-commuting driver Hamiltonian**.

Simplest is a transverse field: $\mathcal{H}_D = -\Gamma \sum_i \sigma_i^x$

Total Hamiltonian:

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

with $s(0) = 0$, $s(\tau) = 1$.



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

Real Experiments:

D-Wave: large number of superconducting qubits:

D-Wave 1, 128 qubits

D-Wave 2, 512 qubits

Runs the QAA.

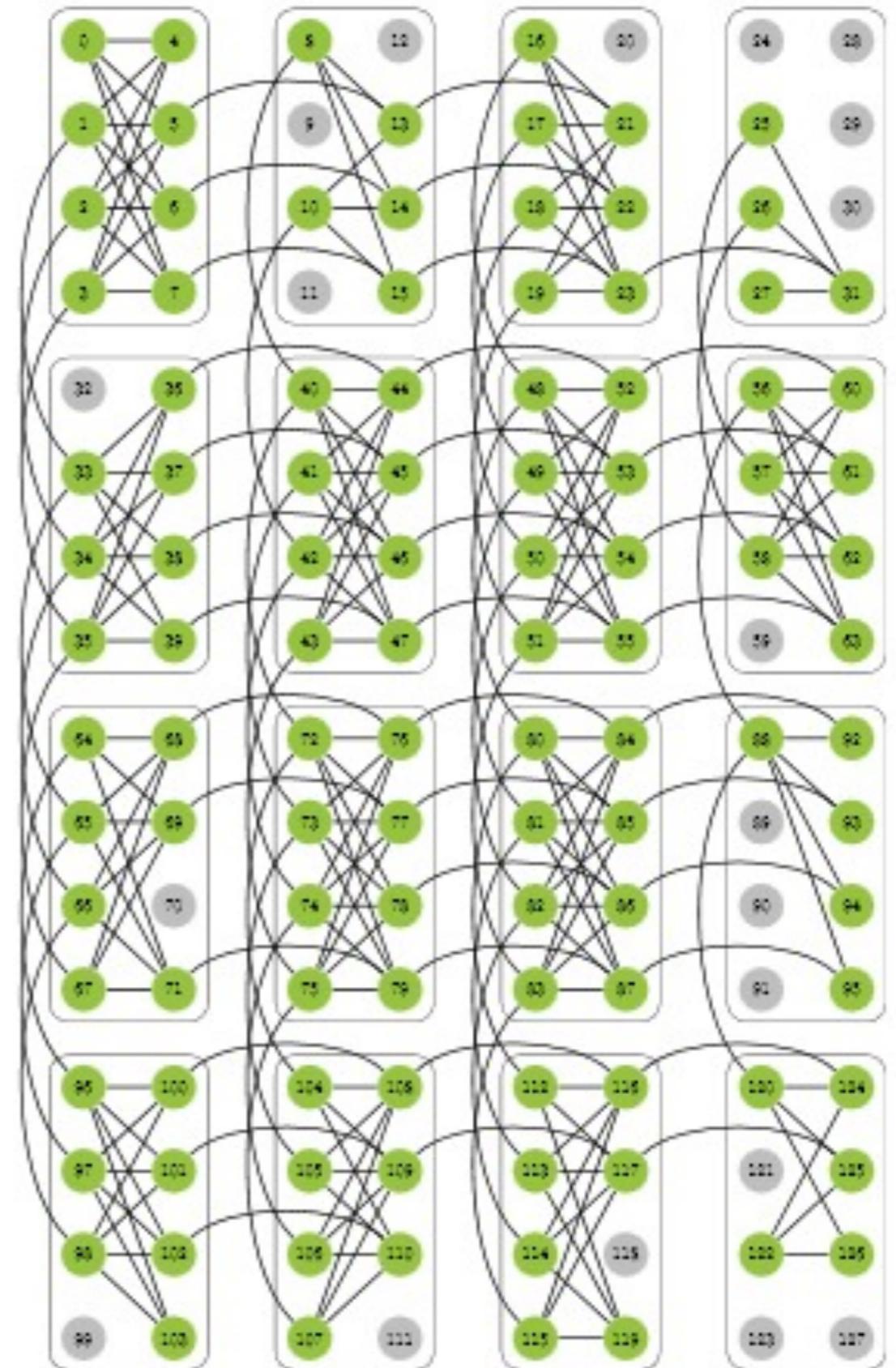
During the run, phase coherence is not maintained, hence call this a **quantum annealer**.

Questions:

- D-Wave has noise and non-zero T , so is it really quantum?
- If it is, then is the D-Wave machine more efficient than a classical computer?



D-Wave



Connections of the qubits form a (2-d) “chimera” graph, see figure for D-Wave 1.

Outline

In this talk I will discuss:

- Results of simulations (QMC) that I've been involved in on **idealized** (quantum) models which are **not coupled to the environment and which are, effectively at $T = 0$** . The idea is to see how the **time to solve the problem increases with system size**.
- Briefly discuss how the difficulties of solving optimization problems with thermal or quantum annealing may be related to **classical and quantum chaos** (c.f. Gutzwiller's work).

Complexity

On a classical computer, the running time for hard problems increases exponentially with problem size N , i.e.

$$\tau \propto \exp(\mu N)$$

Can QA/QAA do better? Unlikely to become polynomial but can it make μ smaller?

In the traditional “gate model” paradigm of QC it is known for certain problems, e.g. integer factoring, that there is a quantum speedup, (if decoherence can be eliminated, which is a big “if”)

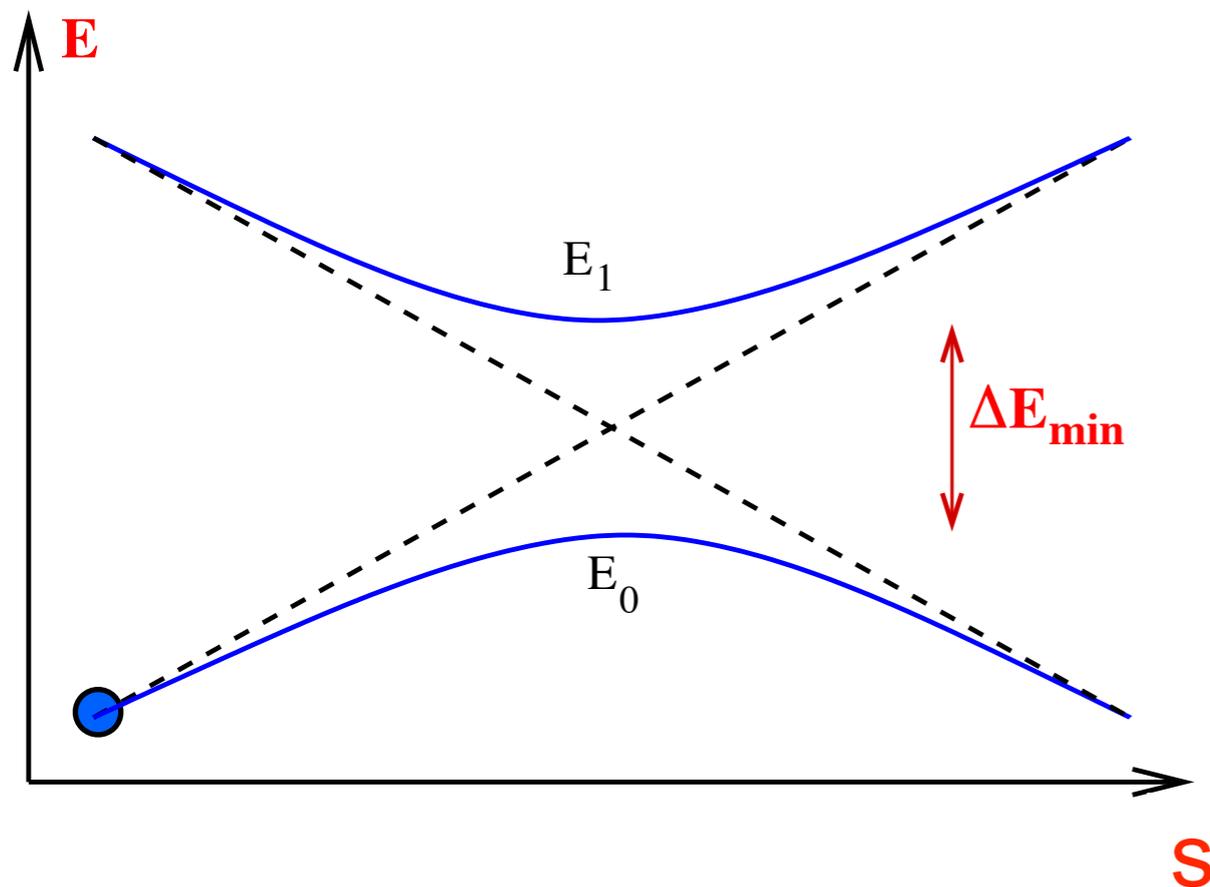
In the QA/QAA paradigm there is no proof that quantum can do better, but also no proof that it can't. **Hence we need numerics.**

Note: there is hope that noise/decoherence doesn't immediately remove the quantum speedup in QA/QAA (if it exists), since it uses quantum tunneling. This is different from the gate model, which uses quantum parallelism.

Quantum Phase Transition



Bottleneck is where the **gap to the first excited state is very small**, for example at a **quantum phase transition (QPT)**



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

Used **QMC** to compute ΔE for different s : $\rightarrow \Delta E_{\min}$

Synopsis: Mind the Gap



iStockphoto.com/cinoby

Quantum computers promise to accelerate some kinds of calculations, but that's only half the story: efficiency requires development of new algorithms.

To apply a quantum computer to a broad class of problems, researchers have developed an algorithm in which the problem to be solved is encoded into the ground state of a Hamiltonian.

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MIND THE GAP

Exponential complexity of the quantum adiabatic algorithm for certain satisfiability problems

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Quantum Monte Carlo

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

But possible “crossover” to exponential at larger sizes?

Want to estimate how the running time varies with size for large sizes.

We therefore have to do a **Quantum Monte Carlo Sampling** of the 2^N states.

QMC can efficiently study only **equilibrium** properties of a quantum system by simulating a **classical model with an extra dimension**, imaginary time, τ , where $0 \leq \tau < 1/T$.
Used a version called the stochastic series expansion (SSE), pioneered by Sandvik.

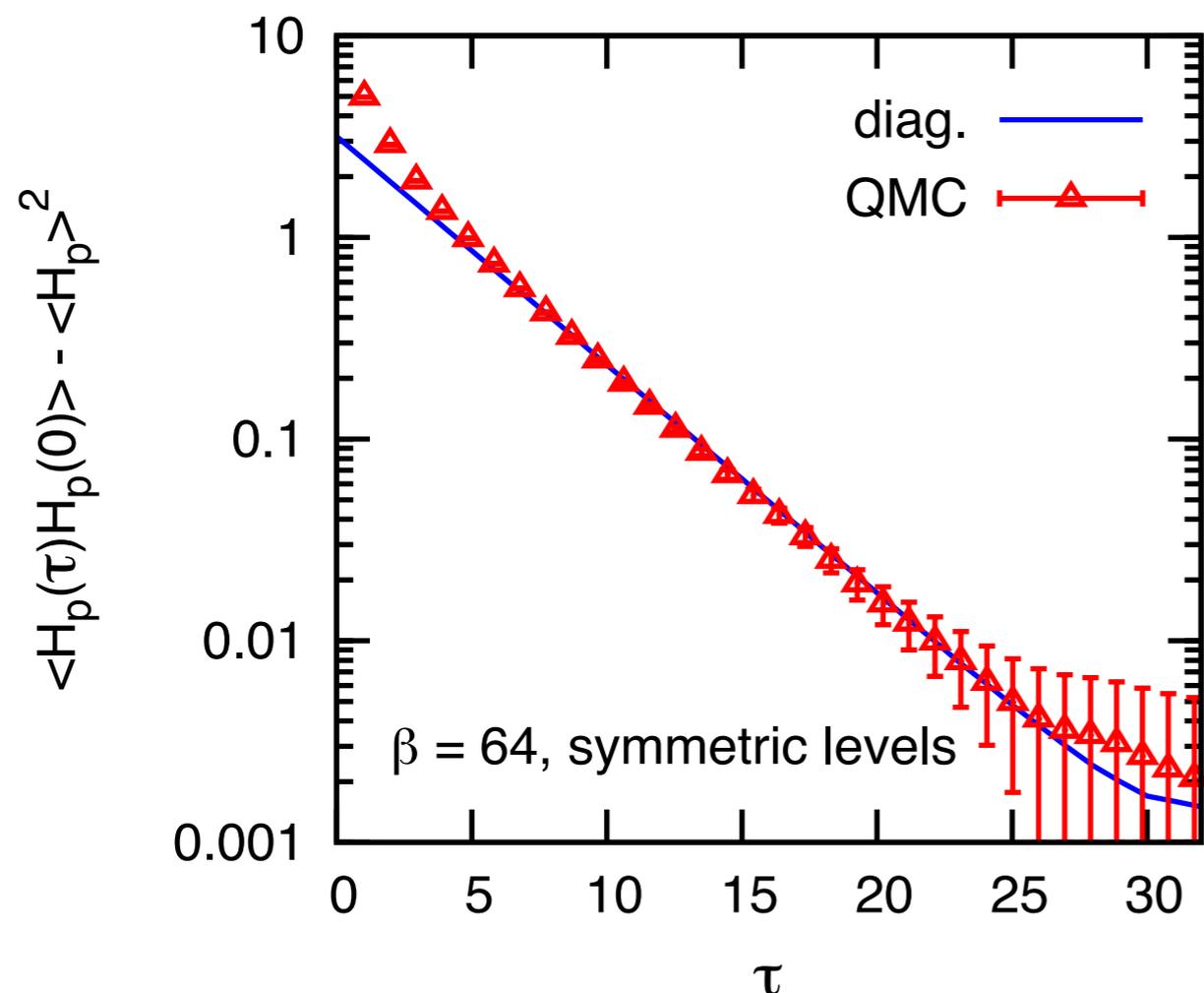
Not perfect, (statistical errors, need to ensure equilibration) but the only numerical method available for large N .

Examples of results with the SSE code

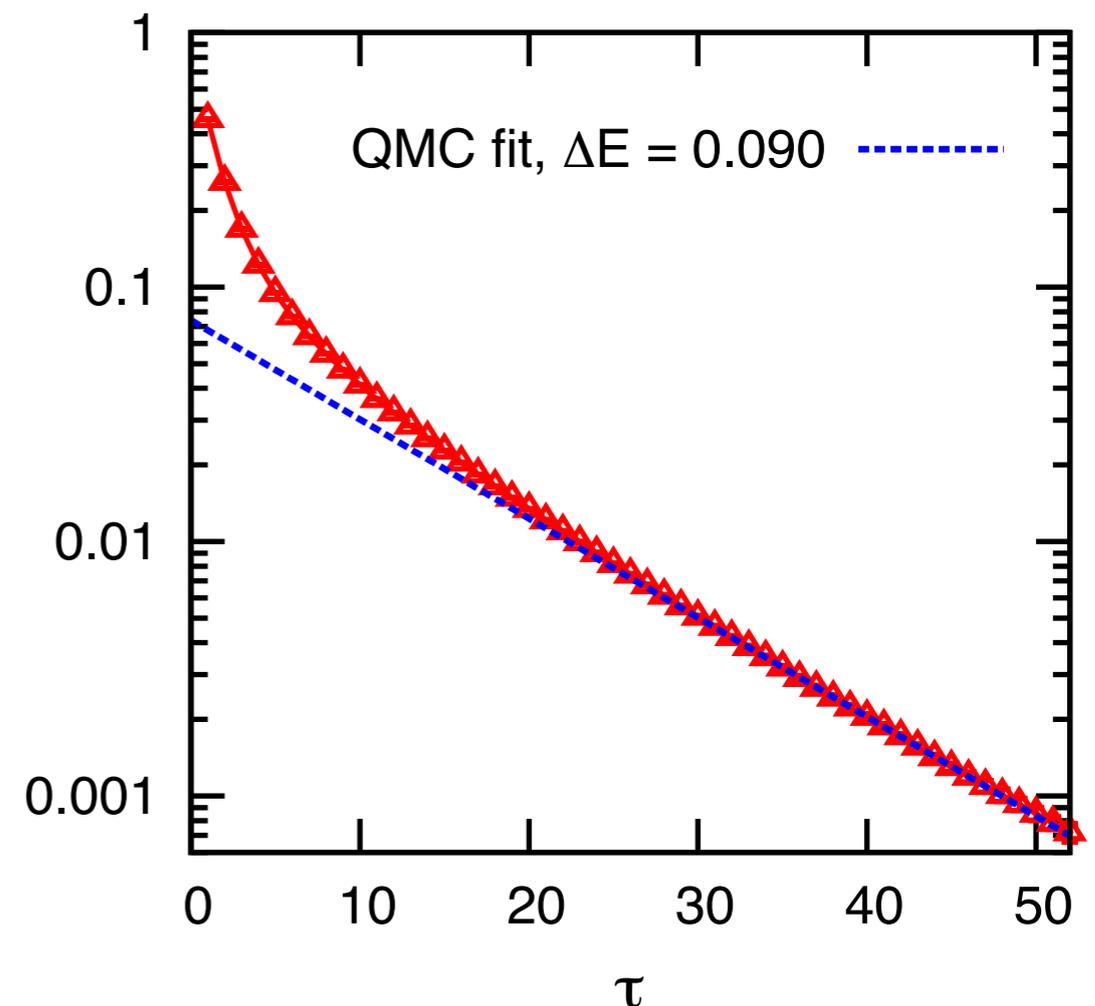
Time dependent correlation functions decay with τ as a **sum of exponentials**

$$\langle A(\tau)A(0) \rangle - \langle A \rangle^2 = \sum_{n \neq 0} |\langle 0|A|n \rangle|^2 \exp[-(E_n - E_0)\tau]$$

For **large τ** only first excited state contributes, \rightarrow **pure exponential decay**

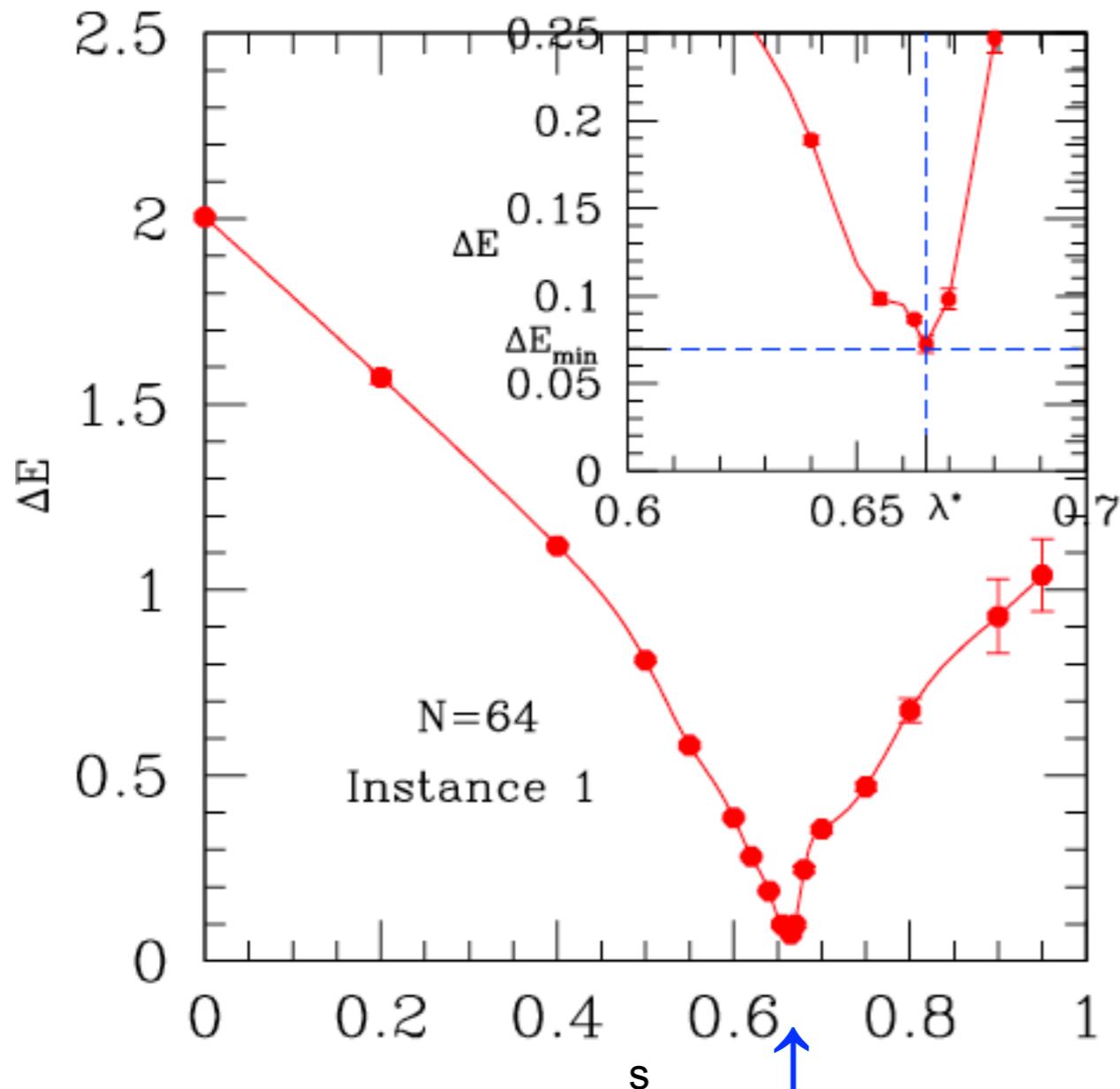


Small size, $N = 24$, excellent agreement with diagonalization.



Large size, $N = 128$, good quality data, slope of straight line \rightarrow gap.

Dependence of gap on s



Mind THIS gap

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.

Results

We studied several models using Quantum Monte Carlo.

We compute the minimum gap and use that to estimate the size dependence of the running time of the QAA using the Landau-Zener formula.

- Several **satisfiability (SAT)** problems
- A **spin glass**. (on a random graph)

We do not include the effects of finite-T and non-thermal noise in the D-Wave machine.

Our aim is to see if there is a quantum speedup in the QA/QAA paradigm of quantum computing in an ideal world where these complications do not occur.

SAT problems

We studied some satisfiability (**SAT**) problems, very popular with computer scientists.

One has **N** bits, and **M** logical conditions (**clauses**) each of which involves a small number of bits.

Question: is there a configuration of the bits which satisfies all the clauses?

If **M** \ll **N** then **yes** (many ways to do it)

If **M** \gg **N** then **no** (always a conflict)

Hence there is a **satisfiability transition** at a critical value of **M/N**. The problem is hard in this region, so we shall **take M/N close to critical value**.

Convert to a problem Hamiltonian **H_P** which is a sum of contributions from each clause:

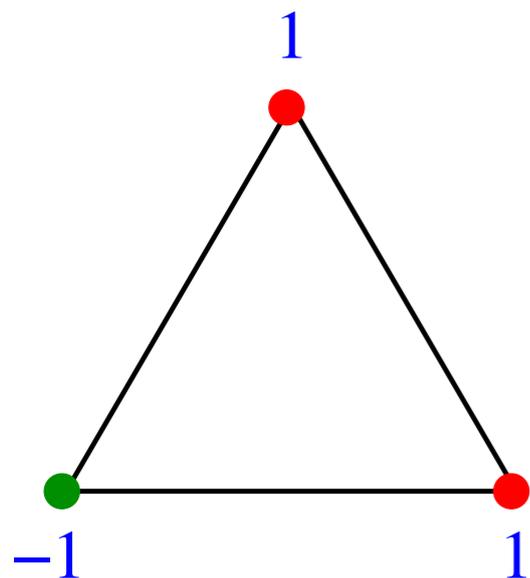
$$\mathcal{H}_P = \sum_{a=1}^M \mathcal{H}_a$$

H_P is chosen such that it is zero if the clause is satisfied and a positive value if not. **Hence the problem is SAT if the ground state energy is zero.**

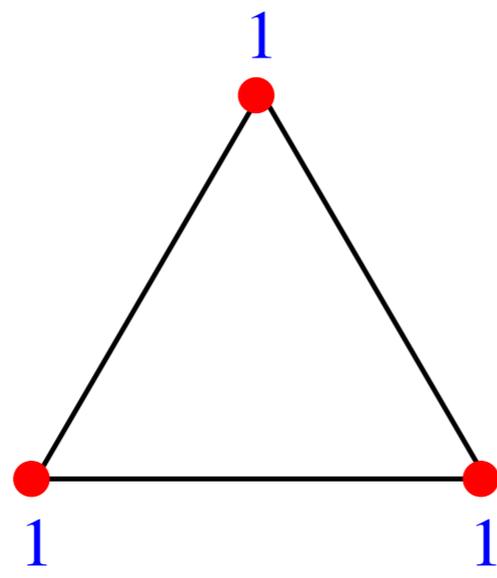
Example of a Satisfiability Problem

- 1-in-3 SAT

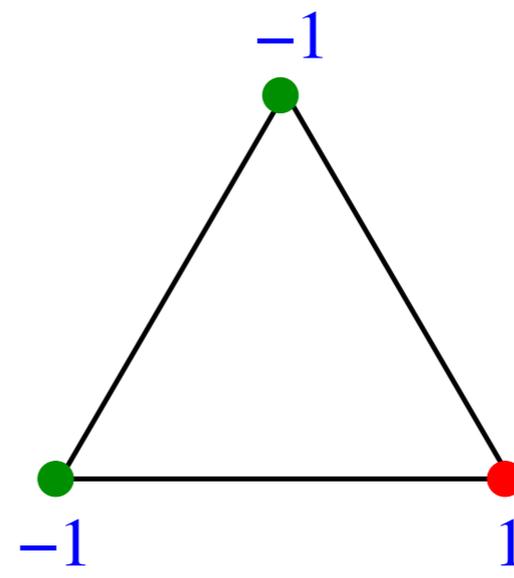
The clause is formed from 3 bits picked at random. The clause is satisfied (has energy 0) if one is 1 and the other two are 0 (in terms of spins one is -1 (green) and the other two are +1 (red)). Otherwise it is not satisfied (the energy is 1).



Satisfied



Unsatisfied

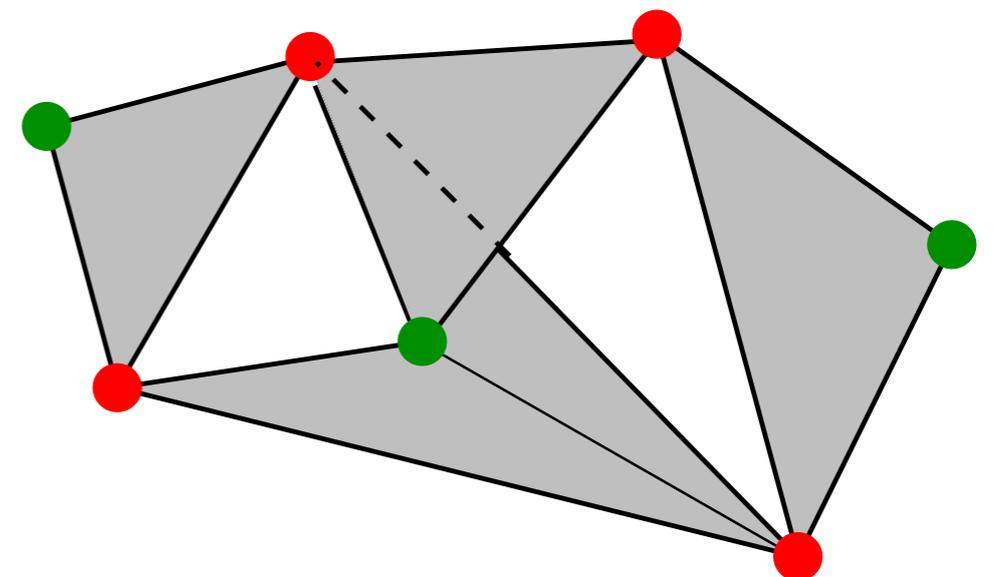


Unsatisfied

Example of a satisfying assignment with $N=7$, $M=5$.

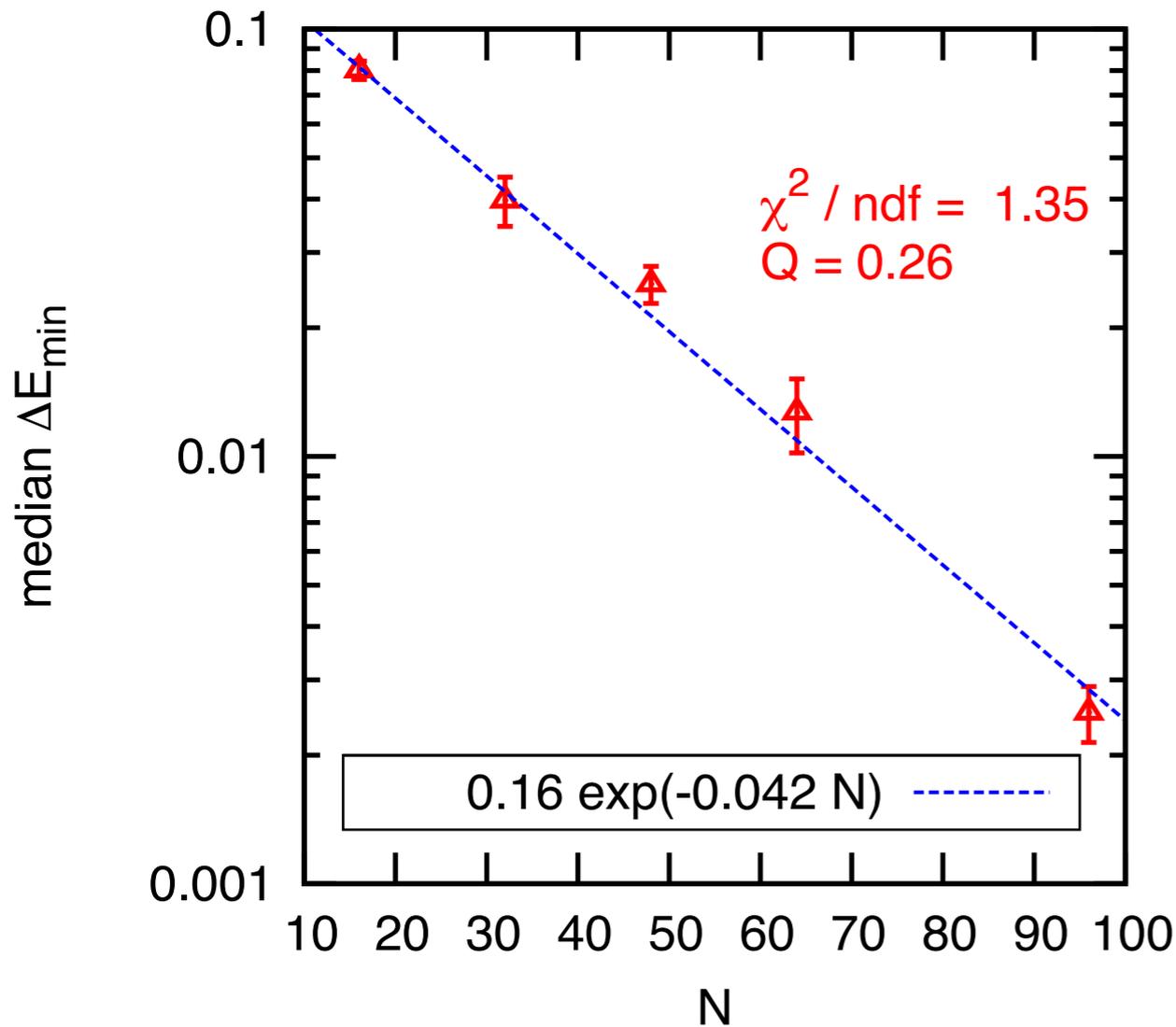
(V. Choi)

$$\mathcal{H}_P = \sum_{\text{clauses}} \left(\frac{\sigma_1^z + \sigma_2^z + \sigma_3^z - 1}{2} \right)^2$$

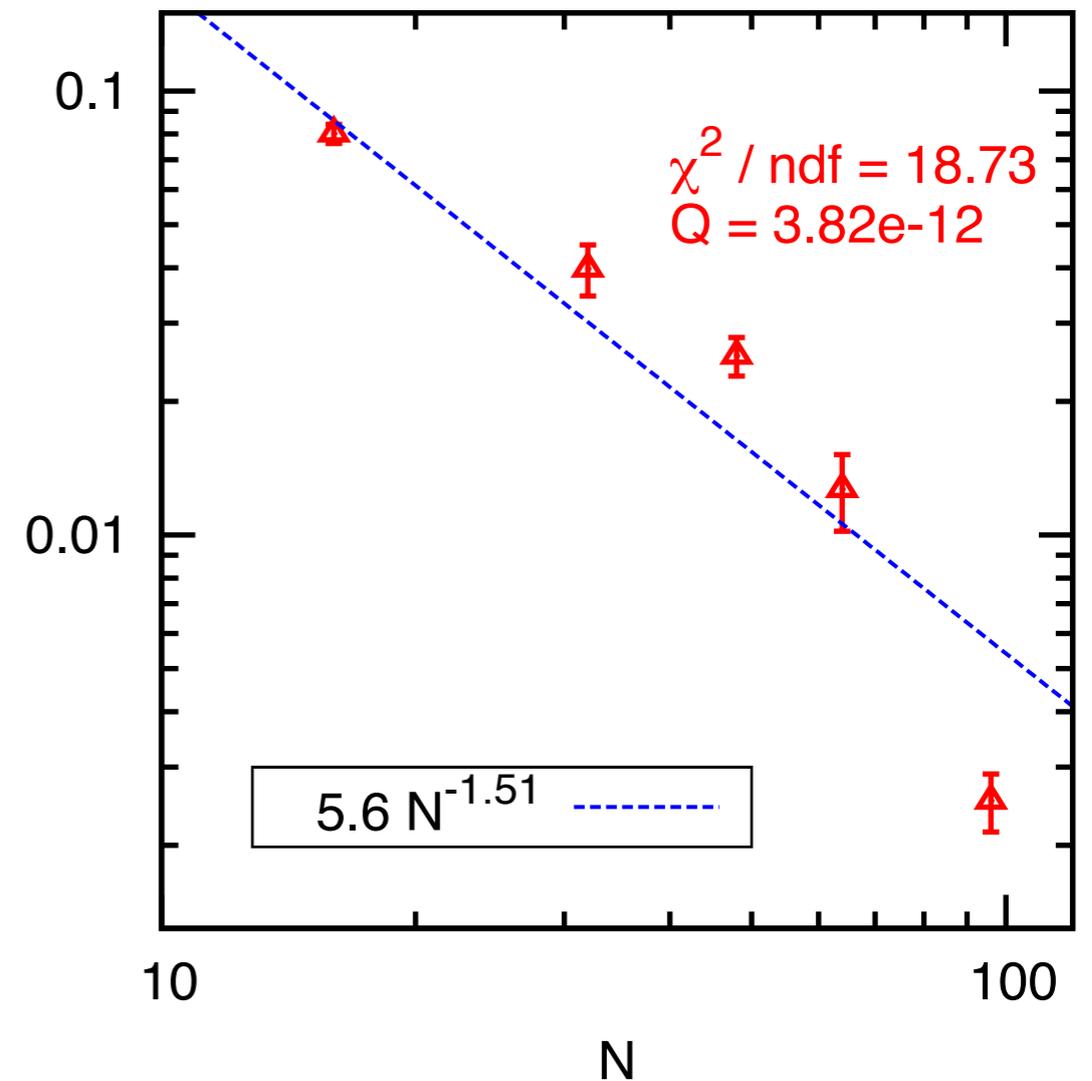


1-in-3 SAT (gap)

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



Exponential fit

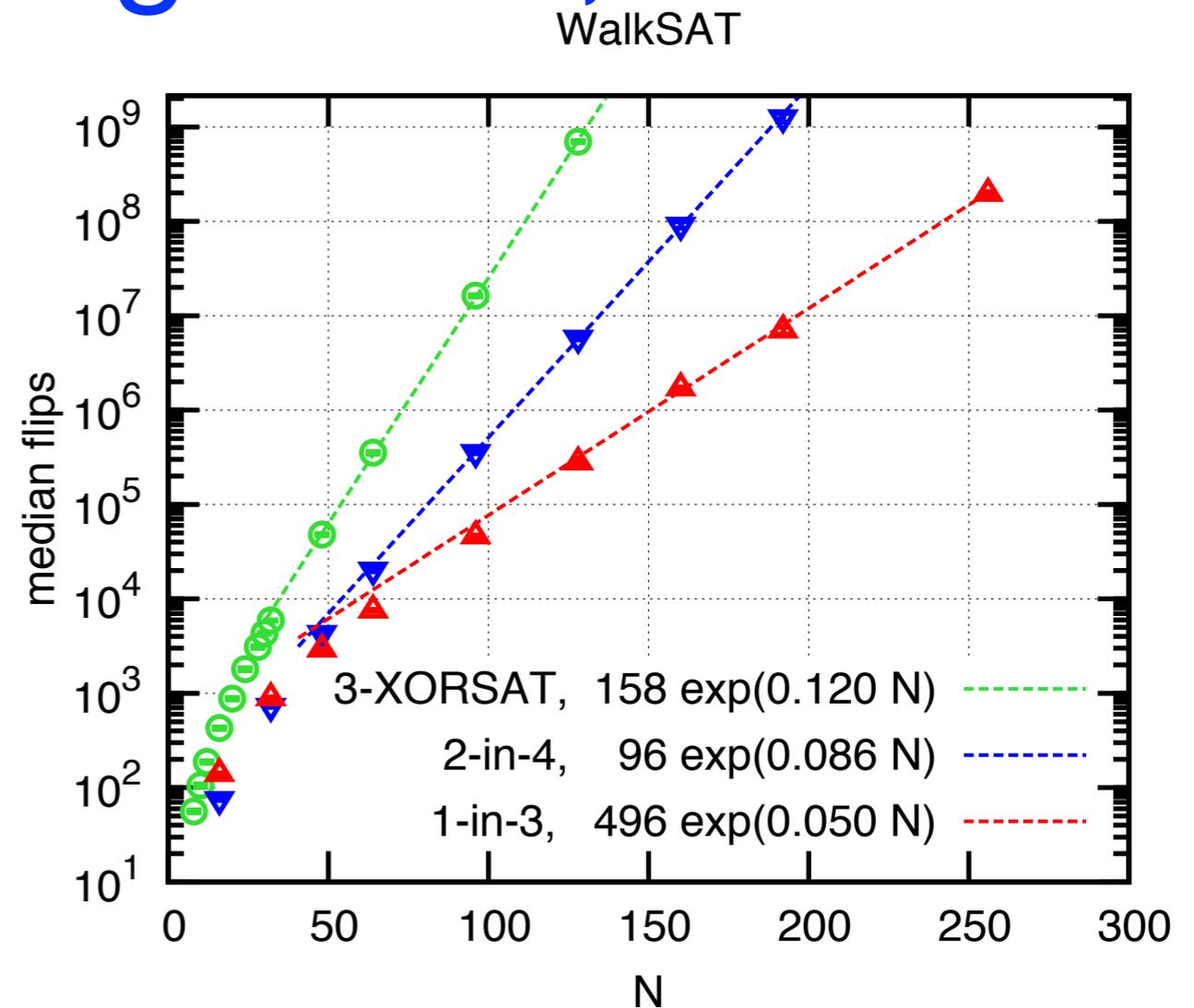
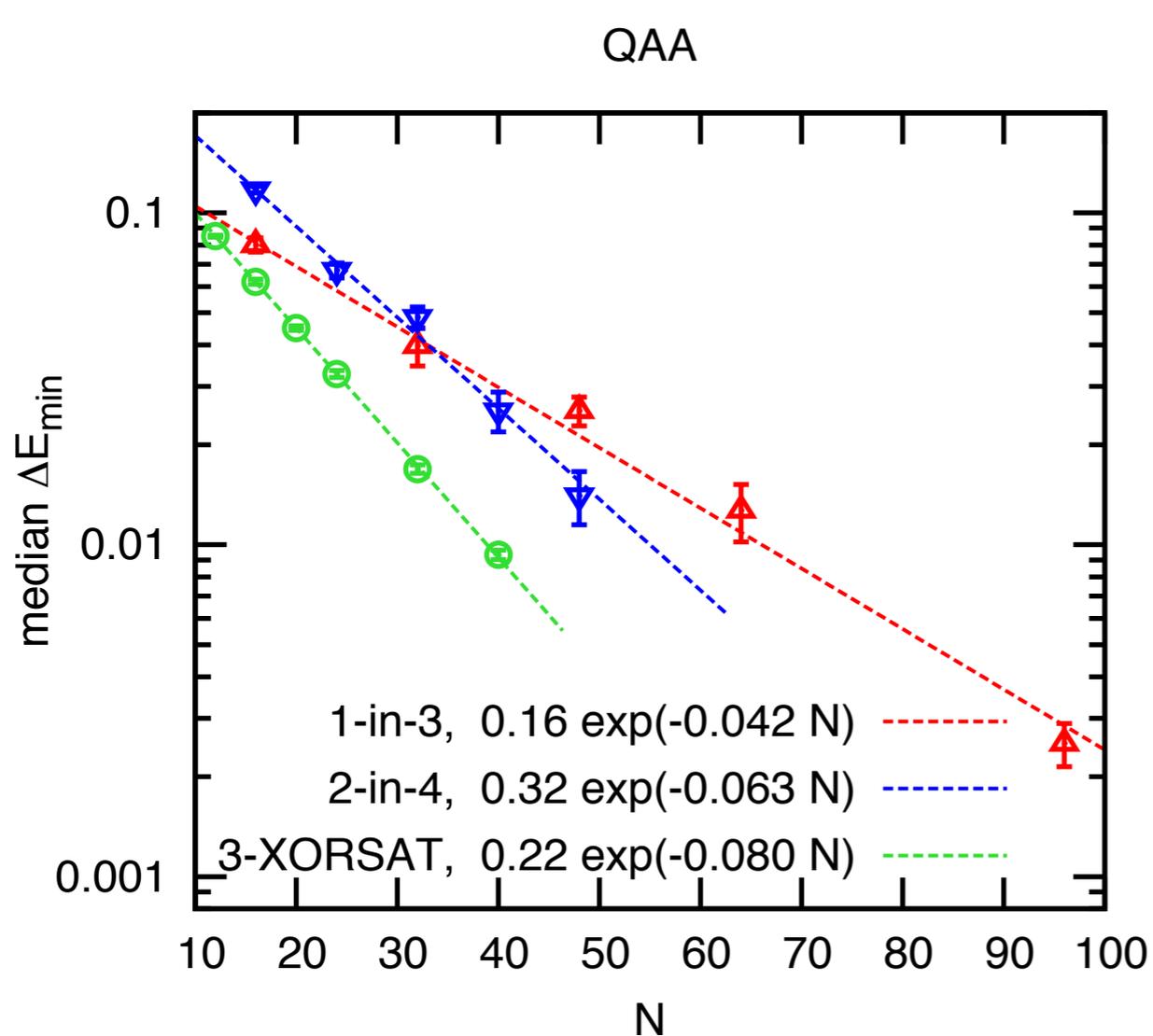


Power law fit

Hen and APY, Phys. Rev. E 84, 061152 (2011)

Clearly the behavior of the minimum gap is exponential

3 SAT models: comparison between QAA and a classical algorithm, WalkSAT



WalkSAT is a classical heuristic algorithm similar in spirit to SA.
Exponential behavior for both QAA and WalkSAT

Problems that are hardest for WalkSAT are hardest for QAA and vice-versa

Summary for SAT models

For **WalkSAT** we find that the number of “flips” is given by

$$\tau \propto \exp(\mu N)$$

and we determine the values for μ .

For the **QAA** we find $\Delta E_{\min} \propto \exp(-c N)$

and we determine the values for c . Running time $\propto 1/(\Delta E_{\min})^2$
so we have $\mu = 2c$ and hence we can compare the values of μ
for the classical and quantum algorithms: (Hen and APY, Phys. Rev. E 84, 061152 (2011))

model	$\mu(\text{QAA})$	$\mu(\text{WalkSAT})$	Ratio
1-in-3 SAT	0.084(3)	0.0505(5)	1.66
2-in-4 SAT	0.126(5)	0.0858(8)	1.47
3-XORSAT	0.159(2)	0.1198(20)	1.32

QAA is always a bit worse (i.e. μ a bit bigger) than WalkSAT.

Bottleneck for SAT is **at** the (first order) quantum phase transition. Transition first order argued by Krzakala et al.

(Digression on) P versus NP

The **hardest** of the three previous models is a **3-spin model (3-XORSAT)** where choose **M** triplets of spins at random and require that the **product** of the three has some specified value,

$$S_{1,\alpha}^z S_{2,\alpha}^z S_{3,\alpha}^z = f_\alpha, \quad (\alpha = 1, 2, \dots, M)$$

where the f_α are specified to be 1 or -1. **Is there a configuration of the spins which satisfies all these M constraints?**

In terms of bits, $z_i = (1 - S_i^z)/2$ the product becomes a **sum**

$$z_{1,\alpha} + z_{2,\alpha} + z_{3,\alpha} = u_\alpha \pmod{2}$$

where the u_α are 1 or 0. These are **LINEAR** equations, **solvable in polynomial time (P)** by e.g. **Gaussian elimination**.

Thus this 3-spin model is in the **category P** of optimization problems, those that can be **SOLVED in polynomial time**.

Computer scientists also discuss a category they call **NP**, problems that can be **VERIFIED in polynomial time**. e.g. a SAT problem, if I give you a spin configuration which I claim is a SAT assignment you can verify this in polynomial time.

More on P and NP

A major problem in science is

Is $P = NP$?

One of the seven Millennium problems of the Clay foundation.

\$1 million prize if you can solve it!

No known polynomial time algorithm for most problems in NP, e.g. 3-SAT, spin glass ground state in $d > 2$.

Probably $P \neq NP$ but no proof. The 3-spin model shows that intuition is not a guide. There are problems which heuristic algorithms find very hard but for which there is a special feature which allows a clever polynomial time algorithm.

Hard to believe that every problem in NP will have such a special feature but no proof, so far, that they don't.

A physicist's problem; a spin glass

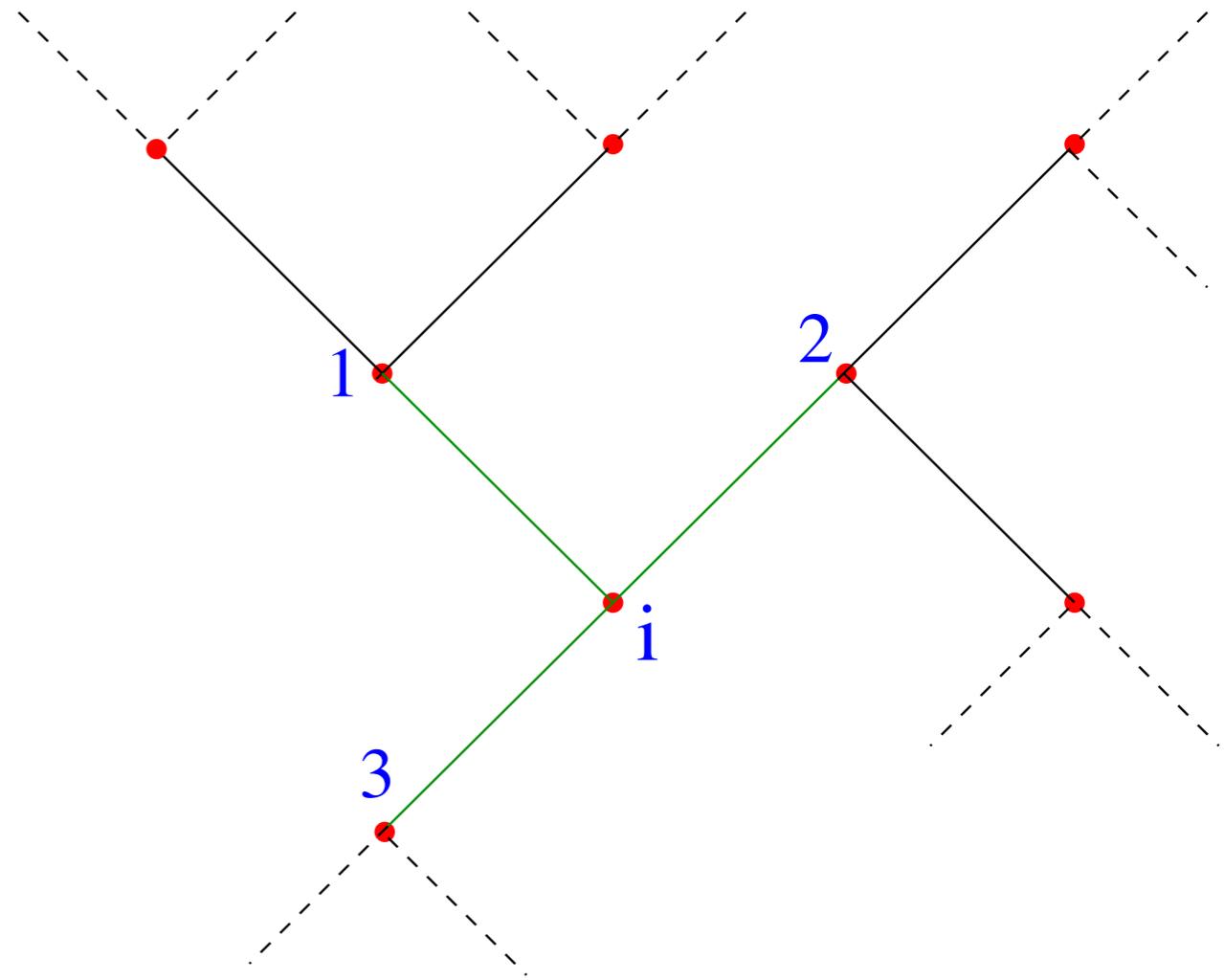
We study a very simple spin glass model, an **anti-ferromagnet** on a **3-regular random graph**.

$$\mathcal{H}_P = \frac{1}{2} \sum_{\langle i,j \rangle} \left(1 + \sigma_i^z \sigma_j^z \right)$$

3-Regular means that each spin is connected to exactly three neighbors.

Spin glasses need **randomness and frustration**. Here we have no disorder in the interactions so these come entirely from the geometry of the (large) loops.

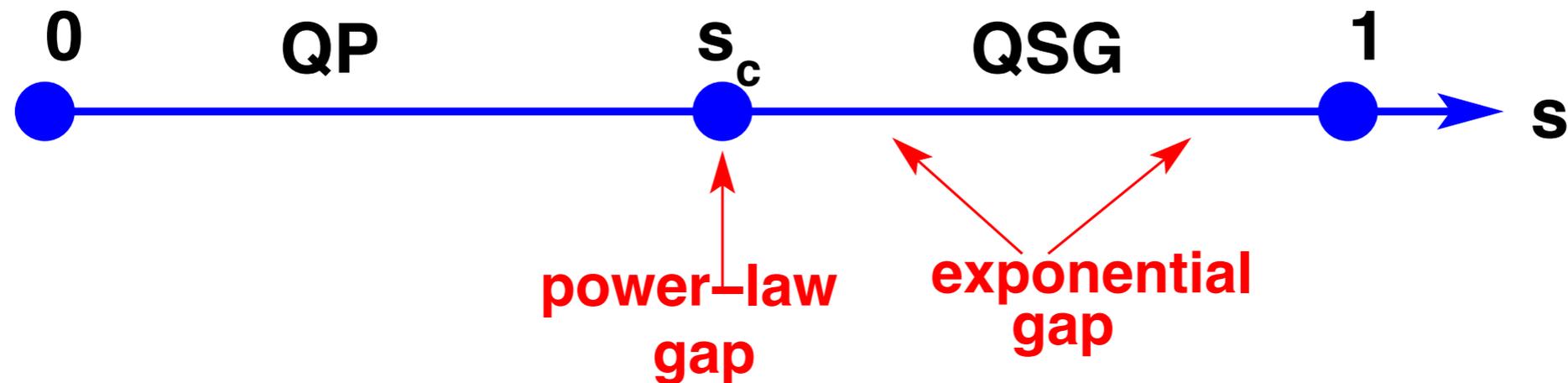
Because of large loops there is **no AF state, only a spin glass** (Zdeborova et al).



Note: there are large loops

Spin glass

Adding the driver Hamiltonian there is a quantum phase transition at $s = s^*$ above which the symmetry is spontaneously broken. This is the quantum spin glass phase.

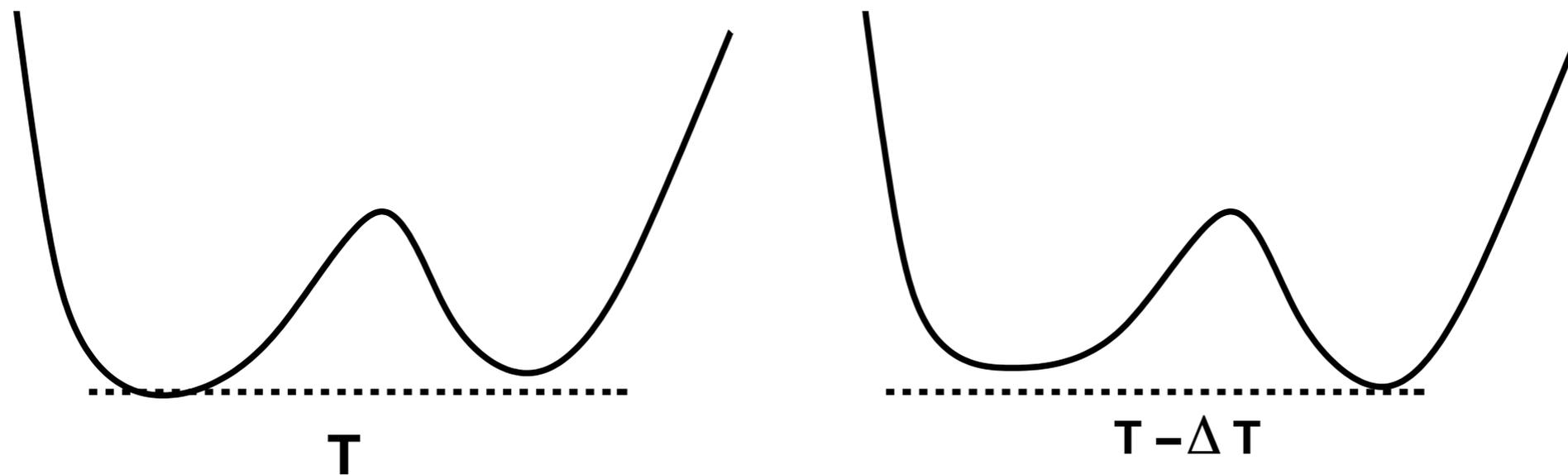


We find an **exponentially small gap** in the spin glass phase, Farhi et al. Phys. Rev, A86, 052334 (2012), (used computer time from Google), (but **power-law at the quantum critical point s_c .**)

We shall argue that the exponentially small gaps are an example of “**chaos**” in the spin glass phase (which we discuss next.)

Classical and quantum chaos in spin glasses

Consider a classical spin glass below the transition temperature. There is a very complicated “energy landscape”. If the temperature is changed by ΔT a different minimum can become the lowest. This is called “temperature chaos”



Effect is rather weak, but present for large sizes.

Problems with temperature chaos are hard to solve by thermal annealing.

What about “quantum chaos”

i.e. “transverse field” chaos.

We have seen that classically hard problems are those with **temperature chaos**.

In quantum annealing (at $T = 0$ and without errors in the bond strengths) presumably the hard samples are those where the spin configuration changes suddenly as a function of the strength of the transverse field, which we call **“quantum chaos”**.

This is our interpretation of the exponentially small gaps found in our QMC simulations of the spin glass on a random graph in the quantum spin glass phase, see earlier part of talk.

Are samples with temperature chaos also the ones with quantum chaos? To my knowledge this is not known but could be determined by QMC simulations.

What about D-Wave?

Is the D-Wave machine doing quantum (or just classical) annealing?

Controversial: don't have access to the system at intermediate times. Also, the system is coupled to the environment which has a non-zero T (e.g. 40mK). It freezes at some value of s so the probabilities at the end can show some resemblance to a Boltzmann distribution even if it underwent quantum evolution to get there.

Is the performance of the D-Wave machine better than that of a classical algorithm?

Can't tell from the D-Wave data because there is a minimum annealing time (due to hardware limitations) which is too fast to be optimal (except for the larger sizes; max. size is 512).

Recent discussion in M. Amin, arXiv:1503.04216

Conclusions

- We have studied the **efficiency of the QAA** neglecting the effects of non-zero temperature and non-thermal noise which are present in the D-Wave machine.
- Even in this ideal world we do **NOT** find the QAA to be more **efficient than an analogous, heuristic, classical algorithm, WalkSAT**. The bottleneck is **AT** the quantum phase transition for the SAT problems, but **IN** the quantum spin glass phase for the spin glass.
- We also discussed the connection between the difficulty of solving optimization problems by thermal or quantum annealing and **classical or quantum chaos** (respectively).

Danke schön