"Mind the Gap"--Could a quantum computer solve optimization problems efficiently?

A.P. Young

http://young.physics.ucsc.edu

UNIVERSITY OF CALIFORNIA SANTA CRUZ

Work supported by

SCIENCE TO SHAPE THE FUTURE OF THE ARMY · ARMY RESEARCH OFFICE · 1951

NATIONAL SECURITY AGENCY · UNITED STATES OF AMERICA

Google

NSF National Science Foundation WHERE DISCOVERIES BEGIN

Talk at Statistical Physics of Quantum Matter, Taipei, July 31, 2013

Collaborators: **I. Hen**, E. Farhi, P. Shor, D. Gosset, A. Sandvik, V. Smelyanskiy, S. Knysh, M. Guidetti.

Synopsis: Mind the Gap

iStockphoto.com/cinoby

Exponential complexity of the quantum adiabatic algorithm for certain satisfiability problems

Itay Hen and A. P. Young
Phys. Rev. E **84**, 061152 (2011)
Published December 29, 2011

Quantum computers promise to accelerate some kinds of calculations in a remarkable manner. But as in present-day classical computing, hardware is only half the story: efficiency requires development of appropriate algorithms, such as the fast Fourier transform.

To apply a quantum computer to a broad class of problems, general-purpose algorithms are needed. One such method is the quantum adiabatic algorithm, in which the problem to be solved is coded into a Hamiltonian H. One prepares the quantum computer in the ground state of a reference Hamiltonian H_R and then has it evolve under a time-dependent Hamiltonian $H(t)$ that gradually switches from H_R to H. If the evolution is slow enough ("adiabatic") the system ends up in the ground state of H, which contains information about the desired solution.

In a paper in *Physical Review E*, Itay Hen and Peter Young of the University of California, Santa Cruz, show that "slow enough" may be very slow indeed. The reason is that the time required for adiabatic evolution depends inversely on the gap in energies between the ground and first excited states of $H(t)$. Using computer simulations, Hen and Young show that for three classes of logic problems, the scaling of the gap is such that the computational time can be expected to grow exponentially with the size of the problem. The authors suggest that it might be possible to optimize the evolution of $H(t)$ to avoid the bottleneck associated with a vanishing gap. – *Ron Dickman*

Synopsis: Mind the Gap

iStockphoto.com/cinoby

Exponential complexity of the quantum adiabatic algorithm for certain satisfiability problems

Itay Hen and A. P. Young
Phys. Rev. E **84**, 061152 (2011)
Published December 29, 2011

Quantum computers promise to accelerate some kinds of calculations in a remarkable manner. But as in present-day classical computing, hardware is only half the story: efficiency requires development of appropriate algorithms, such as the fast Fourier transform.

To apply a quantum computer to a broad class of problems, general-purpose algorithms are needed. One such method is the quantum adiabatic algorithm, in which the problem to be solved is coded into a Hamiltonian H. One prepares the quantum computer in the ground state of a reference Hamil me-dependent Hamiltonian $H(t)$ that gradually switches from H_R to H. If the evolution is slow enough ("adia tate of H, which contains information about the desired solution.

In a p Peter Young of the University of California, Santa Cruz, show that "slow enough" may be very slow indeed. The r c evolution depends inversely on the gap in energies between the ground and first excited states of $H(t)$. Using ow that for three classes of logic problems, the scaling of the gap is such that the computational time can be ex of the problem. The authors suggest that it might be possible to optimize the evolution of $H(t)$ to avoid the bottle *lon Dickman*

Synopsis: Mind the Gap

iStockphoto.com/cinoby

Exponential complexity of the quantum adiabatic algorithm for certain satisfiability problems

Itay Hen and A. P. Young

Ph

Pu

Quantum computers promise to accelerate some kin
only half the story: efficiency requires development c

To apply a quantum computer to a broad class of pro
algorithm, in which the problem to be solved is coded
Hamil me-d
("adia tate

In a p eter
The r c evo
Using ow th
be ex of th
bottle *on D*

d.
an
he

Plan

- Motivation (solving optimization problems on a quantum computer)
- Quantum Monte Carlo (the method used to study large sizes)
- Results for Satisfiability-type problems
- Results for a spin-glass problem
- Conclusions

Motivation

There are some problems which could be solved much more efficiently on an eventual quantum computer than an classical computer.

Most famous example: integer factoring (Shor) important for encryption.

Could a quantum computer also solve optimization problems more efficiently than a classical computer?

Wide range of such problems in science, engineering, and industrial applications, e.g.

- Physics: spin glasses
- Biology: protein folding
- Computer science: satisfiability problems
- Industry: machine learning, image recognition...

Quantum Adiabatic Algorithm

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

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

Make quantum by adding a non-commuting driver Hamiltonian.

Simplest is a transverse field:

$$\mathcal{H}_D = -h \sum_{i=1}^{N} (\sigma_i^x - 1)$$

Total Hamiltonian:

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

with s(0) = 0, s(τ) = 1.

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

Quantum Adiabatic Algorithm

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

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

Make quantum by adding a non-commuting driver Hamiltonian.

Simplest is a transverse field:

$$\mathcal{H}_D = -h \sum_{i=1}^{N} (\sigma_i^x - 1)$$

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 $T \to 0$), it ends in g.s. of problem Hamiltonian,

Experimental Interest

QAA is quantum annealing but directly implemented on the qubits of a quantum computer.

Quantum Adiabatic Algorithm is less sensitive to effects of decoherence than the traditional "circuit model" of quantum computing.

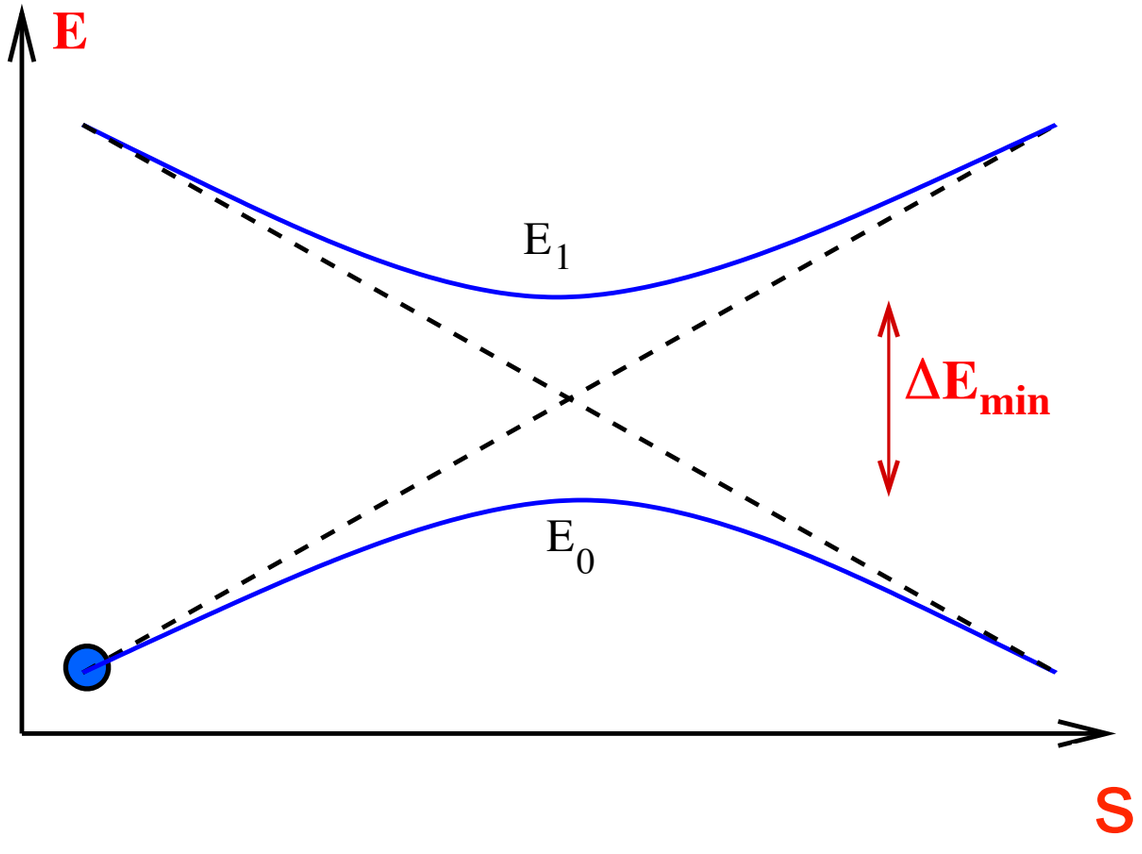
A company, D-Wave, has built a "quantum annealer" using the QAA with 512 superconducting qubits, so there are now starting to be real experiments, as well as theory.

In the experiments, though, coupling to the outside plays a substantial role, unlike in the simulations that I will describe. Effects of coupling to the environment in the QAA need to better understood.

Been shown (Aharonov et al.) that quantum adiabatic evolution can solve any problem that the circuit model can solve (though not necessarily in a natural way.) (Polynomially equivalent.)

Quantum Phase Transition

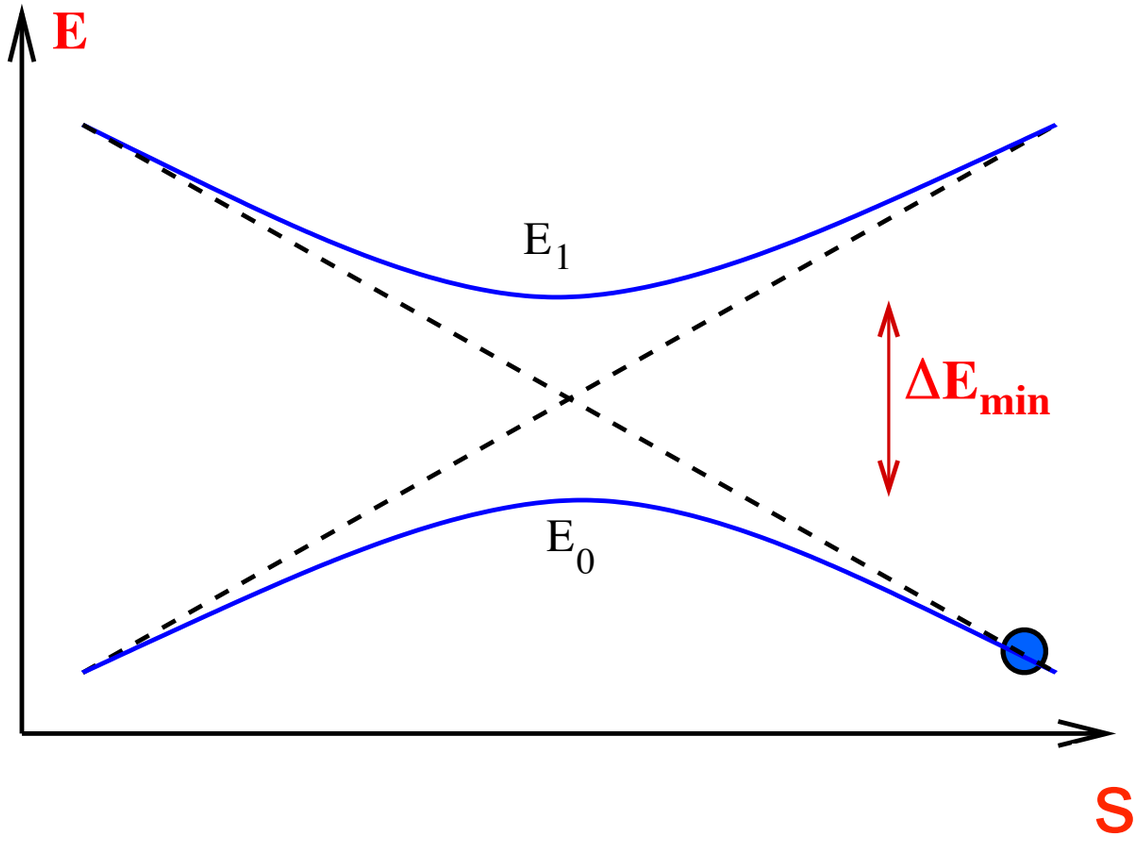
Bottleneck is likely to be a **quantum phase transition** (QPT) where the gap to the first excited state is very small



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

Quantum Phase Transition

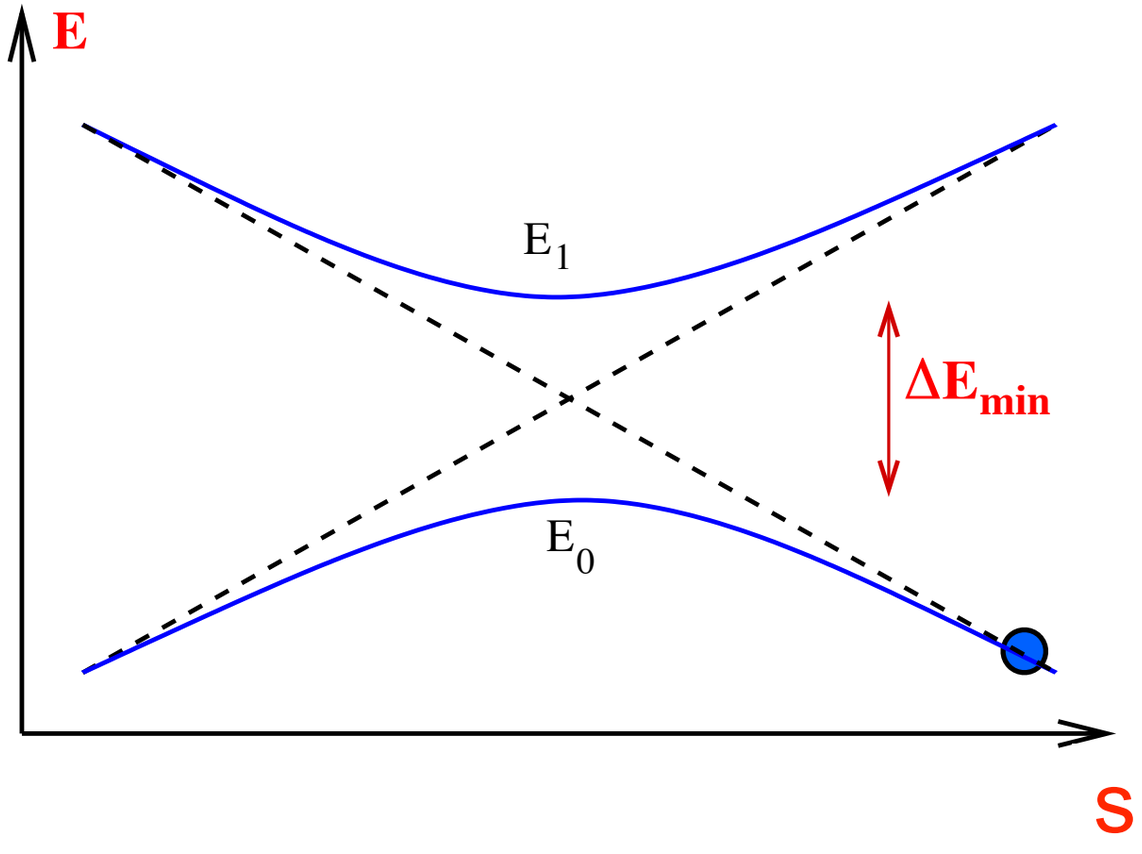
Bottleneck is likely to be a **quantum phase transition** (QPT) where the gap to the first excited state is very small



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

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}

Used QMC to compute ΔE for different s: → ΔE_{min}

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 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.

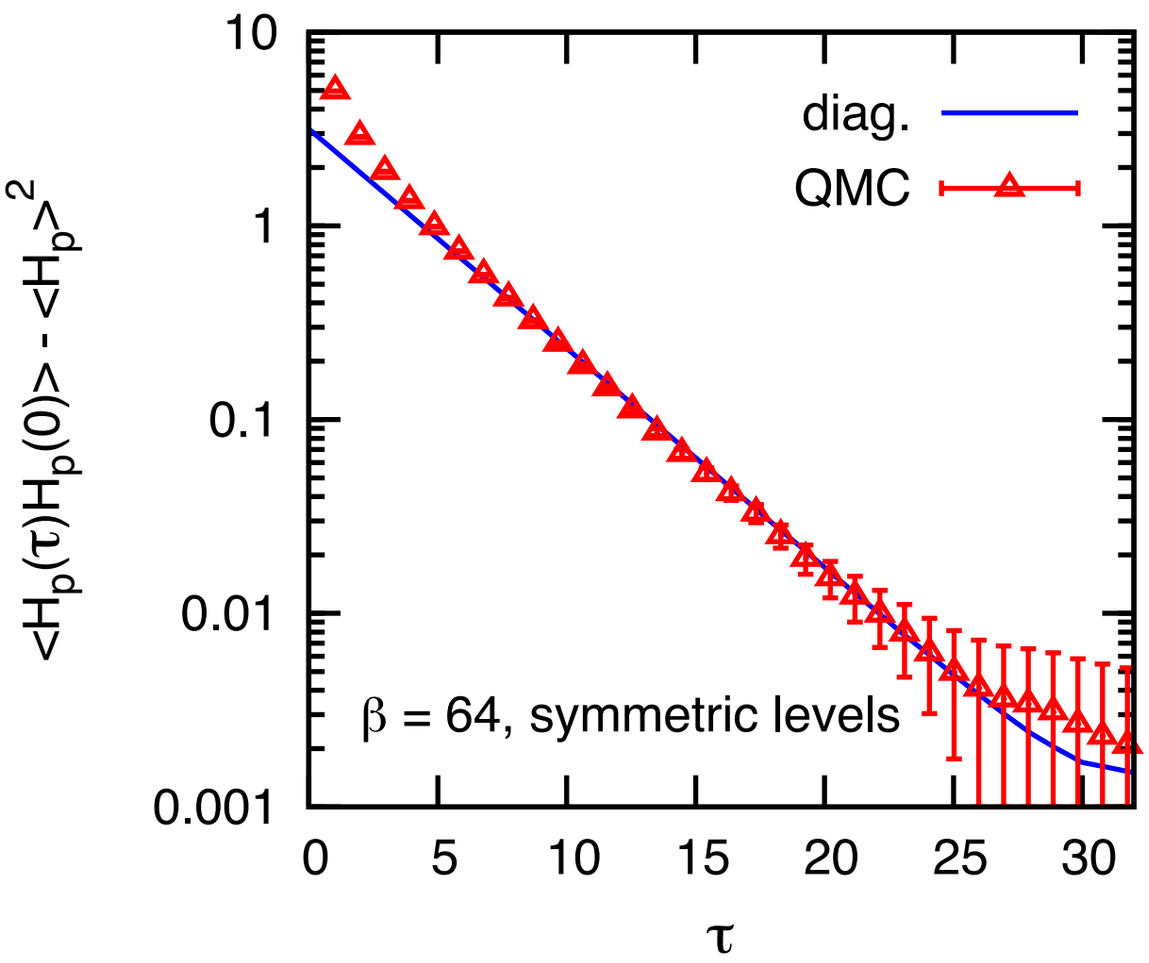
QMC $\rightarrow \Delta E_{min}$. **Use size dependence of ΔE_{min} to get size dependence of running time in the QAA, $\sim 1/(\Delta E_{min})^2$**

Examples of results with the SSE code

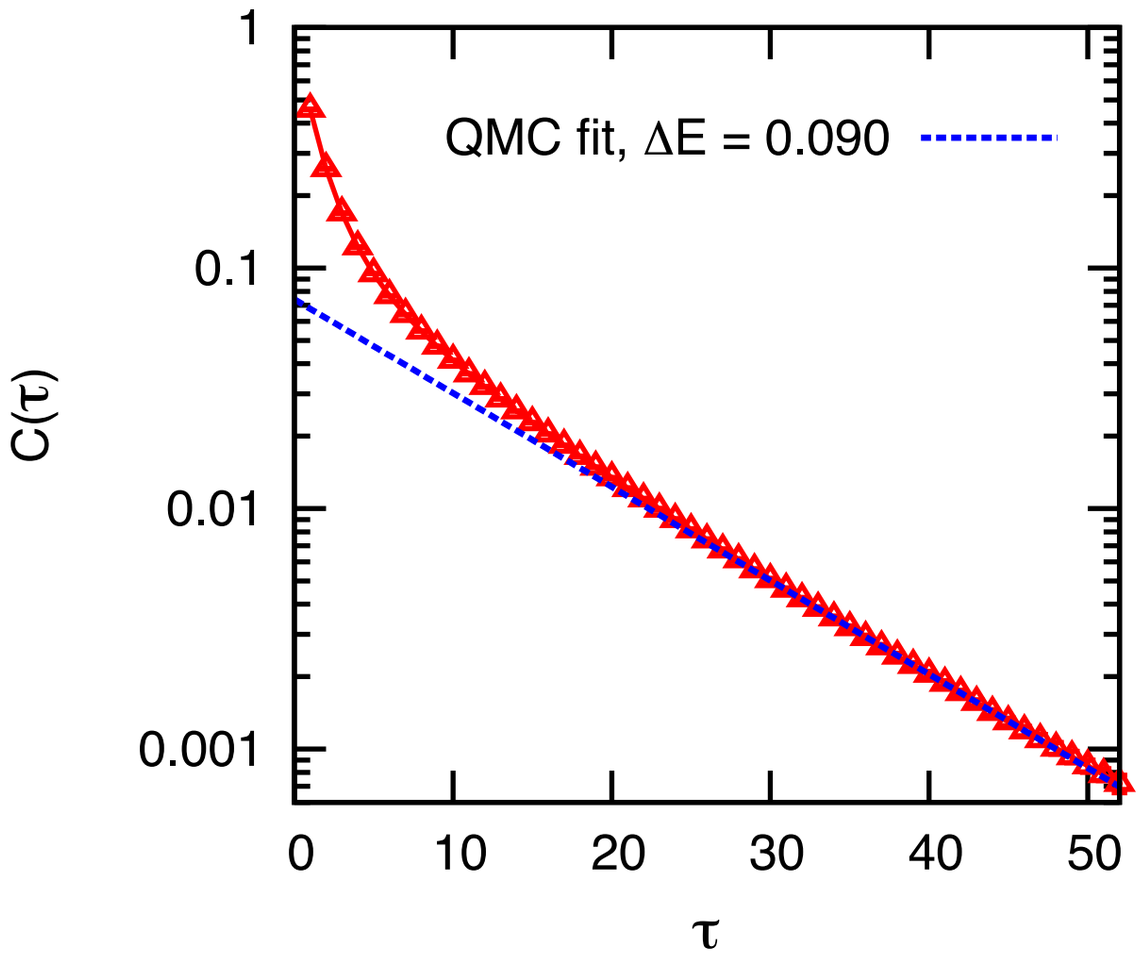
Time dependent correlation functions decay with τ as a sum of exponentials

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

For large τ only first excited state contributes, → pure exponential decay

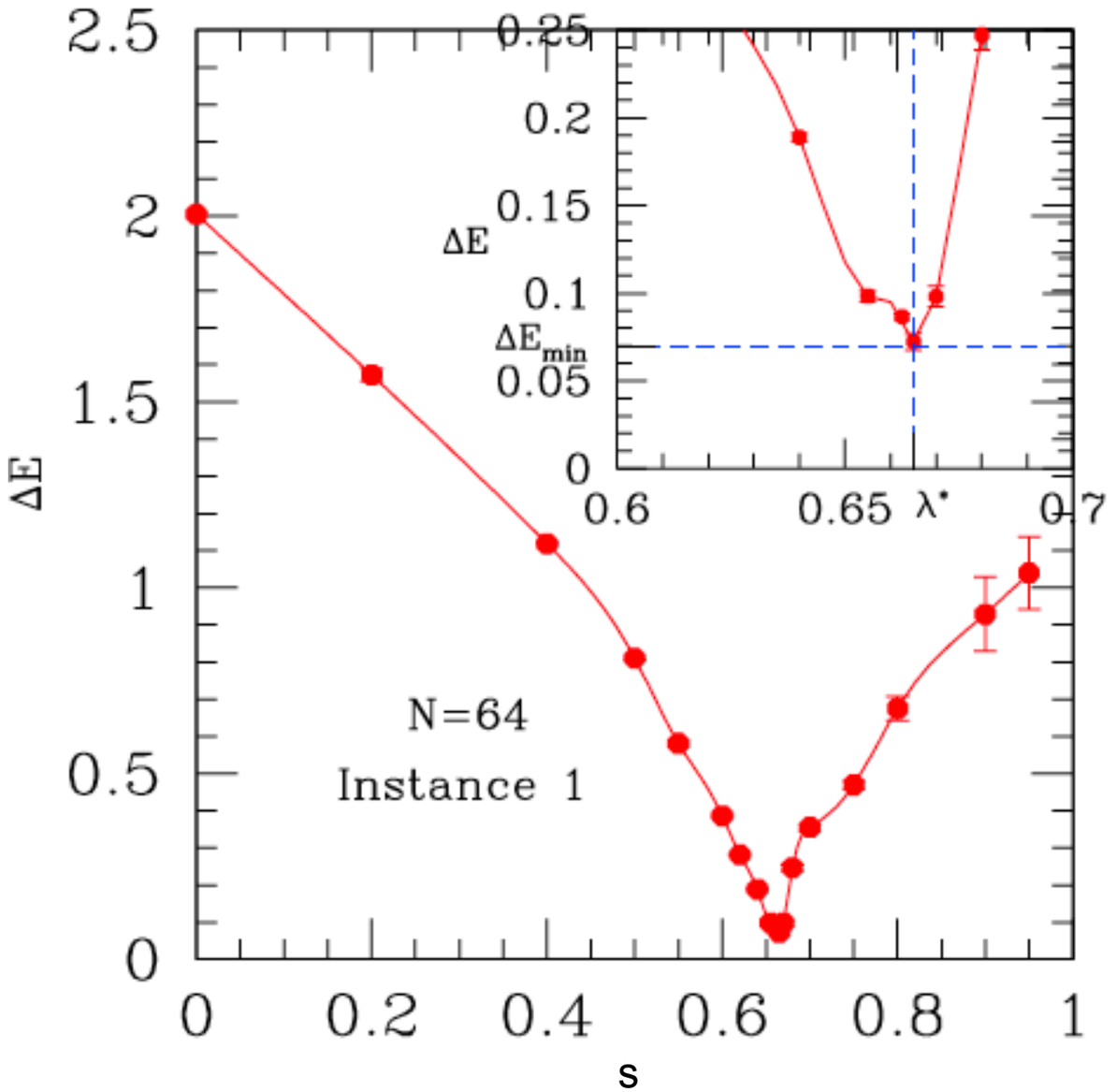


Small size, N= 24, excellent agreement with diagonalization.



Large size, N = 128, good quality data, slope of straight line → gap.

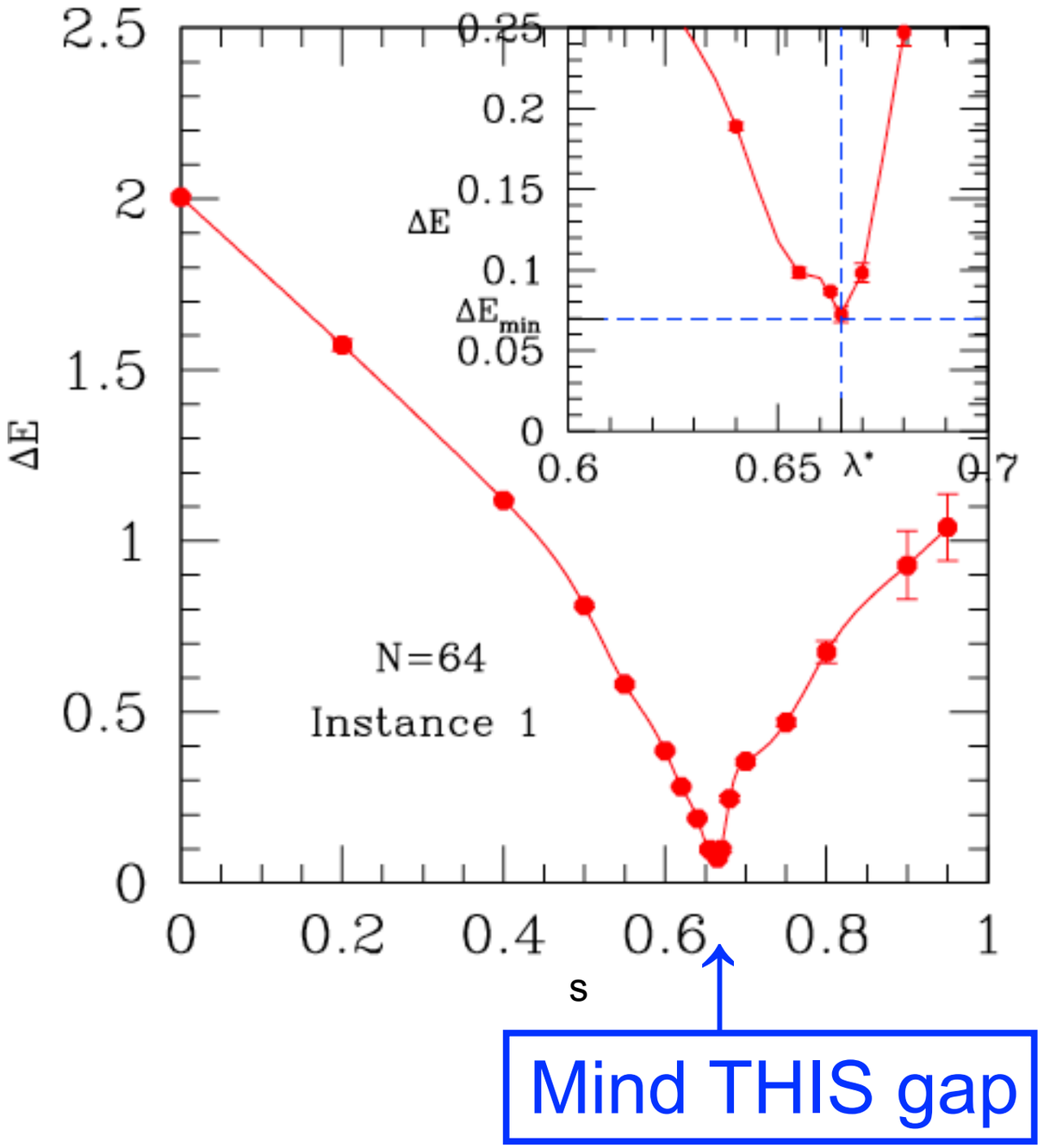
Dependence of gap on s



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.

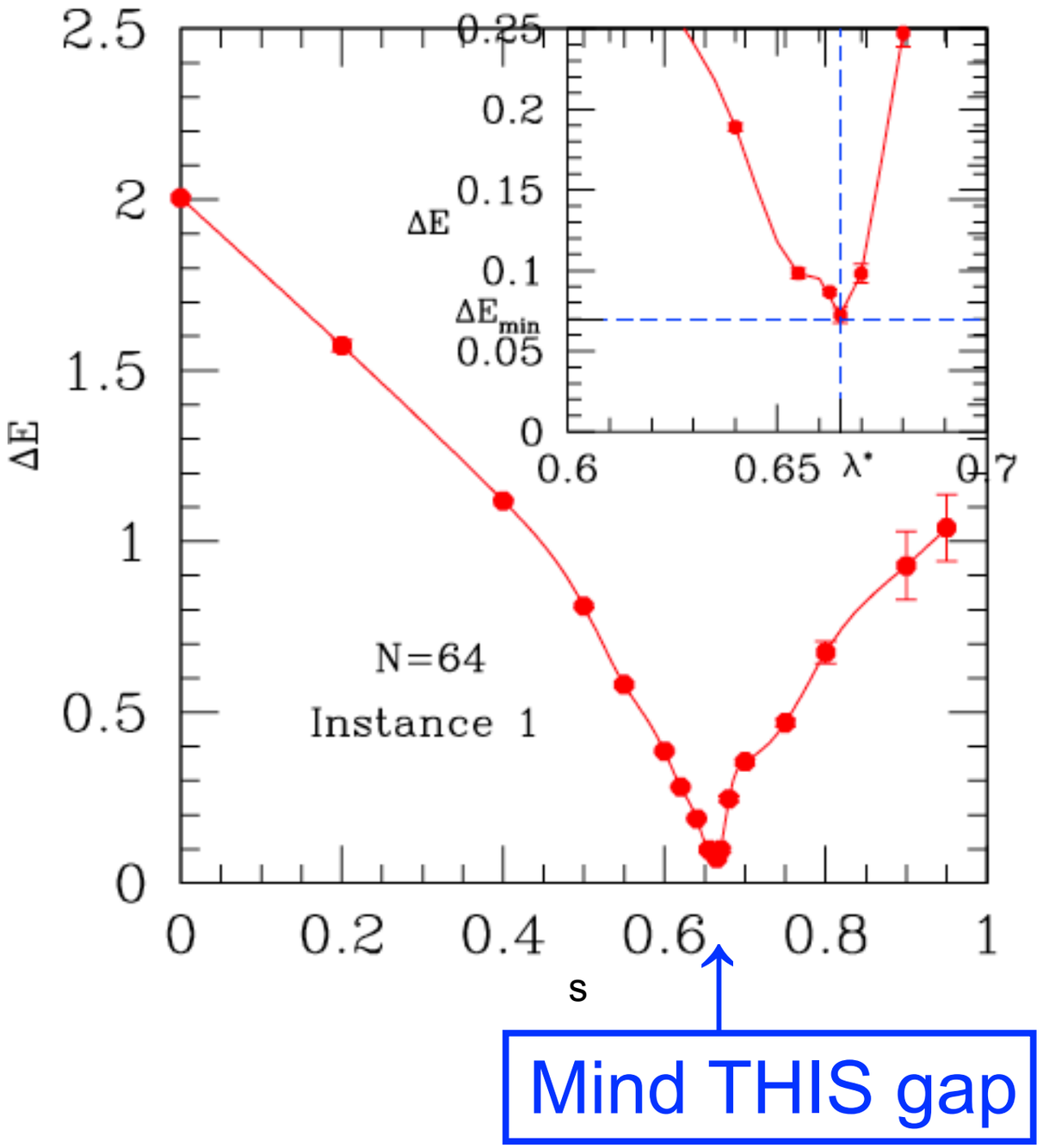
Dependence of gap on s



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.

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.

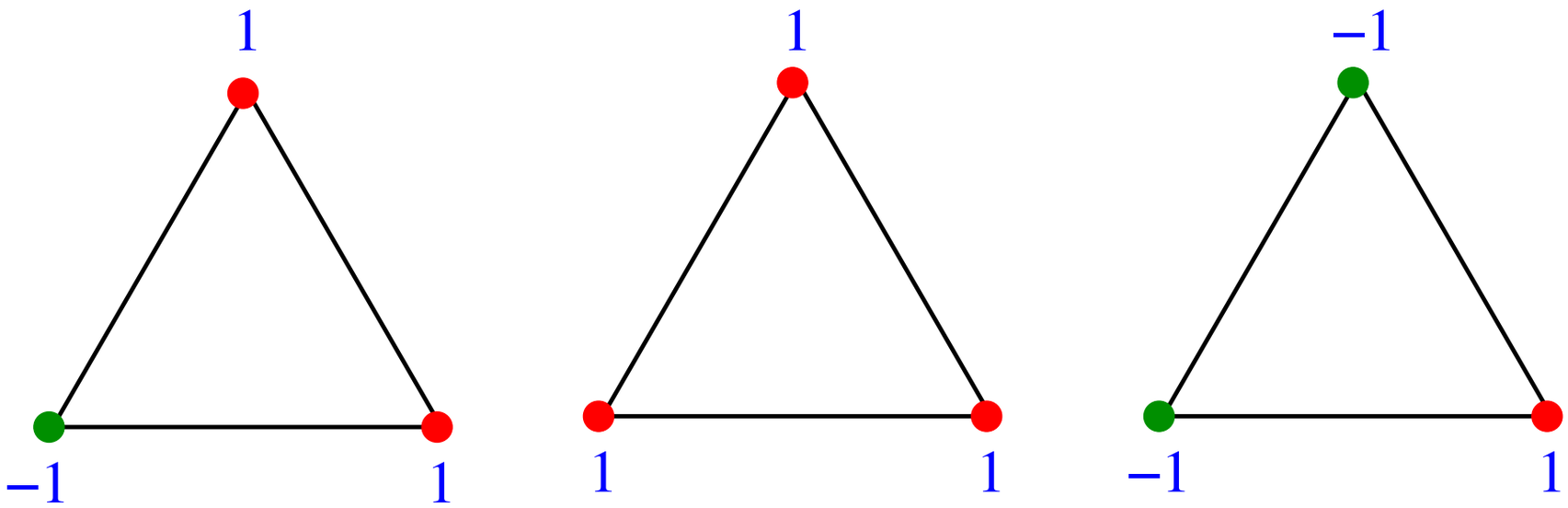
We take the ratio of M/N to be at the satisfiability threshold, and study instances with a "unique satisfying assignment" (USA).
(so gap to 1st excited state has a minimum whose value indicates the complexity.)

These SAT problems are "NP-complete", a category of hard problems for which the time is exponential with classical algorithms, at least in the worst case.

Satisfiability Problems II

- "Locked" 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).

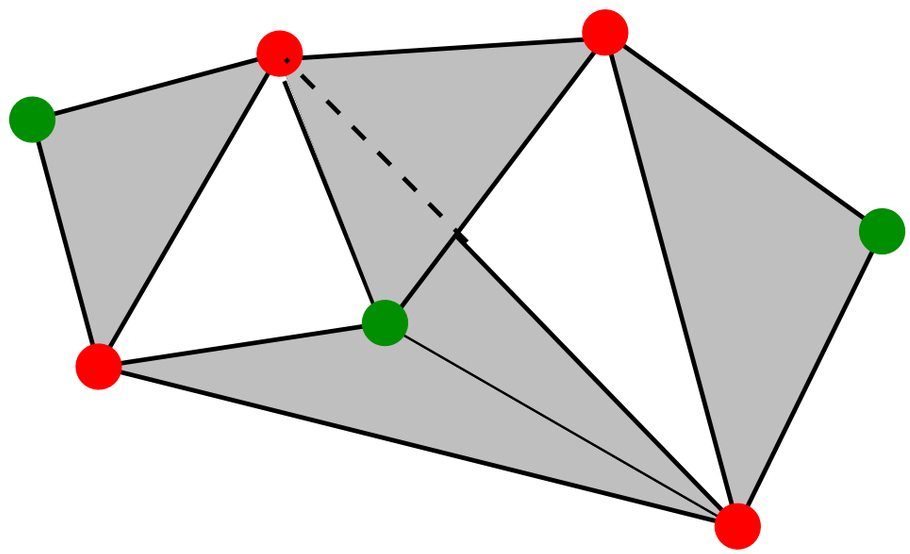


Satisfied **Unsatisfied** **Unsatisfied**

Connections between spins form a **random graph** (no local xgeometry). d→∞

Example of a satisfying assignment with N=7, M = 5.
(V. Choi)

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



Satisfiability Problems III

- 3-spin model (3-regular 3-XORSAT)
  3-regular means that each bit is in exactly three clauses. 3-XORSAT means that the clause is satisfied if the sum of the bits (mod 2) is a value specified (0 or 1) for each clause.
  In terms of spins σ^z (= ±1) we require that the **product** of the three σ^z's in a clause is specified (+1 or -1).

$$\mathcal{H}_P = \sum_{\alpha=1}^{M} \frac{1}{2}\left(1 - J_\alpha\, \sigma^z_{\alpha,1}\sigma^z_{\alpha,2}\sigma^z_{\alpha,3}\right)$$

(Is at SAT threshold.)

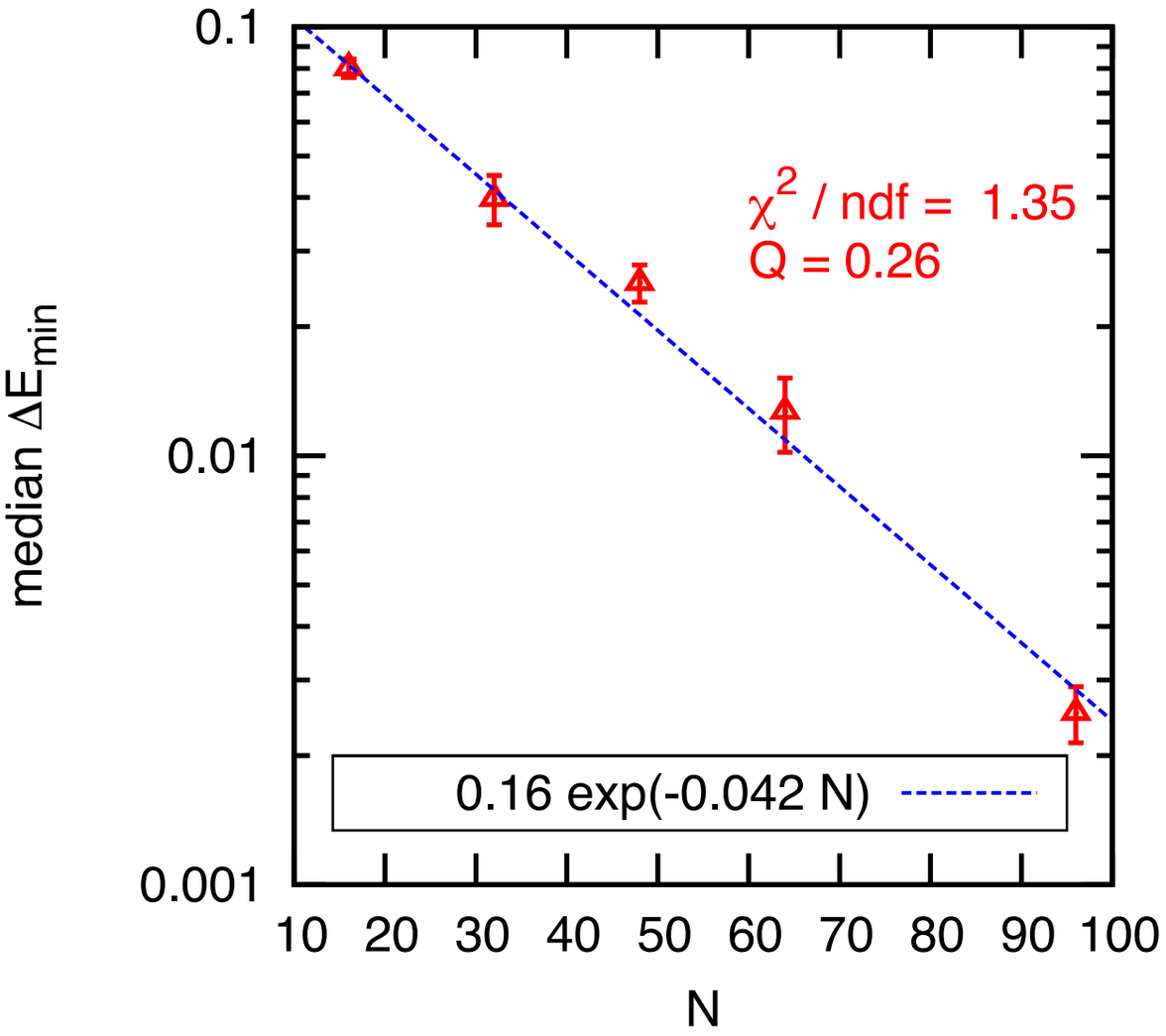
This 3-spin problem can be solved by linear algebra (Gaussian elimination) since, in terms of bits, 0 or 1

$$b_{\alpha,1} + b_{\alpha,2} + b_{\alpha,3} = J_\alpha, \quad (\mathbf{mod}\ 2)$$

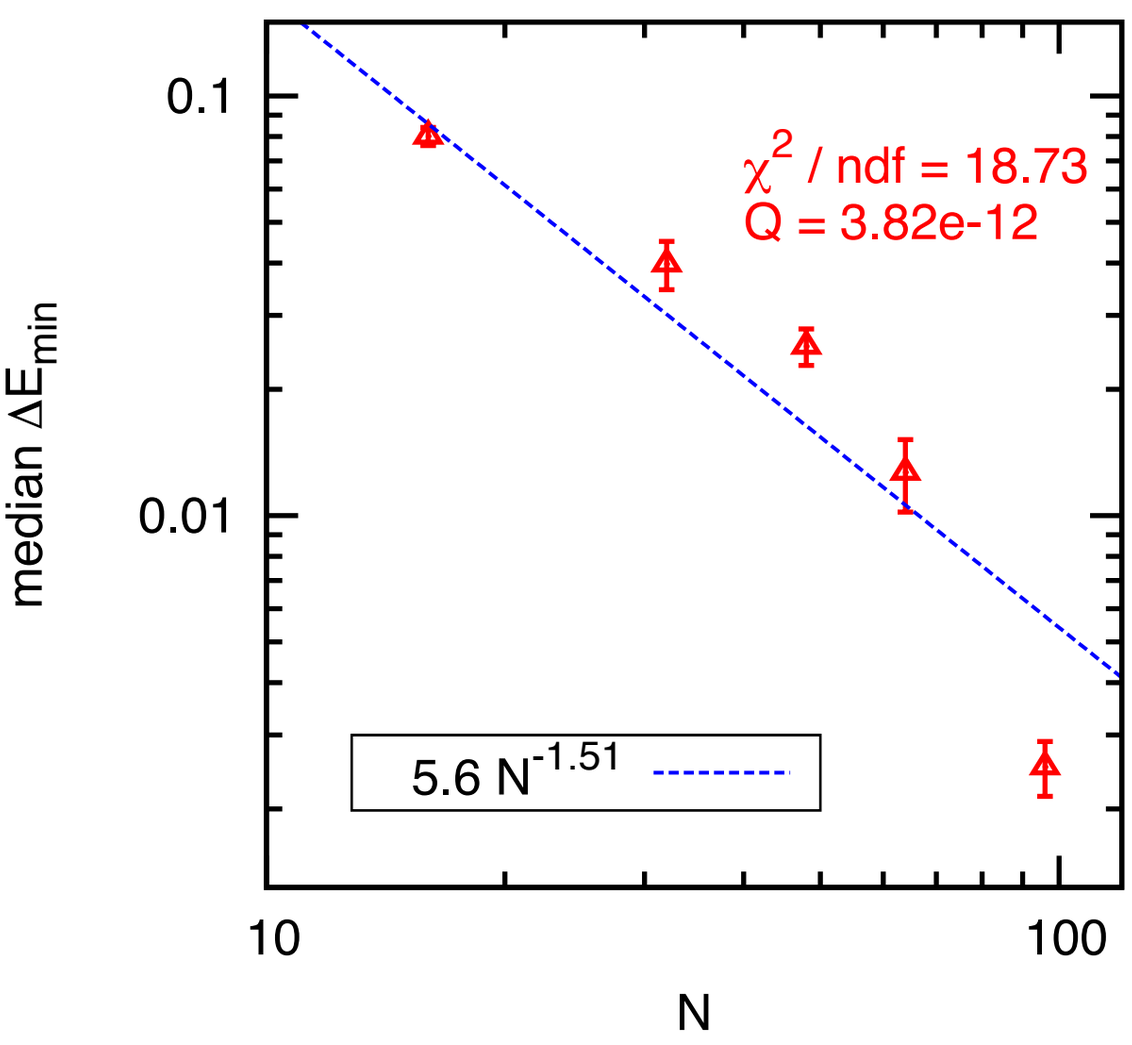
and so is in P (the class of problems that can be solved in polynomial time). Nonetheless we will see that it is very hard for heuristic algorithms (quantum and classical).

Locked 1-in-3 SAT

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.

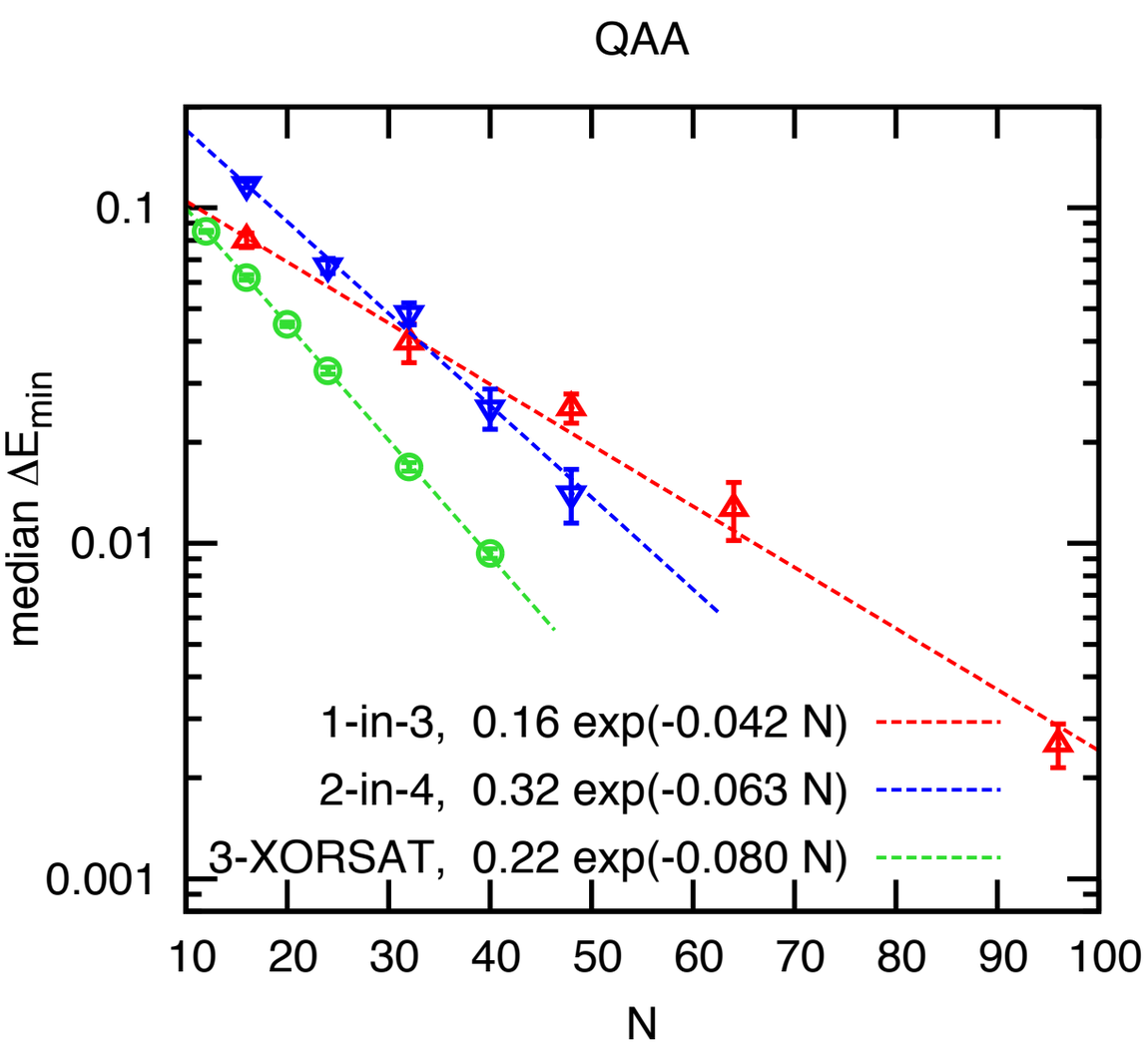
For QAA, Landau-Zener theory states that the time is proportional to $1/(\Delta E_{min})^2$ (neglecting N dependence of matrix elements).

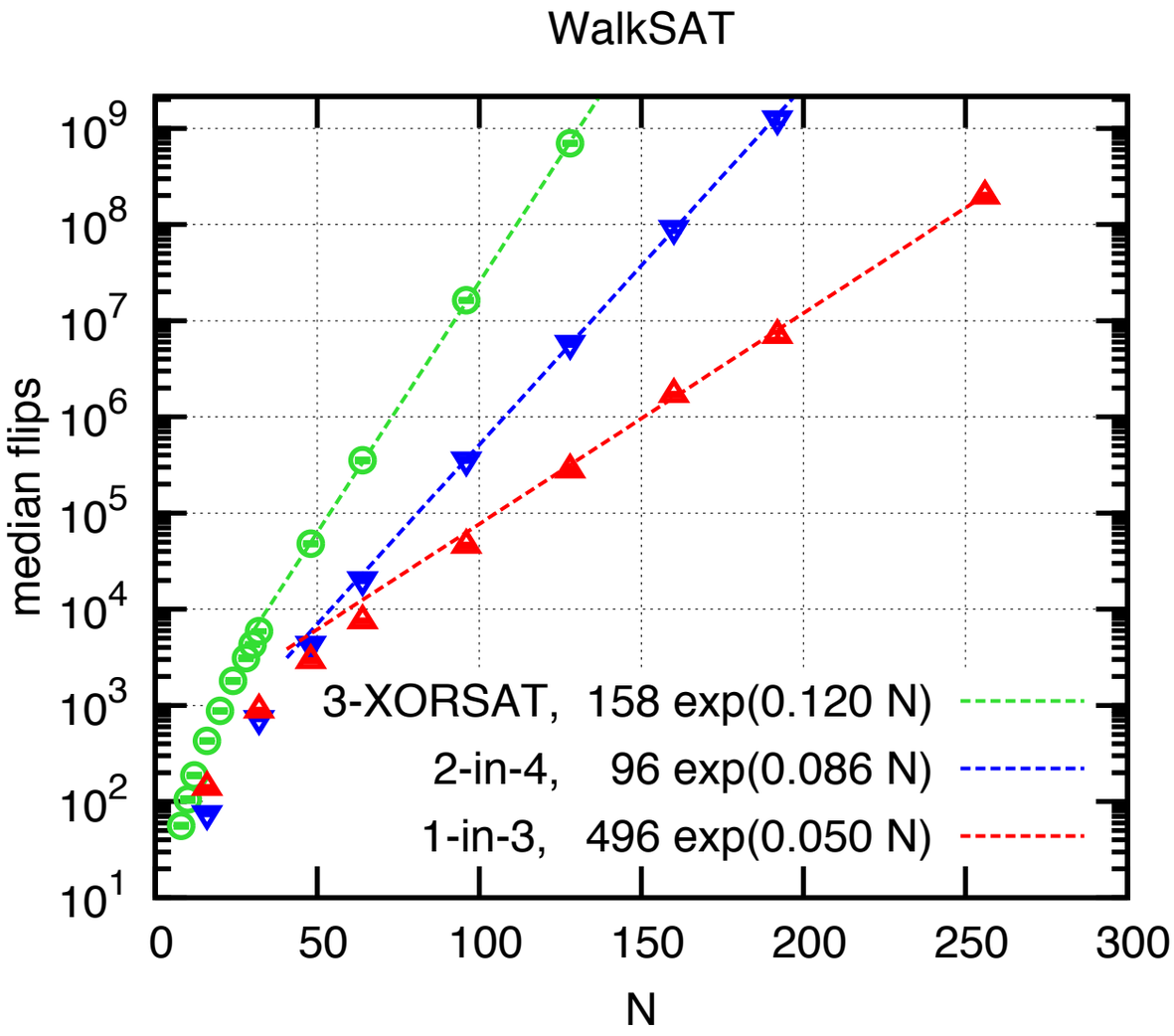
For WalkSAT the running time is proportional to number of "bit flips".

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 (a 3-spin Hamiltonian) is the hardest, and locked 1-in-3 SAT the easiest.

Curious that the hardest problem for these heuristic algorithms is the one with a polynomial time algorithm (complexity class P).

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**.

A “spin glass” on a random graph:

For simplicity we put the spins a **regular random graph**, each site having exactly three neighbor (3-regular). Spins prefer to be antiparallel, an antiferromagnet (but see next slide)

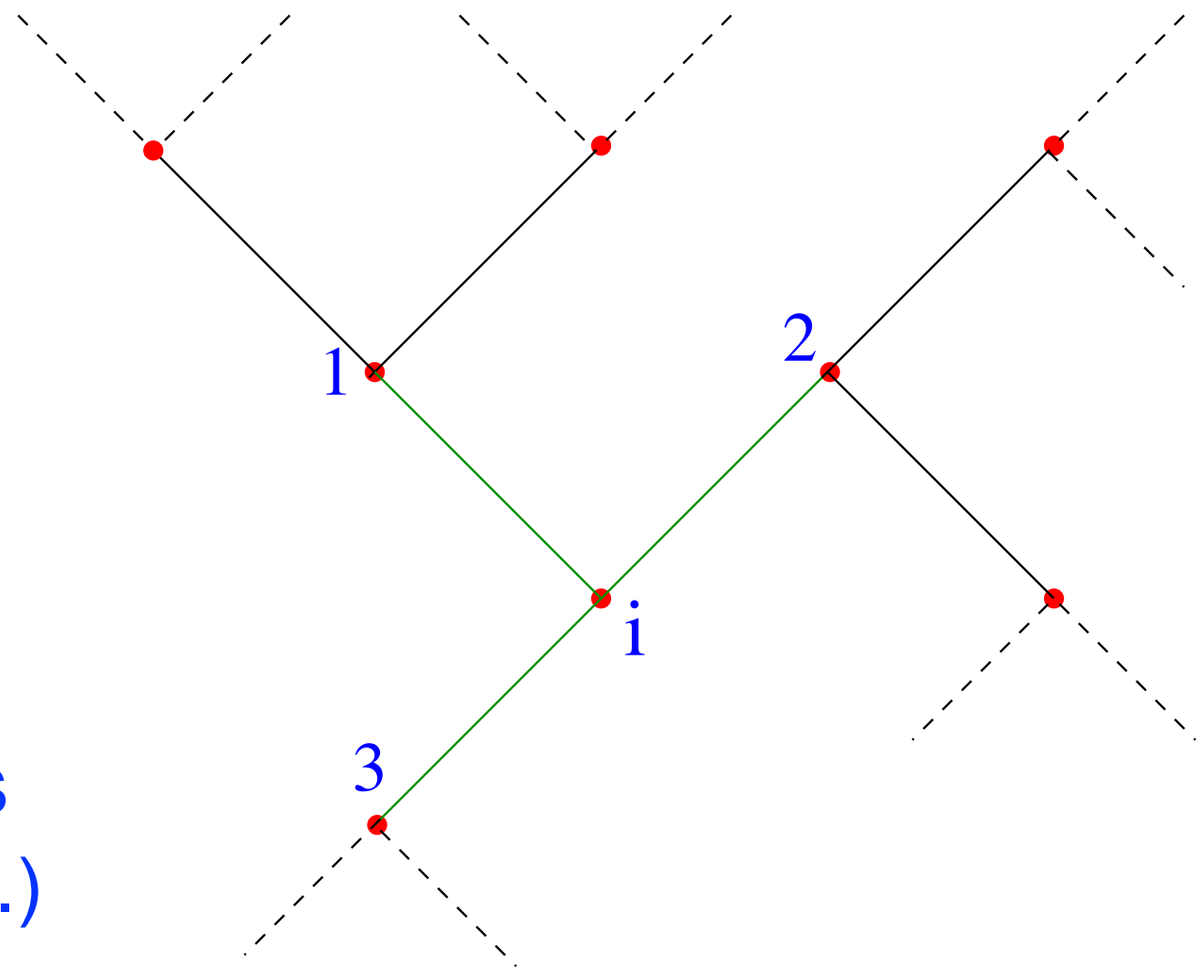
The problem Hamiltonian is

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

Note the symmetry under

$$\sigma_i^z \rightarrow -\sigma_i^z,\ \forall i$$

“Replica” theory indicates that these 2-SAT-like problems are **different** from K-SAT problems for K > 2. (Hence we study it here.)



Note: there are large loops

Spin Glass on a random graph: II

Cannot form an “up-down” antiferromagnet because of loops of odd length. In fact, it is a “spin glass”, a system with disorder and “frustration” (here no disorder in bonds, only geometry)

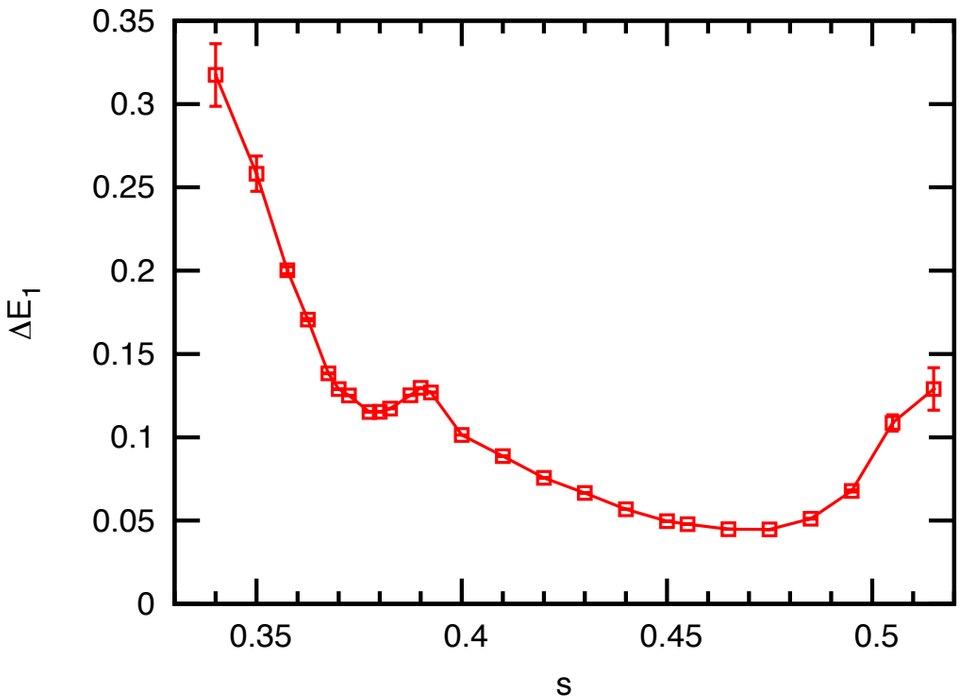
Adding the driver Hamiltonian there is a quantum phase transition at $s = s^*$ above which the symmetry is spontaneously broken.

Did “cavity” calculations (Gosset, Zamponi), semi-analytical approach in which the thermodynamic limit has been taken, but needs approximations in the spin glass phase for $s > s^*$. These calculations find $s^* \cong 0.36$

Also investigated the problem by QMC near s^* ($s \leq 0.5$).

(Just considered instances with a “unique satisfying assignment”, apart from the degenerate state related by flipping all the spins. These are exponentially rare.)

Spin glass" on a random graph: III



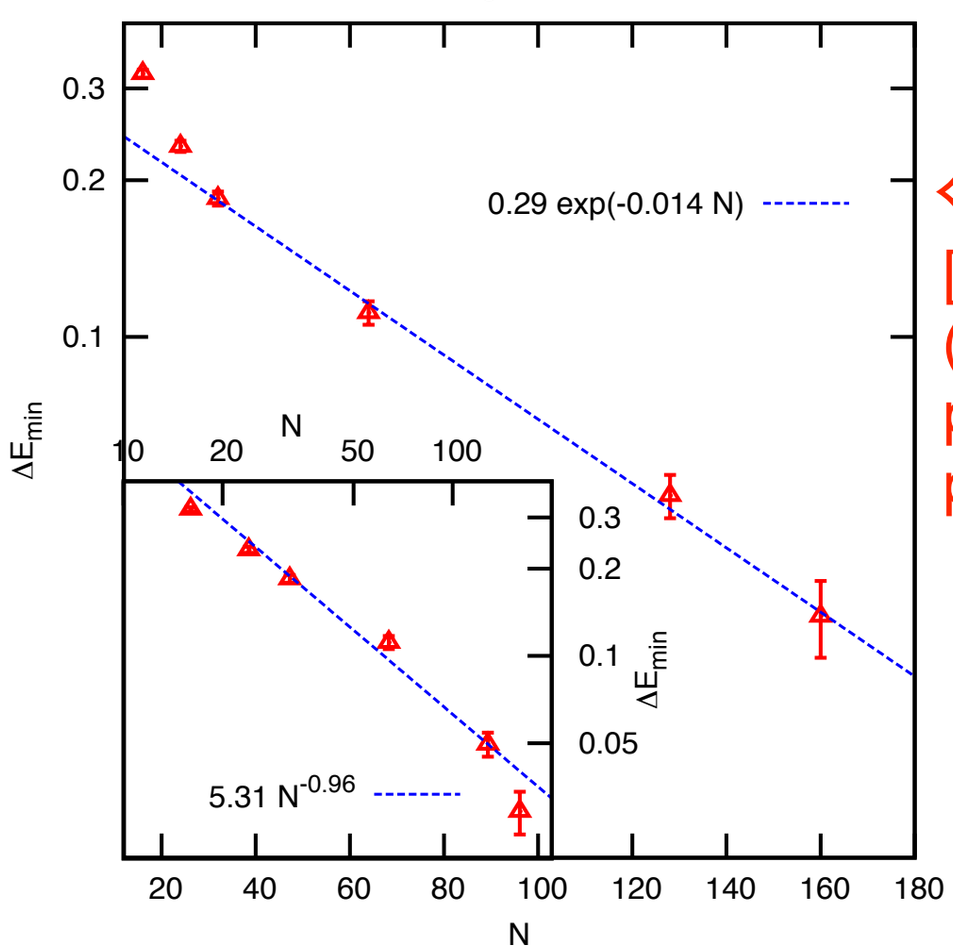
For larger sizes, a fraction of instances have **two minima**, one fairly close to s^* ($\simeq$ 0.36) and other at larger s in the spin glass phase.

⇐ Figure shows an example for N = 128.

Hence did 2 analyses

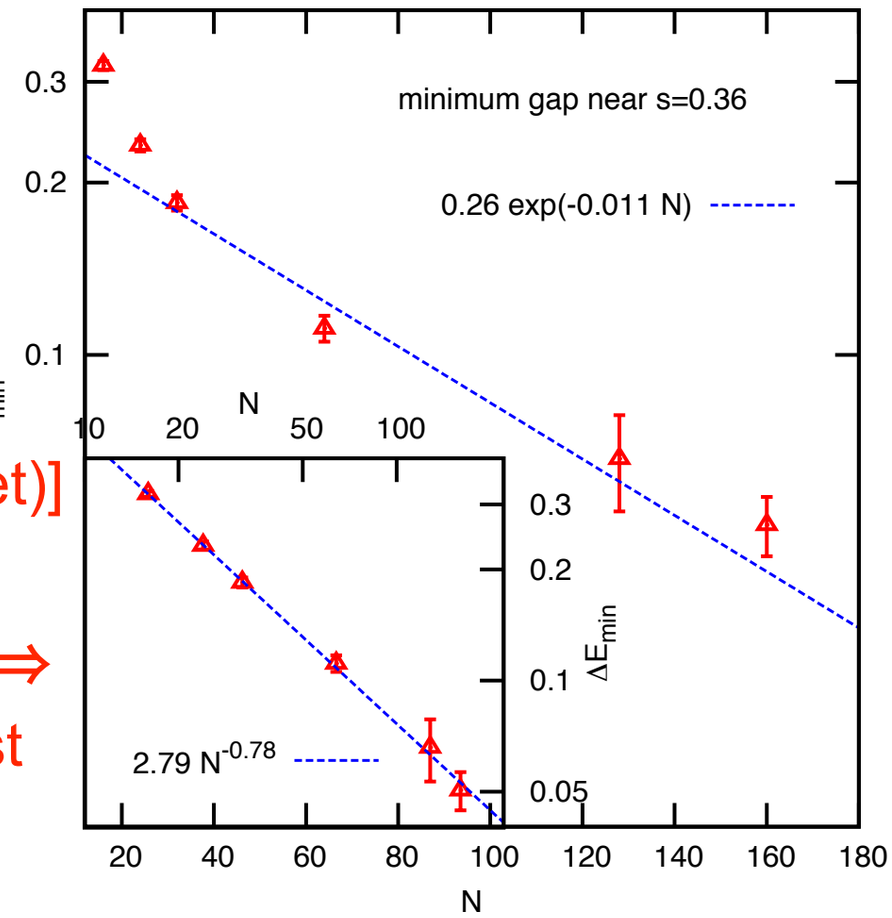
(i) Global minimum in range (up to s=0.5)

(ii) If two minima, just take the local minimum near s^*.



⇐Global
[exponential (main figure) preferred over power-law (inset)]

Local⇒
[power-law best (inset)]



Conclusions

Conclusions

- Simple application of QAA gives exponential running time.
  Not faster than a classical algorithm.

Conclusions

- Simple application of QAA gives exponential running time.
  Not faster than a classical algorithm.
  The bottleneck is:

Conclusions

- Simple application of QAA gives exponential running time.
  Not faster than a classical algorithm.
  The bottleneck is:
  - At the (first order transition) for SAT problems

Conclusions

- Simple application of QAA gives exponential running time.
  Not faster than a classical algorithm.
  The bottleneck is:
  - At the (first order transition) for SAT problems
  - In the spin glass phase, beyond the transition, in the spin glass model

Conclusions

- Simple application of QAA gives exponential running time.
  Not faster than a classical algorithm.
  The bottleneck is:
  - At the (first order transition) for SAT problems
  - In the spin glass phase, beyond the transition, in the spin glass model
- What about other models?

Conclusions

- Simple application of QAA gives exponential running time.
  Not faster than a classical algorithm.
  The bottleneck is:
  - At the (first order transition) for SAT problems
  - In the spin glass phase, beyond the transition, in the spin glass model
- What about other models?
- Perhaps the QAA could be useful to get an approximate ground state. (For some problems, even this is difficult).

Conclusions

- Simple application of QAA gives exponential running time. Not faster than a classical algorithm.
  The bottleneck is:
  - At the (first order transition) for SAT problems
  - In the spin glass phase, beyond the transition, in the spin glass model
- What about other models?
- Perhaps the QAA could be useful to get an approximate ground state. (For some problems, even this is difficult).
- I have just described the simplest implementation of the QAA. Perhaps if one could find clever paths in Hamiltonian space one could do better. A subject for future research.

Conclusions

- Simple application of QAA gives exponential running time. Not faster than a classical algorithm.
  The bottleneck is:
  - At the (first order transition) for SAT problems
  - In the spin glass phase, beyond the transition, in the spin glass model
- What about other models?
- Perhaps the QAA could be useful to get an approximate ground state. (For some problems, even this is difficult).
- I have just described the simplest implementation of the QAA. Perhaps if one could find clever paths in Hamiltonian space one could do better. A subject for future research.

Thank you