

“Mind the gap”

Solving optimization problems with a quantum computer

A.P. Young

<http://physics.ucsc.edu/~peter>



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Work supported by



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WHERE DISCOVERIES BEGIN

NASA future technologies conference, January 17-21, 2012

Collaborators: Itay Hen, see poster and Phys. Rev. E, 061152 (2011)

E. Farhi, P. Shor, D. Gosset, A. Sandvik, V. Smelyanskiy, S. Knysh, M. Guidetti.

Synopsis: Mind the Gap



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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 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 . 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*

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MIND THE GAP

Synopsis: Mind the Gap



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Quantum computers promise to accelerate some tasks, but it's only half the story: efficiency requires developing new algorithms.

To apply a quantum computer to a broad class of problems, an algorithm in which the problem to be solved is

under a bound

and adiabatic algorithm scaling with the size of the problem. —

MIND THE GAP

Exponential complexity of the quantum adiabatic algorithm for certain satisfiability problems

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Plan

Question: What could we do with an eventual quantum computer in addition to Shor and Grover?

Here: compare the efficiency of a proposed **quantum** algorithm with that of a **classical** algorithm for solving optimization and “constraint satisfaction” problems

Will use the **Quantum Monte Carlo** (QMC) Method to study the **Quantum Adiabatic Algorithm** (QAA) for large sizes, and compare with a classical algorithm (**WALKSAT**).

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 $= -h \sum (\sigma_i^x - 1)$

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

\mathcal{T} is the running time

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

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

Quantum Phase Transition

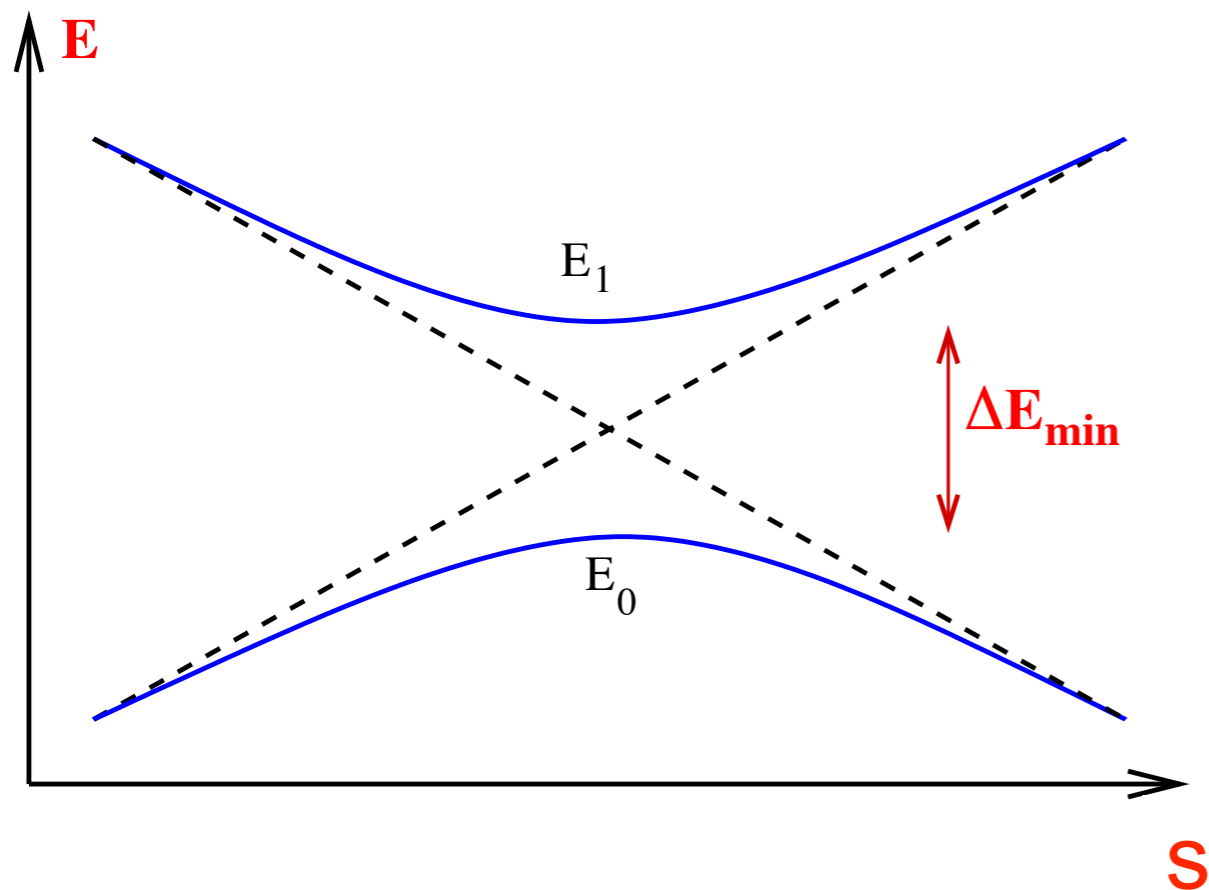


Bottleneck is likely to be a quantum phase transition (QPT) where the gap to the first excited state is very small

Quantum Phase Transition



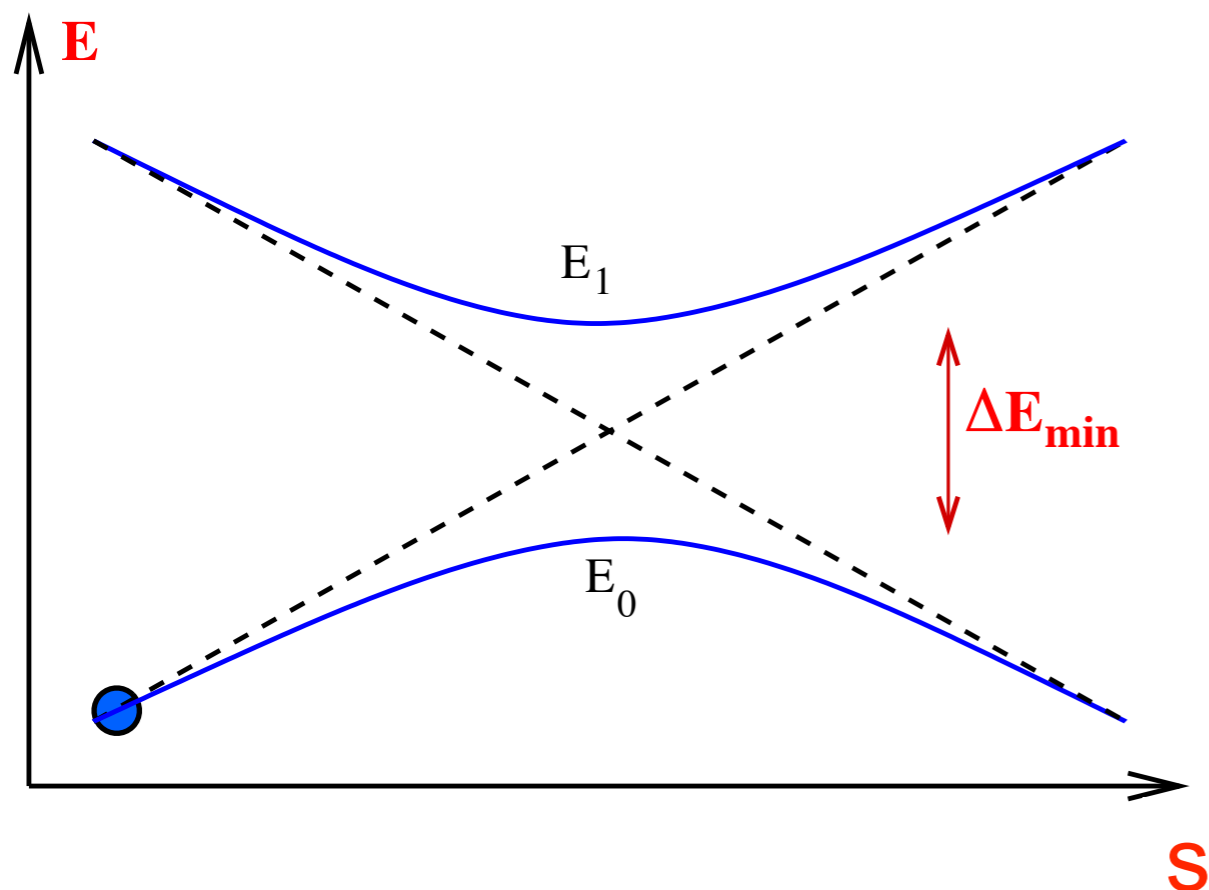
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Quantum Phase Transition



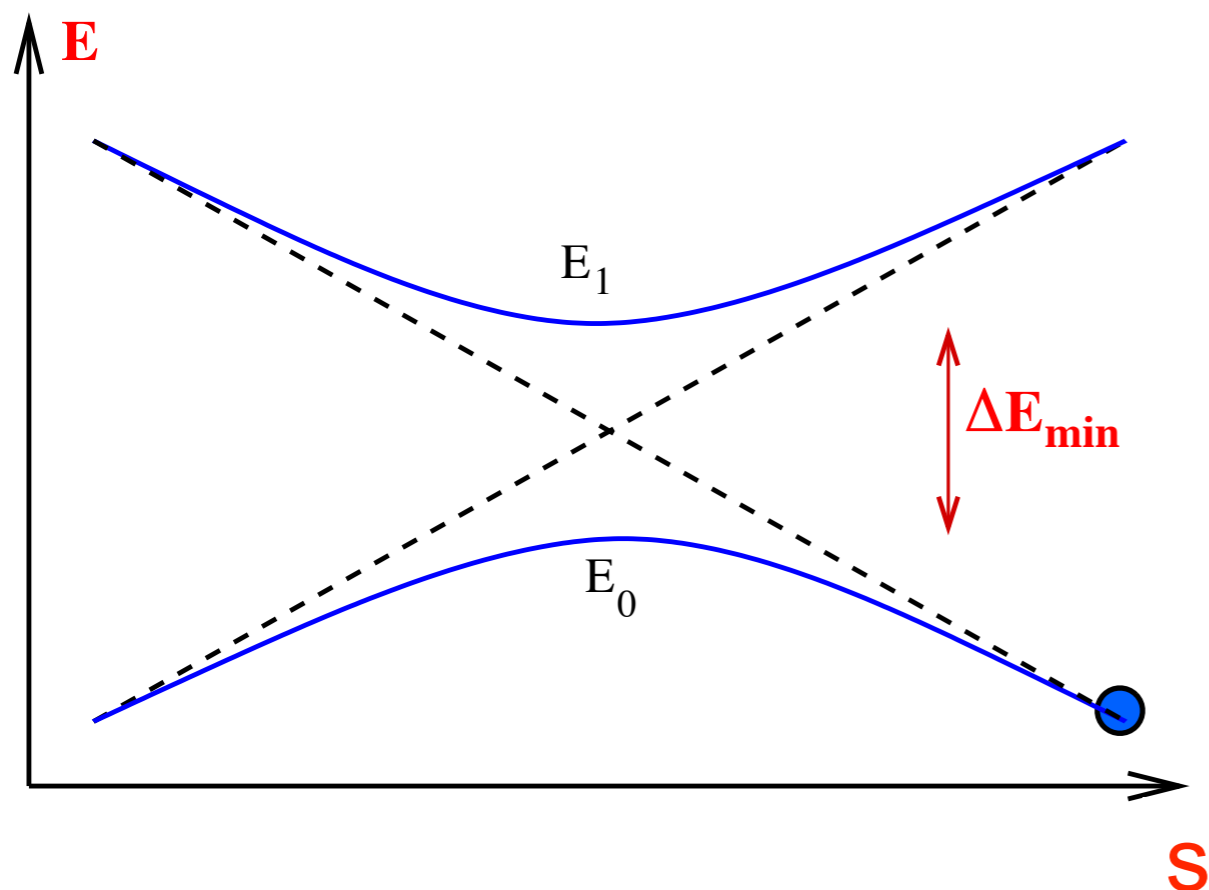
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Quantum Phase Transition



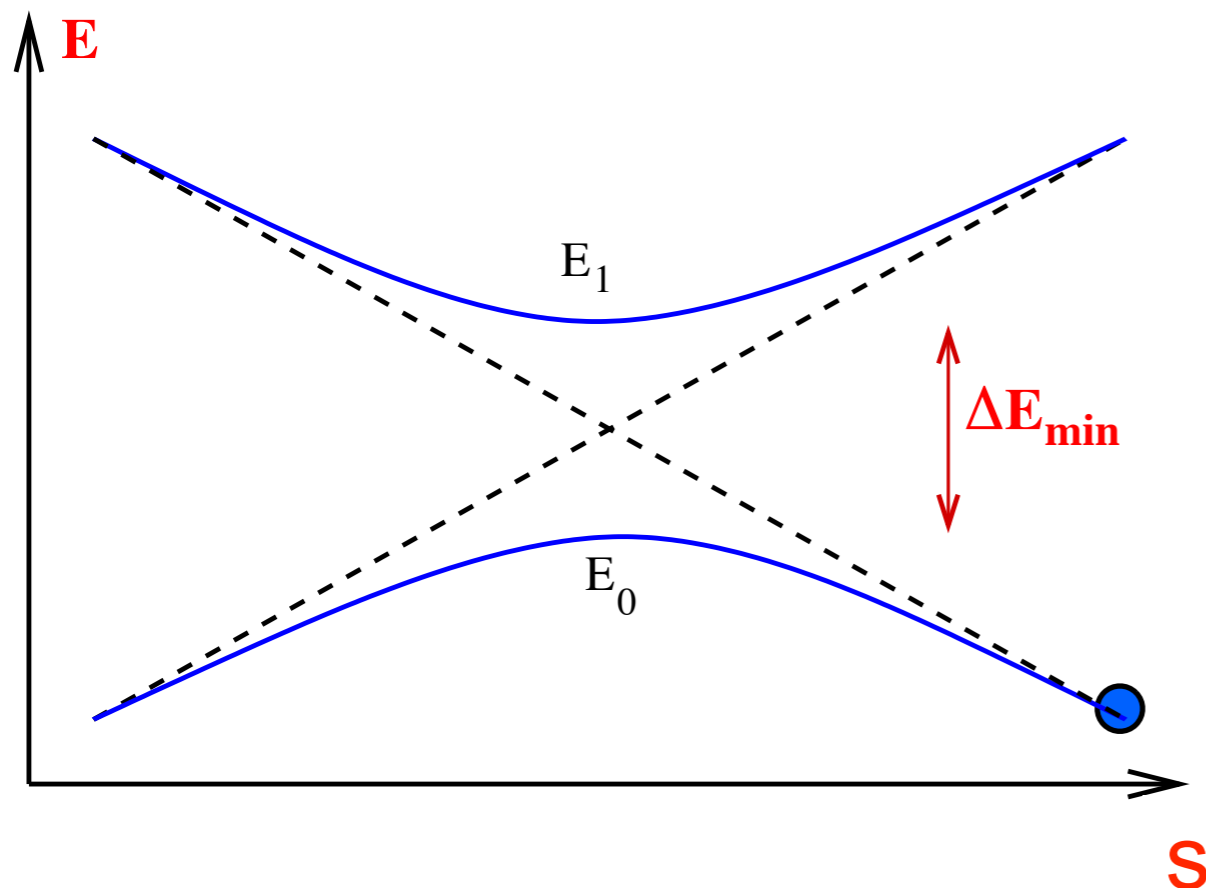
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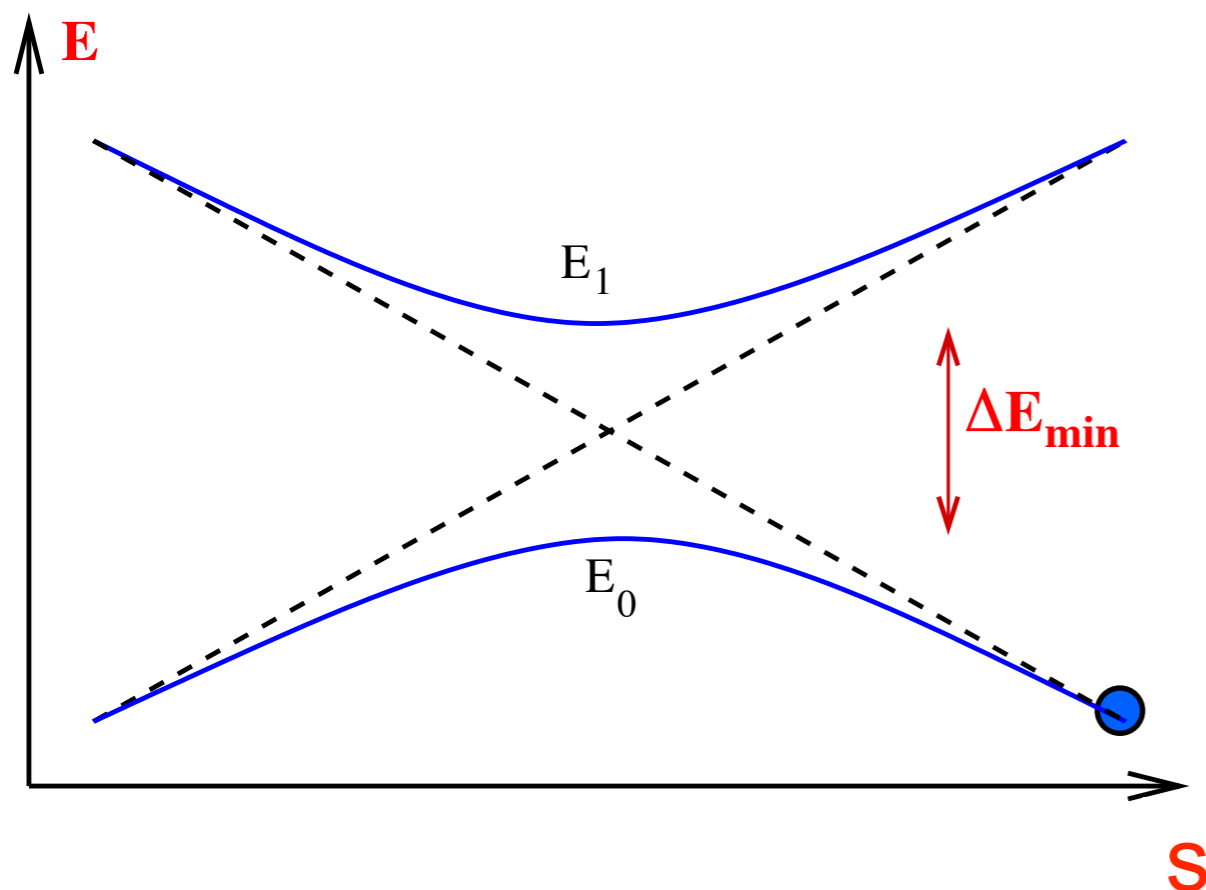


Landau Zener Theory:
To stay in the ground state the time needed is proportional to ΔE_{\min}^{-2}

Quantum Phase Transition



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

Using QMC compute ΔE for different s : $\rightarrow \Delta E_{\min}$

Quantum Monte Carlo

We do a **sampling** of the 2^N states (so statistical errors).

Study **equilibrium** properties of a quantum system by simulating a **classical model with an extra dimension**, imaginary time, τ , where $0 \leq \tau < 1/T$.

Not perfect, but the only numerical method available for large N .

We use the “**stochastic series expansion**” method for Quantum Monte Carlo simulations which was pioneered by Anders Sandvik.

$$Z \equiv \text{Tr} e^{-\beta \mathcal{H}} = \sum_{n=0}^{\infty} \frac{\text{Tr} (-\beta \mathcal{H})^n}{n!}$$

Stochastically sum the terms in the series.

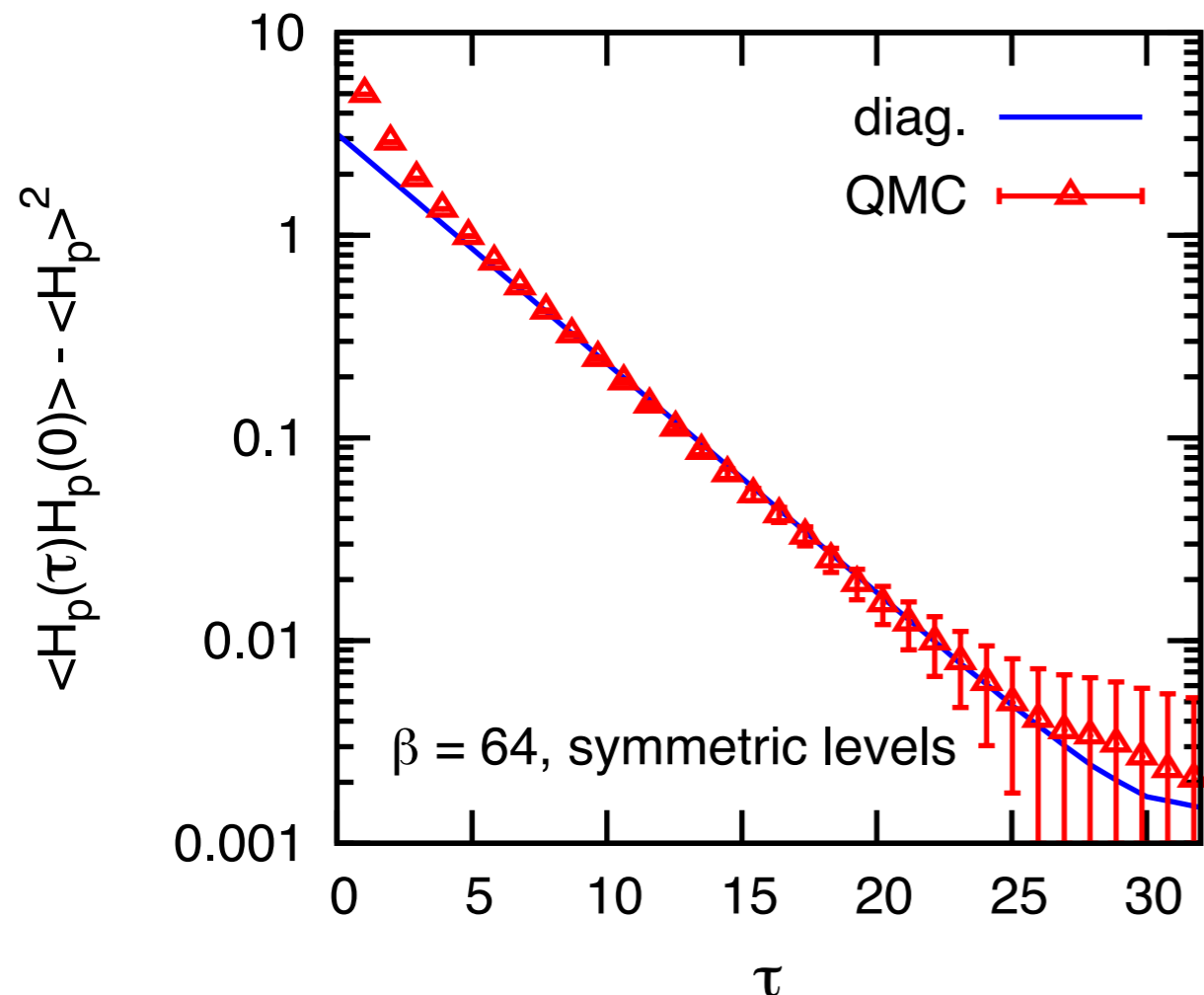
Examples of results with the SSE code

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

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

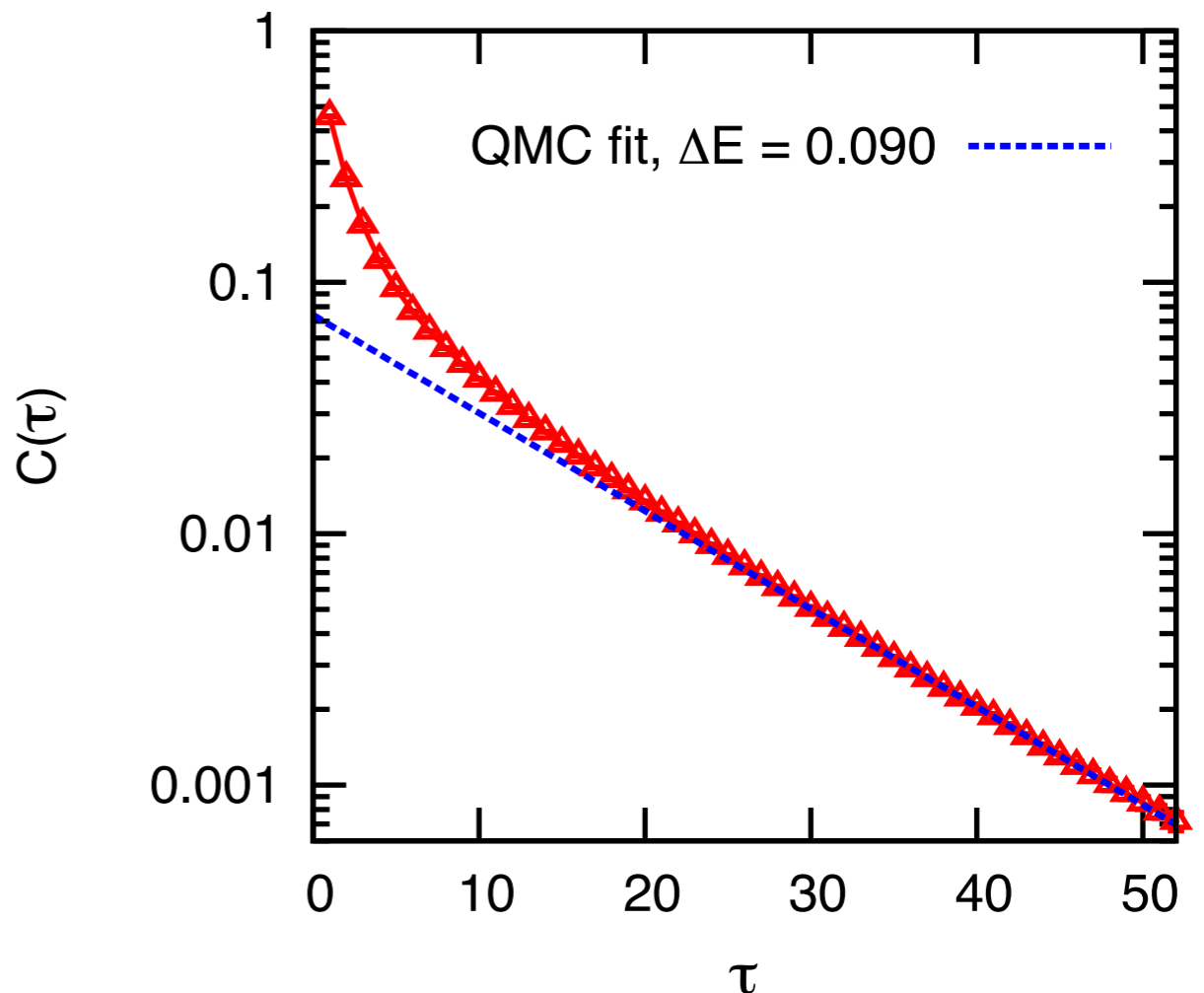
For **large τ** only first excited state contributes, \rightarrow **pure exponential decay**

3-reg MAX-2-XORSAT, N=24



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

3-reg MAX-2-XORSAT, N = 128



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

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.)

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 **1 is one and the other two are zero**. Otherwise it is not satisfied (and the energy is 1).

- **Locked 2-in-4 SAT**

Similar to 1-in-3 but the **clause has 4 bits and is satisfied if 2 of them are one**. (This has bit-flip symmetry).

“Locked” means that each bit is in at least two clauses, and flipping one bit in a satisfying assignment makes it unsatisfied.

Satisfiability threshold at **critical value of M/N** . We work at this threshold, (hard, Kirkpatrick and Selman) and take instances with a **“USA”**. These seem to be a **finite fraction** of whole ensemble even for **$N \rightarrow \infty$** .

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 $\sigma^z (= \pm 1)$ we require that the **product of the three σ^z 's in a clause is specified (+1 or -1)**.

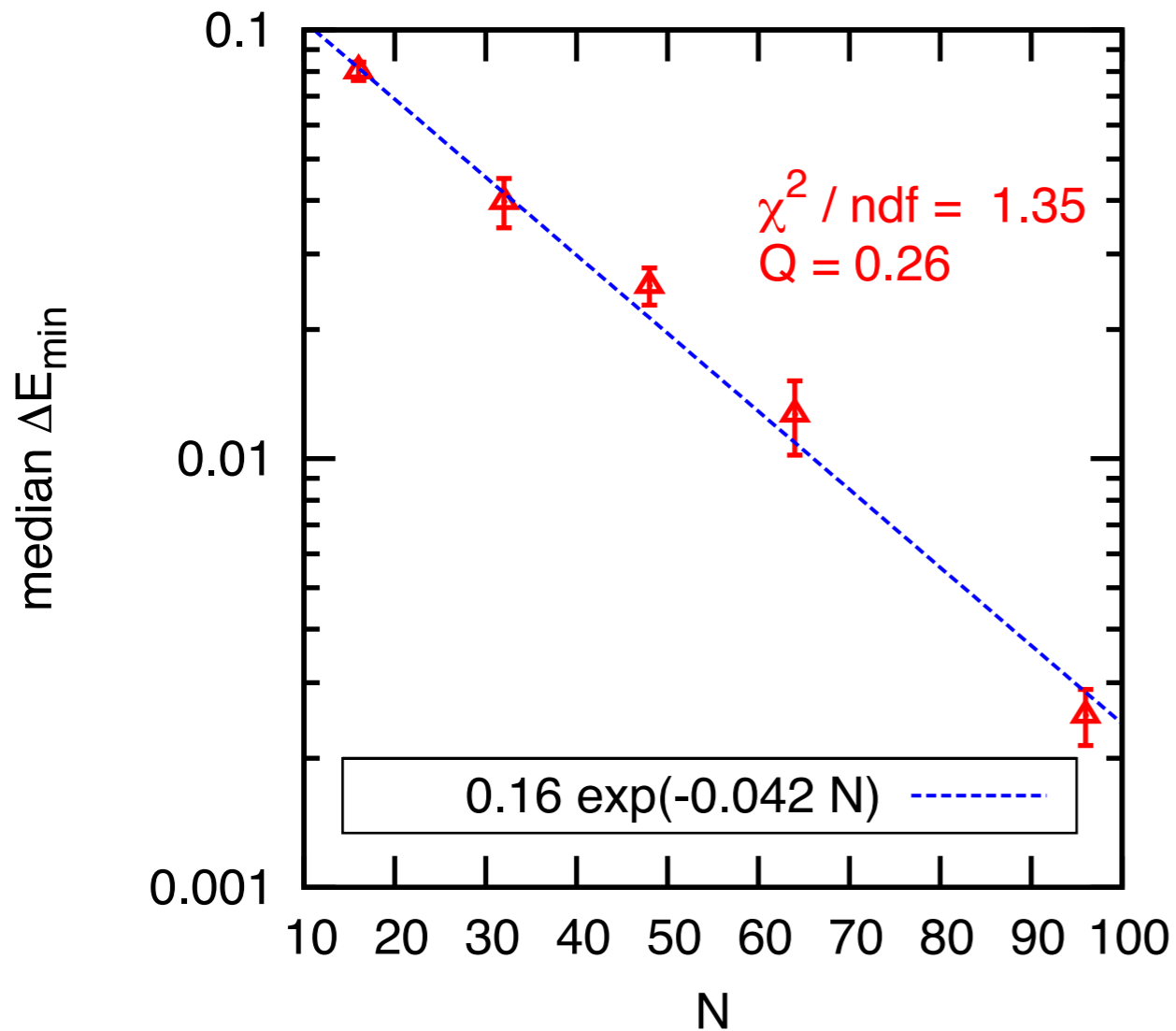
$$\mathcal{H}_P = \sum_{\alpha=1}^M \frac{1}{2} \left(1 - J_{\alpha} \sigma_{\alpha,1}^z \sigma_{\alpha,2}^z \sigma_{\alpha,3}^z \right)$$

(Is at SAT threshold.)

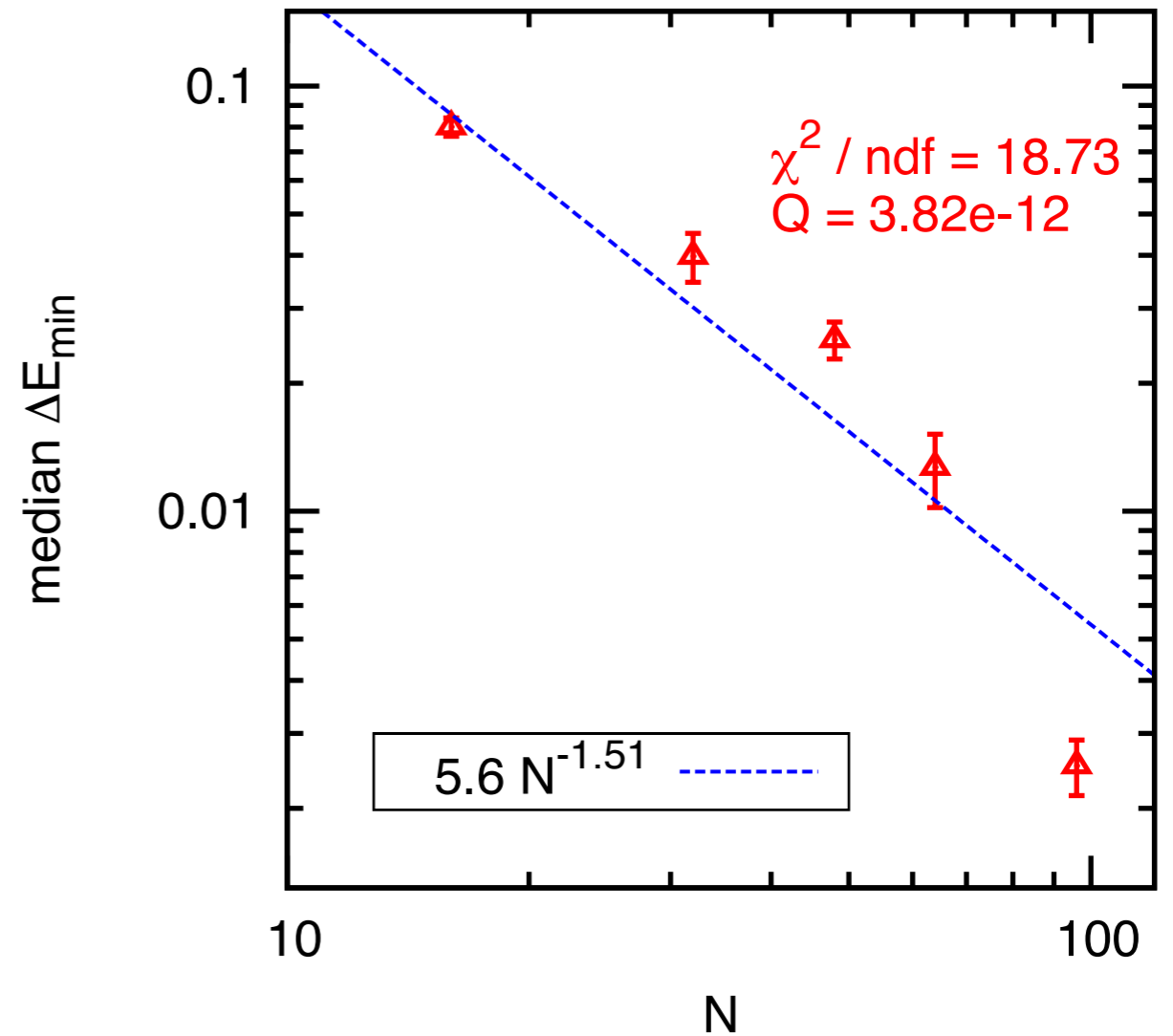
This SAT problem can be solved by linear algebra (**Gaussian elimination**) **and so is in P**. Nonetheless we will see that it is **very hard** for heuristic algorithms (quantum and classical).

Locked 1-in-3

Plots of the median minimum gap



Exponential fit

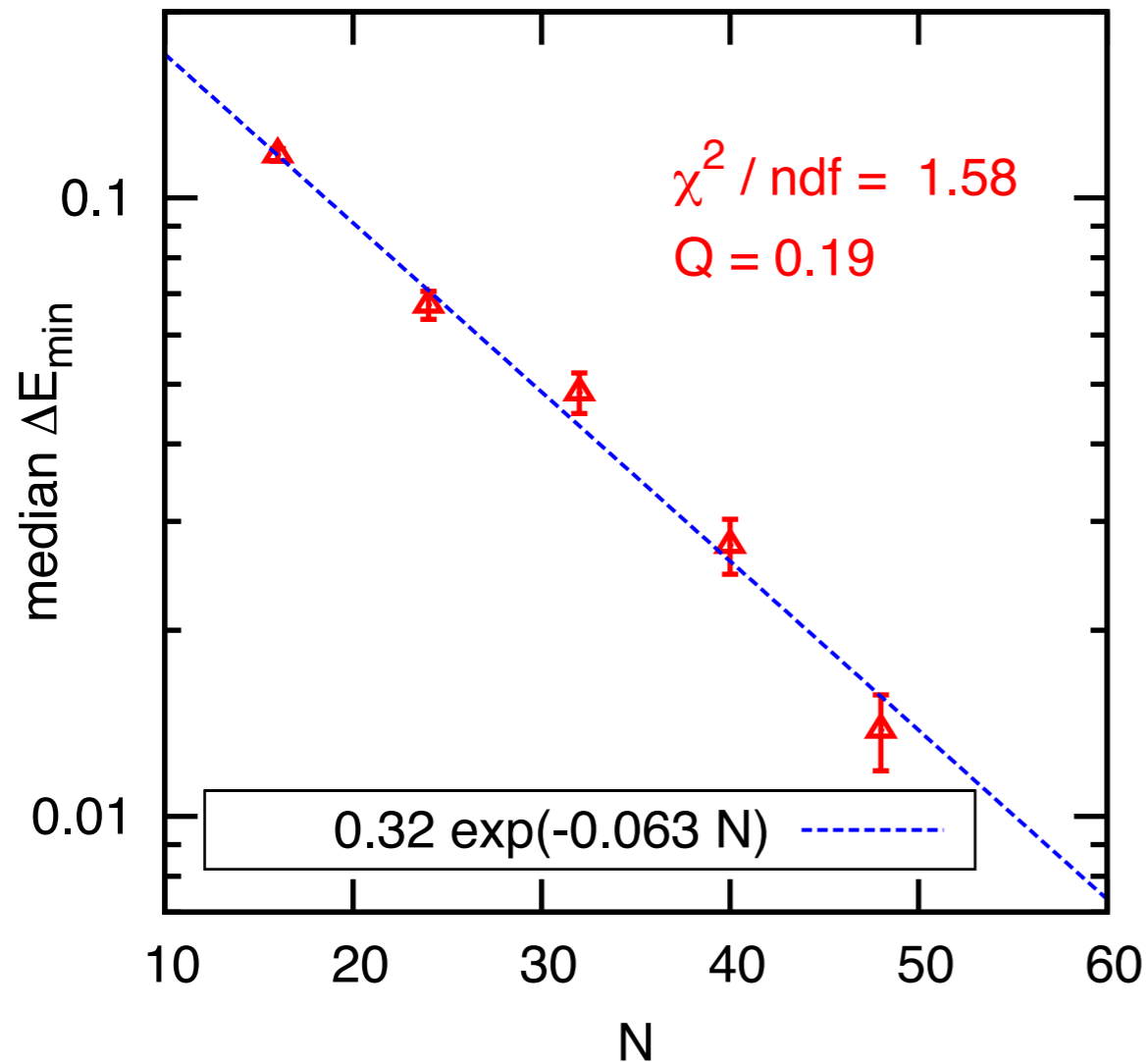


Power law fit

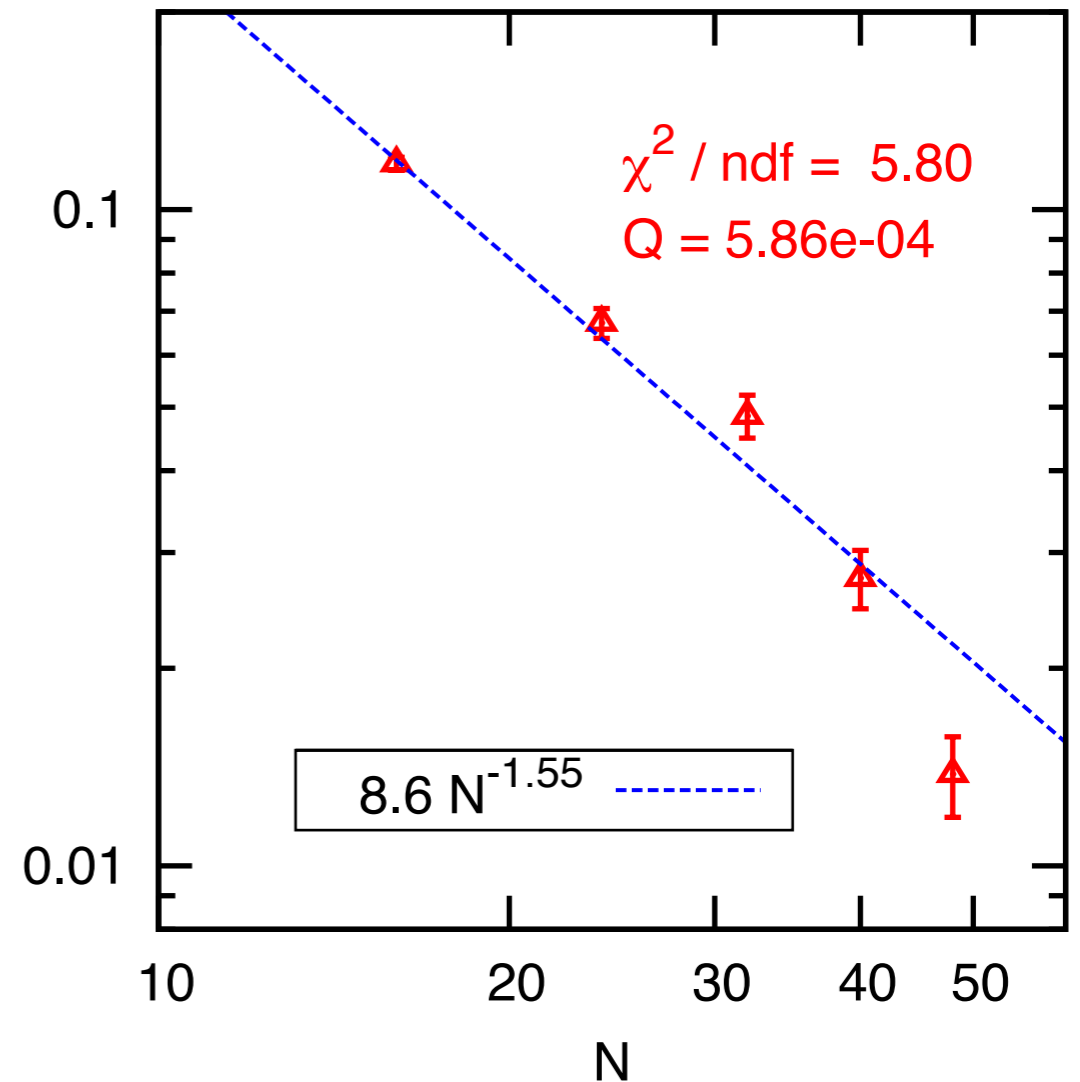
Clearly the behavior of the minimum gap is exponential

Locked 2-in-4

Plots of the median minimum gap



Exponential fit

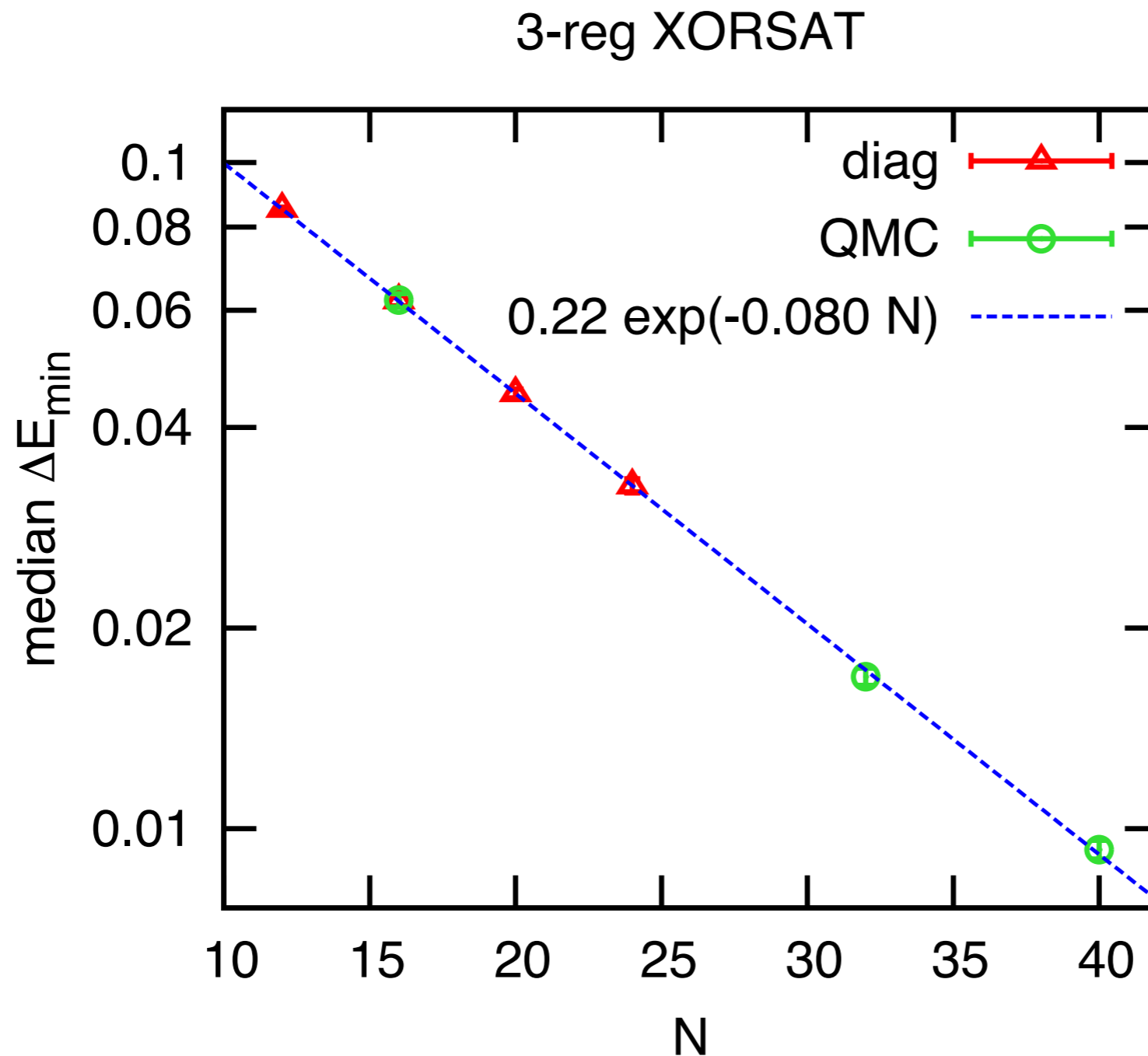


Power law fit

The exponential fit is much better.

3-Reg 3-XORSAT

Exponential (i.e. log-lin) plot of the median minimum gap



Clearly the minimum gap is exponential, even for small N

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).

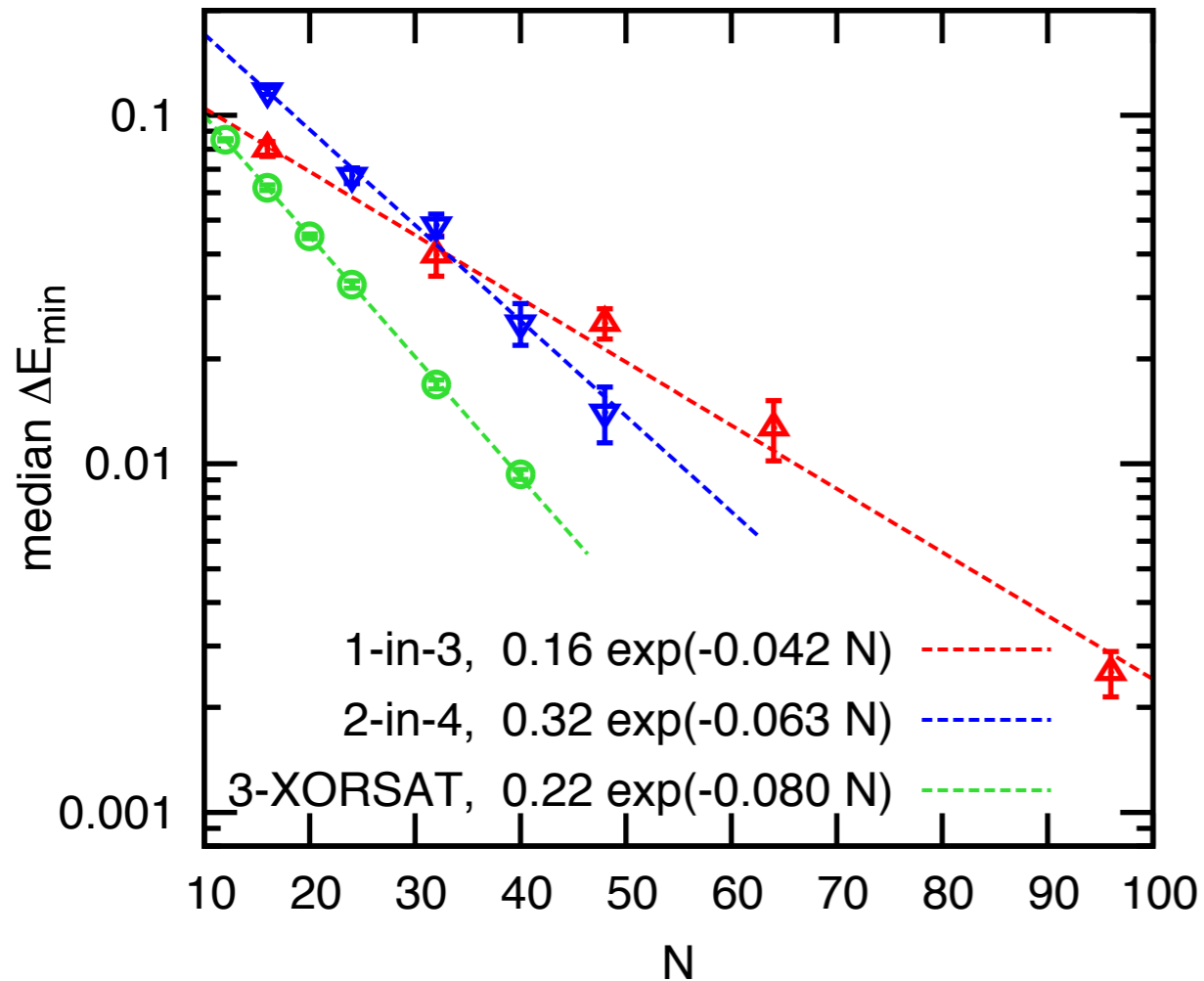
For WalkSAT the running time is proportional to number of “**bit flips**”.

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

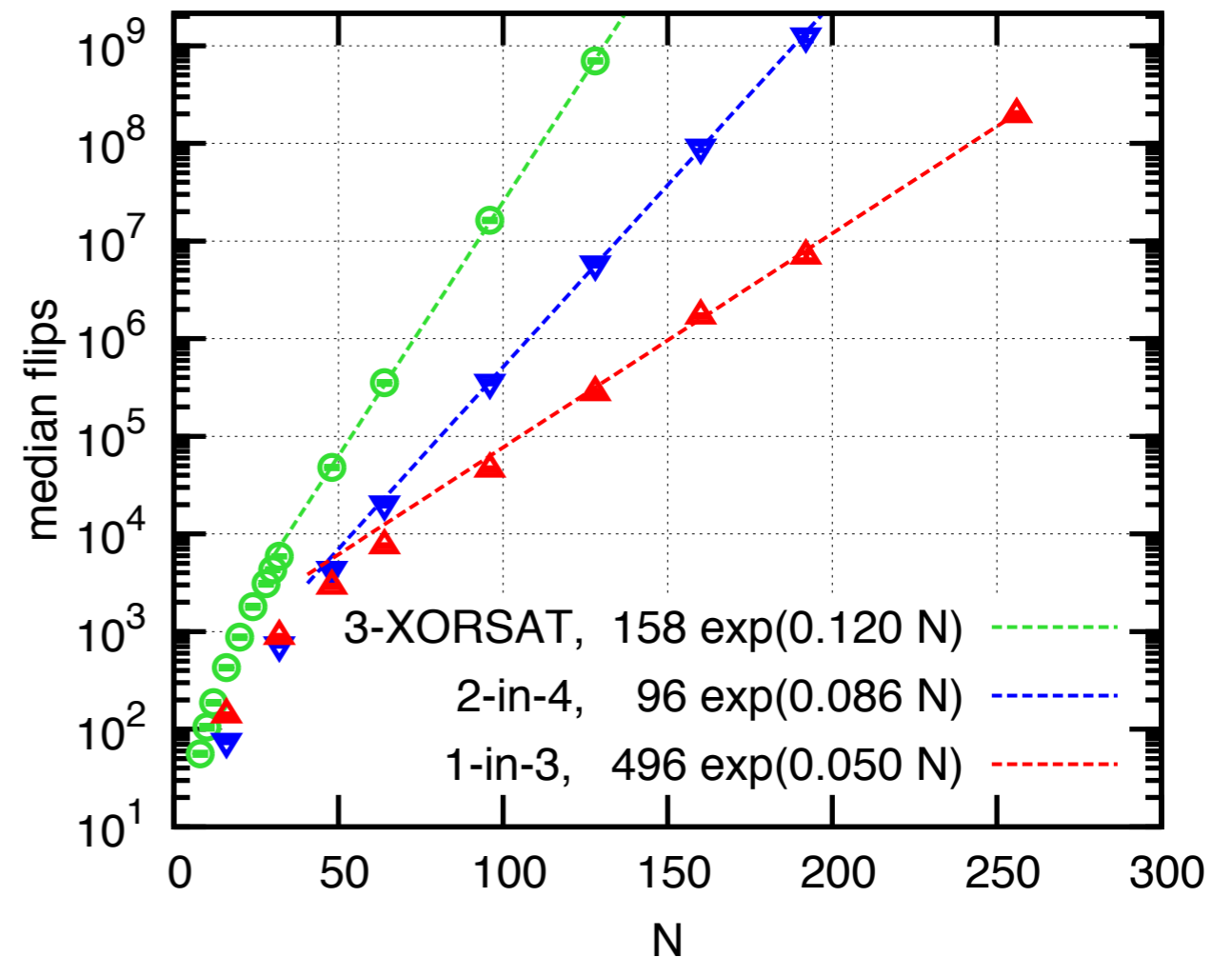
We will compare the values of μ among the different models and between QAA and WalkSAT.

Comparison with a classical algorithm, WalkSAT: II

QAA



WalkSAT



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

Values of μ
(where time \sim
 $\exp[\mu N]$).

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.**

3-Reg MAX-2-XORSAT: I

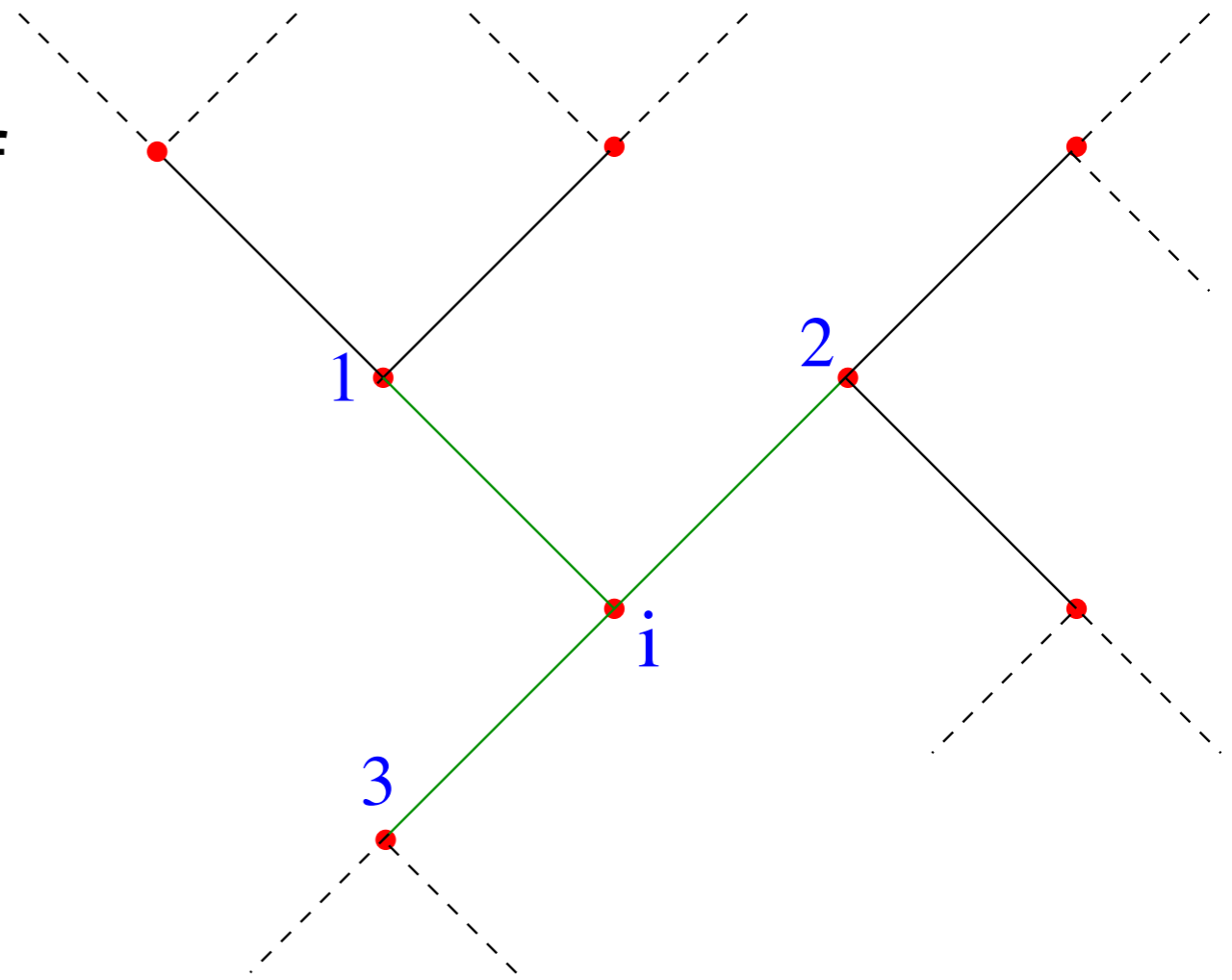
We have also studied one “MAX” (i.e. optimization) problem.

MAX means we are in the UNSAT phase, and want to find the configuration with the least number of unsatisfied clauses.

The “2” in 2-XORSAT means each clause has 2 bits. “Replica” theory indicates that 2-SAT-like problems are different from K-SAT problems for $K > 2$.

We take the “antiferromagnet” version, i.e. the energy is zero if the bits are different (otherwise it is 1).

3-Regular means that it bit is in three clauses, i.e. has 3 “neighbors” connected to it. The connected pairs are chosen at random.



Note: there are large loops

3-Reg MAX-2-XORSAT: II

The problem Hamiltonian is (i.e. antiferro. on random graph)

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

Note the **symmetry** under $\sigma_i^z \rightarrow -\sigma_i^z, \forall i$

Cannot form an “up-down” antiferromagnet because of loops of odd length. In fact, it is a “**spin glass**”.

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

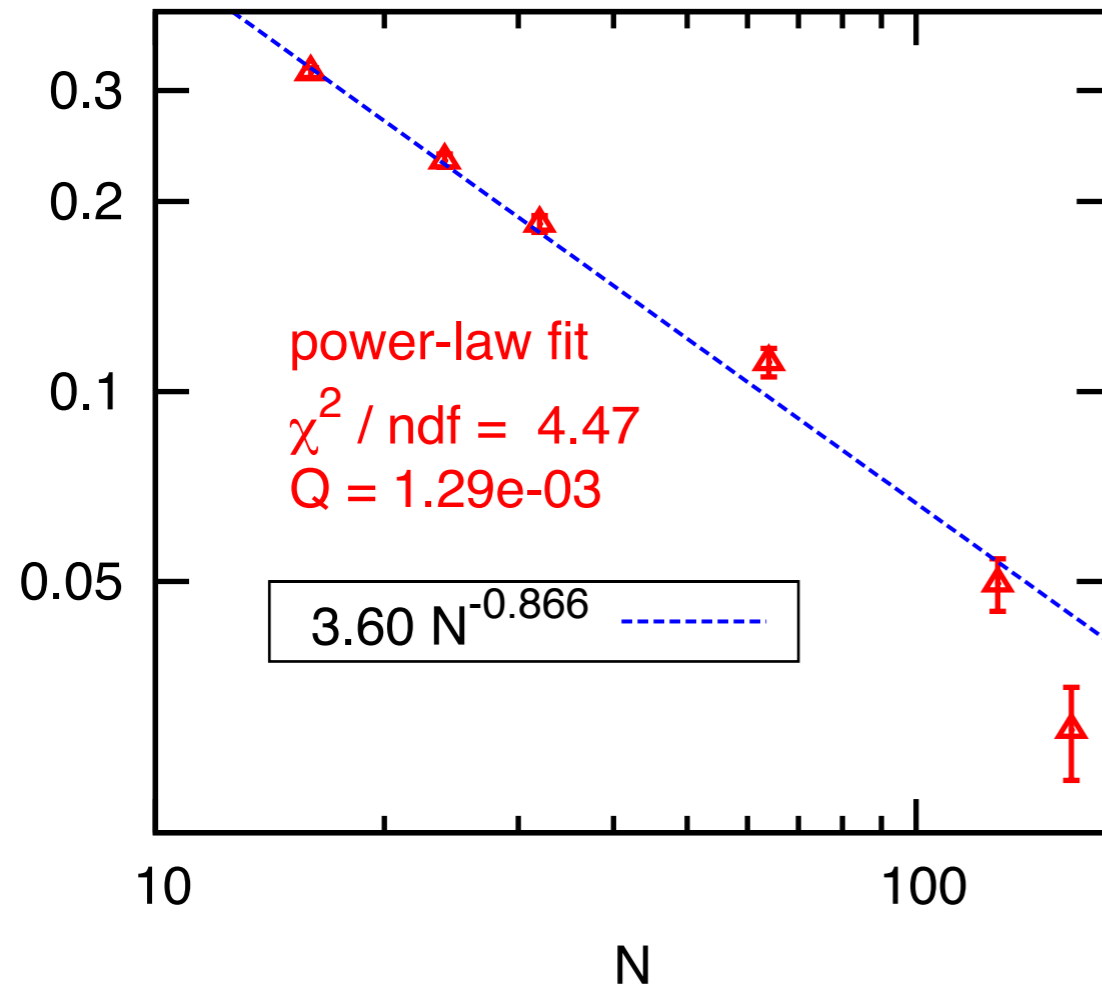
“Cavity” calculations (Gosset) find $s^* \cong 0.36$

So far, have just investigated the problem **near s^*** . Also just considered instances with a “**unique satisfying assignment**” (apart from the degenerate state related by flipping all the spins).

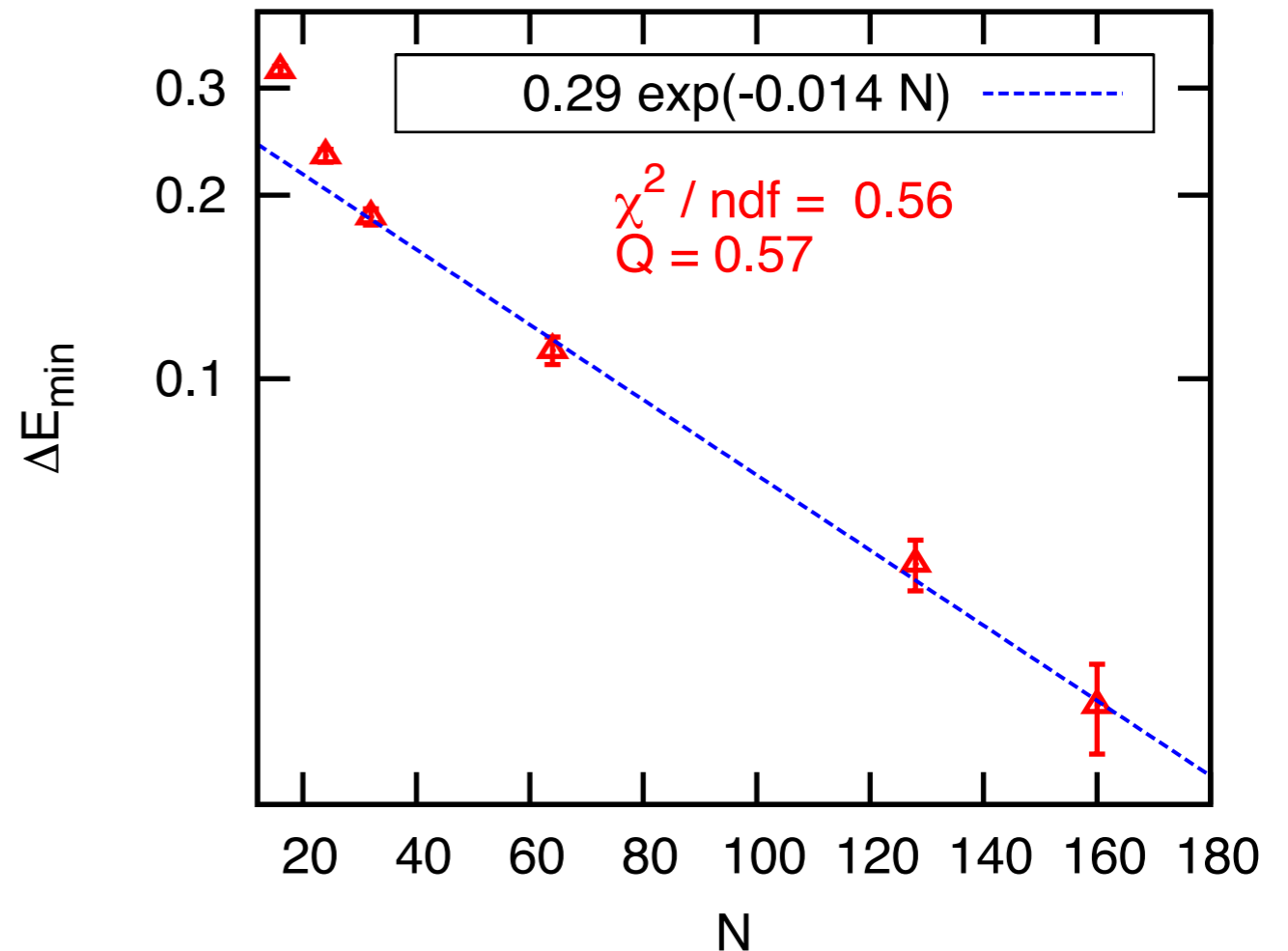
3-Reg MAX-2-XORSAT: III

Median minimum gap for intermediate values of s

3-reg MAX-2-XORSAT



3-reg MAX-2-XORSAT



Power-law fit

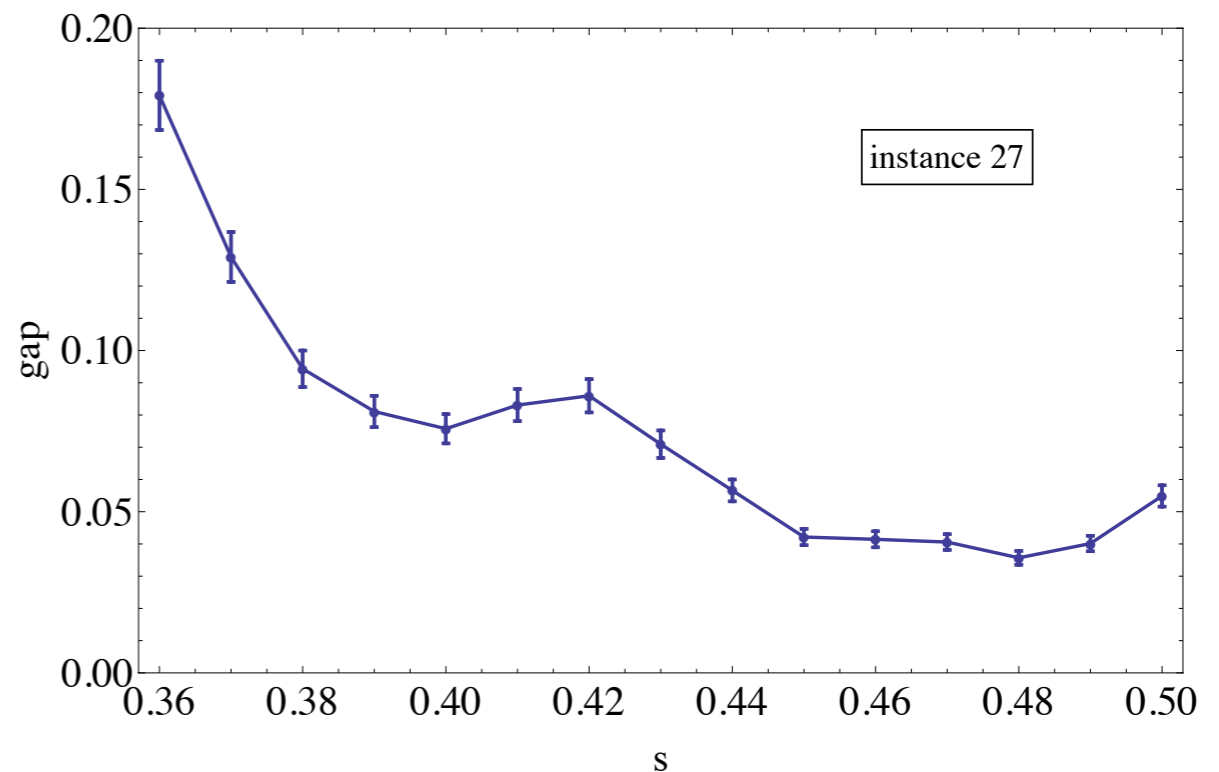
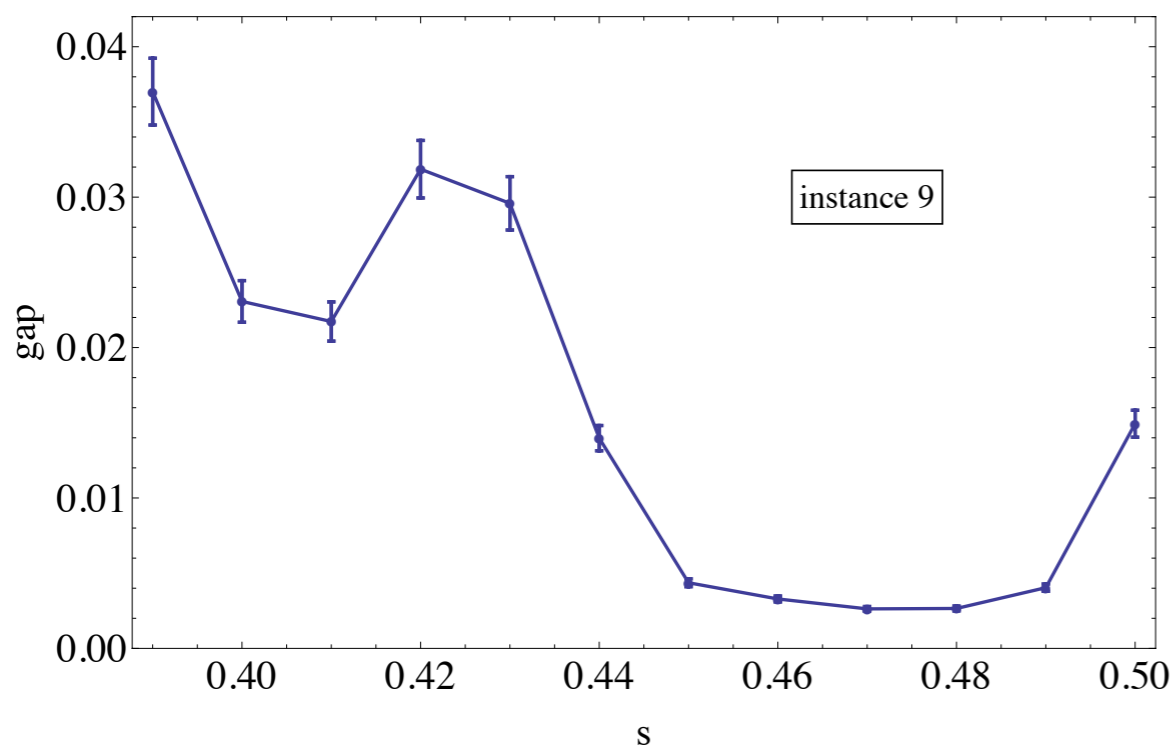
Exponential fit omitting 1st 2 points

Quantum Phase transition is at $s \approx 0.36$ ("cavity" method).

Data shows the minimum gap in region $0.36 \leq s \leq 0.50$.
Looks **exponential** at large sizes.

3-Reg MAX-2-XORSAT: IV

Small sizes have just one minimum, near $s = 0.36$. Larger sizes have additional, deeper minima at larger s , in the “spin glass” phase. Figures below are for two instances of $N = 160$.

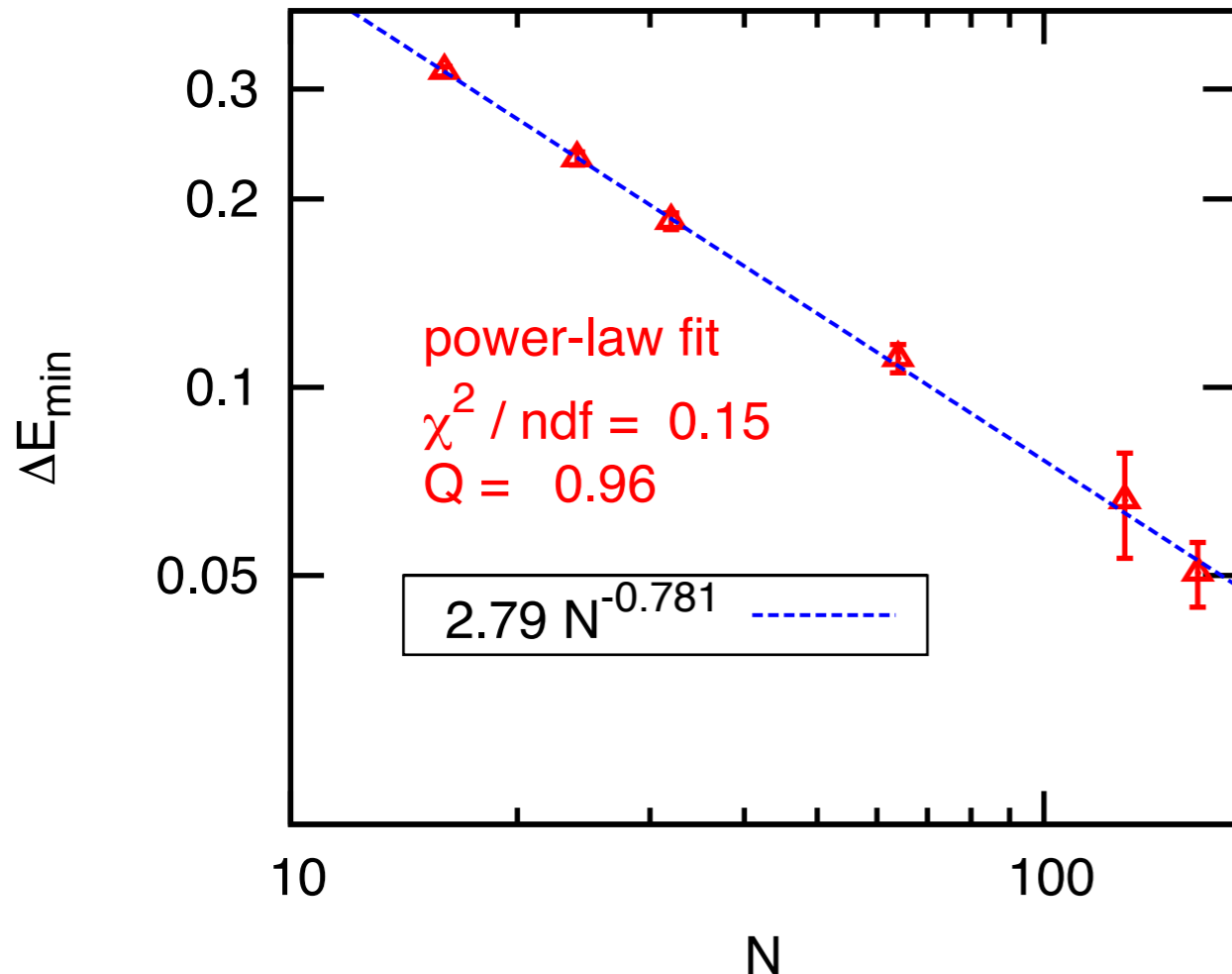


Previous slide shows data for the deepest minimum in the range $0.36 \leq s \leq 0.50$. Next slide shows data for the minimum closest to $s = 0.36$ (if there is more than 1).

3-Reg MAX-2-XORSAT: V

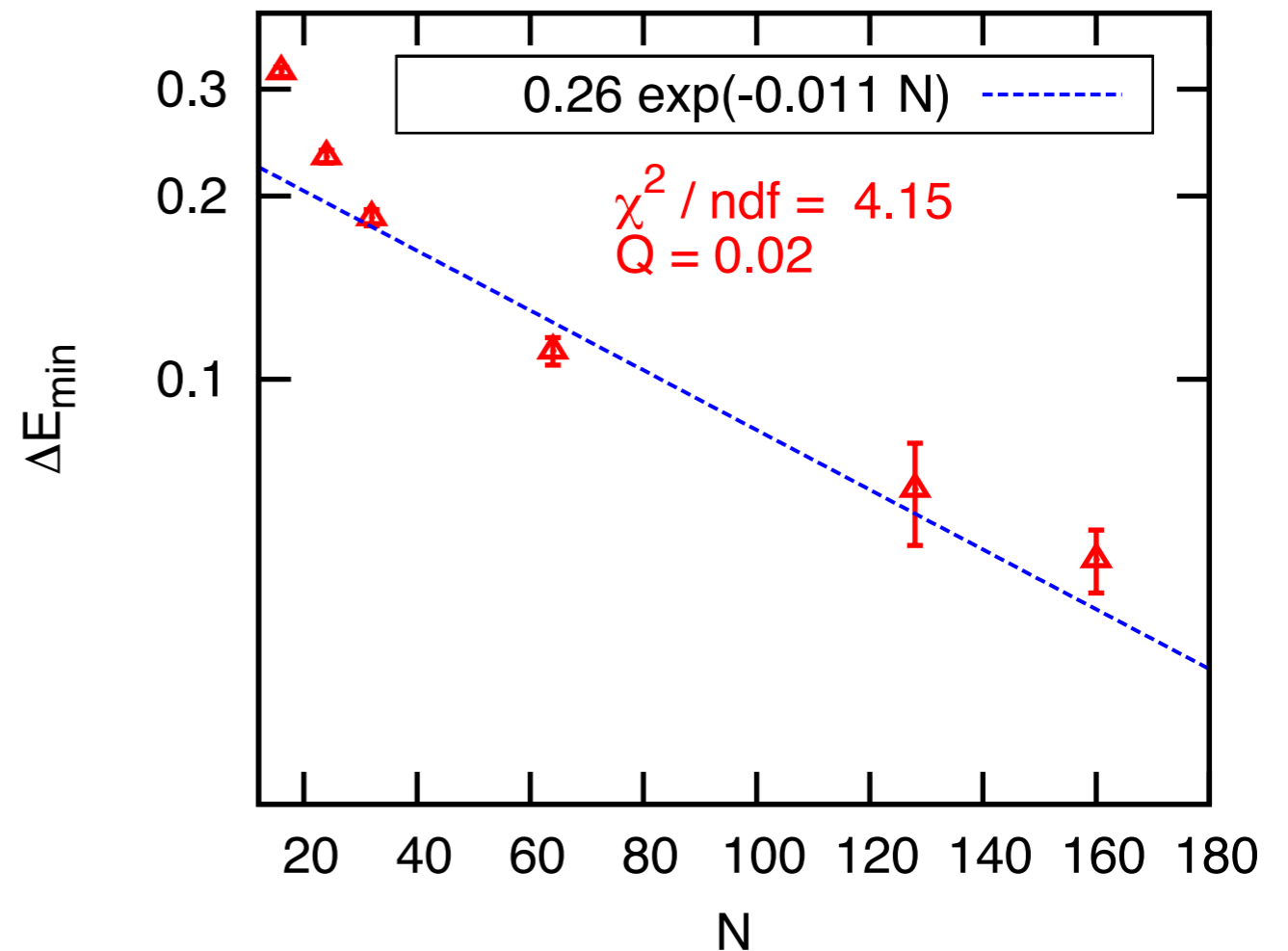
Median minimum gap near $s = 0.36$ (the quantum critical point)

3-reg MAX-2-XORSAT (near 0.36)



Power-law fit

3-reg MAX-2-XORSAT (near 0.36)



Exponential fit omitting 1st 2 points

The data close to the critical point seems to be **power-law**, at least for this range of sizes.

Conclusions

- Simple application of QAA gives exponentially small gaps for SAT problems with a USA.
- An optimization problem, MAX-2-SAT, seems to have polynomial gaps near the quantum critical point, but exponentially small gaps at larger s (in the spin glass phase)
- Need to see if the exponentially small gap can be removed by
 - repeatedly running the algorithm with different random values for the transverse fields (and costs).
 - trying to find a clever way to optimize the path in Hamiltonian space “on the fly” during the simulation to increase the minimum gap.
 - considering random instances rather than instances with a USA.