

The Quantum Adiabatic Algorithm

A.P. Young

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



SANTA CRUZ

Work supported by



National Science Foundation
WHERE DISCOVERIES BEGIN

Talk at SMQS-IP2011, Jülich, October 18, 2011

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Collaborators:

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Collaborators: See also poster by I. Hen and [arXiv:1109.6872](https://arxiv.org/abs/1109.6872)
V. Smelyanskiy, S. Knysh, I. Hen, E. Farhi, D. Gosset, A. Sandvik, M. Guidetti

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

- The **Quantum Adiabatic Algorithm** (QAA)
- The **Quantum Monte Carlo Method** (QMC)
- The Models Studied
- Results
- Comparison with a classical algorithm (**WALKSAT**)
- Conclusions

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 ?

Early Numerics

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

But possible “crossover” to exponential at larger sizes?

Need techniques from statistical physics, **Monte Carlo**.

Quantum Phase Transition

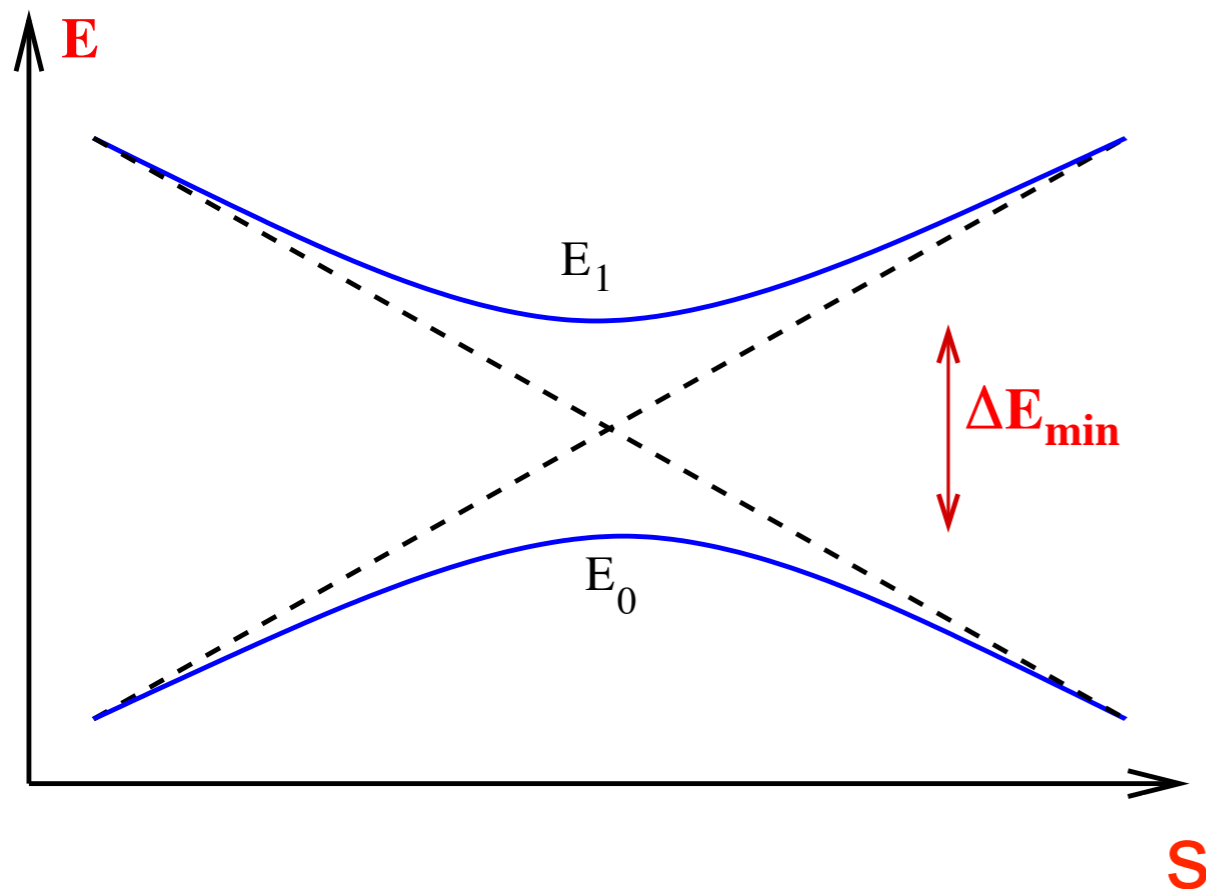


Bottleneck is likely to be a quantum phase transition (QPT) where the gap to the first excited state is very small

Quantum Phase Transition



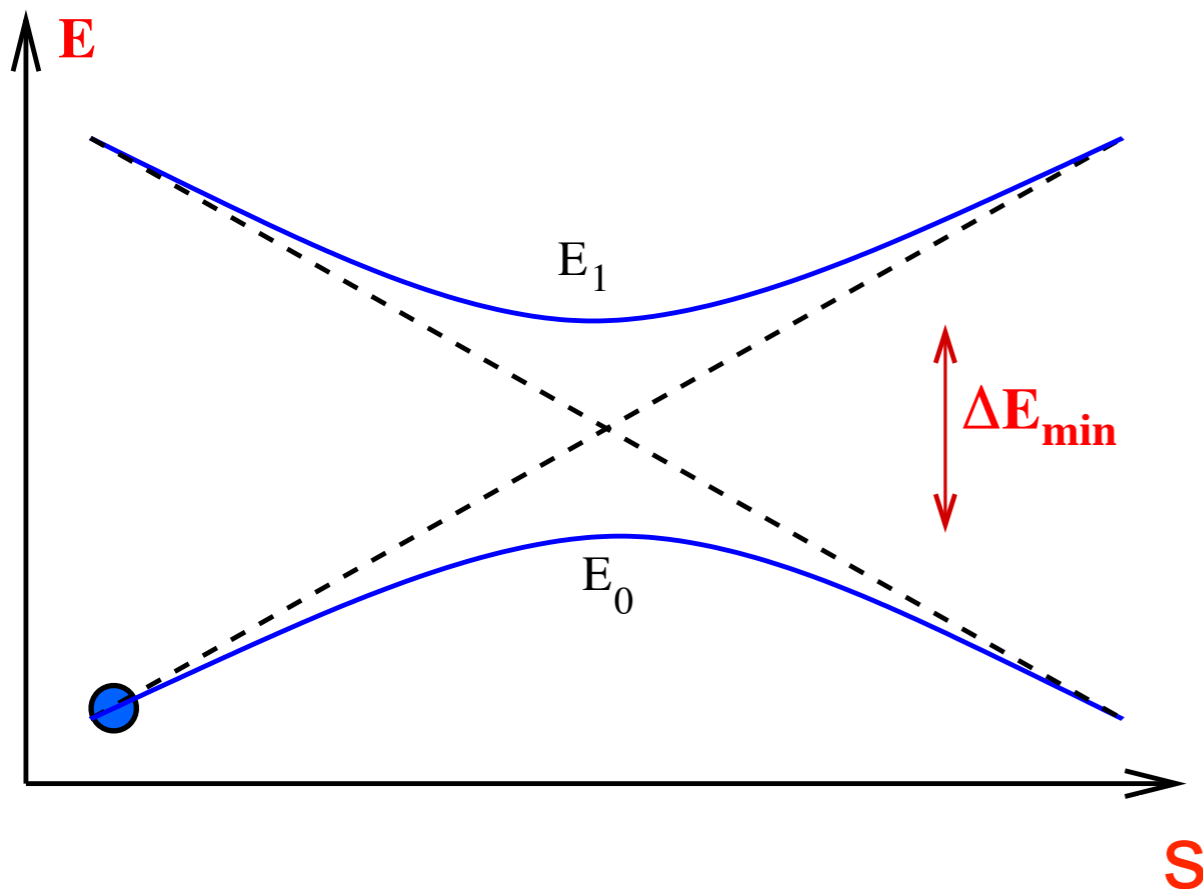
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Quantum Phase Transition



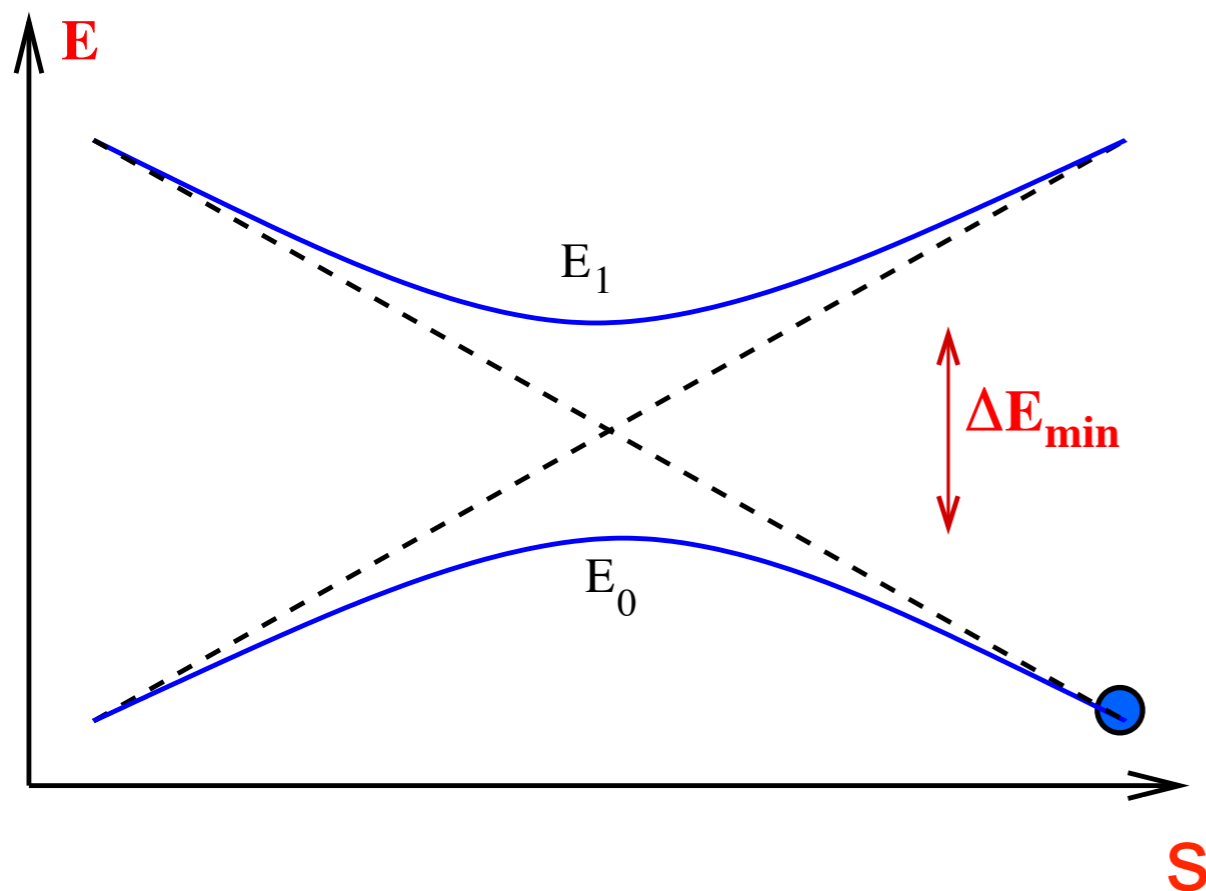
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Quantum Phase Transition



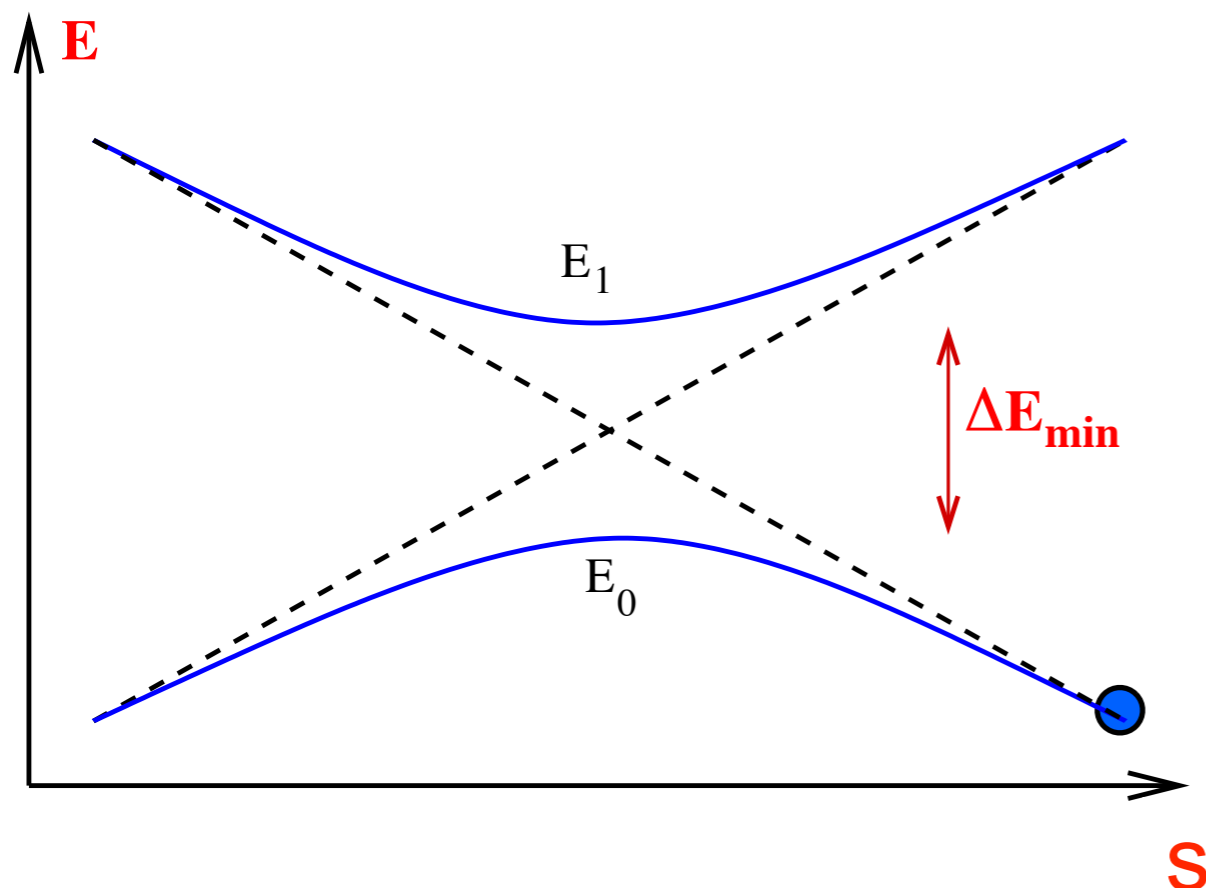
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Quantum Phase Transition



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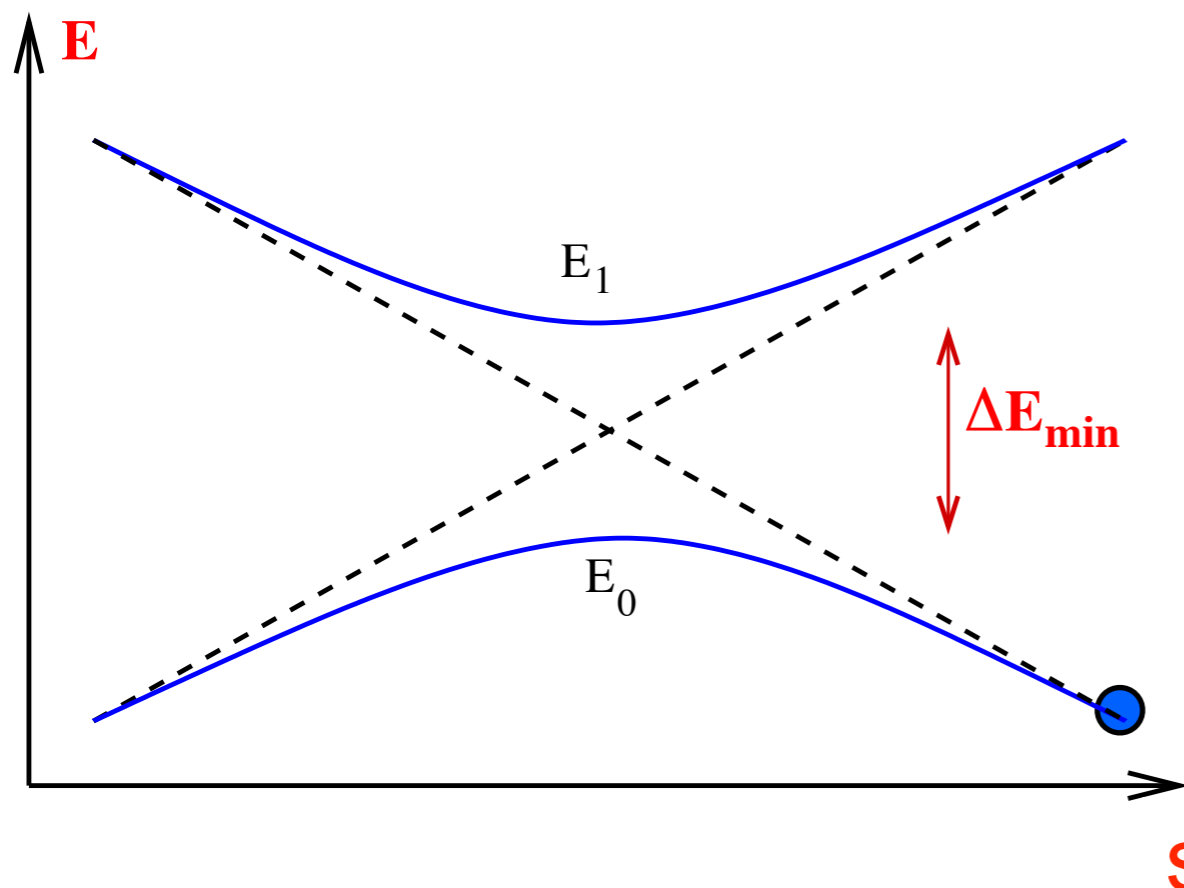


Landau Zener Theory:
To stay in the ground state the time needed is proportional to ΔE_{\min}^{-2}

Quantum Phase Transition



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 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.

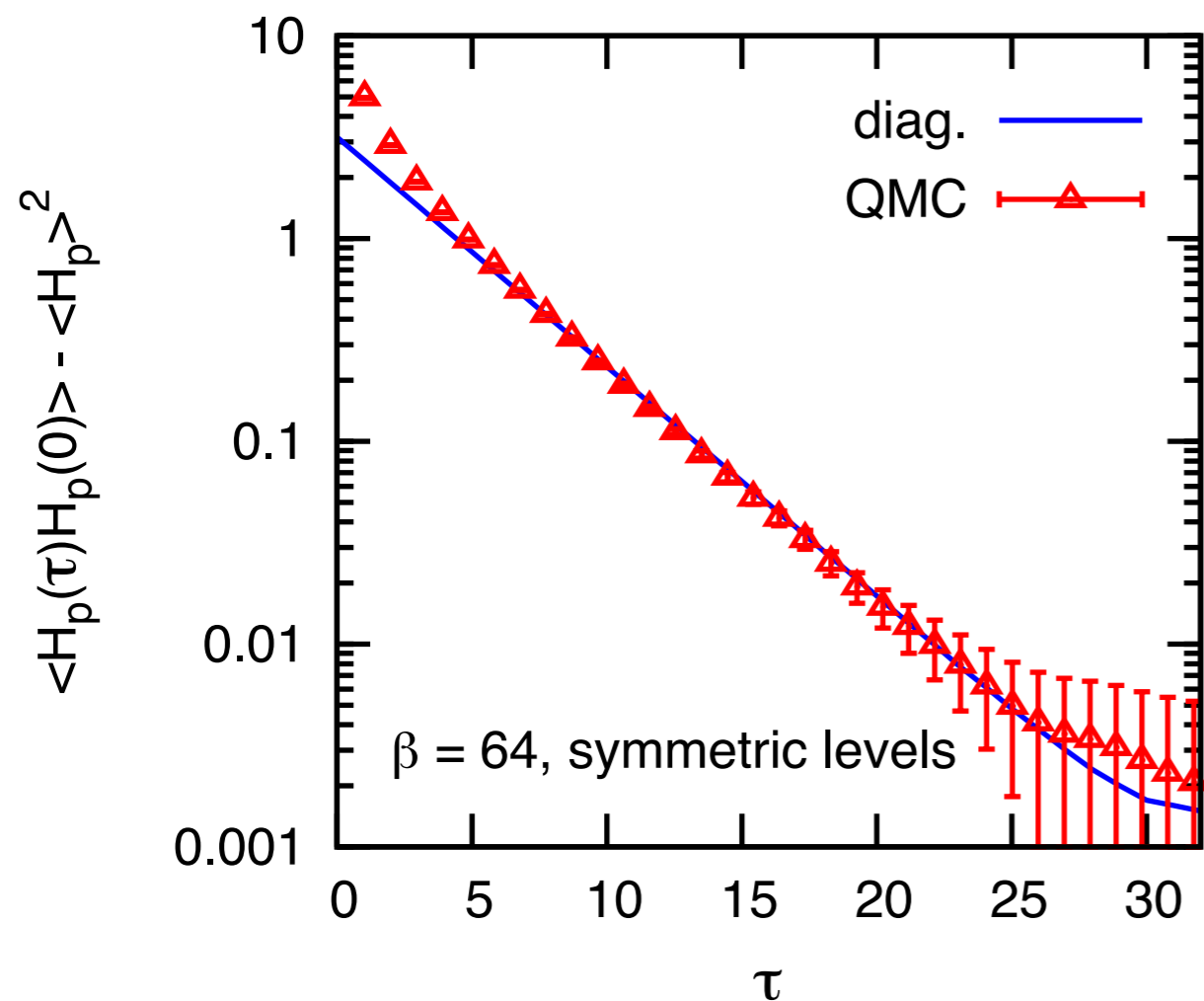
Examples of results with the SSE code

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

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

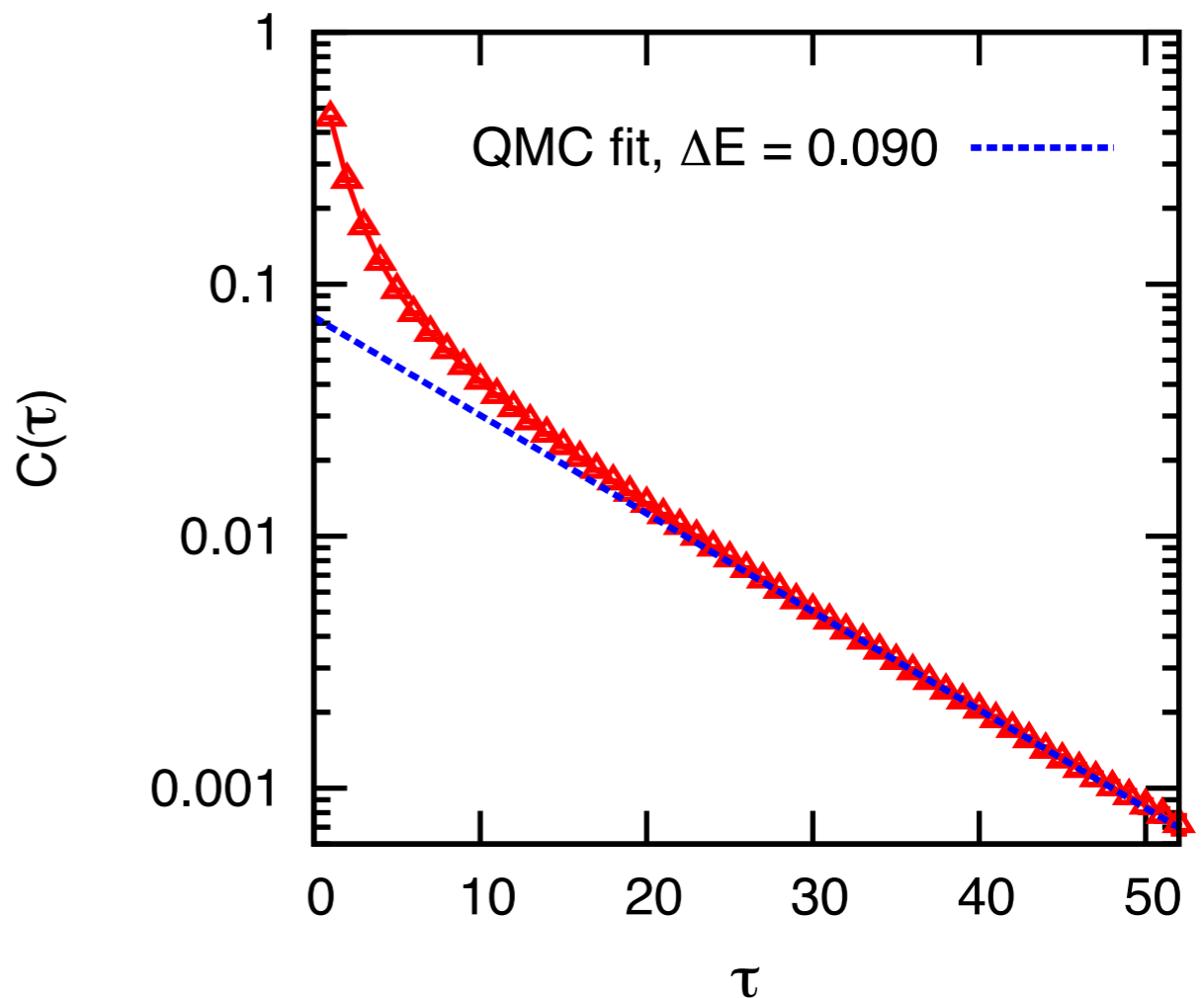
For **large τ** only first excited state contributes, \rightarrow **pure exponential decay**

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)**.

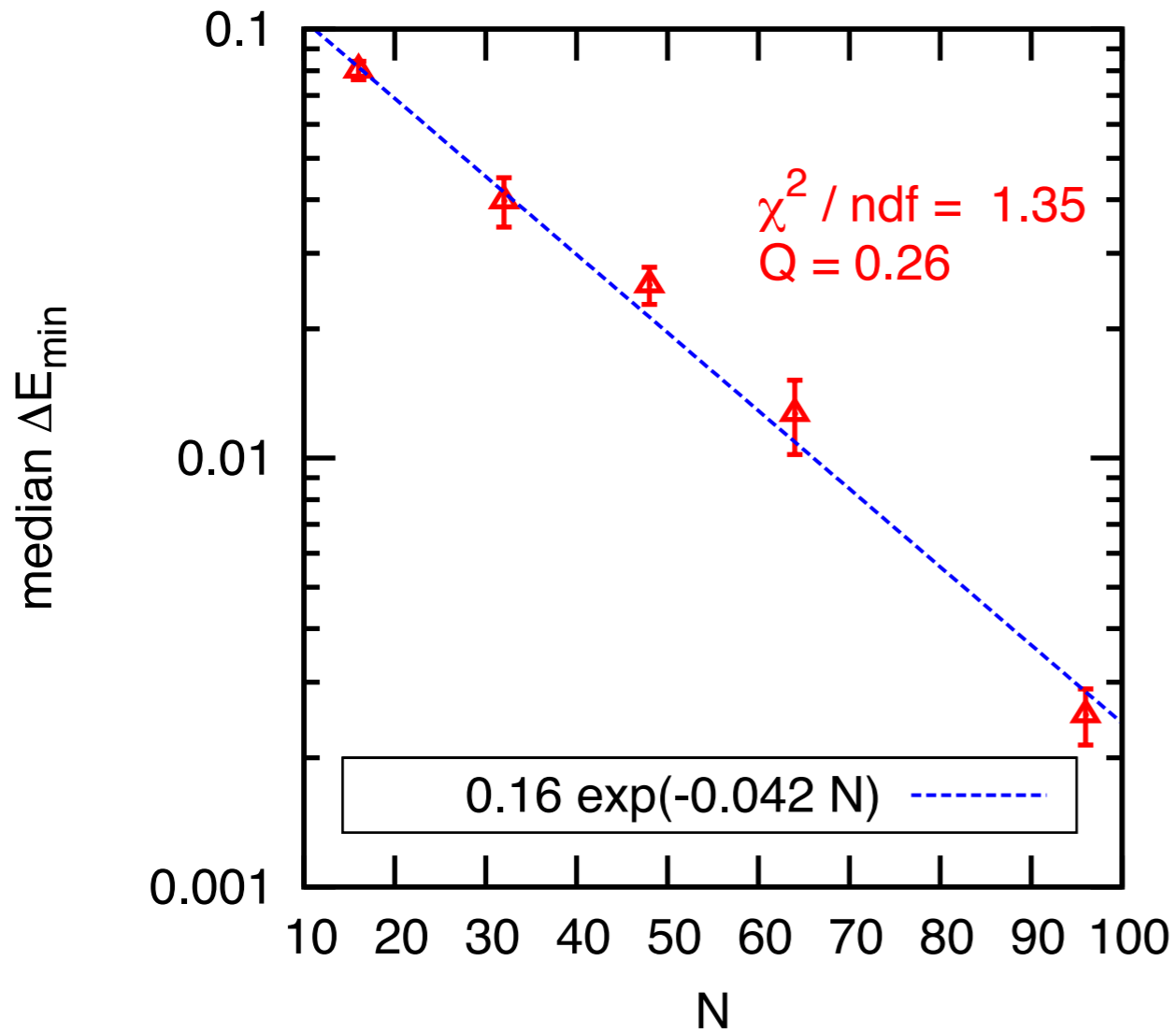
$$\mathcal{H}_P = \sum_{\alpha=1}^M \frac{1}{2} \left(1 - J_{\alpha} \sigma_{\alpha,1}^z \sigma_{\alpha,2}^z \sigma_{\alpha,3}^z \right)$$

(Is at SAT threshold.)

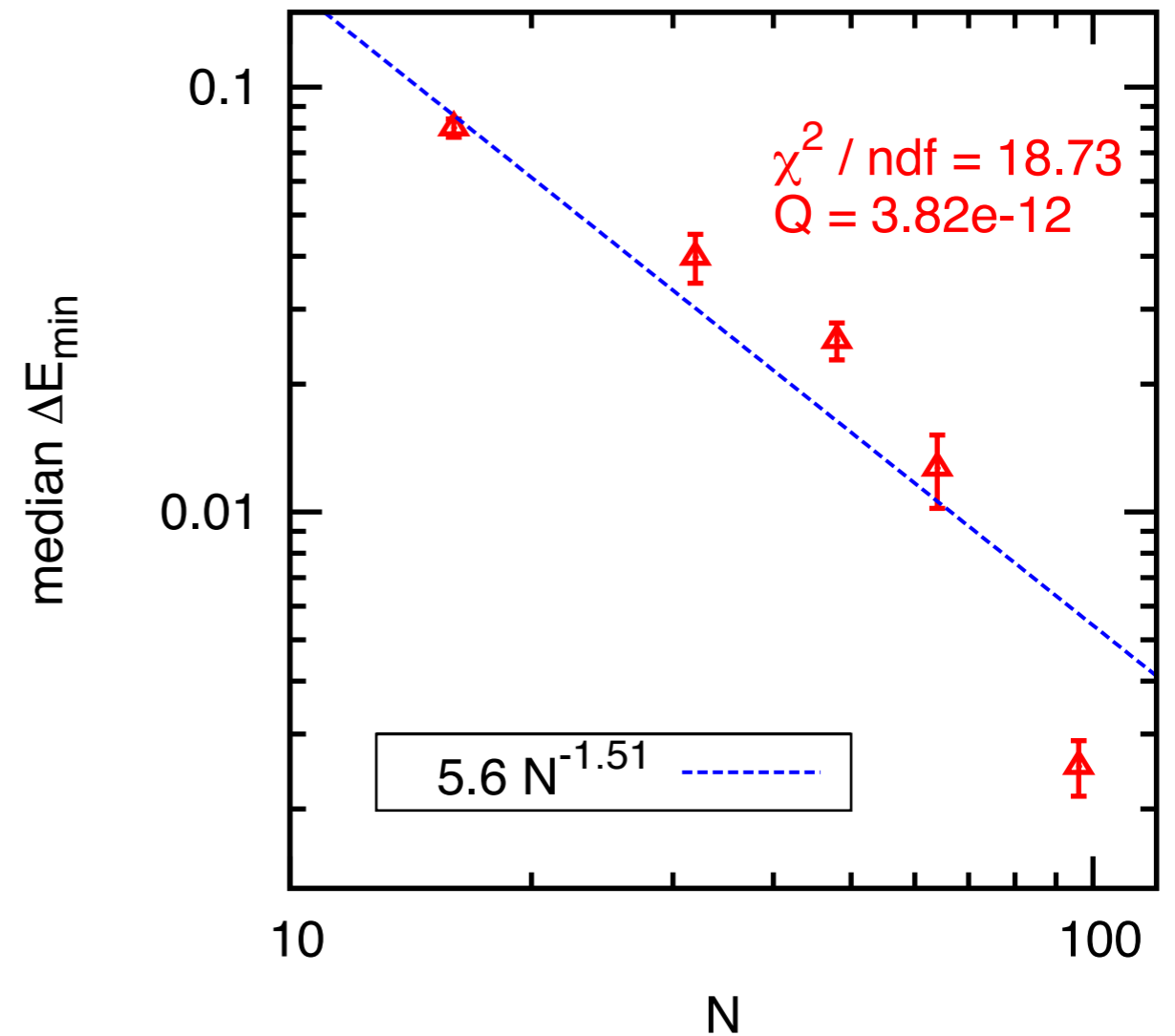
This SAT problem can be solved by linear algebra (**Gaussian elimination**) **and so is in P**. Nonetheless we will see that it is **very hard** for heuristic algorithms (quantum and classical).

Locked 1-in-3

Plots of the median minimum gap



Exponential fit

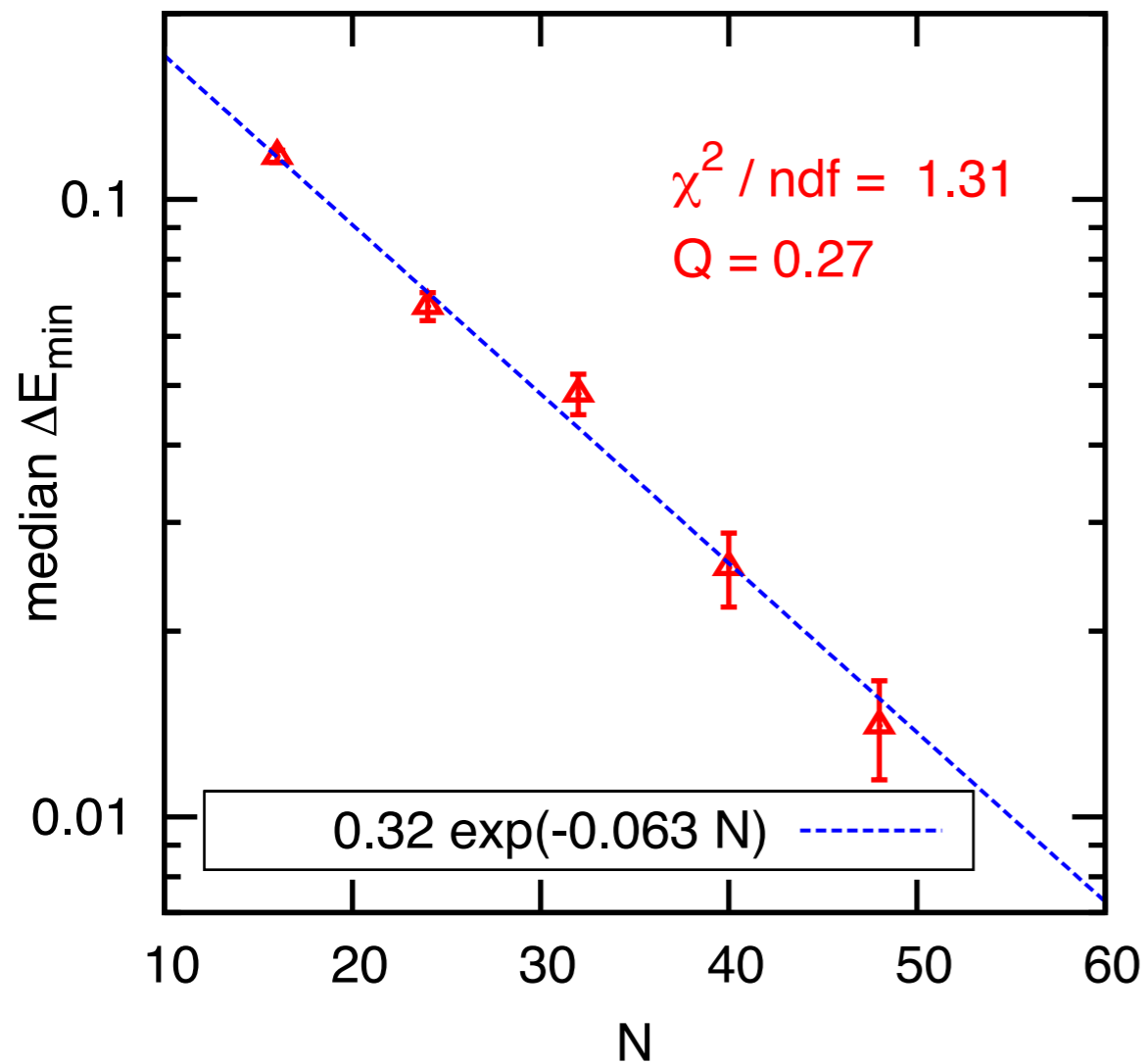


Power law fit

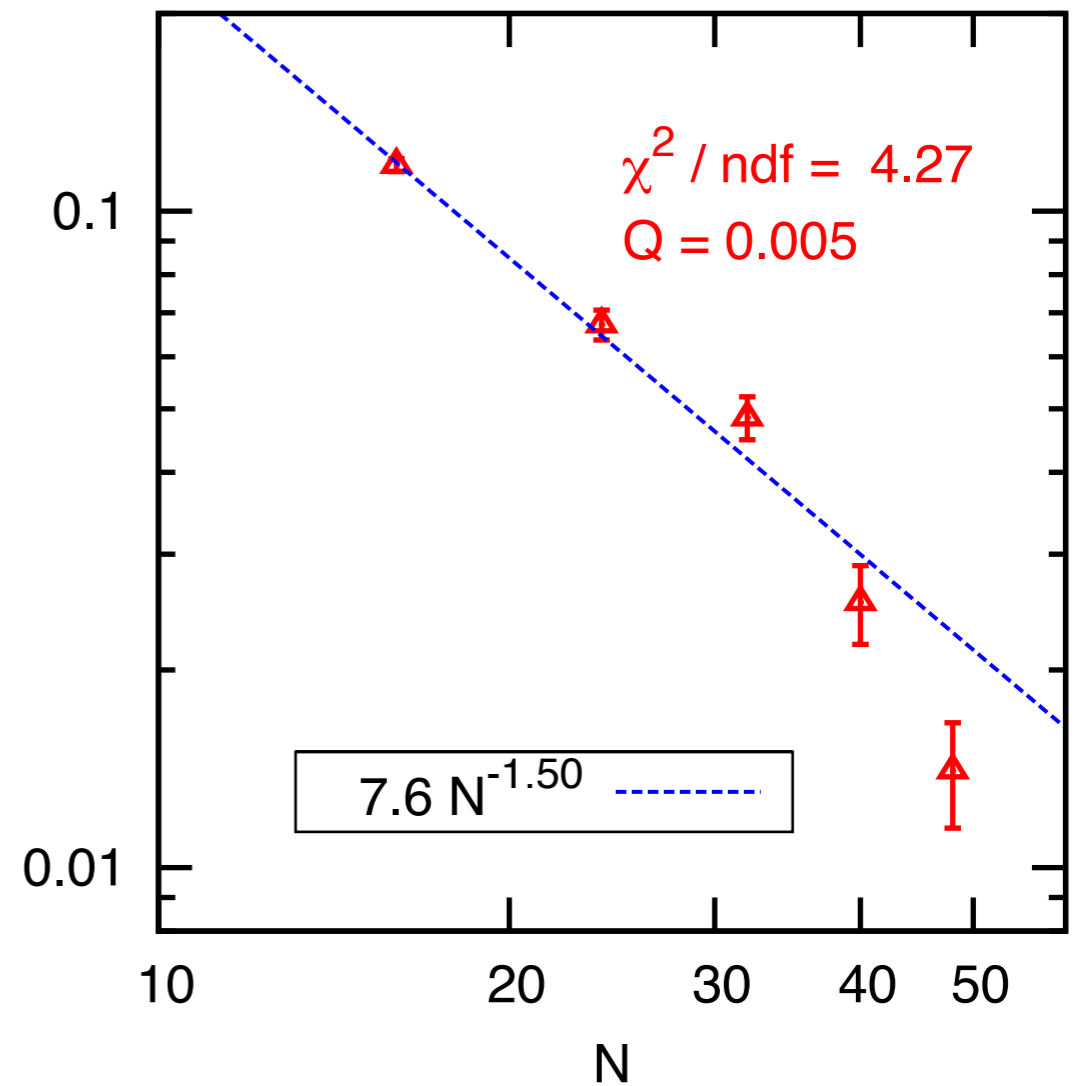
Clearly the behavior of the minimum gap is exponential

Locked 2-in-4

Plots of the median minimum gap



Exponential fit

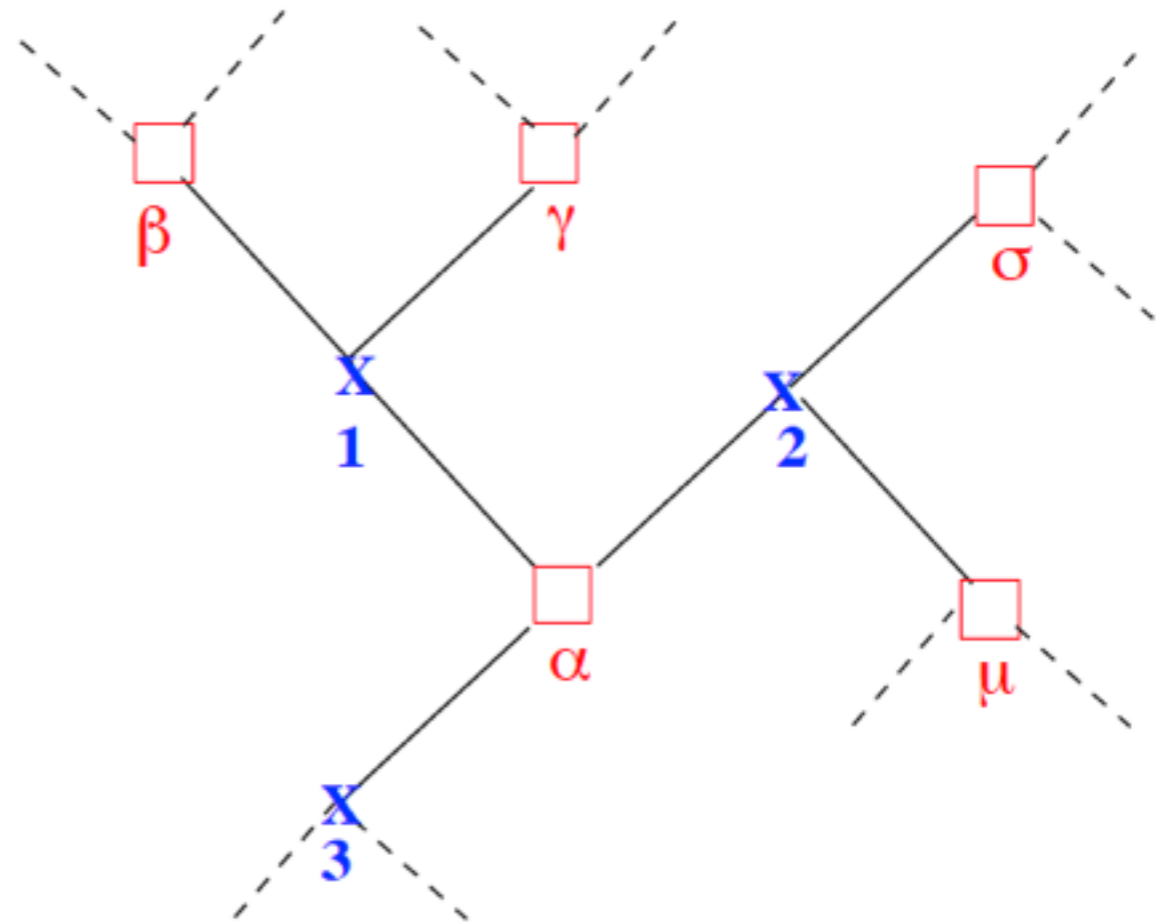
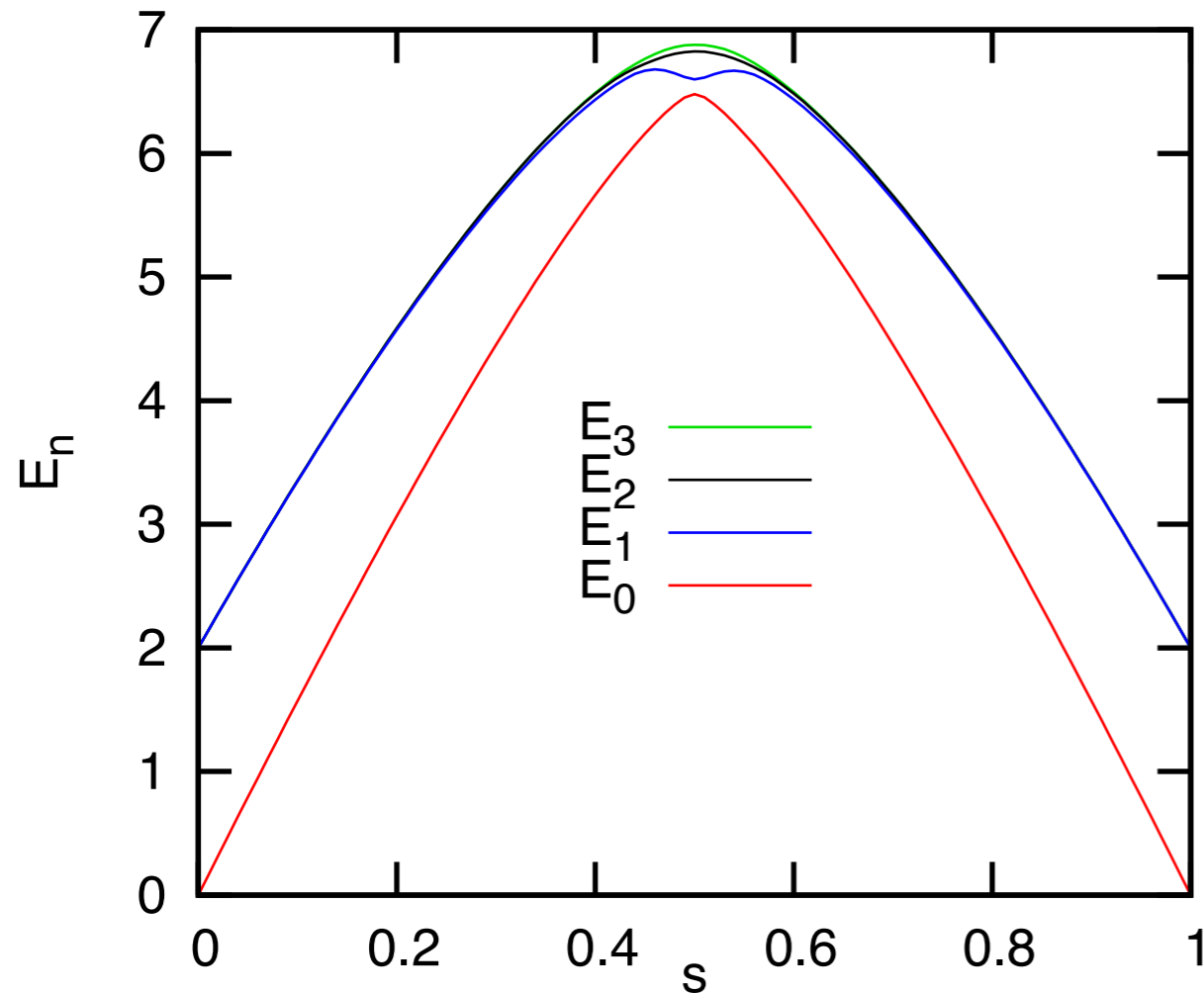


Power law fit

The exponential fit is much better. Will improve the data to confirm the exponential behavior.

3-Reg 3-XORSAT (3-spin model): I

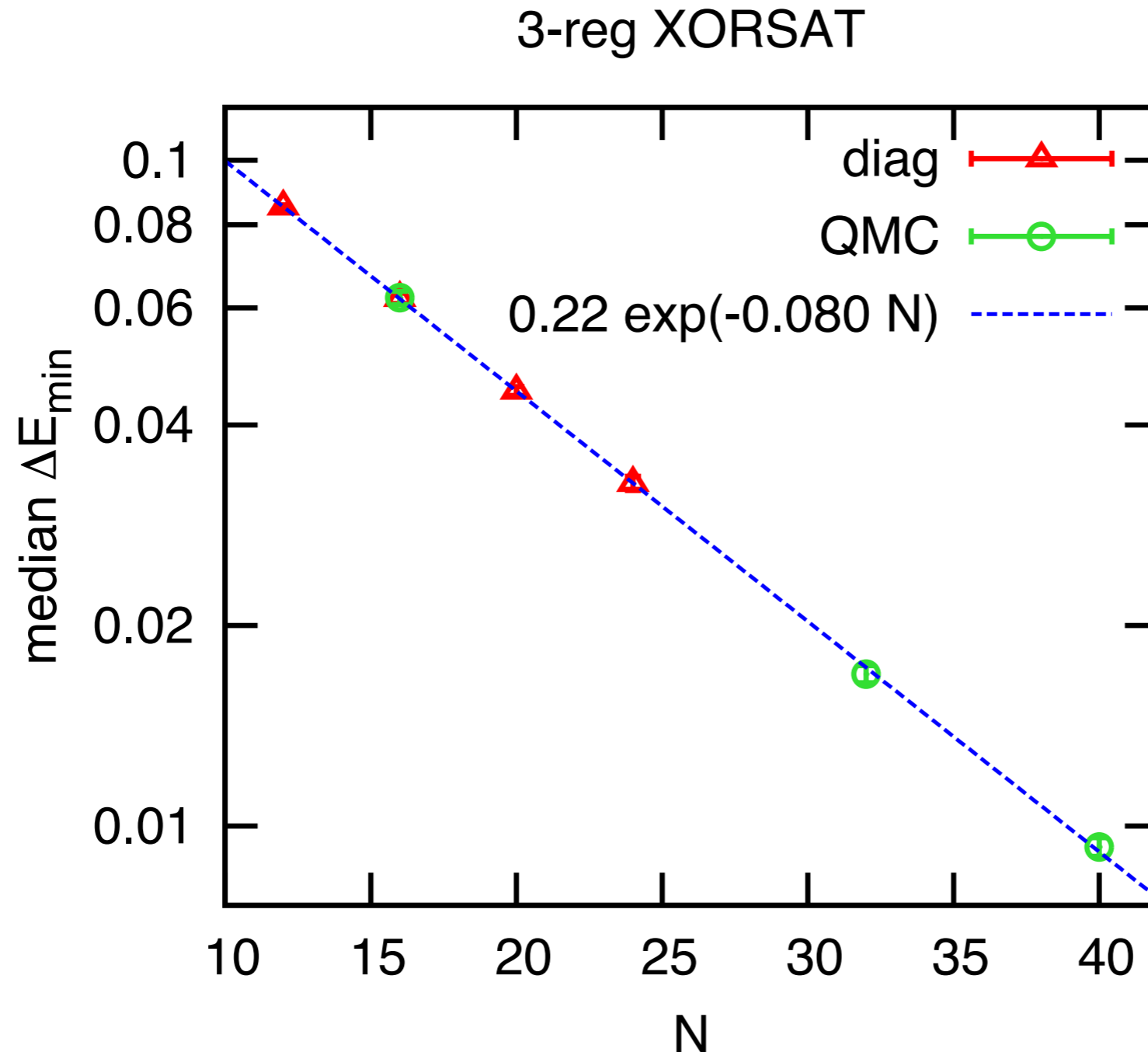
3-reg XORSAT (1 instance, N = 16)



Curves for energies on left are very close to symmetric about $s = 1/2$. There is an **exact duality** $\mathcal{H}(s) = \mathcal{H}^{\text{Dual}}(1 - s)$ where the dual lattice interchanges the clauses and bits (i.e. is a different member of the ensemble), see the “**factor graph**” above right. Hence the phase transition is **exactly** at the **self dual point** $s=1/2$.

3-Reg 3-XORSAT: II

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).

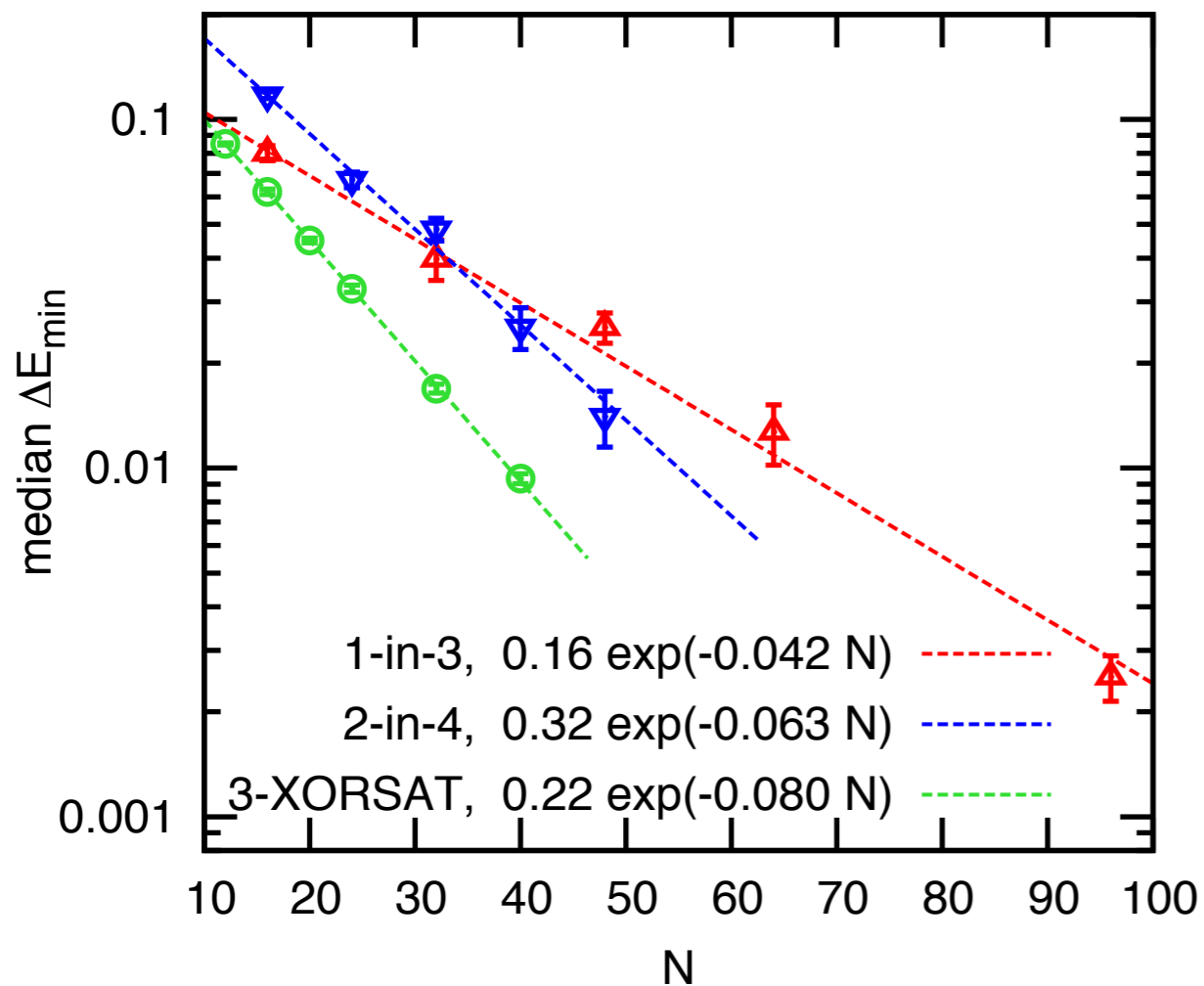
For WalkSAT the running time is proportional to number of “**bit flips**”.

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

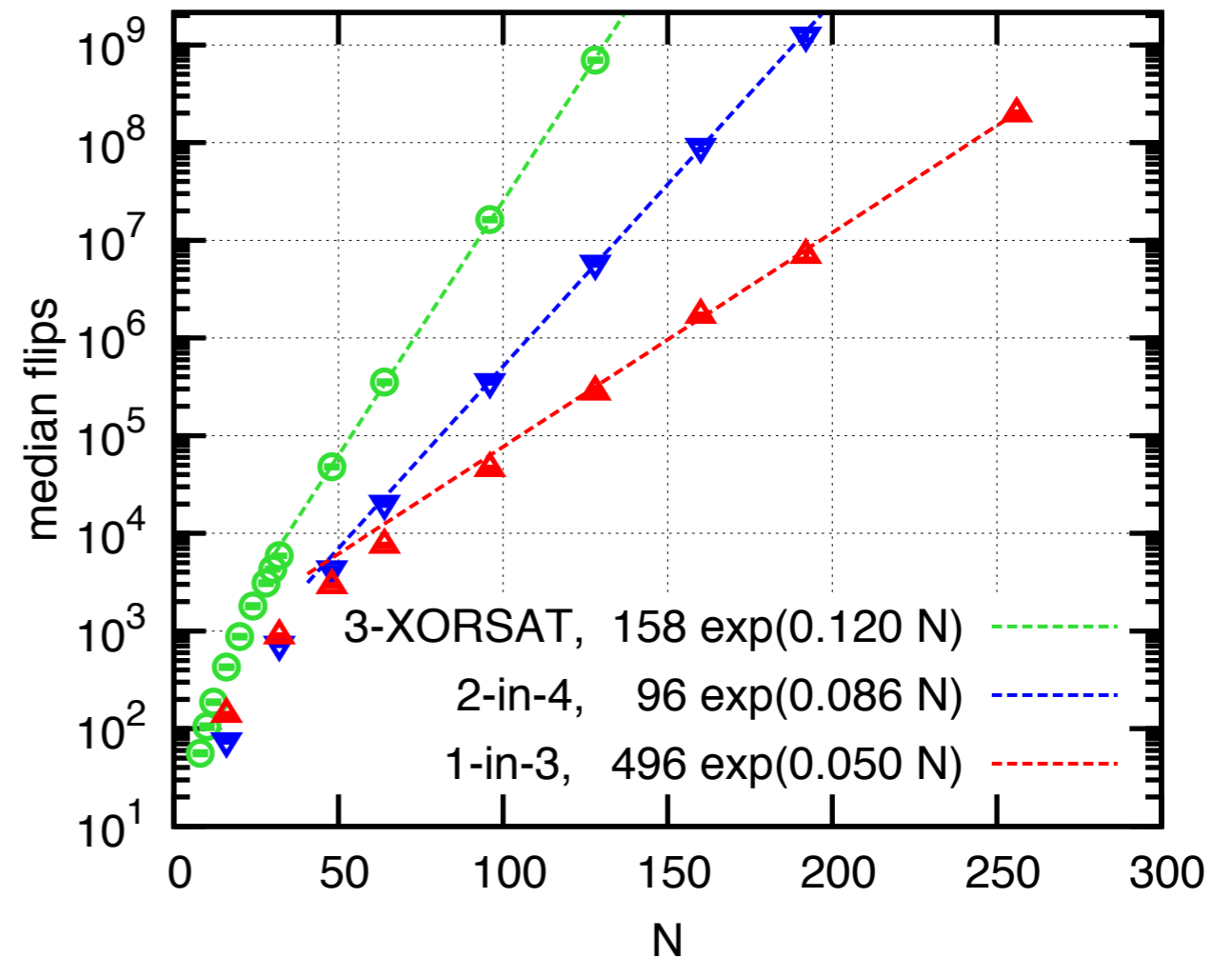
We will compare the values of μ among the different models and between QAA and WalkSAT.

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

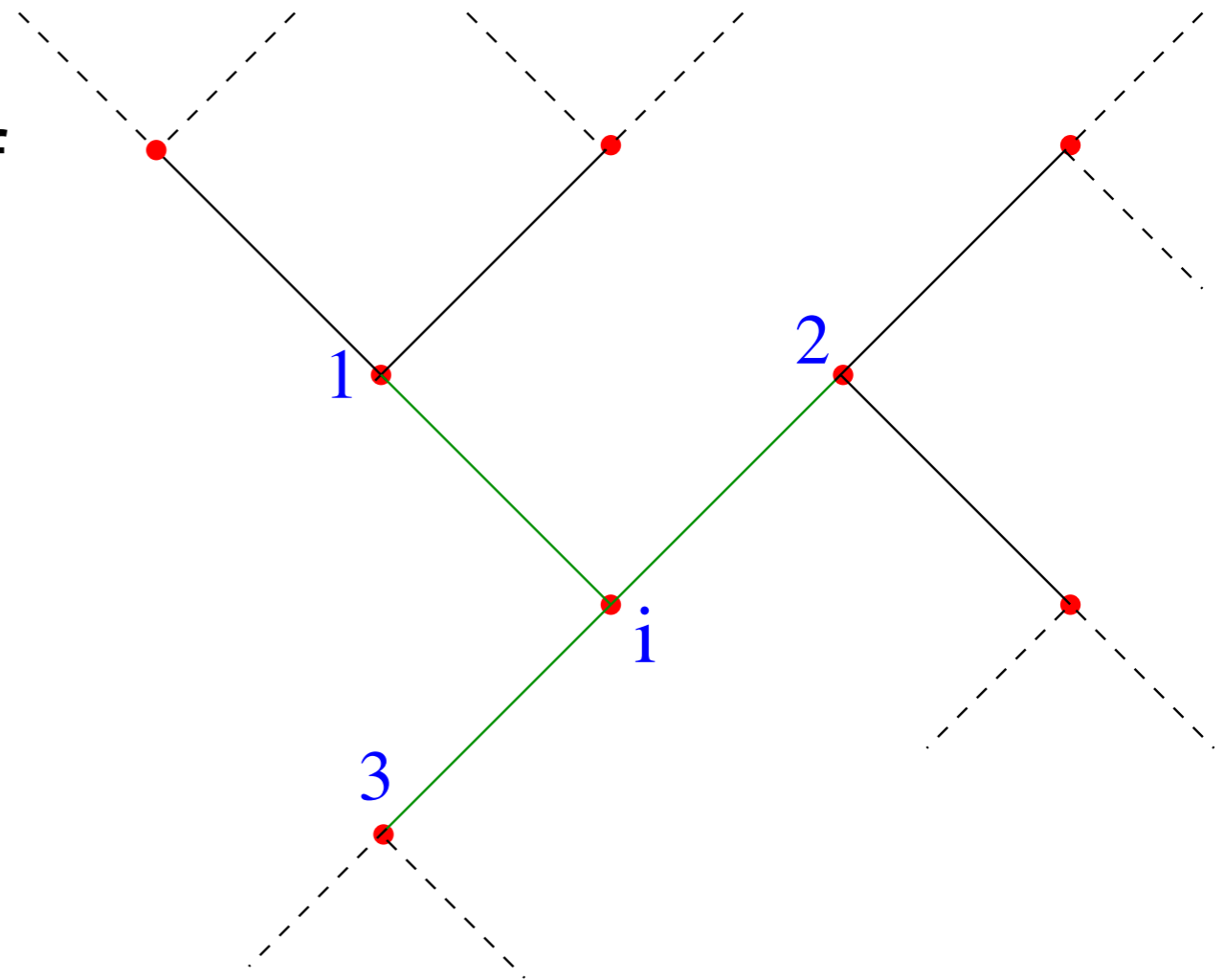
We have also studied one “MAX” (i.e. optimization) problem.

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**.

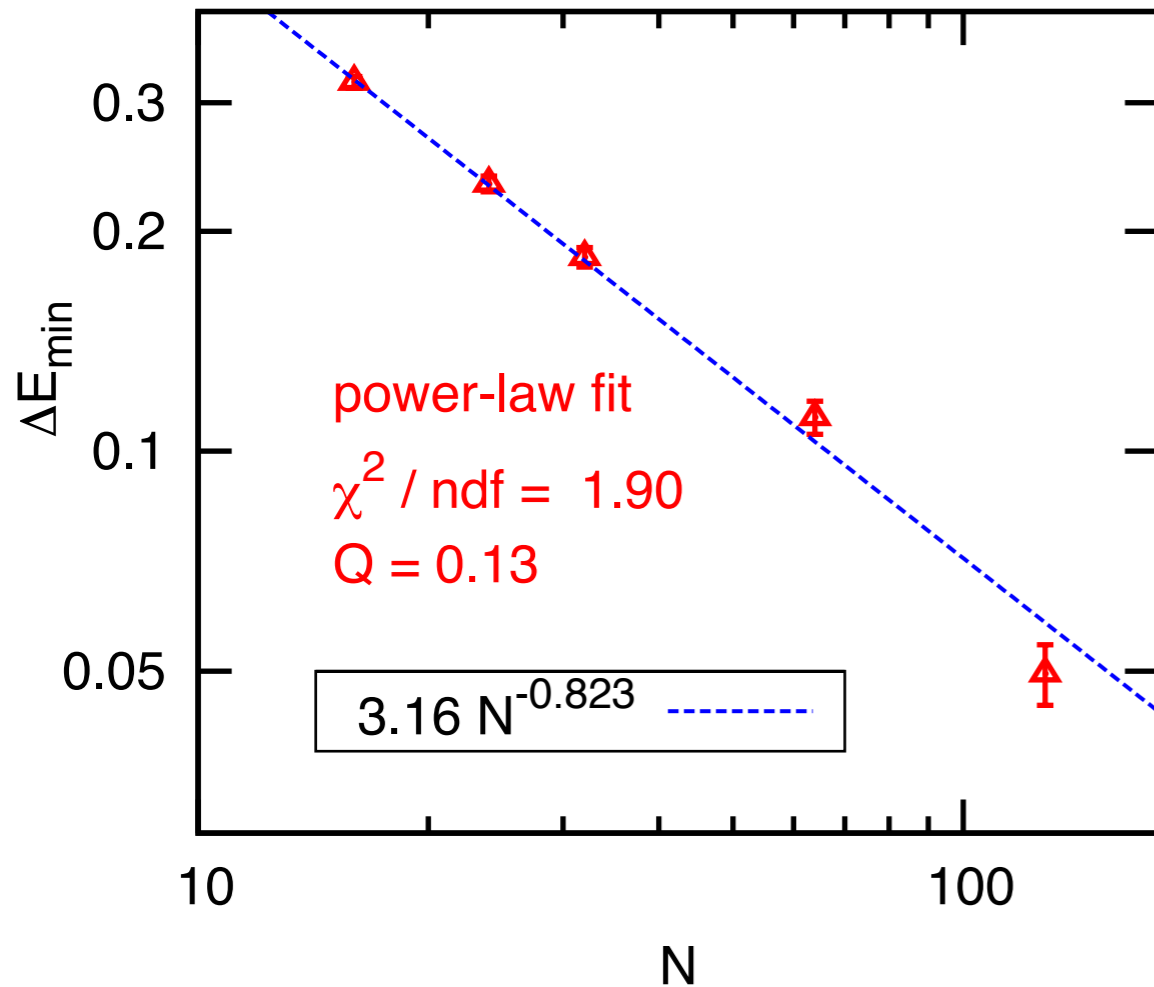
“Cavity” calculations (Gosset) find $s^* \cong 0.36$

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

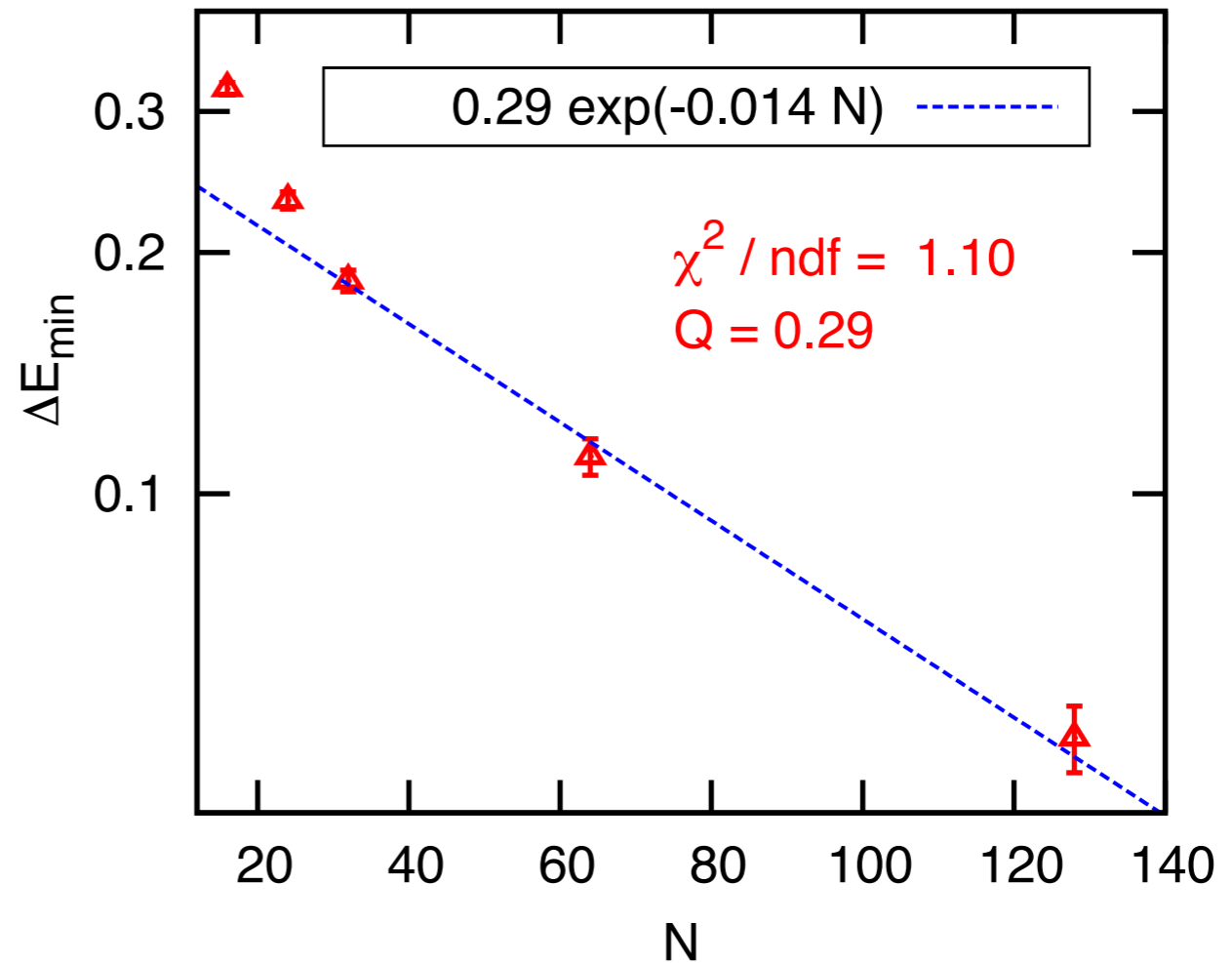
Median minimum gap in the vicinity of the quantum transition

3-reg MAX-2-XORSAT



Power-law fit

3-reg MAX-2-XORSAT



Exponential fit omitting 1st 2 points

Looks like power law, but exponential (plus corrections at small sizes) can't be excluded. Larger sizes will be done to check.

Conclusions

- Simple application of QAA gives exponentially small gaps for SAT problems with a USA.
(same conclusion as in the talk by Thomas Neuhaus).
- An optimization problem, MAX-2-SAT, looks more promising, but needs data at larger sizes to be sure.
- 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.