Quantum annealing in imaginary time

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C. De Grandi, A. Polkovnikov, A.W. Sandvik, PRB 84, 224303 (2011)
C.-W. Liu, A. Polkovnikov, A.W. Sandvik, PRB 87, 174302 (2013)
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C.-W. Liu, A. Polkovnikov, A.W. Sandvik, PRL 114, 147203 (2015)

Outline

Introduction

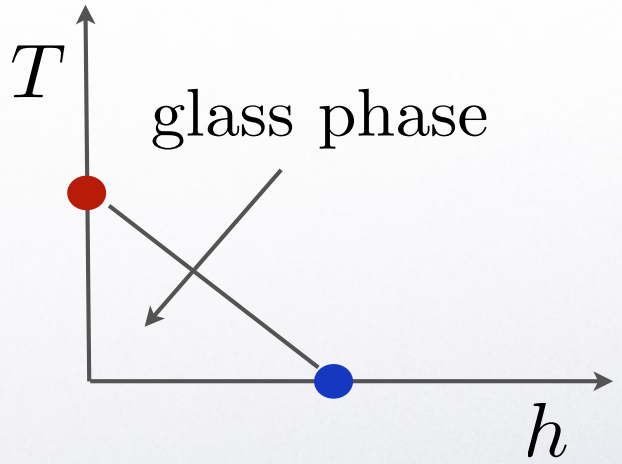
- Quantum annealing for quantum computing/optimization
- Transverse-field Ising model, quantum phase transition

Quantum dynamics in real and imaginary time

- Exact numerical solutions for small systems
- Dynamical quantum Monte Carlo in imaginary time

Dynamic scaling at phase transitions

- Kibble-Zurek velocity scaling
- Demonstration for classical Ising model



Quantum spin glass transition

- Imaginary-time QMC and KZ scaling
- Implications for quantum computing

[Going all the way to the classical spin-glass ground state]

- Scaling of success probability in real and imaginary time
- Problem hardness in real and imaginary time

Thermal and Quantum Annealing

Simulated (Thermal) Annealing

Reduce T as a function of time in a Monte Carlo simulation
- efficient way to equilibrate a simulation
- powerful as optimization algorithm

Quantum Annealing

Reduce quantum fluctuations as a function of time
- start with simple quantum system H_0 (s=0):
- end with a complicated classical potential H_1 (s=1)

$$H(s) = (1-s)H_0 + sH_1 \qquad [H_0, H_1] \neq 0$$

$$s = s(t) = vt, \quad v = 1/t_{\max}$$

Adiabatic Theorem:

For small v, the system stays in the ground state of H[s(t)]

Can quantum annealing be more efficient than thermal annealing?

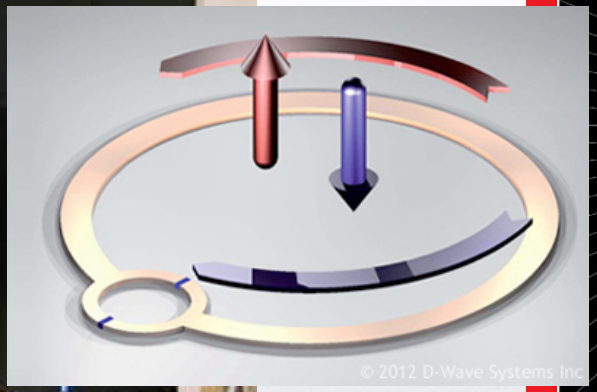
Kadowaki, Nishimory (PRE 1998), Farhi et a (Science 2002),….

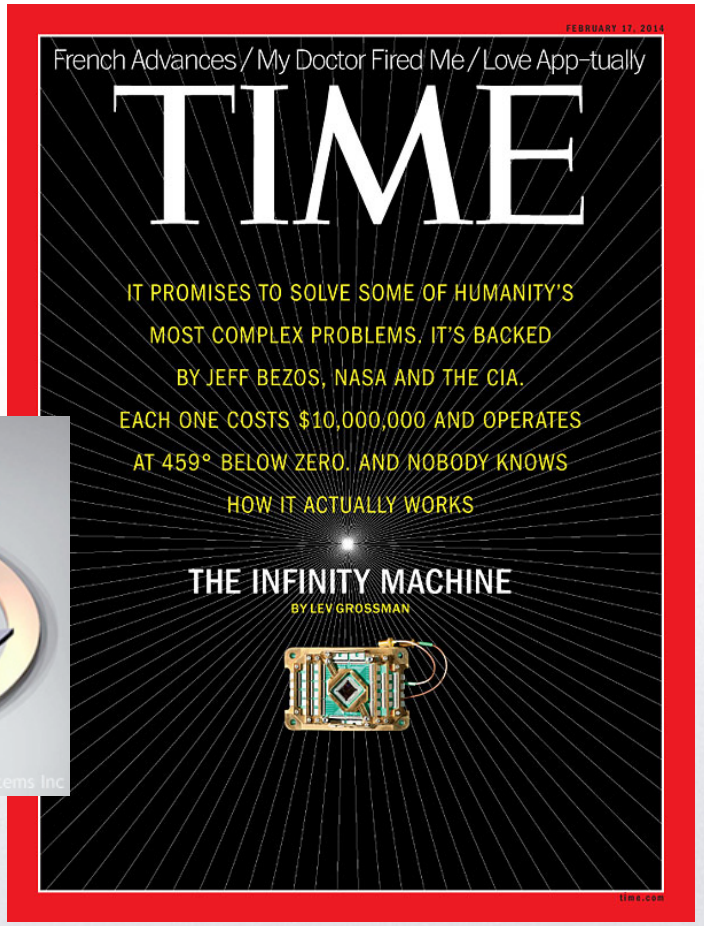
Useful paradigm for quantum computing?

Quantum Annealing & Quantum Computing

The D-wave "quantum annealer"; ~1000 flux qubits

- Claimed to solve some hard optimization problems
- Is it really doing quantum annealing?
- **Is quantum annealing really better than simulated annealing (on a classical computer)?**





Hamiltonian implemented in D-wave quantum annealer....

Hamiltonian of the D-Wave Device

Solves optimization problems mapped onto frustrated Ising model

$$H_1 = \sum_{i=1}^{N}\sum_{j=1}^{N} J_{ij}\sigma_i^z\sigma_j^z, \quad \sigma_i^z \in \{-1,+1\}$$

Interactions J_{ij} are programmable
- restricted to "Chimera lattice"

$$H_0 = -\sum_{i=1}^{N}\sigma_i^x = -\sum_{i=1}^{N}(\sigma_i^+ + \sigma_i^-)$$

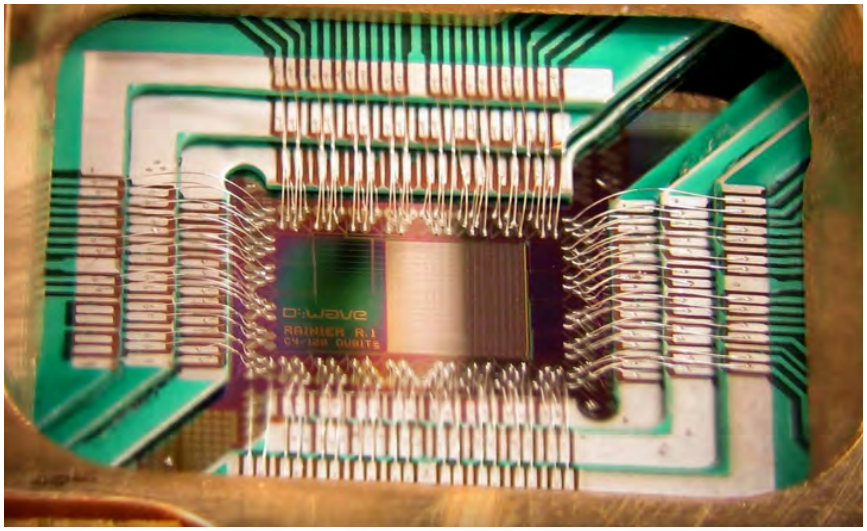
$$[H_0, H_1] \neq 0$$

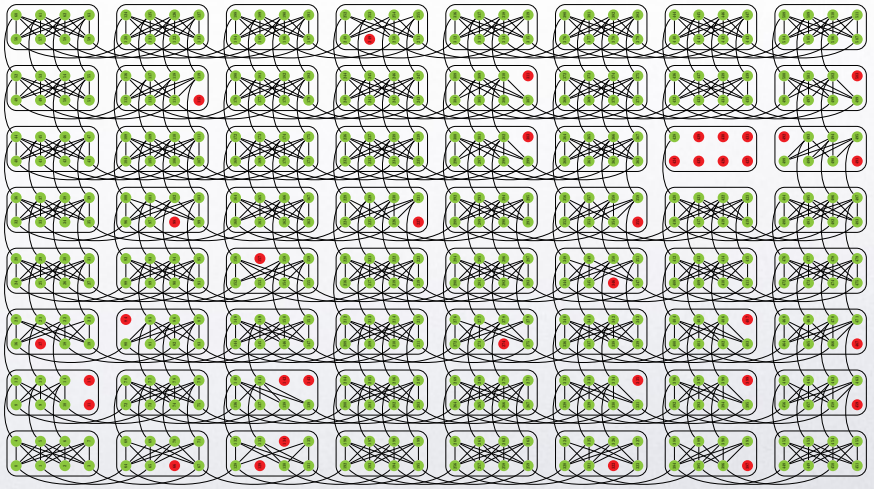
Tune the strength of the field

$$H(s) = (1-s)H_0 + sH_1$$

$$s = s(t) = vt, \quad v = 1/t_{\max}$$

adiabatically from s=0 to s=1





D-wave Chimera-lattice setup, picture from Martin-Mayor & Hen, arXiv:1502.02494

→ Studies of dynamics of transverse-field Ising models

Quantum Phase Transition

One can expect a quantum phase transition in the system

$$H(s) = (1-s)H_0 + sH_1 \qquad [H_0, H_1] \neq 0$$

Ground state changes qualitatively as s changes
- trivial (easy to prepare) for s=0
- complex (solution of hard optimization problem) at s=1

→ **expect a quantum phase transition at some $s=s_c$**

as in the clean transverse-field Ising ferromagnet

$$H(s) = -s\sum_{\langle ij\rangle}\sigma_i^z\sigma_{i+1}^z - (1-s)\sum_{i=1}^{N}\sigma_i^x \qquad (N\to\infty)$$

- trivial x-oriented ferromagnet at s=0 (→→→)
- z-oriented (↑↑↑ or ↓↓↓, symmetry broken) at s=1
- s_c=1/2 in 1D, appr. 0.25 in 2D

Have to pass through s_c and beyond adiabatically

How long does it take (versus problem size N)?

Quantum Dynamics

Time evolution

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle$$

Time evolution operator with time-dependent H

$$U(t,t_0) = T_t \exp\left[i\int_{t_0}^{t} dt' H[s(t')]\right]$$

Difficult to study numerically for a many-body system

- exact diagonalization of small systems
- DMRG/MPS/TEBD for 1D systems (moderate sizes and times)

Alternative approach:

Schrödinger dynamics in imaginary time $t=i\tau$

$$|\Psi(\tau)\rangle = U(\tau,\tau_0)|\Psi(\tau_0)\rangle \qquad U(\tau,\tau_0) = T_\tau \exp\left[-\int_{\tau_0}^{\tau} d\tau' H[s(\tau')]\right]$$

Can be implemented in Quantum Monte Carlo

De Grandi, Polkovnikov, Sandvik, PRB2011

What can imaginary time tell us about real-time dynamics?

Real and imaginary time quantum dynamics

Example: linear ramp of transverse-field Ising ferromagnet

$$H(s) = -s \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - (1-s) \sum_{i=1}^{N} \sigma_i^x \qquad s \in [0,1], \quad s = vt$$

2D square-lattice system; $N=L^2$

Start from eigenstate of H(s=0) at t=0

- Instantaneous ground state: $|\Psi_0(t)\rangle = |\Psi_0(s[t])\rangle$

- Actual state during evolution: $|\Psi(t)\rangle$

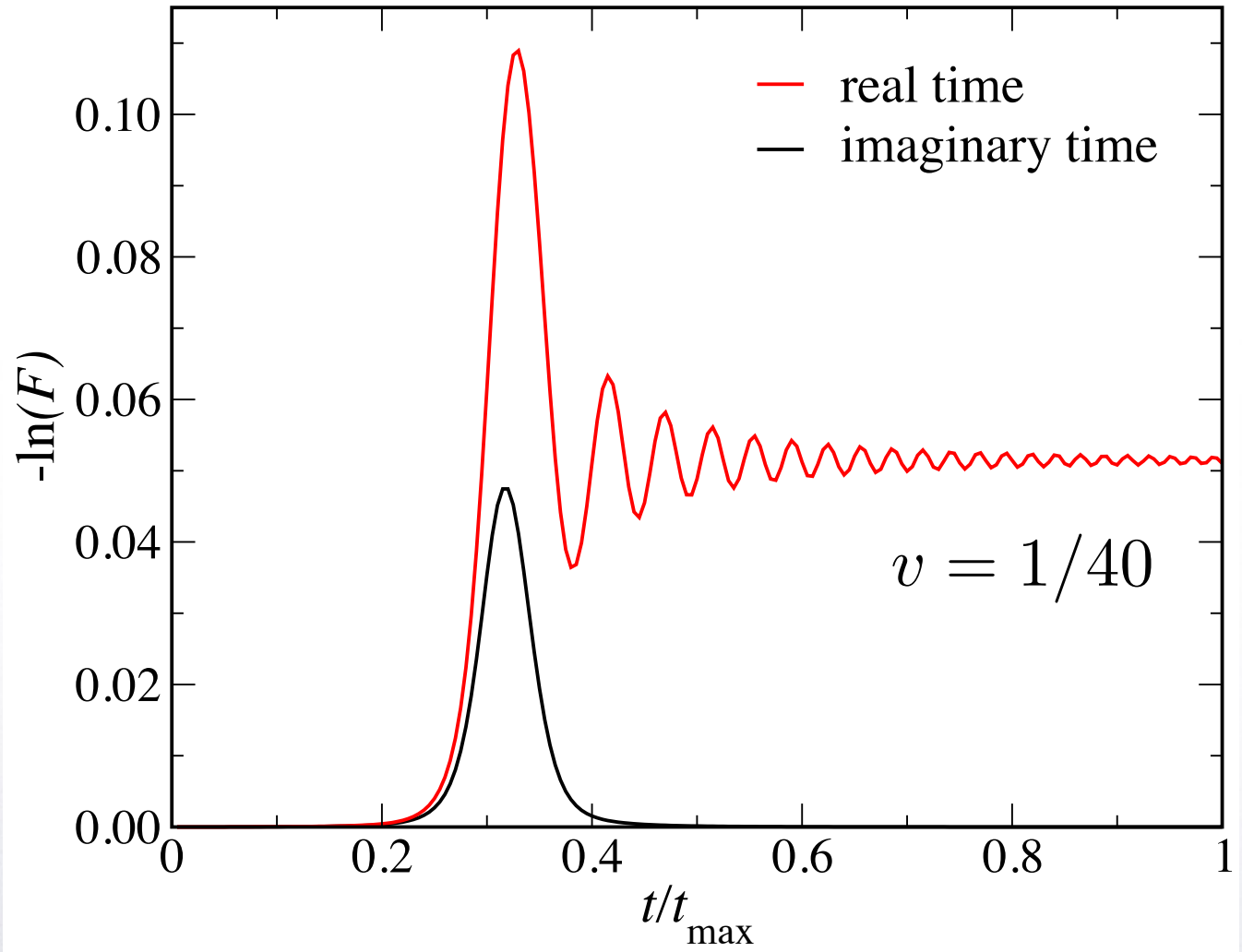
Distance between these states given by log-fidelity

$$-\ln[F(t)] = -\frac{1}{2} \ln\left(|\langle \Psi_0(t)|\Psi(t)\rangle|^2\right)$$

Integrate Schrödinger equation numerically for small L
- compare real and imaginary time

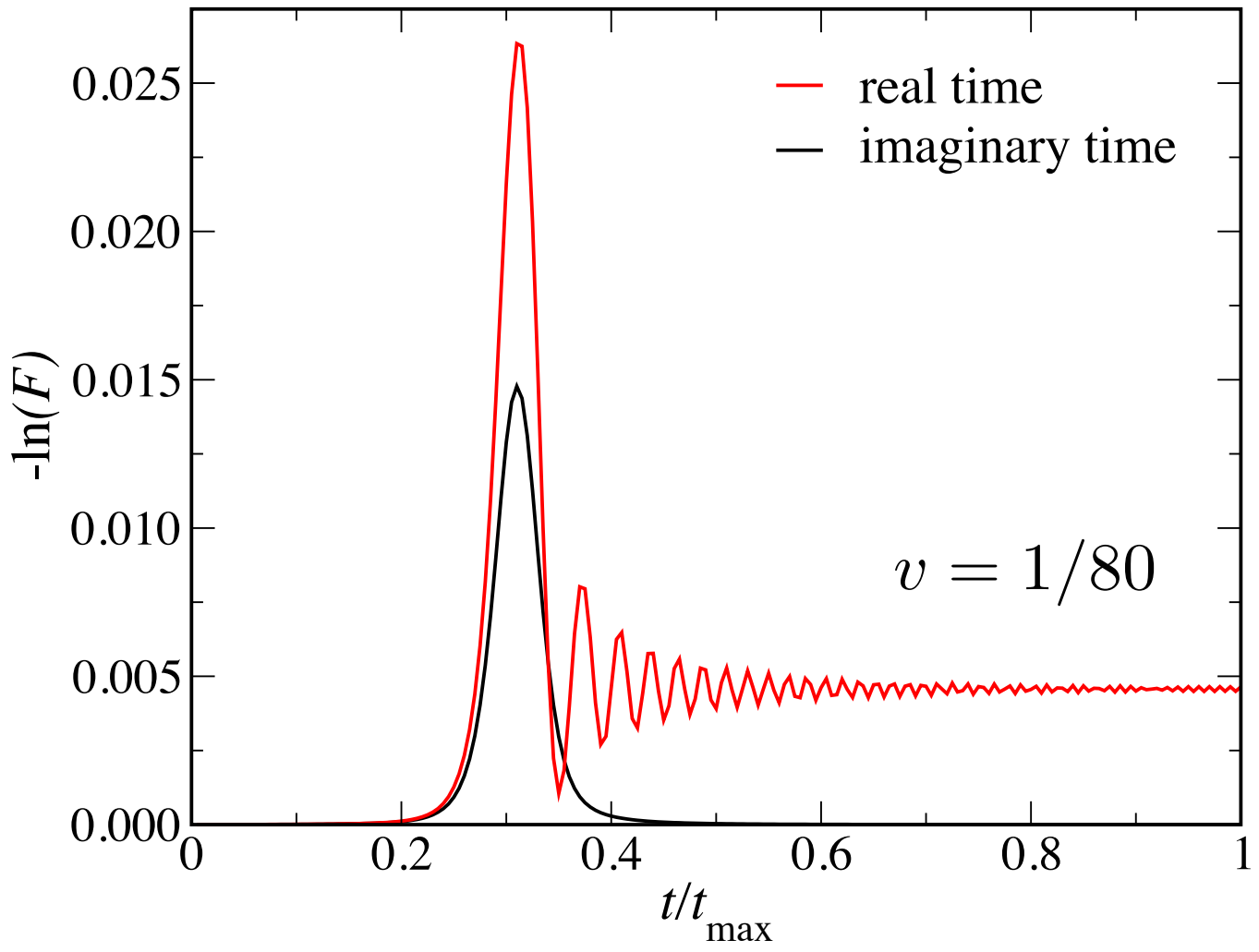
How different? Which one is more adiabatic?

Example: 4×4 lattice



Main peak reflects quantum phase transition at $S_c \approx 0.25$

Example: 4×4 lattice



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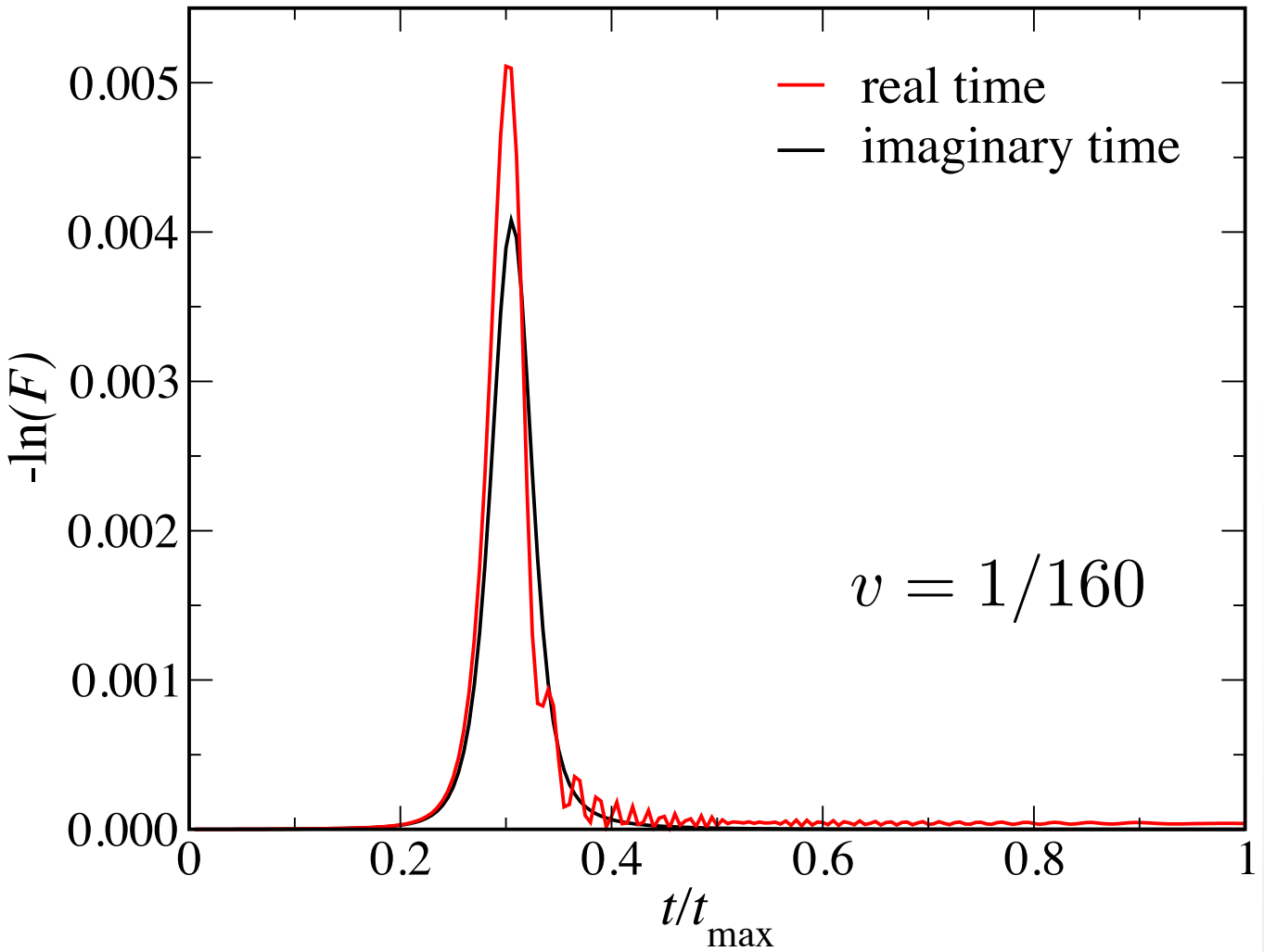
Imaginary time more efficient in reaching ground state for $s \to 1$

Example: 4×4 lattice



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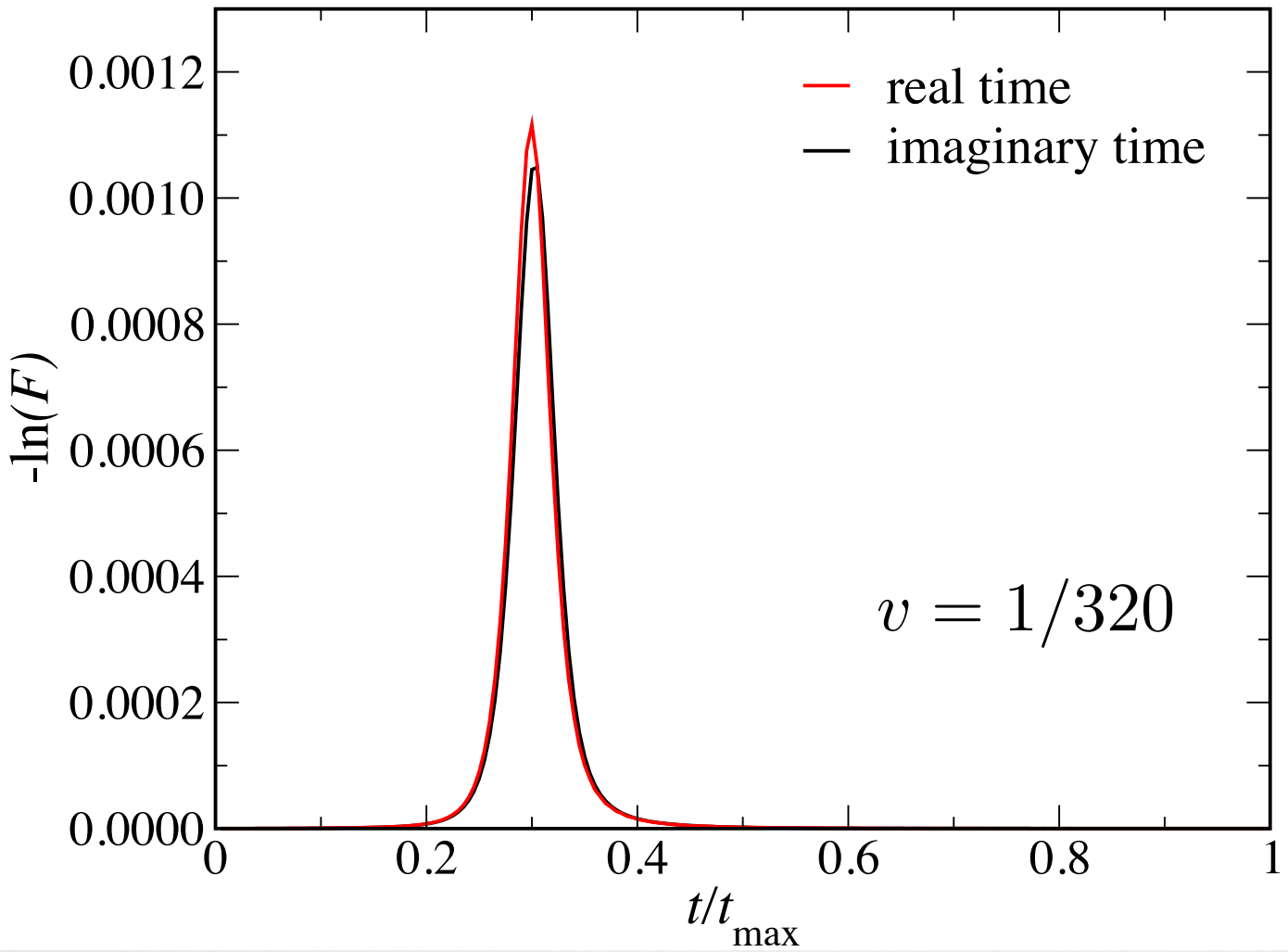


Differences between real and imaginary time are of order v^2 or v^3 (depends on observable)

Same dynamic susceptibilities accessed in real and imaginary time

Dynamic exponent z is same in real and imaginary time

De Grandi, Polkovnikov, Sandvik, PRB 2011

Use imaginary time for large systems

Quantum Monte Carlo Algorithm

Schrödinger dynamic in imaginary time t=iτ

$$|\Psi(\tau)\rangle = U(\tau,\tau_0)|\Psi(\tau_0)\rangle \qquad U(\tau,\tau_0) = T_\tau \exp\left[-\int_{\tau_0}^{\tau} d\tau' H[s(\tau')]\right]$$

Implemented in quantum Monte Carlo as:

$$|\Psi(\tau)\rangle = \sum_{n=0}^{\infty}\int_{\tau_0}^{\tau} d\tau_n \int_{\tau_0}^{\tau_n} d\tau_{n-1}\cdots\int_{\tau_0}^{\tau_2} d\tau_1[-H(\tau_n)]\cdots[-H(\tau_1)]|\Psi(0)\rangle$$

Simpler scheme: evolve with just a H-product

(Liu, Polkovnikov, Sandvik, PRB 2013)

$$|\Psi(s_M)\rangle = H(s_M)\cdots H(s_2)H(s_1)|\Psi(0)\rangle, \quad s_i = i\Delta_s, \quad \Delta_s = \frac{s_M}{M}$$

Time unit is $\propto 1/N$, velocity is $v \propto N\Delta_s$

Difference in v-dependence between product evolution and imaginary-time Schrödinger dynamics is $O(v^2)$ - same critical scaling behavior, dynamic susceptibilities

How is this method implemented?

QMC Algorithm Illustration

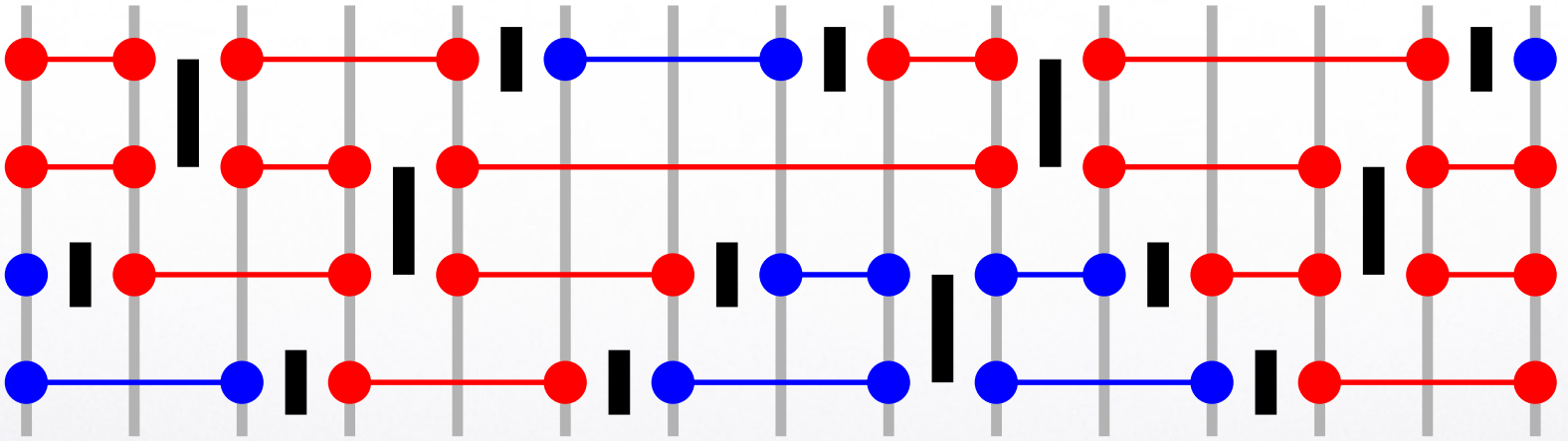
Transverse-field Ising model: 2 types of operators:

$$H_1(i) = -(1-s)(\sigma_i^+ + \sigma_i^-)$$

$$H_2(i,j) = -s(\sigma_i^z \sigma_j^z + 1)$$

Represented as "vertices"

MC sampling of networks of vertices



$N = 4$

$M = 7$

$$\langle \Psi(0) | H(s_1) \cdots H(s_7) | H(s_7) \cdots H(s_1) | \Psi(0) \rangle$$

Simple extension of ground-state projector QMC (fixed H)

Analyze results versus velocity v and system size

Dynamic QMC Illustration

Test on clean 2D Ising model in transverse field

Using H-product dynamics

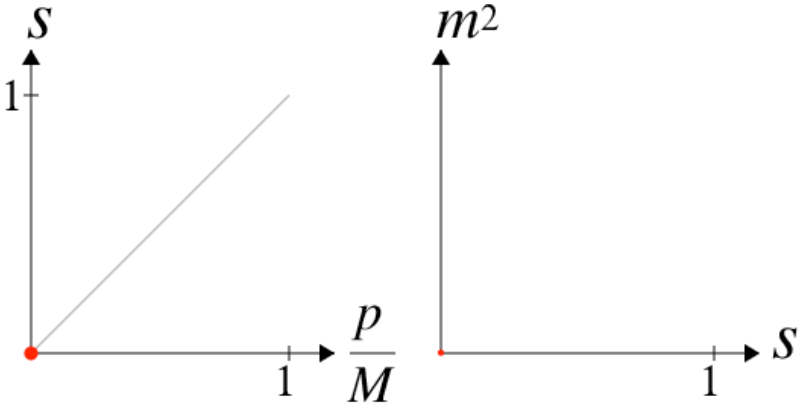
"Asymmetric" expectation values

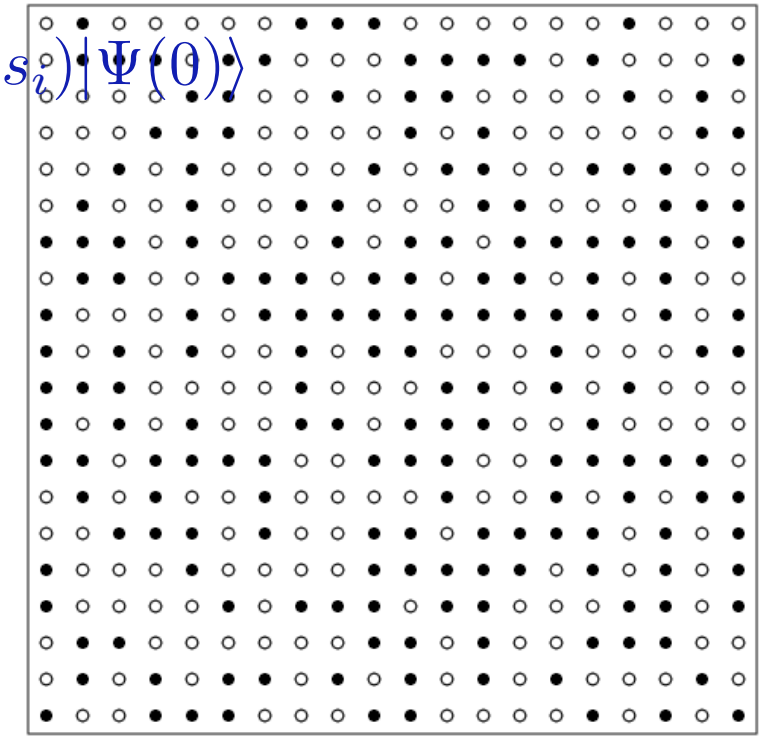
$$\langle A \rangle_k = \frac{\langle \Psi(0) | \prod_{i=M}^{1} H(s_i) \prod_{i=k}^{M} H(s_i) A \prod_{i=1}^{k} H(s_i) | \Psi(0) \rangle}{\langle \Psi(0) | \prod_{i=M}^{1} H(s_i) \prod_{i=k}^{M} H(s_i) \prod_{i=1}^{k} H(s_i) | \Psi(0) \rangle}$$

Same leading-order (in v) behavior as conventional expectation values

Computational advantage:
All s=values in one simulation!

Animation of single configuration





Collect data, do scaling analysis...

Dynamic Critical Exponent and Gap

Dynamic exponent z at a phase transition
- relates time and length scales

At a continuous transition (classical or quantum):

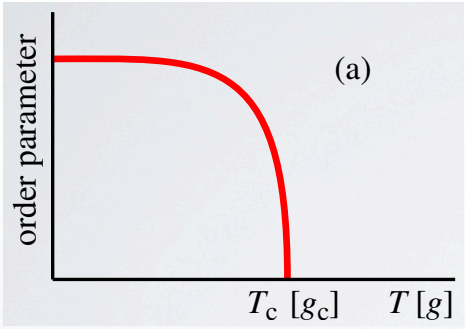
- large (divergent) correlation length

$$\xi_r \sim |\delta|^{-\nu}, \quad \xi_t \sim \xi_r^z \sim |\delta|^{-\nu z}$$

δ = distance from critical point (in T or other param)

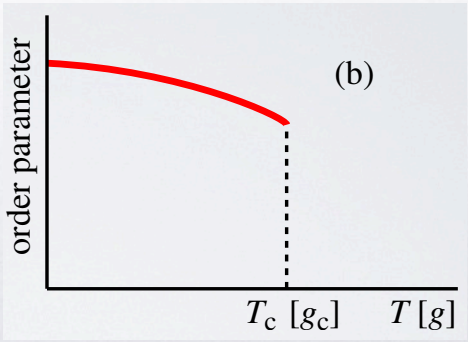
Continuous quantum phase transition
- excitation gap at the transition
  depends on the system size and z as

$$\Delta \sim \frac{1}{L^z} = \frac{1}{N^{z/d}}, \quad (N = L^d)$$



Exponentially small gap at a first-order (discontinuous) transition

$$\Delta \sim e^{-aL}$$



Important issue for quantum annealing!

P. Young et al. (PRL 2008)

Exactly how does z enter in the adiabatic criterion?

Kibble-Zurek Velocity and Scaling

The adiabatic criterion for passing through a continuous phase transition involves exponents z and ν:

Must have v < v_{KZ}, with

$$v_{\mathrm{KZ}} \sim L^{-(z+1/\nu)}$$

Same criterion for classical and quantum phase transitions

- adiabatic (quantum)
- quasi-static (classical)

Kibble 1978
- defects in early universe
Zurek 1981
- classical phase transitions
Polkovnikov 2005 + others
- quantum phase transitions

Generalized finite-size scaling hypothesis

$$A(\delta, v, L) = L^{-\kappa/\nu} g(\delta L^{1/\nu}, v L^{z+1/\nu})$$

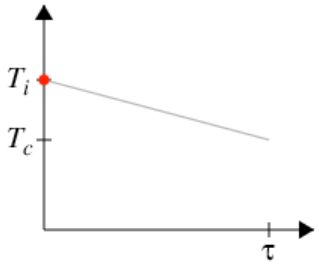
δ = distance from critical point (in T or other param)

$$A(\delta, v, N) = N^{-\kappa/\nu'} g(\delta N^{1/\nu'}, v N^{z'+1/\nu'}), \quad \nu' = d\nu, \; z = z/d$$

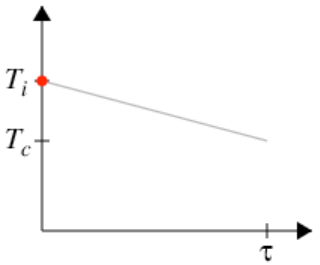
Will use for spin glasses of interest in quantum computing

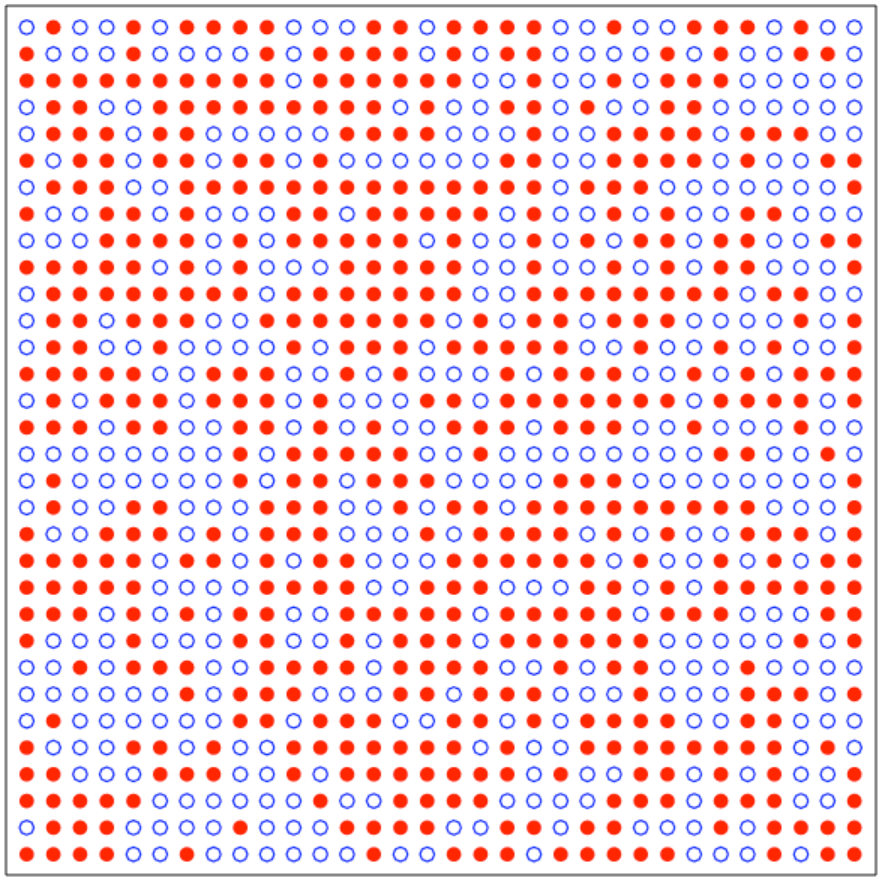
Apply to well-understood classical system first...

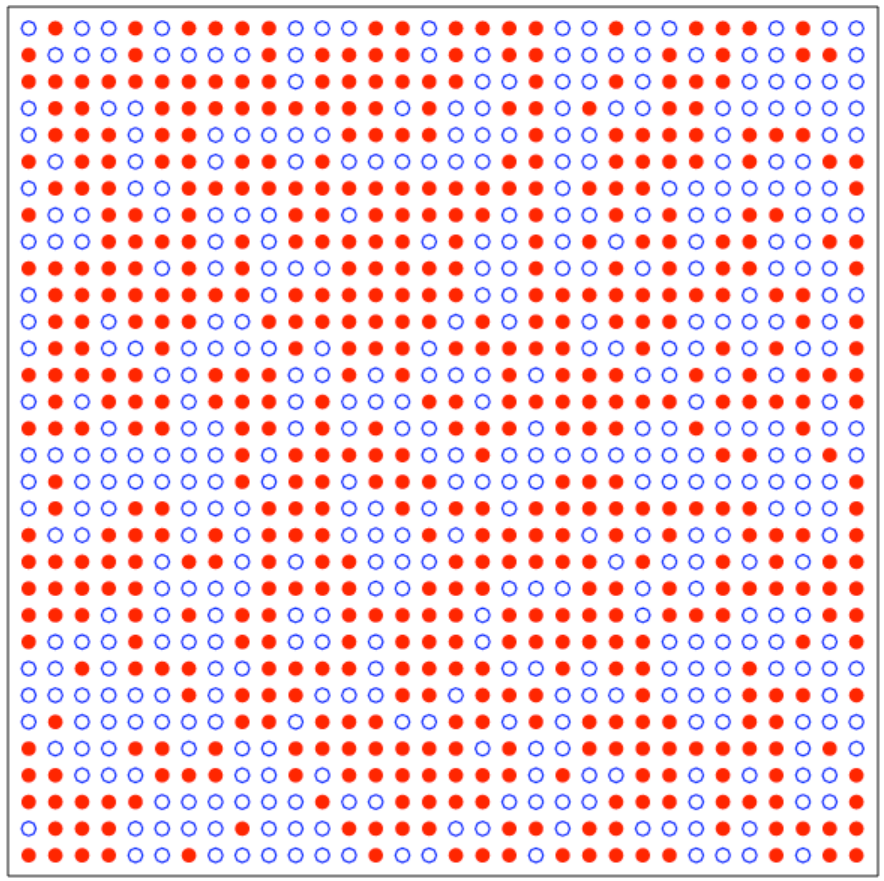
Classical simulated annealing



2D classical Ising Metropolis MC simulations





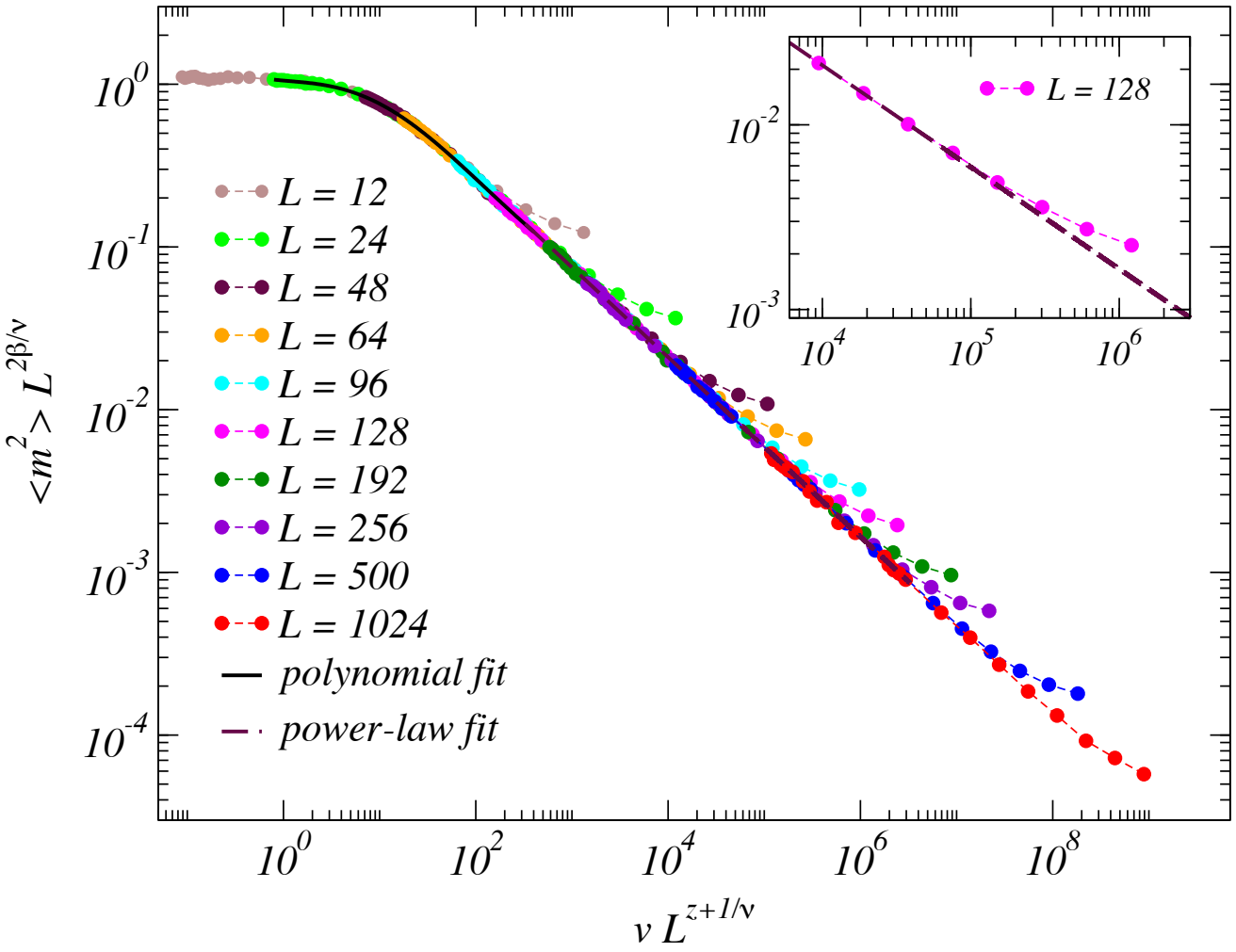


Repeat many times, collect averages, analyze,....

Velocity Scaling, 2D Ising Model

Repeat process many times, average data for $T=T_c$

$$\langle m^2(\delta = 0, v, L)\rangle = L^{-2\beta/\nu} f(vL^{z+1/\nu})$$



Used known 2D Ising exponents $\beta=1/8$, $\nu=1$

Adjusted z for optimal scaling collapse

Result:

$z \approx 2.1767(5)$

consistent with values obtained in other ways

Liu, Polkovnikov, Sandvik, PRB 2014

Can also be done for quantum systems in imaginary time

2D Transverse-Ising, Scaling Example

$$A(\delta, v, L) = L^{-\kappa/\nu} g(\delta L^{1/\nu}, v L^{z+1/\nu}) \qquad z = 1, \nu \approx 0.70$$

If z, ν known, s_c not: use

$$v L^{z+1/\nu} = \text{constant}$$

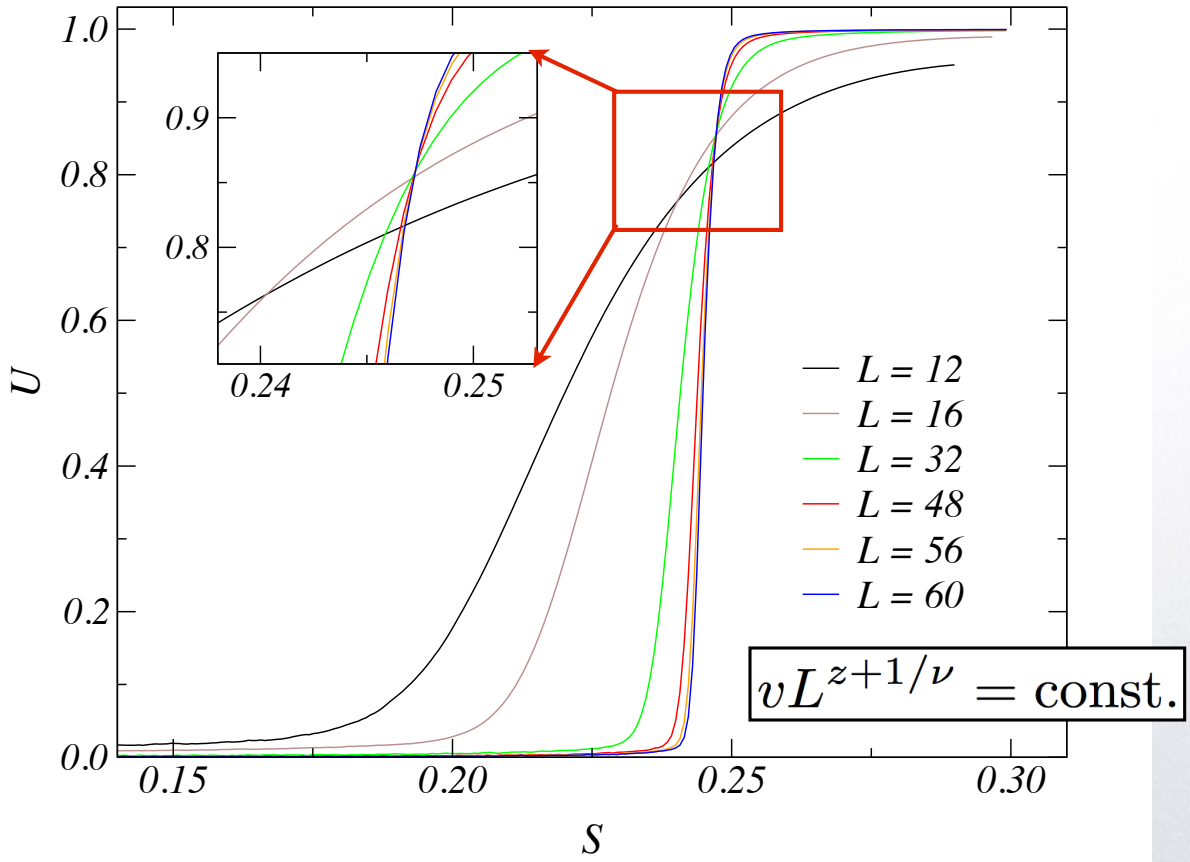
for 1-parameter scaling

Example: Binder cumulant

$$U = \frac{3}{2}\left(1 - \frac{1}{3}\frac{\langle m_z^4 \rangle}{\langle m_z^2 \rangle^2}\right)$$

Step function should form, jump from U=0 to 1 at s_c
- crossing points for finite system size

$$U(s, L, v) = U\left((s - s_c)L^{1/\nu}, v L^{z+1/\nu}\right)$$

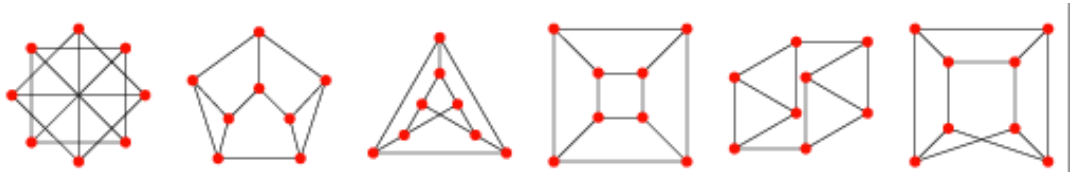


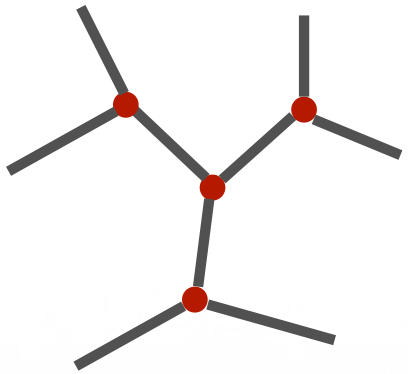
Do similar studies for quantum spin glasses

3-regular graphs with anti-ferro couplings

N spins, randomly connected, coordination-number 3

N=8





Classical model has mean-field glass transition
- Tc known exactly (Krazakala et al.)

The quantum model was studied by

Farhi, Gosset, Hen, Sandvik, Shor, Young, Zamponi, PRA 2012

- $s_c \approx 0.37$ from quantum cavity approximation
- QMC consistent with this s_c, power-law gaps at s_c

More detailed studies with quantum annealing

Edwards-Anderson spin-glass order parameter

$$q = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^z(1)\sigma_i^z(2)$$

(1) and (2) are independent simulations (replicas)

Analyze $\langle q^2 \rangle$ using QMC and velocity scaling

Extracting Quantum-glass transition

Using Binder cumulant

$$U(s, v, N) = U[(s - s_c)N^{1/\nu'}, vN^{z'+1/\nu'}]$$

But now we don't know the exponents. Use

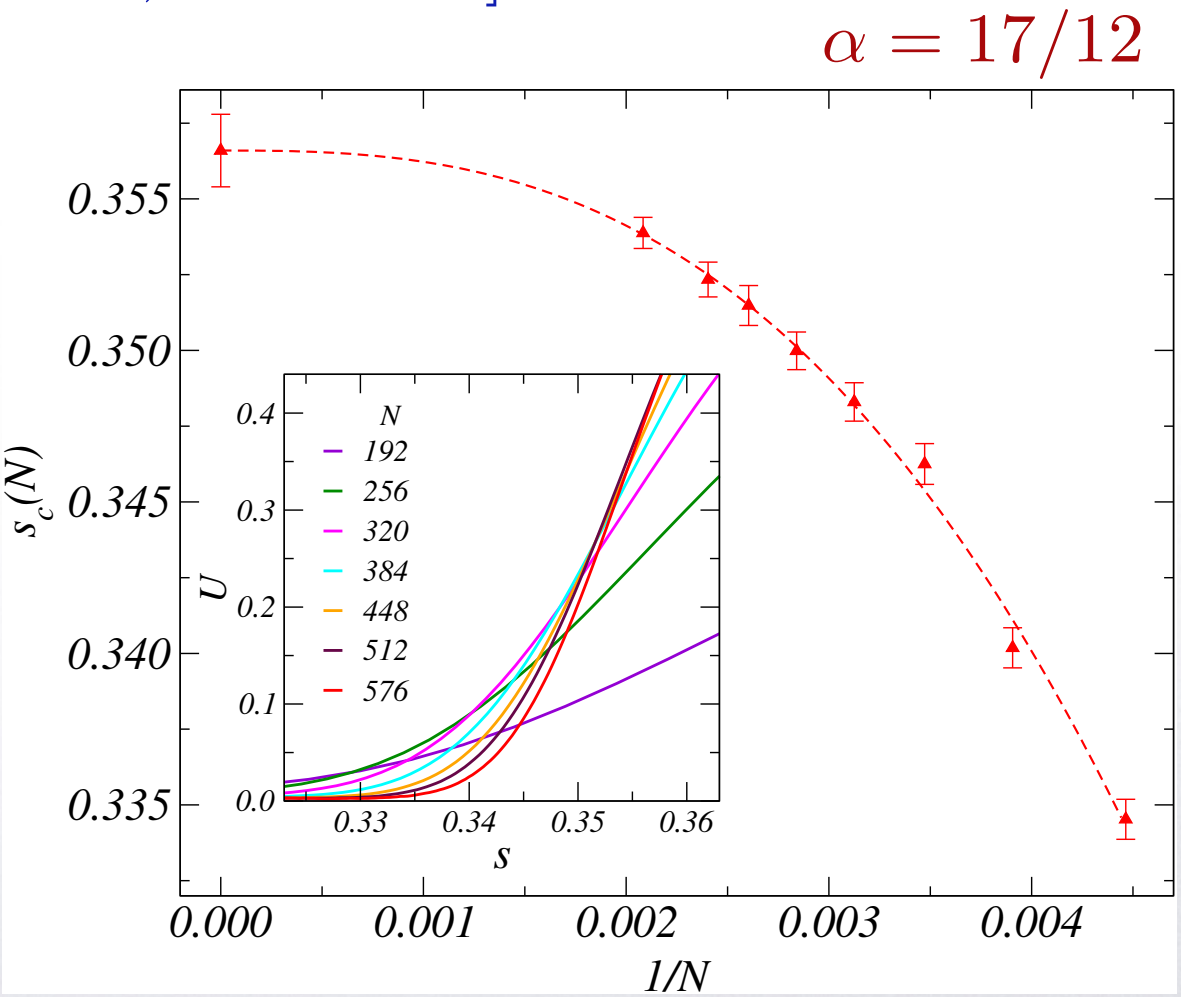
$$v \propto N^{-\alpha}, \quad \alpha > z' + 1/\nu'$$

- do several α
- check for consistency

Best result for α=17/12

s_c = 0.3565 +/- 0.0012

Consistent with previous work, but smaller errors



Next, critical exponents...

Velocity Scaling at the Glass Transition

Study evolution to s_c
- several system sizes N
- several velocities

$\beta/\nu' \approx 0.43(2)$
$z'+1/\nu' \approx 1.3(2)$

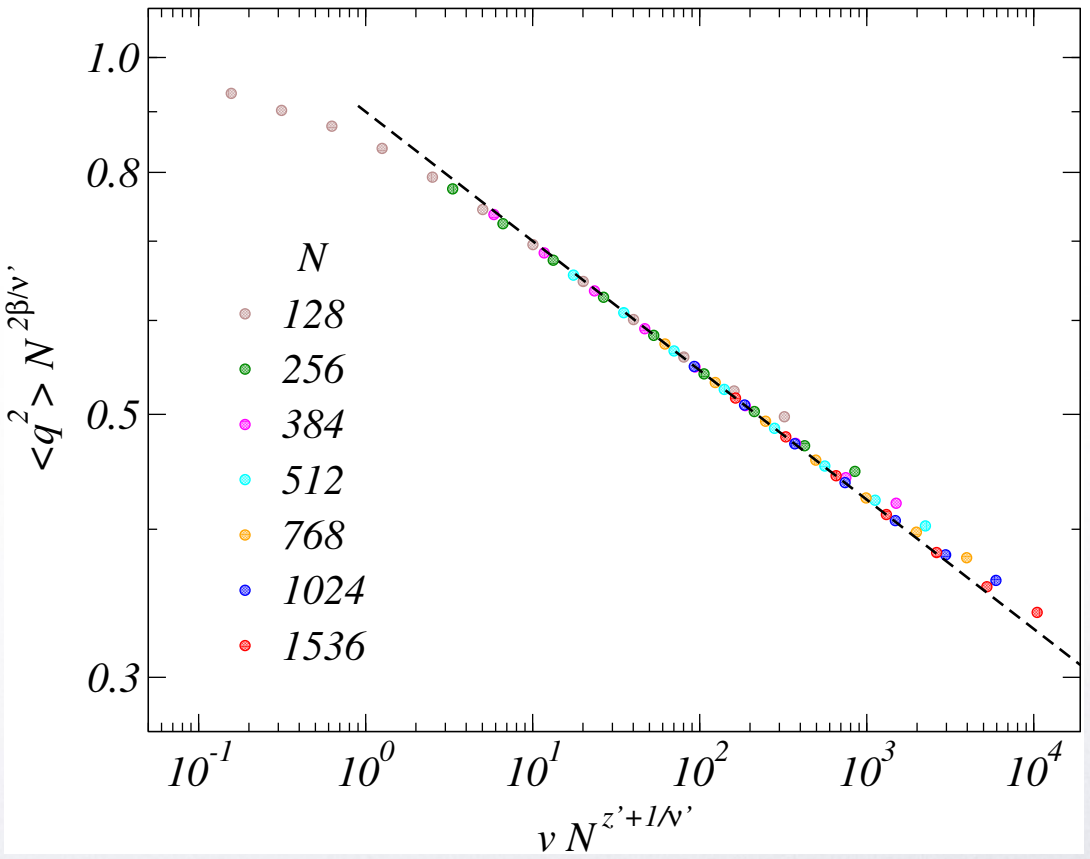
Differ from values expected for d=∞:
(Read, Sachdev, Ye, 1995)

$\beta/\nu' = 1/2$
$z'+1/\nu' = 3/4$

Fully connected model (SK)
- velocity scaling gives

$\beta/\nu' \approx 0.47(3)$
$z'+1/\nu' \approx 0.8(1)$

$$\langle q^2(s_c)\rangle \propto N^{-2\beta/\nu'} f(vN^{z'+1/\nu'})$$



Why is 3-regular model different?

Significance of the exponents?

Relevance to Quantum Computing

The time needed to stay adiabatic up to s_c scales as

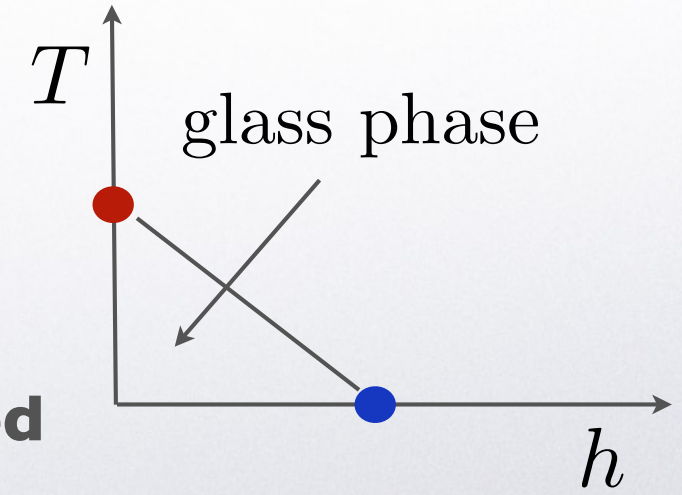
$$t \sim N^{z'+1/\nu} \qquad z' + 1/\nu' \approx 1.3$$

Reaching s_c, the degree of ordering scales as

$$\sqrt{< \langle q^2 \rangle >} \sim N^{-\beta/\nu'} \qquad \beta/\nu' \approx 0.43$$

Let's compare with the know classical exponents
(finite-temperature transition of 3-regular random graphs)

Classical	**Quantum**
$\beta/\nu' = 1/3$	**$\beta/\nu' \approx 0.43$**
$z'+1/\nu' = 1$	**$z'+1/\nu' \approx 1.3$**



- **It takes longer for quantum annealing to reach its critical point**
- **And the state is further from ordered (further from the optimal solution)**

Proposal: Do velocity scaling with the D-wave machine!