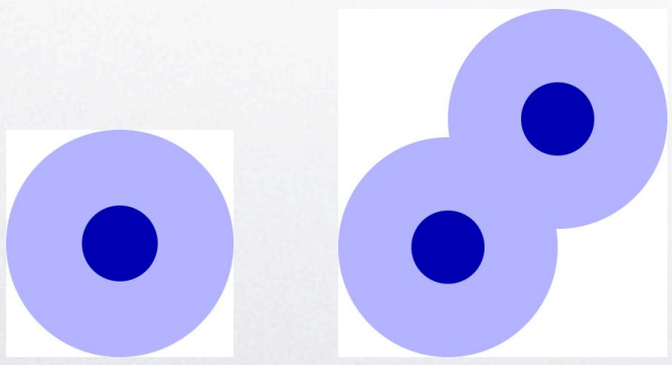
Lecture 4:
Out-of-equilibrium quantum Monte Carlo simulation and quantum annealing

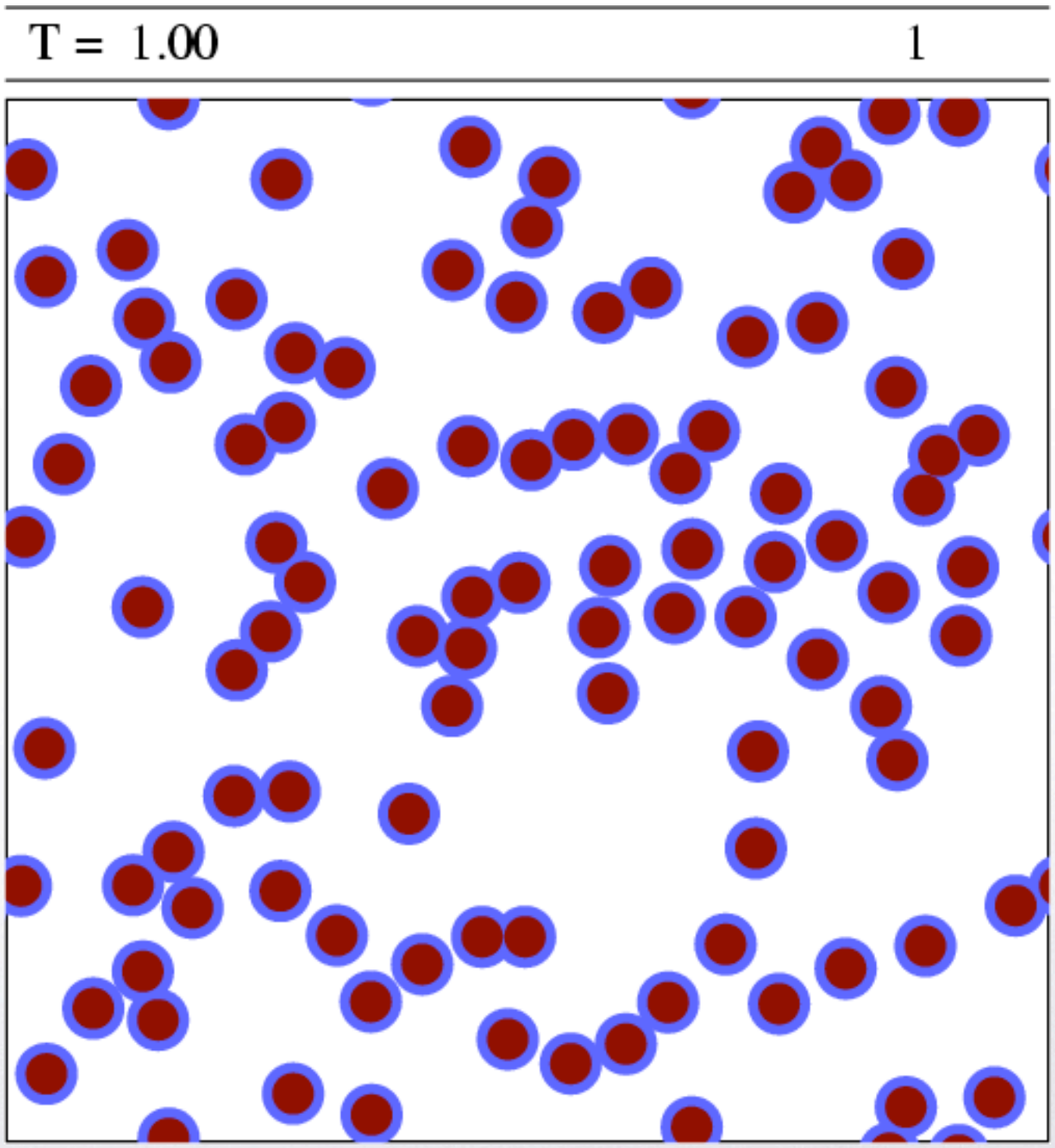
Anders W Sandvik, Boston University

Monte Carlo Simulations

Example: Particles with hard and soft cores (2 dim)

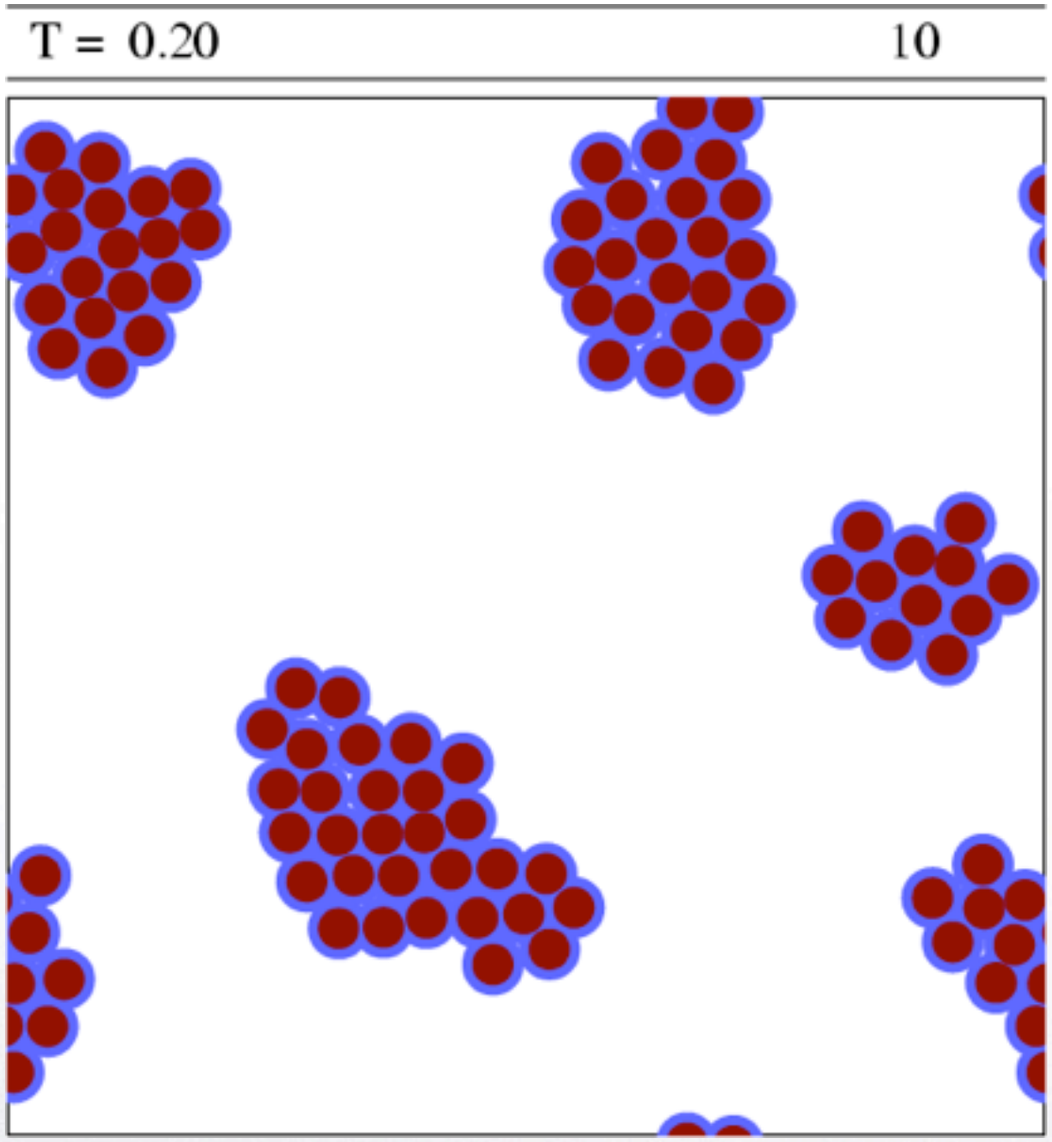
$$V(r) = \begin{cases} \infty, & r <\leq r_1 \\ -V, & r_1 < r \leq r_2 \\ 0, r > r_2 \end{cases}$$

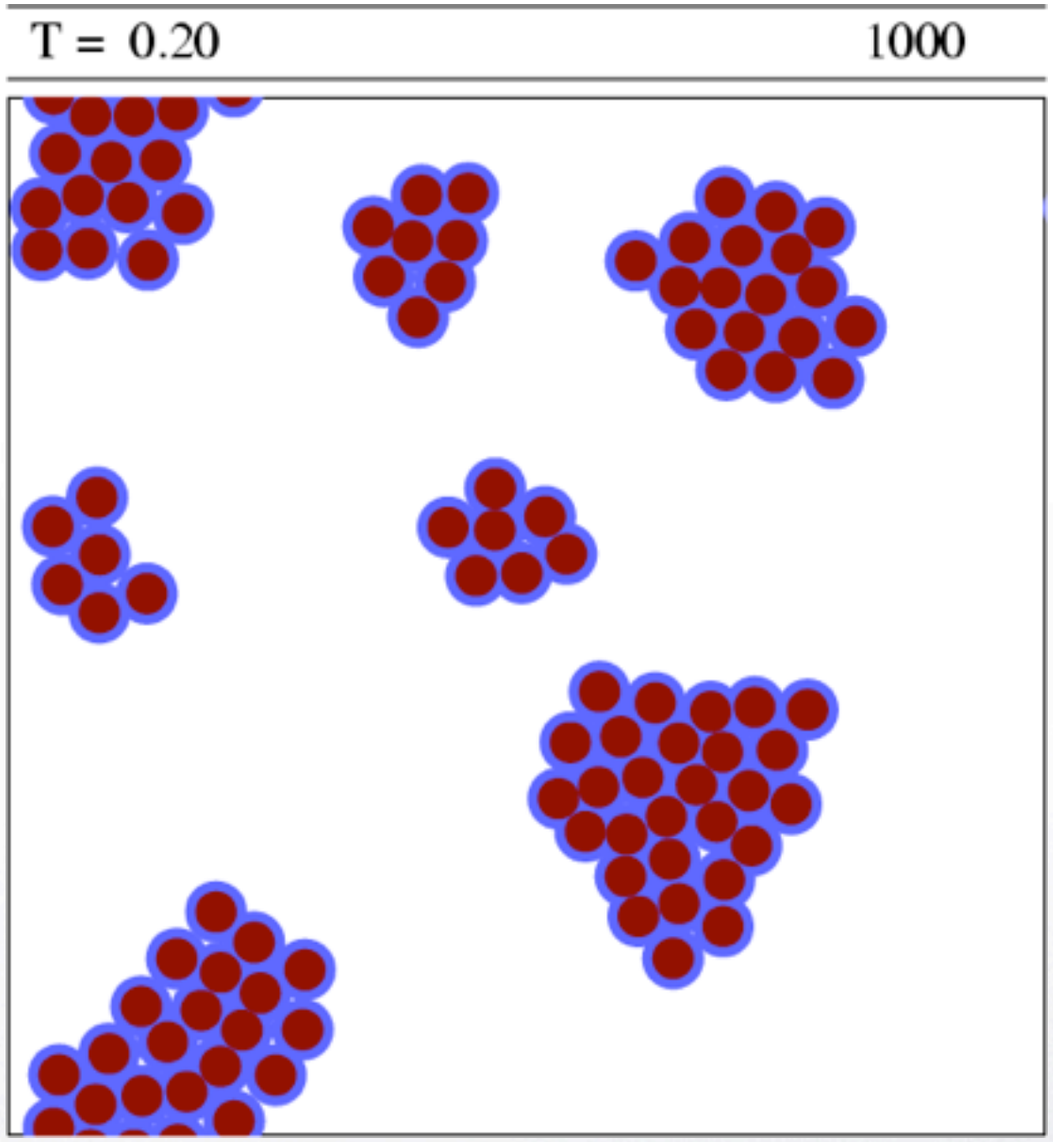




What happens when the temperature is lowered ?

Monte Carlo Simulations





Transition into liquid state has taken place
Slow movement & growth of droplets
- simulation is not strictly equilibrated

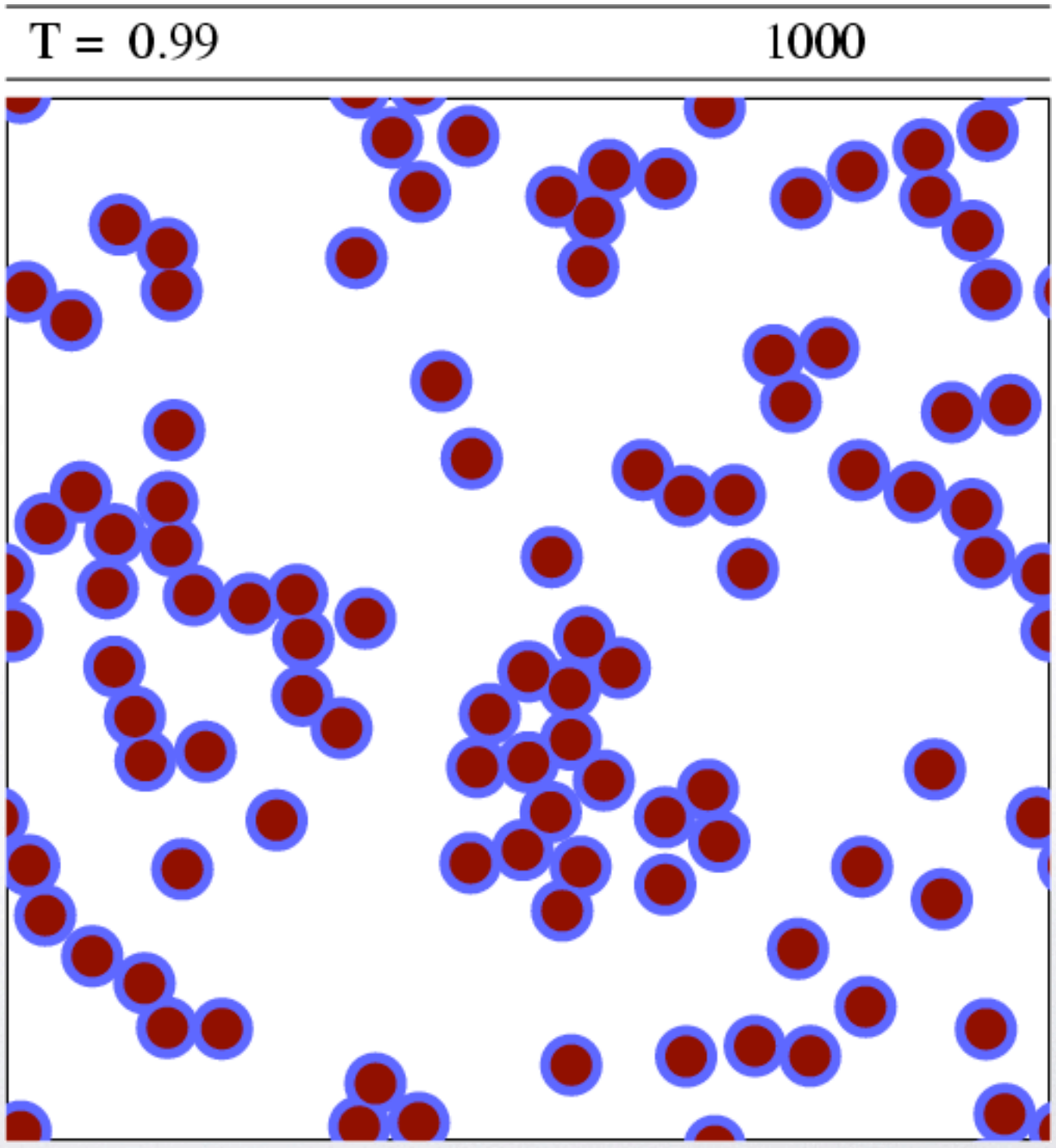
Is there a better way to reach equilibrium at low T?

Simulated Annealing

Annealing: Removal of crystal defects by heating followed by slow cooling

Simulated Annealing: MC simulation with slowly decreasing T
- Can help to reach equilibrium faster

Optimization method: express optimization of many parameters as minimization of a cost function, treat as energy in MC simulation



Similar scheme in quantum mechanics?

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?

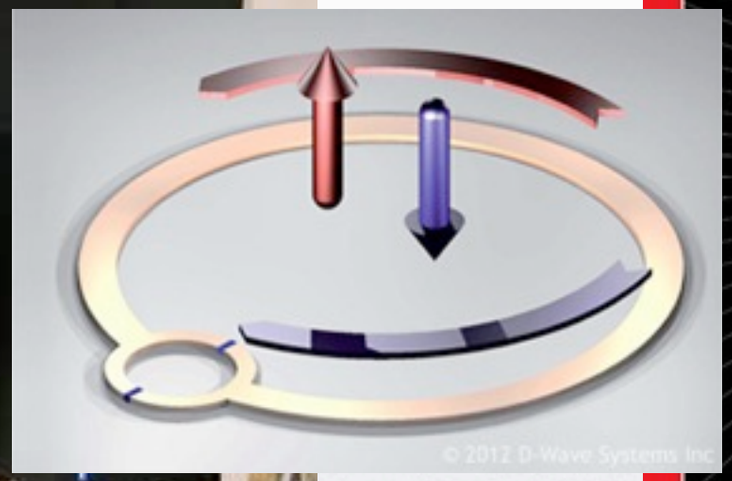
Ray, Chakrabarty,Chakrabarty (PRB 1989), Kadowaki, Nishimory (PRE 1998),...

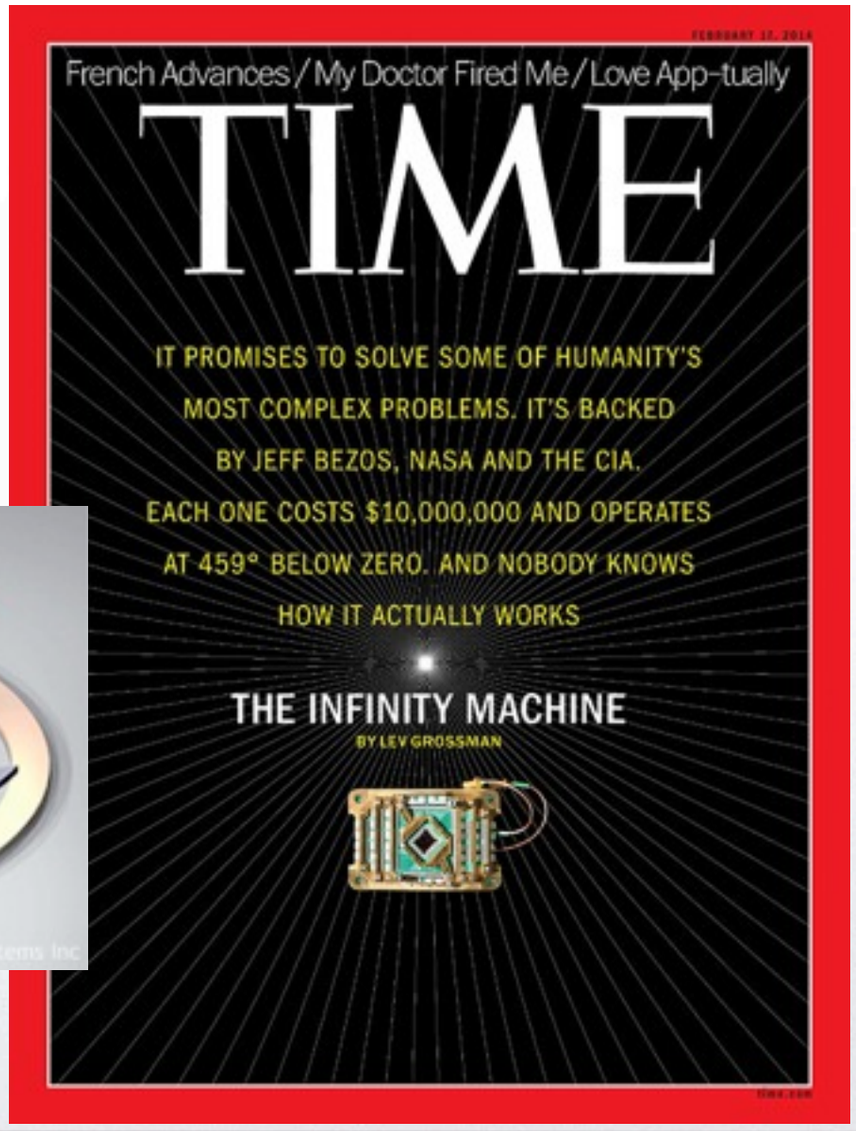
Useful paradigm for quantum computing?

Quantum Annealing & Quantum Computing

The D-wave "quantum annealer"; 512 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

Hard optimization problems map 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"

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

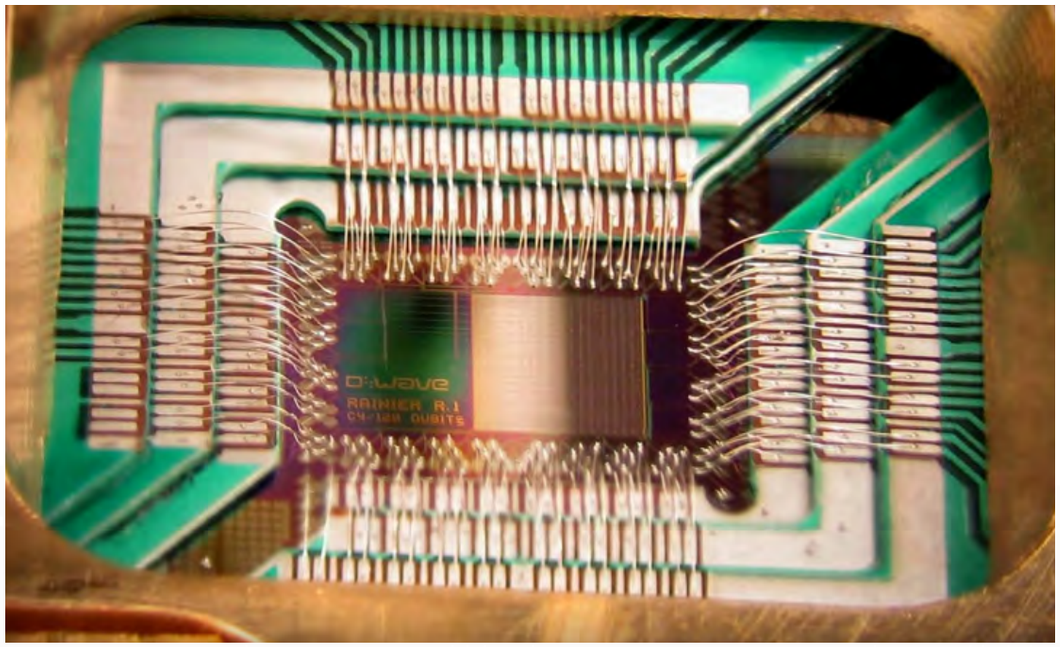
$$[H_0, H_1] \neq 0$$

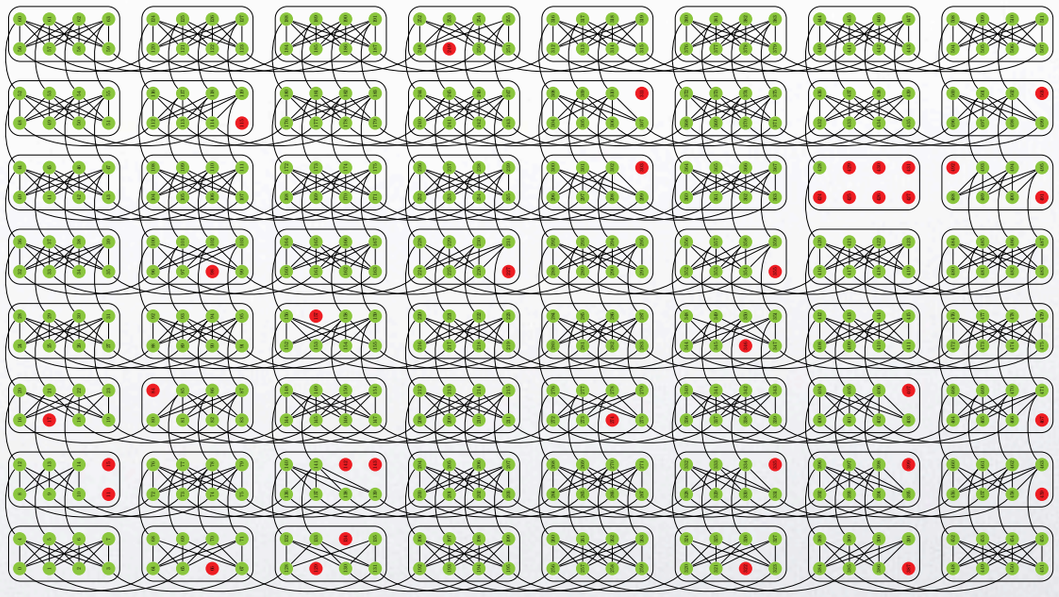
Tune the strength of the field

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

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

adiabatically from s=0 to s=1





Chimera lattice, 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)?

Landau-Zener Problem

Single spin in magnetic field, with mixing term

$$H = -h\sigma^z - \epsilon\sigma^x = -h\sigma^z - \epsilon(\sigma^+ + \sigma^-)$$

Eigen energies are

$$E = \pm\sqrt{h^2 + \epsilon^2}$$

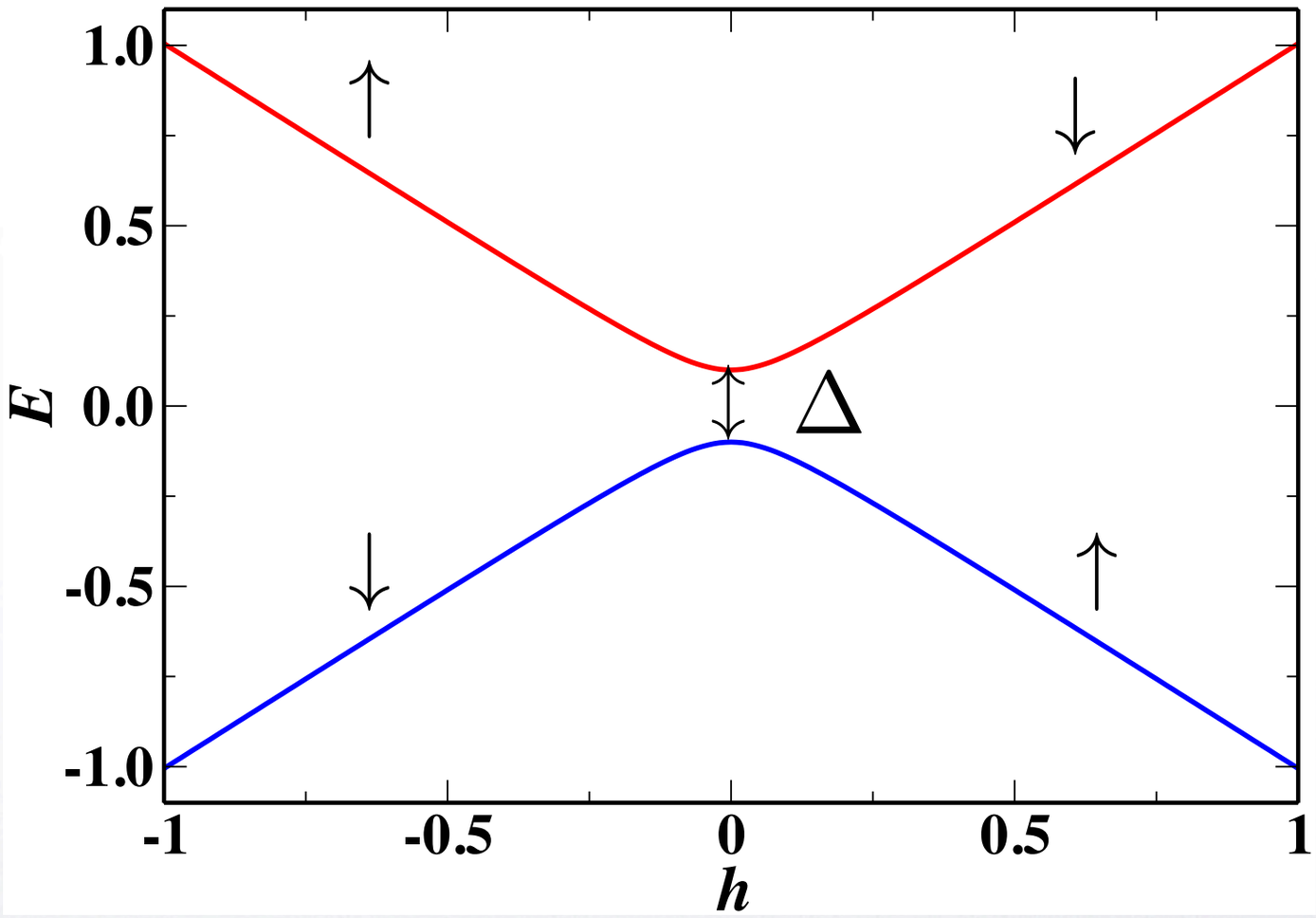
Smallest gap: Δ=2ε

Time-evolution:

$$h(t) = -h_0 + vt$$

To stay adiabatic when crossing h=0, the velocity must be

$$v < \Delta^2 \quad (\text{time} > \Delta^{-2})$$



Suggests the smallest gap is important in general
- but states above the gap play role in many-body system

What can we expect at a quantum phase transition?

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

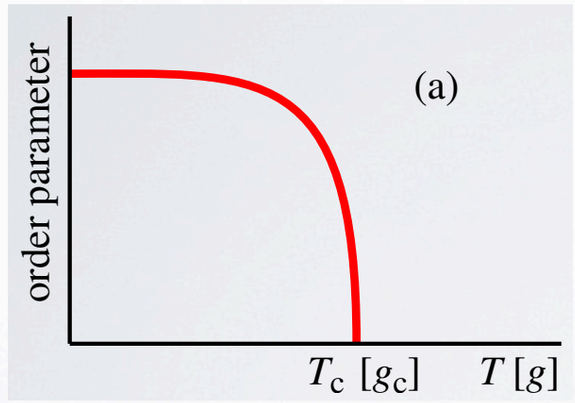
$$\xi_r \sim |\delta|^{-\nu}, \qquad \xi_t \sim \xi_r^z \sim |\delta|^{-\nu z}$$

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

Continuous quantum phase transition

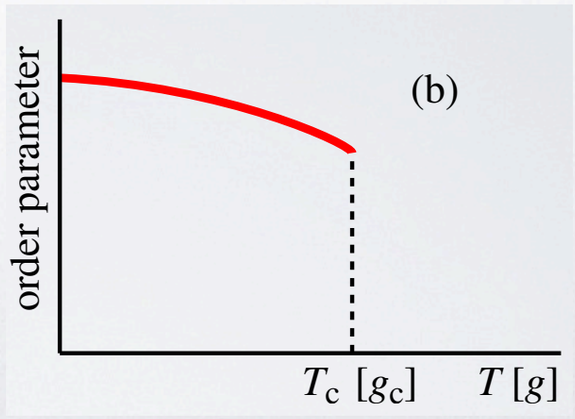
- excitation gap at the transition depends on the system size and z as

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



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
- quantum phase transitions

Generalized finite-size scaling hypothesis

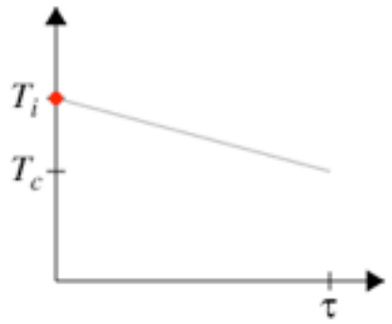
$$A(\delta, v, L) = L^{-\kappa/\nu} g(\delta L^{1/\nu}, v L^{z+1/\nu})$$

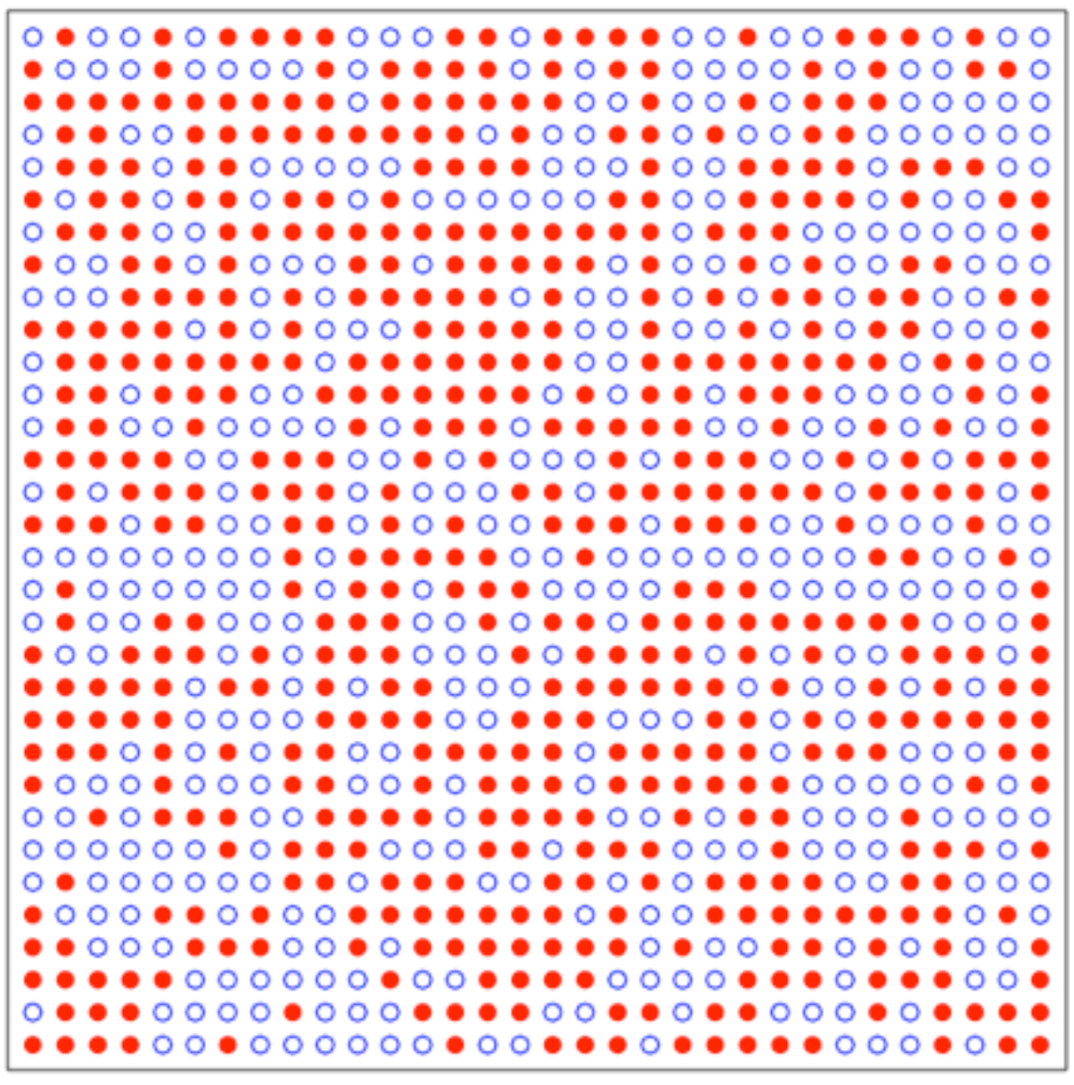
$$A(\delta, v, N) = N^{-\kappa/\nu'} g(\delta N^{1/\nu'}, v N^{z'+1/\nu'}), \quad \nu' = d\nu, \; z = z/d$$

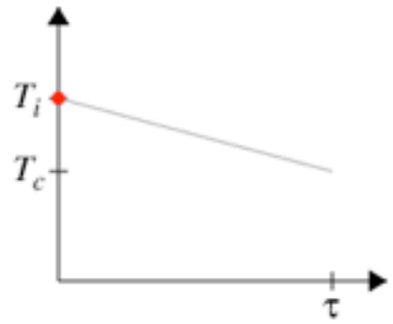
Will use for spin glasses of interest in quantum computing

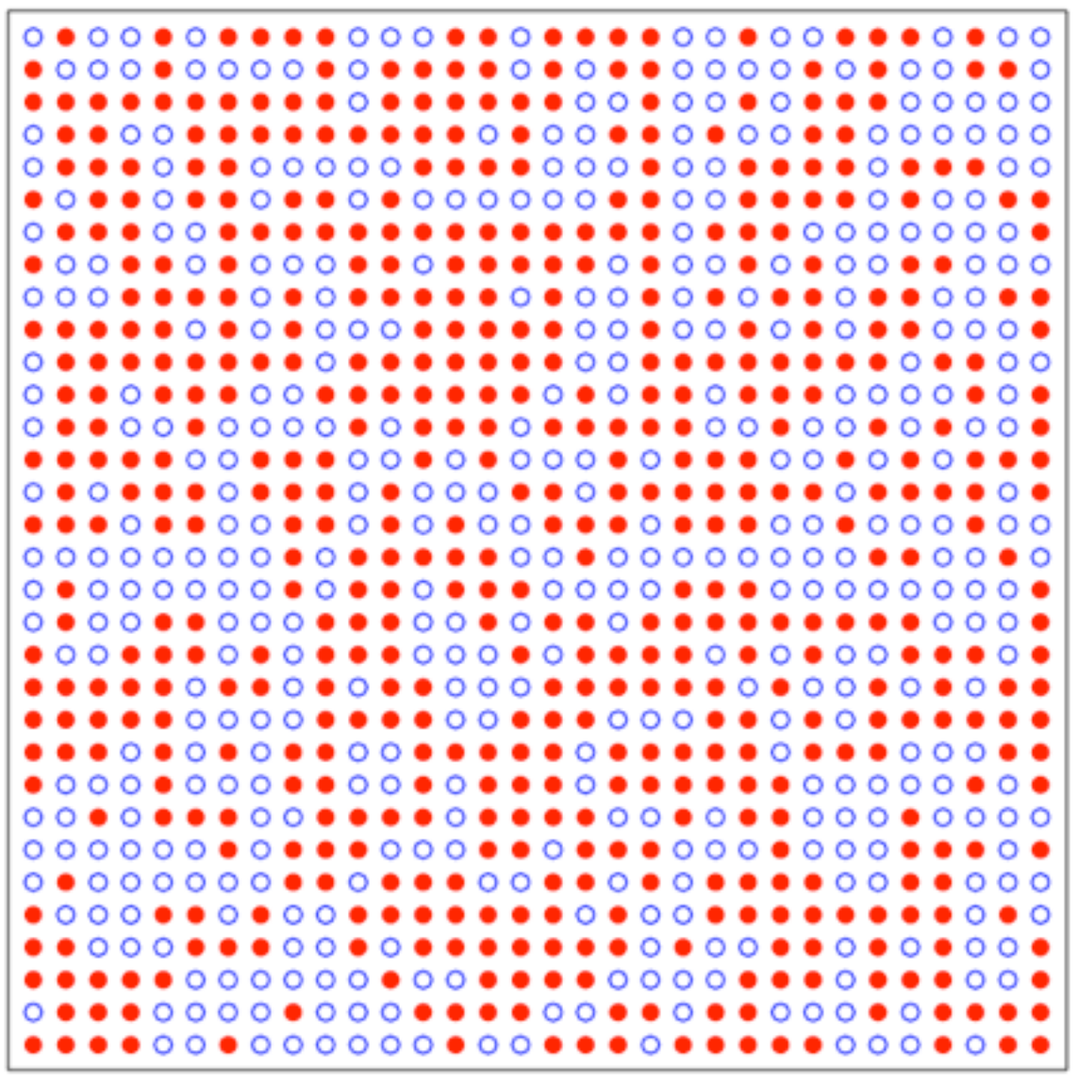
Apply to well-understood classical system first...

Fast and Slow Classical Ising Dynamics







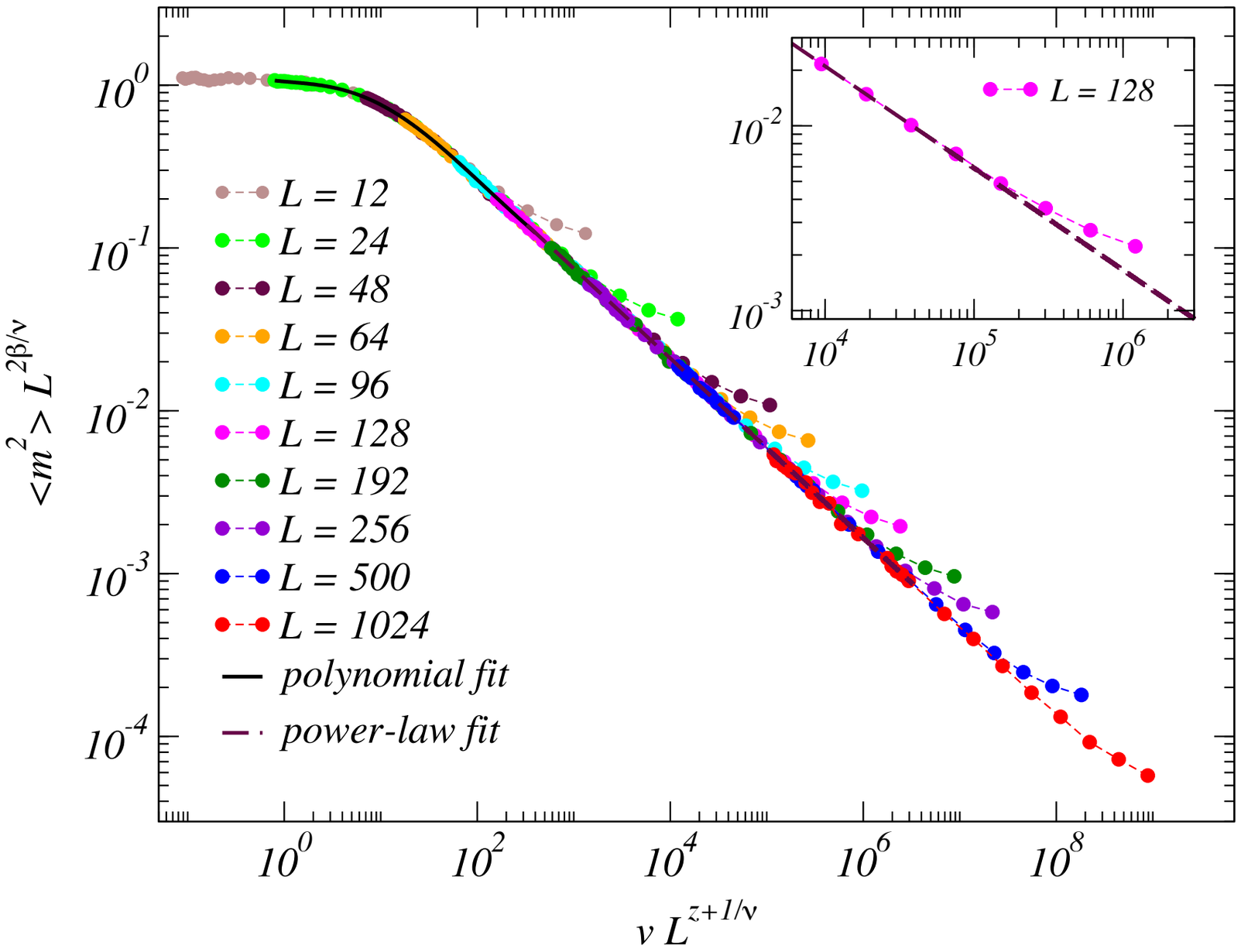


Repeat many times, collect averages, analyze,....

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 β=1/8, ν=1

Adjusted z for optimal scaling collapse

<u>Result: z ≈2.17</u> consistent with values obtained in other ways

Liu, Polkovnikov, Sandvik, PRB 2014

Can we do something like this for quantum models?

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 for 1D systems (moderate sizes and times)

Alternative approach:

Schrödinger dynamics in imaginary time t=iτ

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

Can be implemented in Quantum Monte Carlo

De Grandi, Polkovnikov, Sandvik, PRB2011

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

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

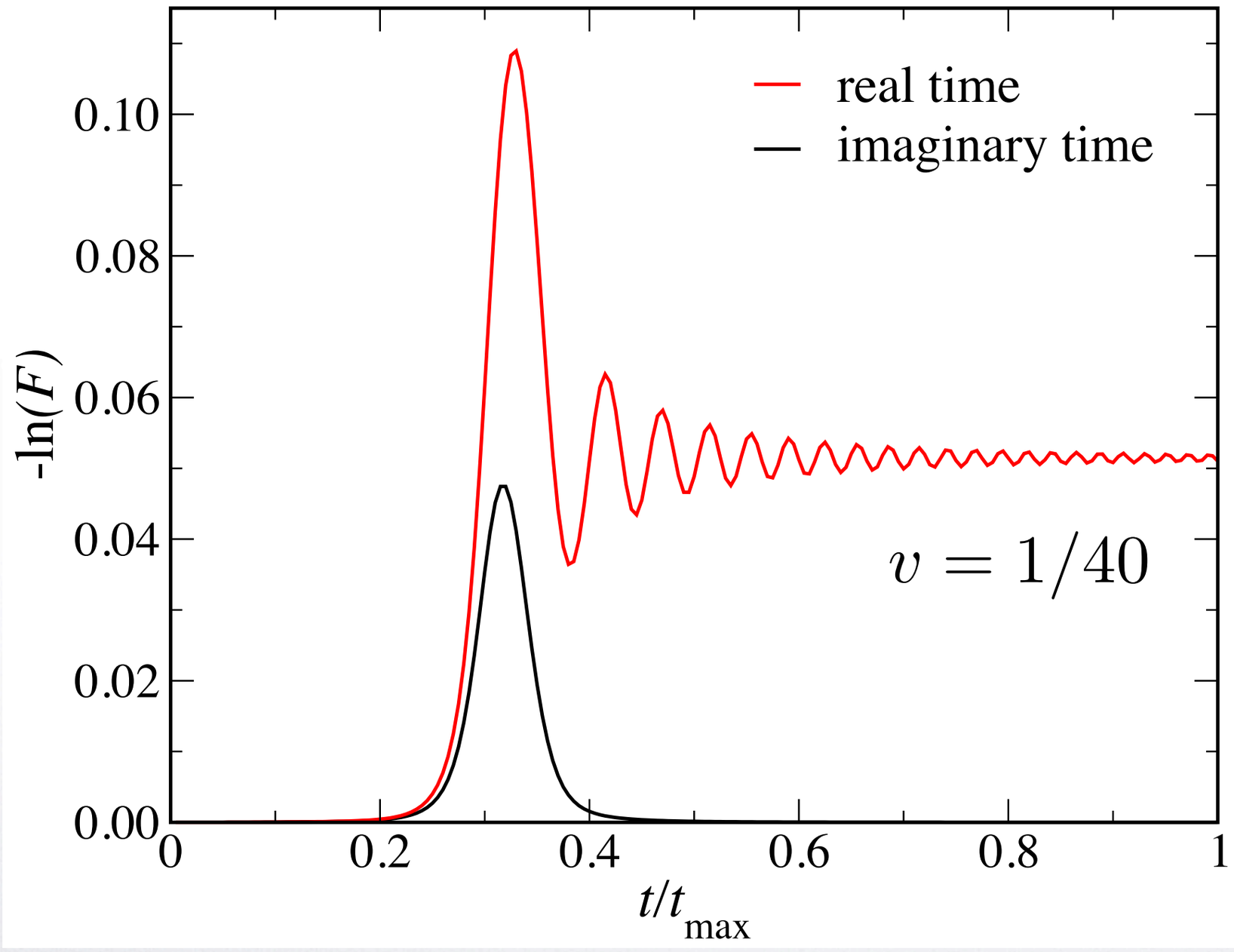
$$-\ln[F(t)] = -\frac{1}{2} \ln\left(|\langle \Psi_0(t)|\Psi(t)\rangle|^2\right)$$

Integrate Schrödinger equation numerically for small L

- compare real and imaginary time

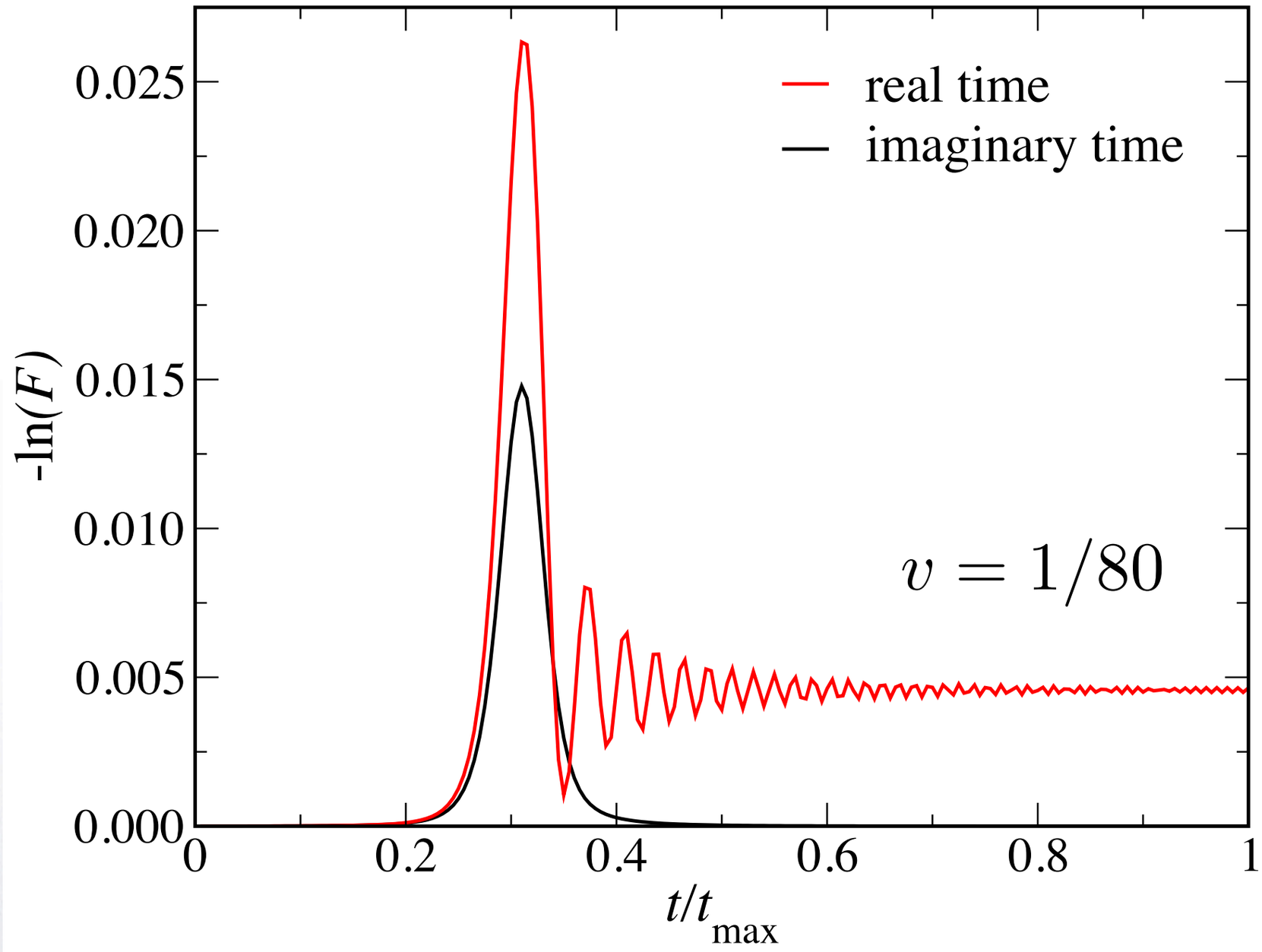
How different? Which one is more adiabatic?

Example: 4×4 lattice



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

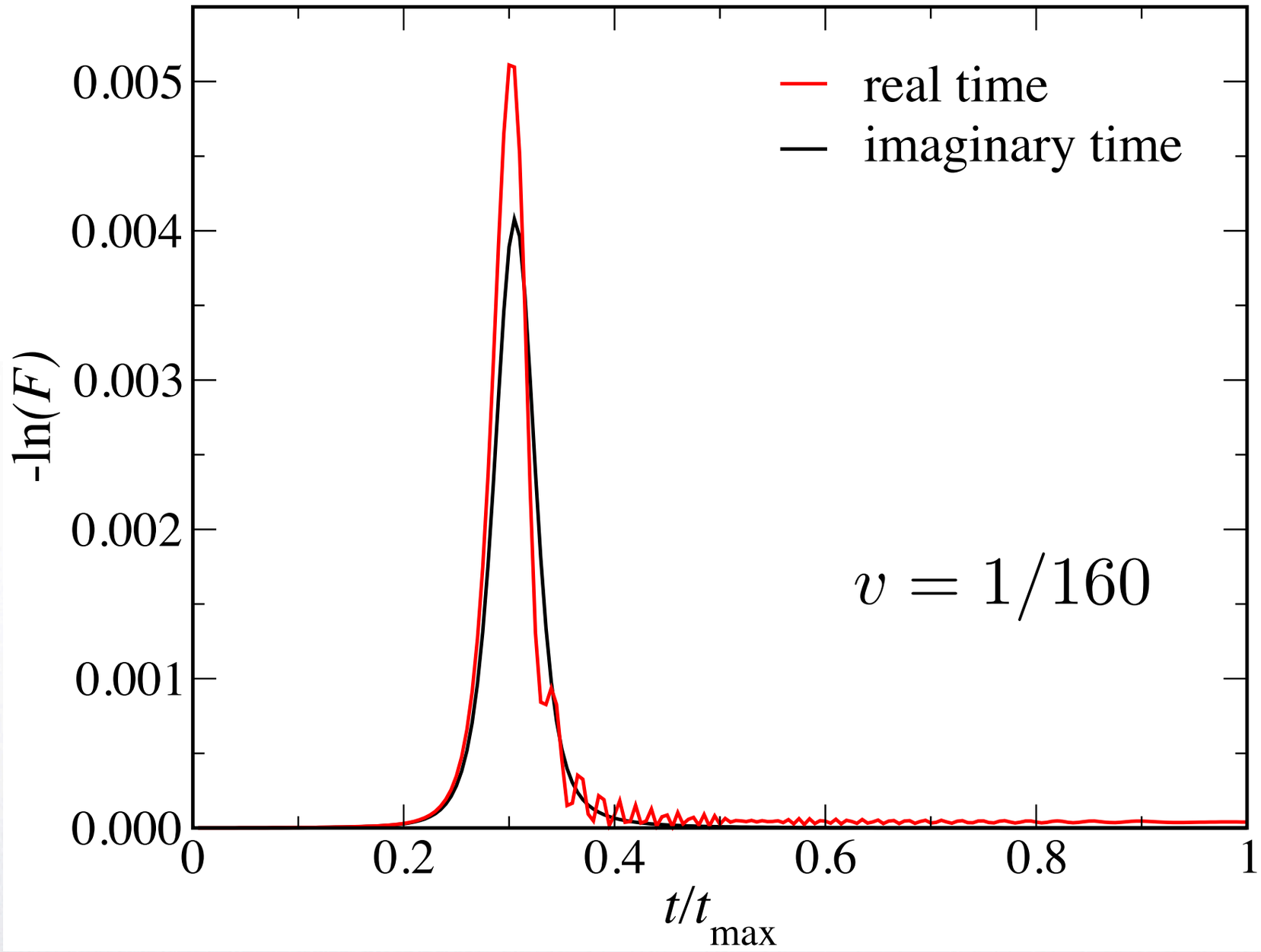
Example: 4×4 lattice



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

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

Example: 4×4 lattice



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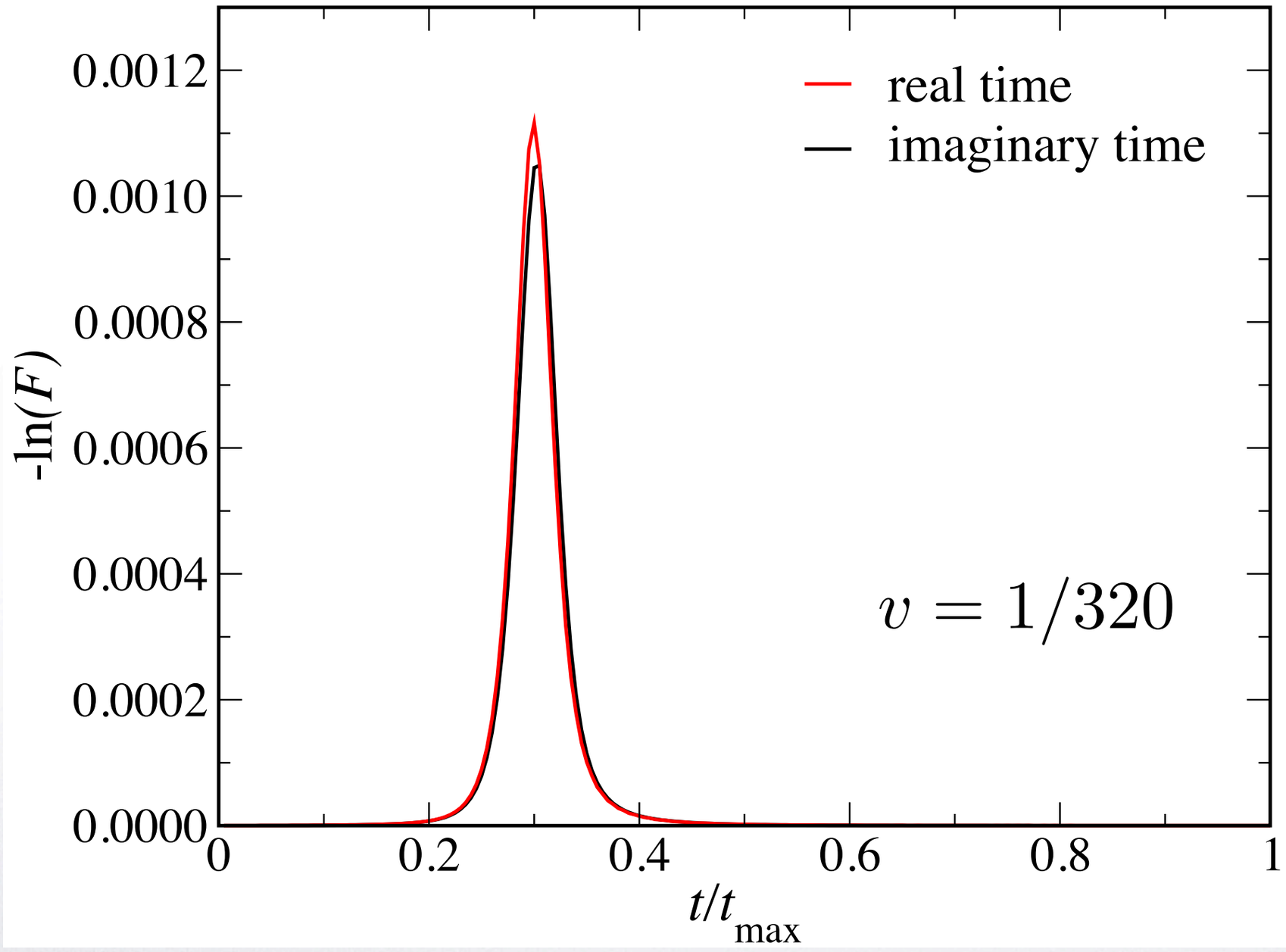


Differences between real and imaginary time come in only at order v^3

Same dynamic susceptibility 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 ∝ 1/N, velocity is $v \propto N\Delta_s$

Difference in v-dependence between product evolution and imaginary-time Schrödinger dynamics is O(v²)
- same critical scaling behavior, dynamic susceptibilities

How is this method implemented?

QMC Algorithm Illustration

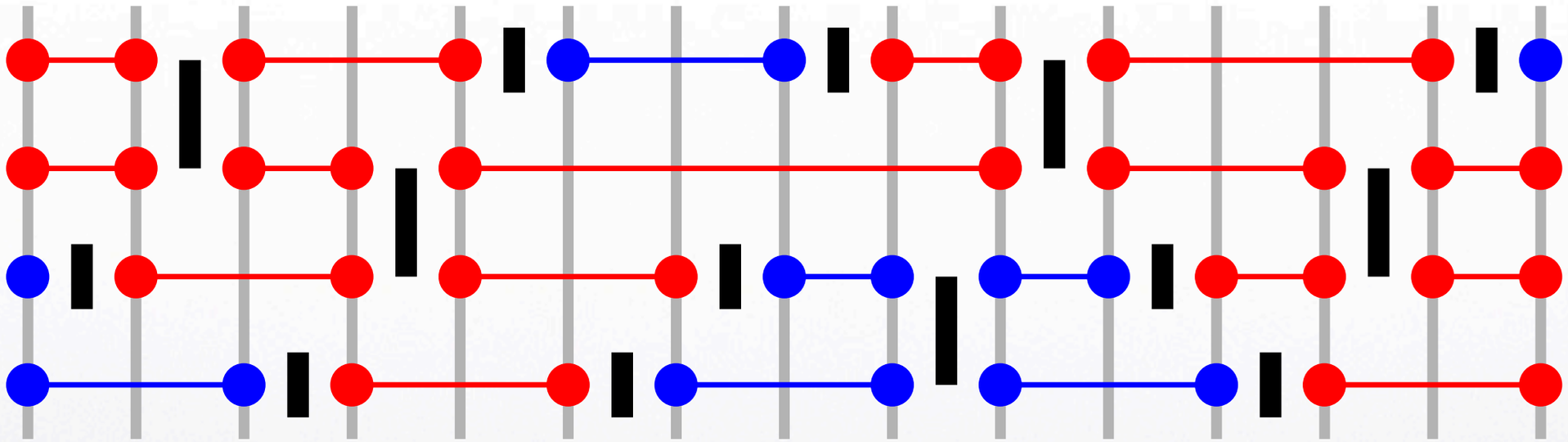
Transverse-field Ising model: 2 types of operators:

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

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

Represented as "vertices"

MC sampling of networks of vertices



Similar to ground-state projector QMC

How to analyze results versus velocity v?

Dynamic Critical Exponent and Gap

Dynamic exponent z at a phase transition

- relates time and length scales

At a continuous transition (classical or quantum):

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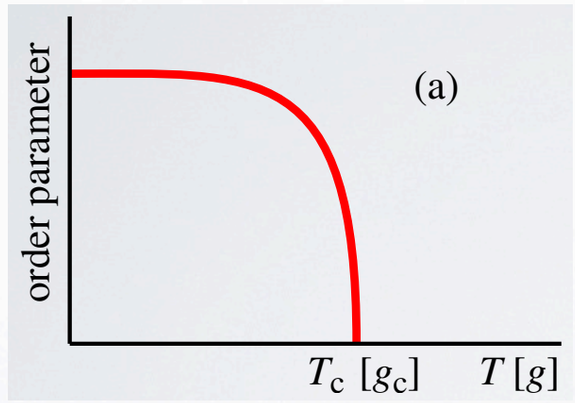

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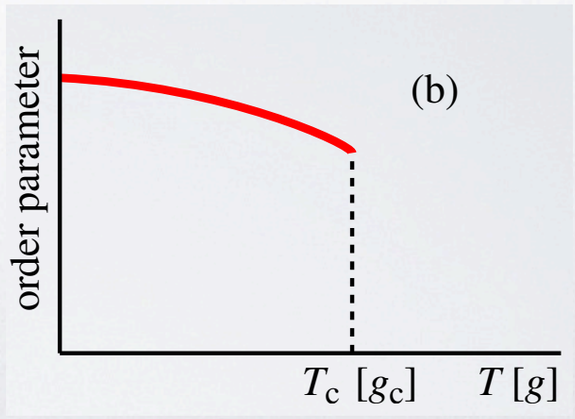

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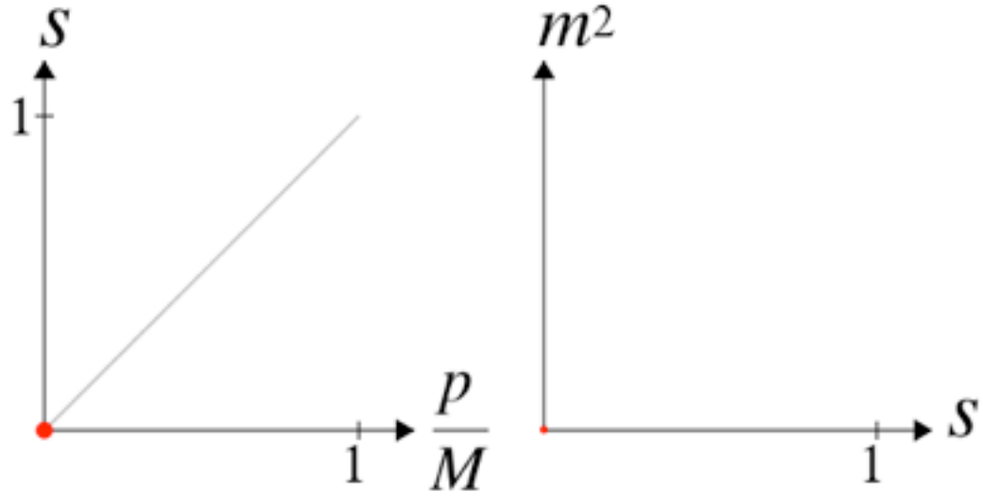
Will use for spin glasses of interest in quantum computing

Apply to well-understood classical system first...

Kibble-Zurek scaling in imaginary time

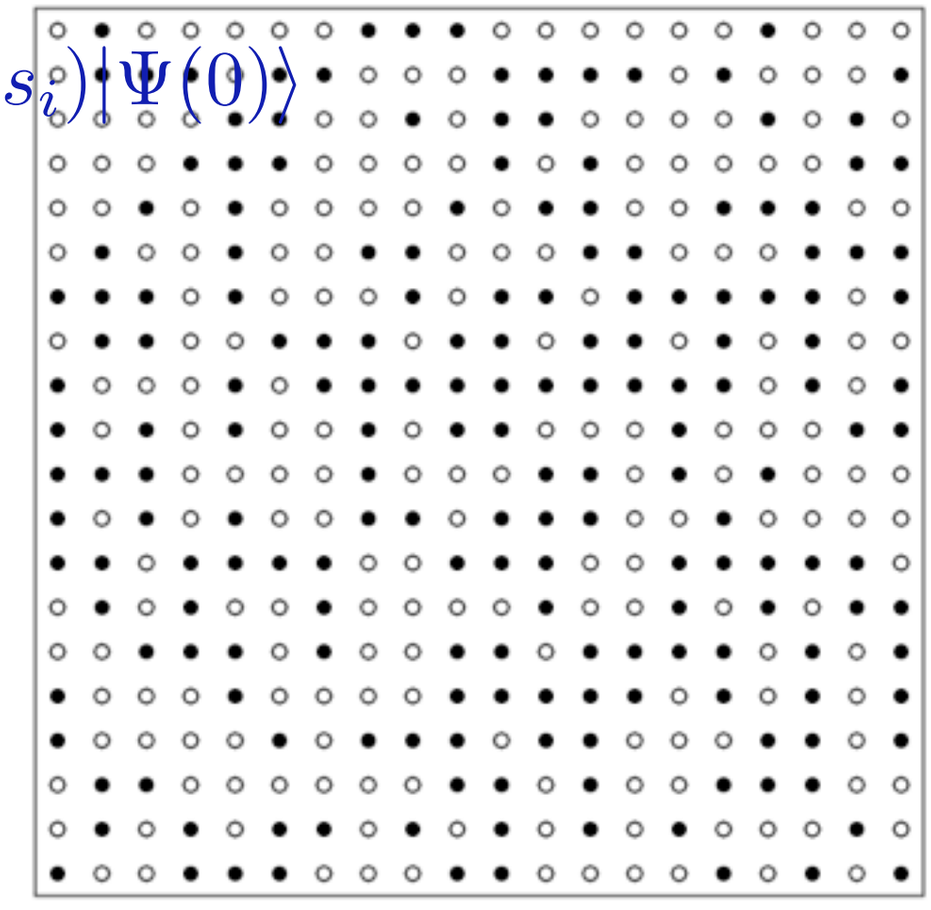
Test on clean 2D Ising model in transverse field



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...

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

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

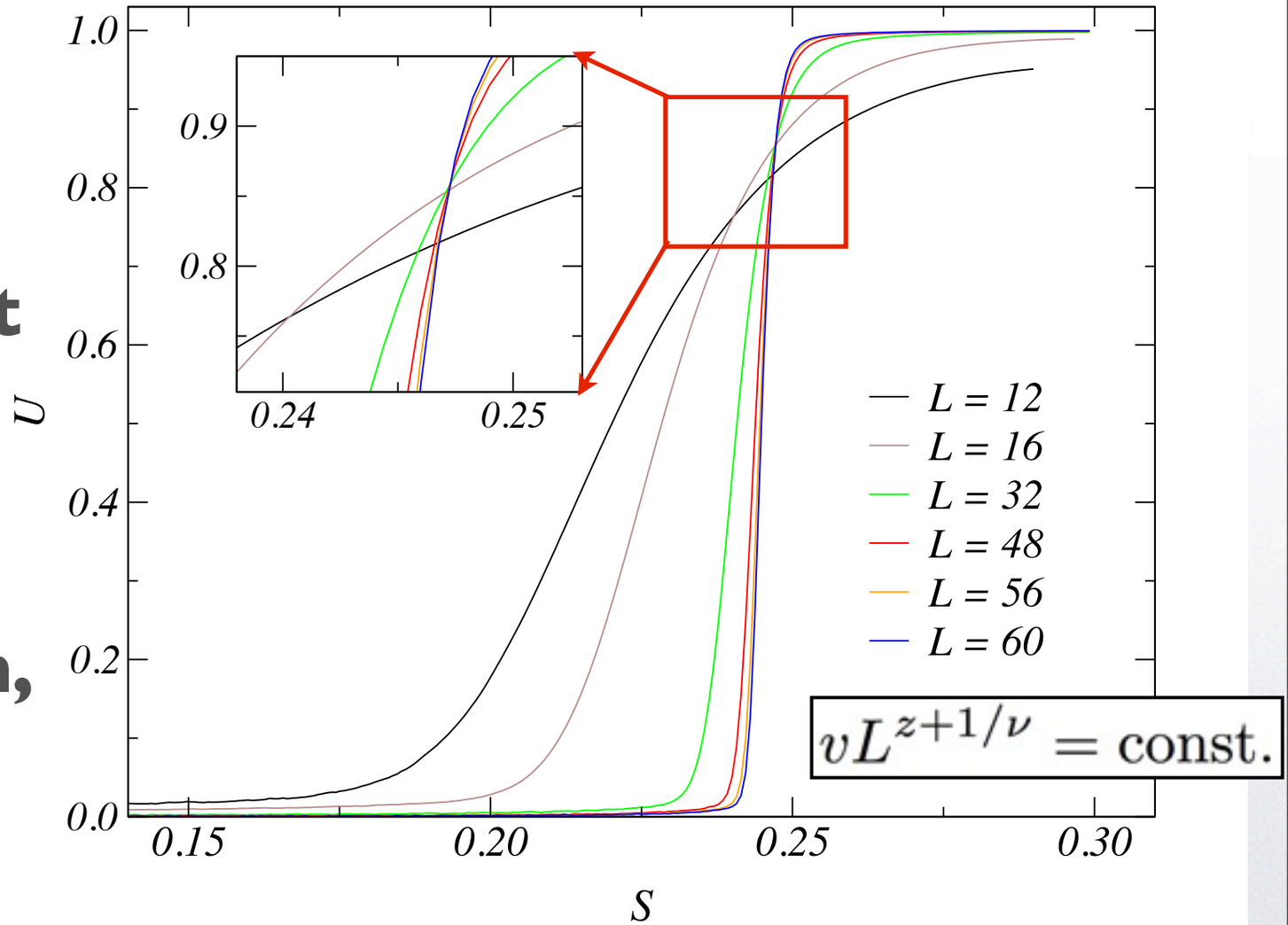
for 1-parameter scaling

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 fromU=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

Note on QMC Simulation Dynamics

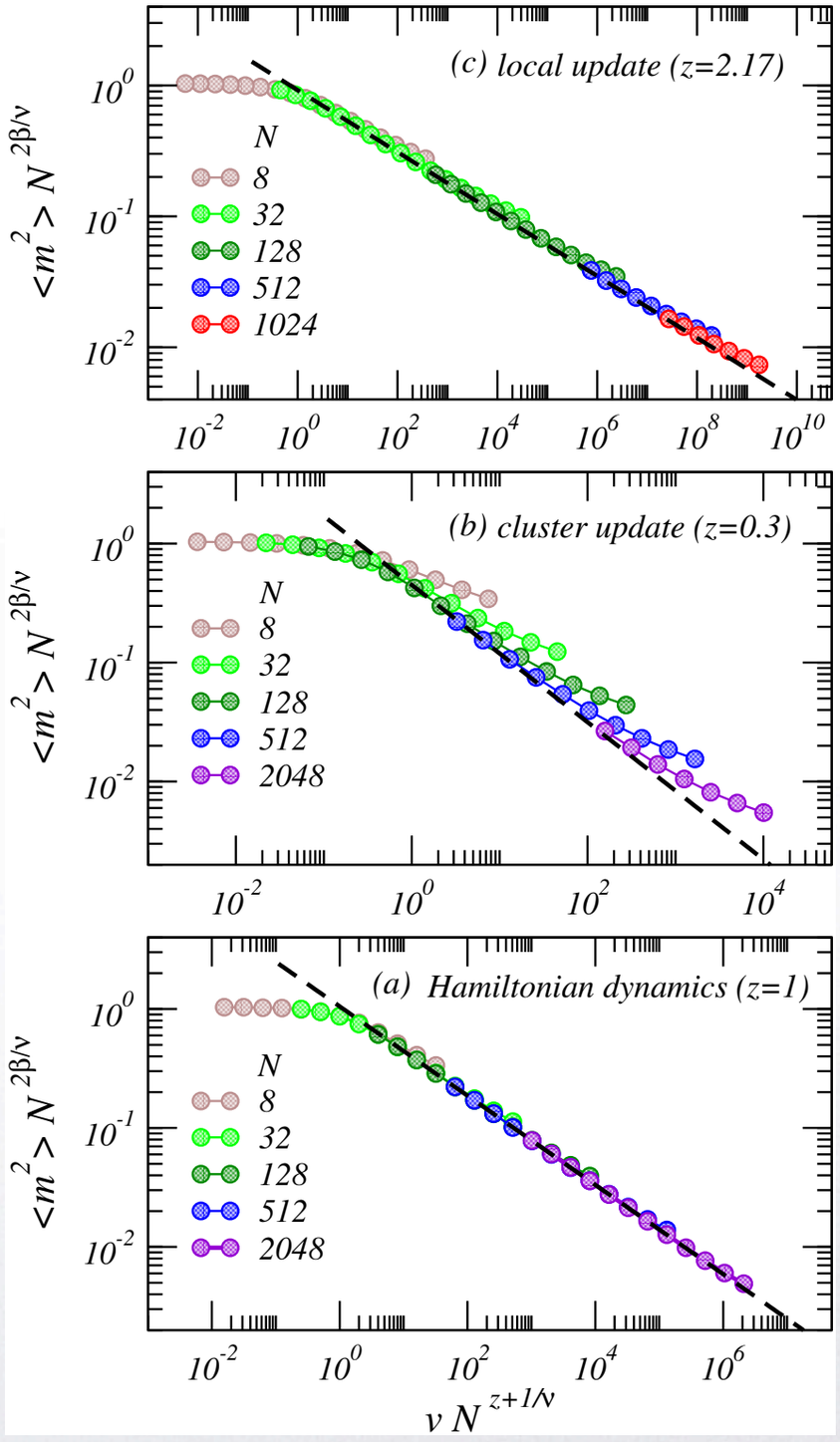
Recent work claimed the D-wave machine shows behavior similar to "simulated quantum annealing"
[S. Boixio, M. Troyer et al., Nat. Phys. 2014]

H(s) evolved in simulation time

Is this the same as Hamiltonian quantum dynamics?

NO! Only accesses the dynamics of the QMC method

Demonstration for 1D Ising model with transverse field shows this
z =1 for true Hamiltonian dynamics
z = 2.17 or z=0.30 for simulation-time dynamics (local or cluster updates)

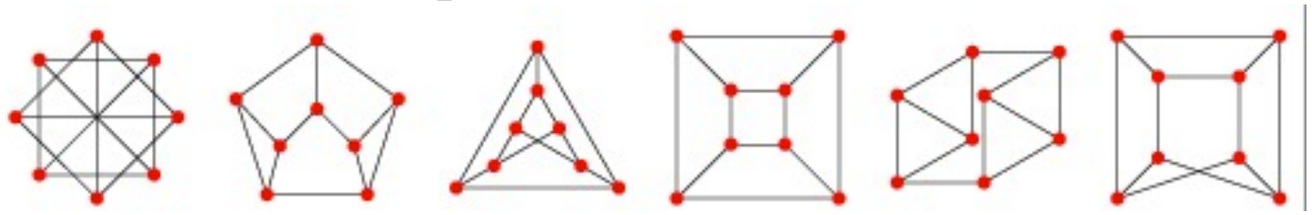


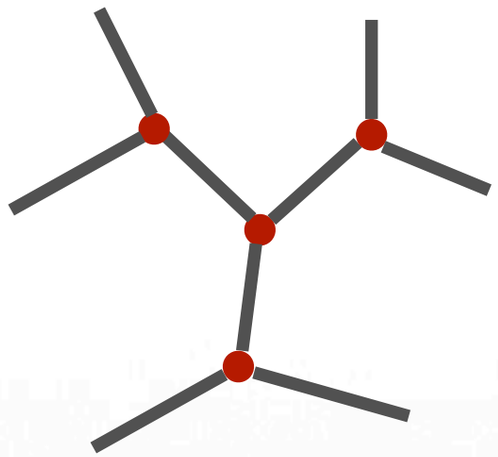
Imaginary-time method = true Hamiltonian dynamics

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 recently:

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

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

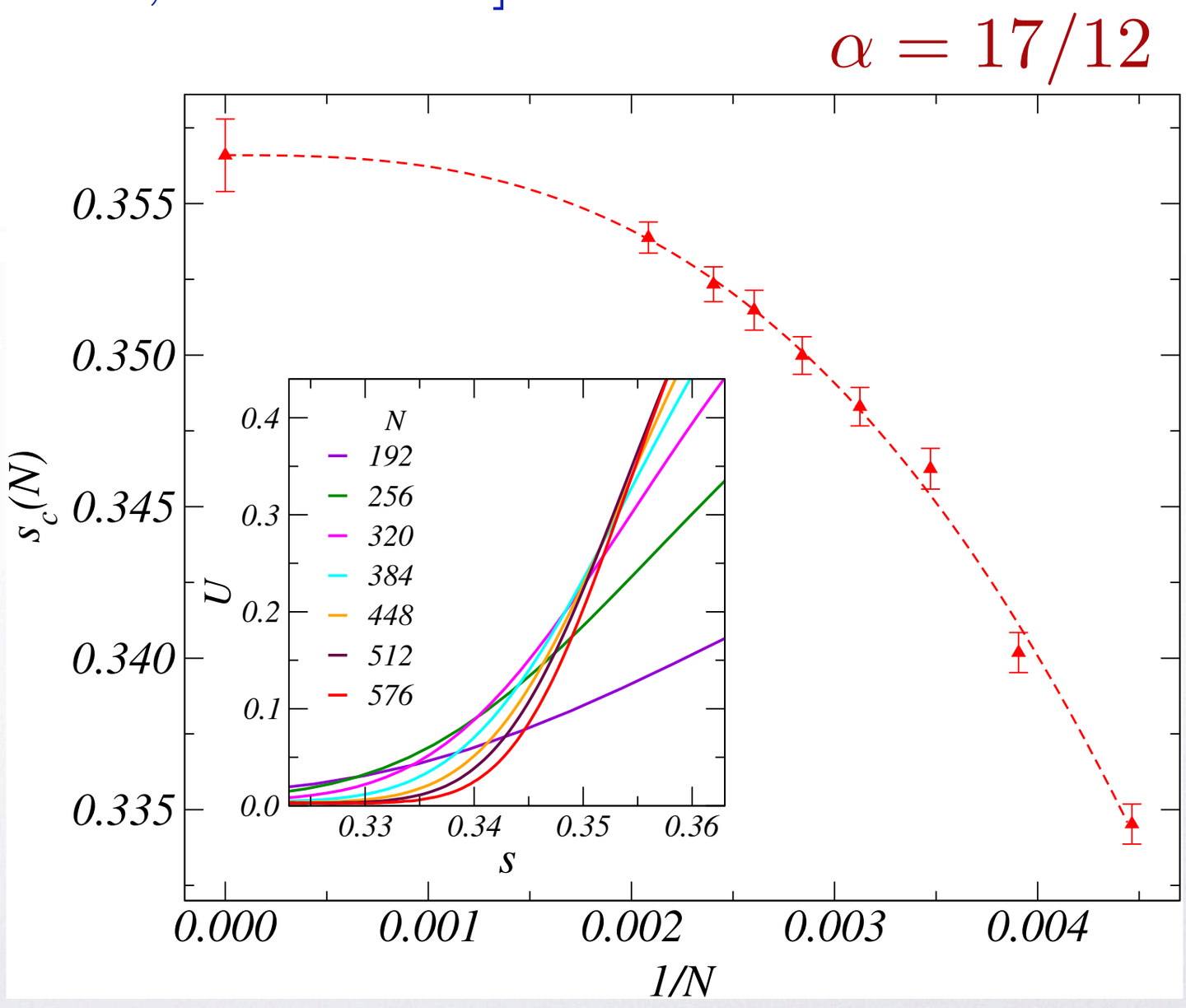
- do several α

- 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

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

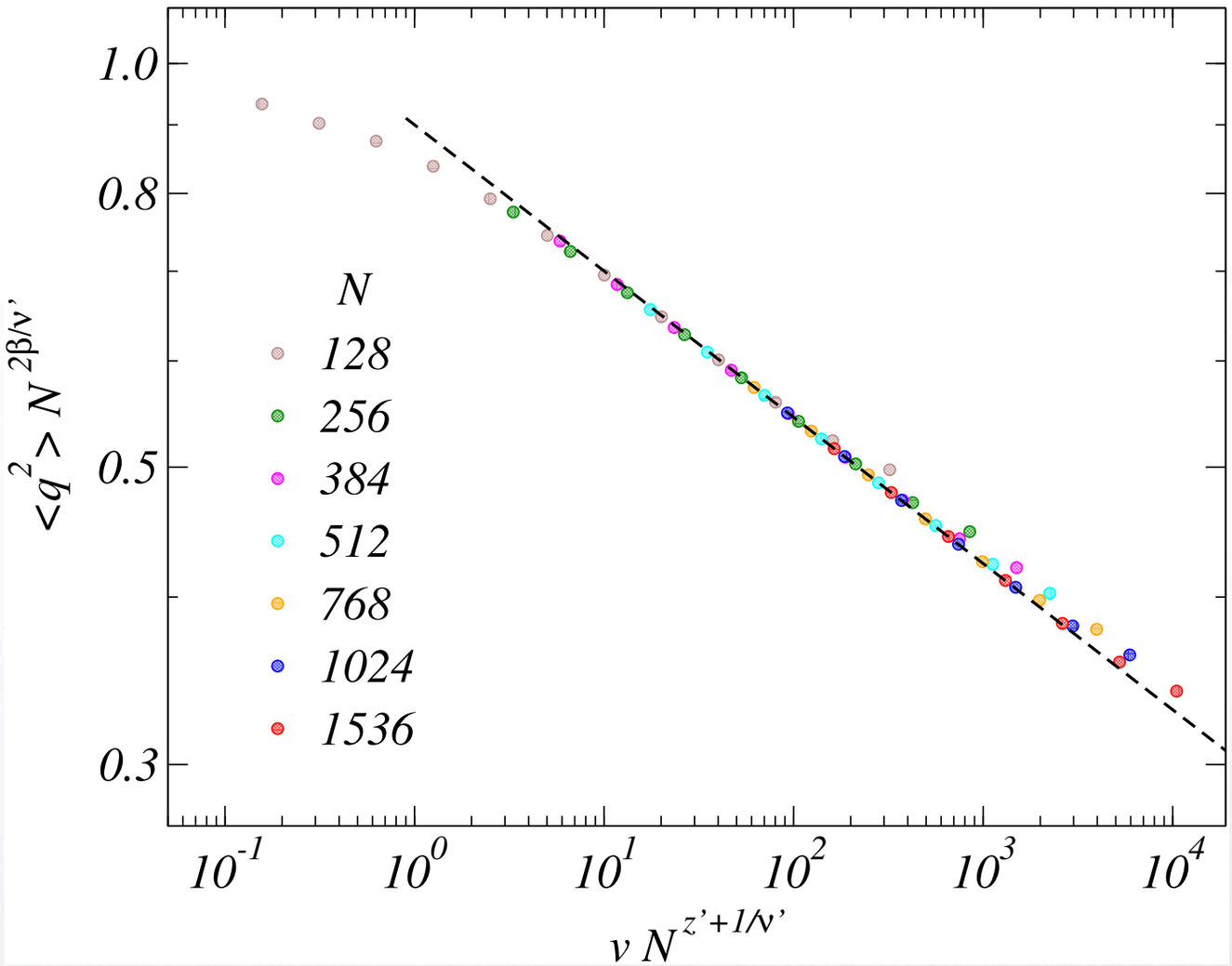
Same as fully connected (Sherrington-Kirkpatrick)?

$\beta/\nu' \approx 0.42(2)$
$z'+1/\nu' \approx 1.4(2)$

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

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

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



Why disagreement?
- log corrections?

Significance of the exponents

Relevance to Quantum Computing

The time needed to stay adiabatic up to s_c scales as

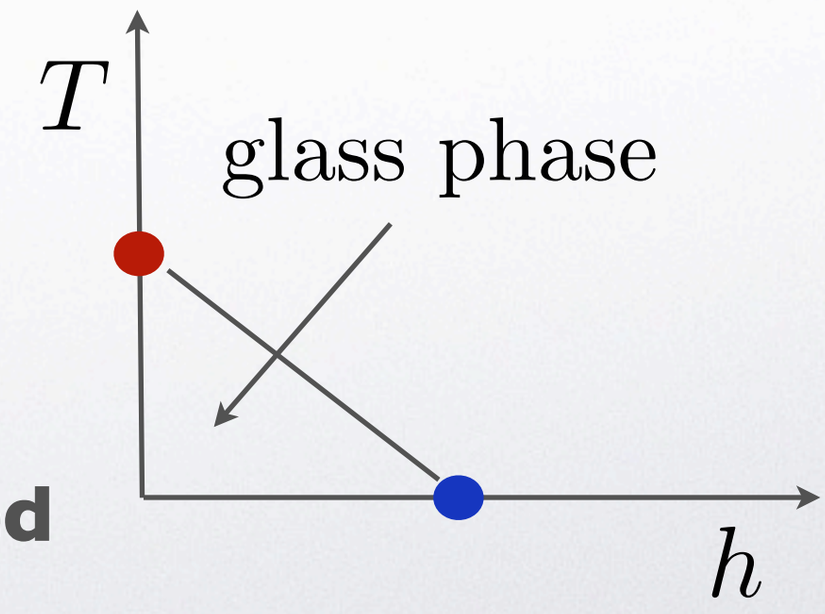
$$t \sim N^{z'+1/\nu} \qquad z' + 1/\nu' \approx 1.3$$

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**
β/ν' = 1/3	**β/ν' ≈ 0.43**
z'+1/ν' = 1	**z'+1/ν' ≈ 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!