Quantum and classical annealing in spin glasses and quantum computing

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C.-W. Liu, A. Polkovnikov, A. W. Sandvik, arXiv:1409.7192

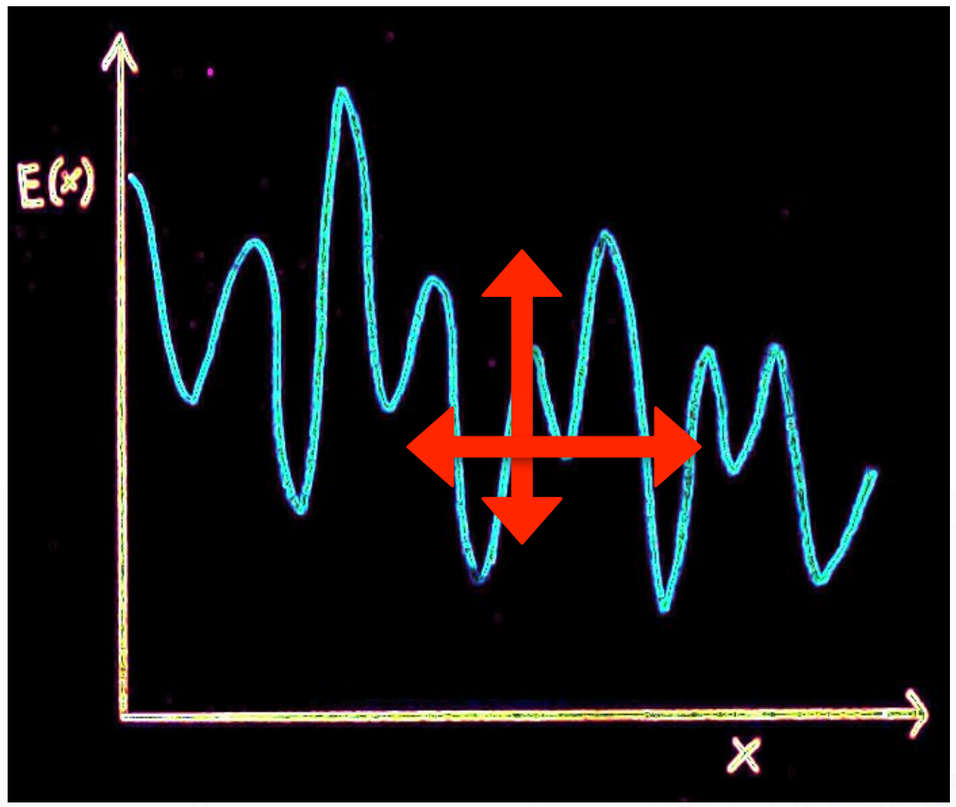
Outline

Classical (thermal) fluctuations

versus

Quantum fluctuations (tunneling)

- **Computational studies of model systems (spin glasses)**
- **Relevance for adiabatic quantum computing**

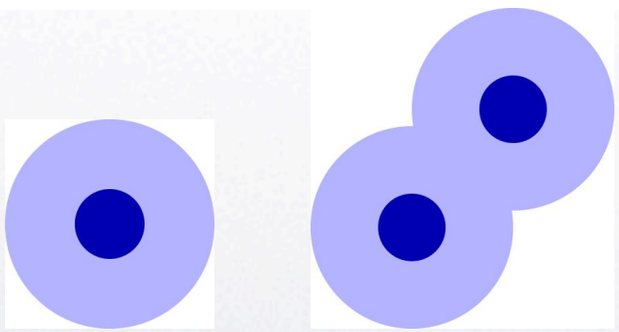


- **Monte Carlo simulations and simulated annealing**
- **Quantum annealing for quantum computing**
- **Classical and quantum spin glasses**
- **Dynamical critical scaling**

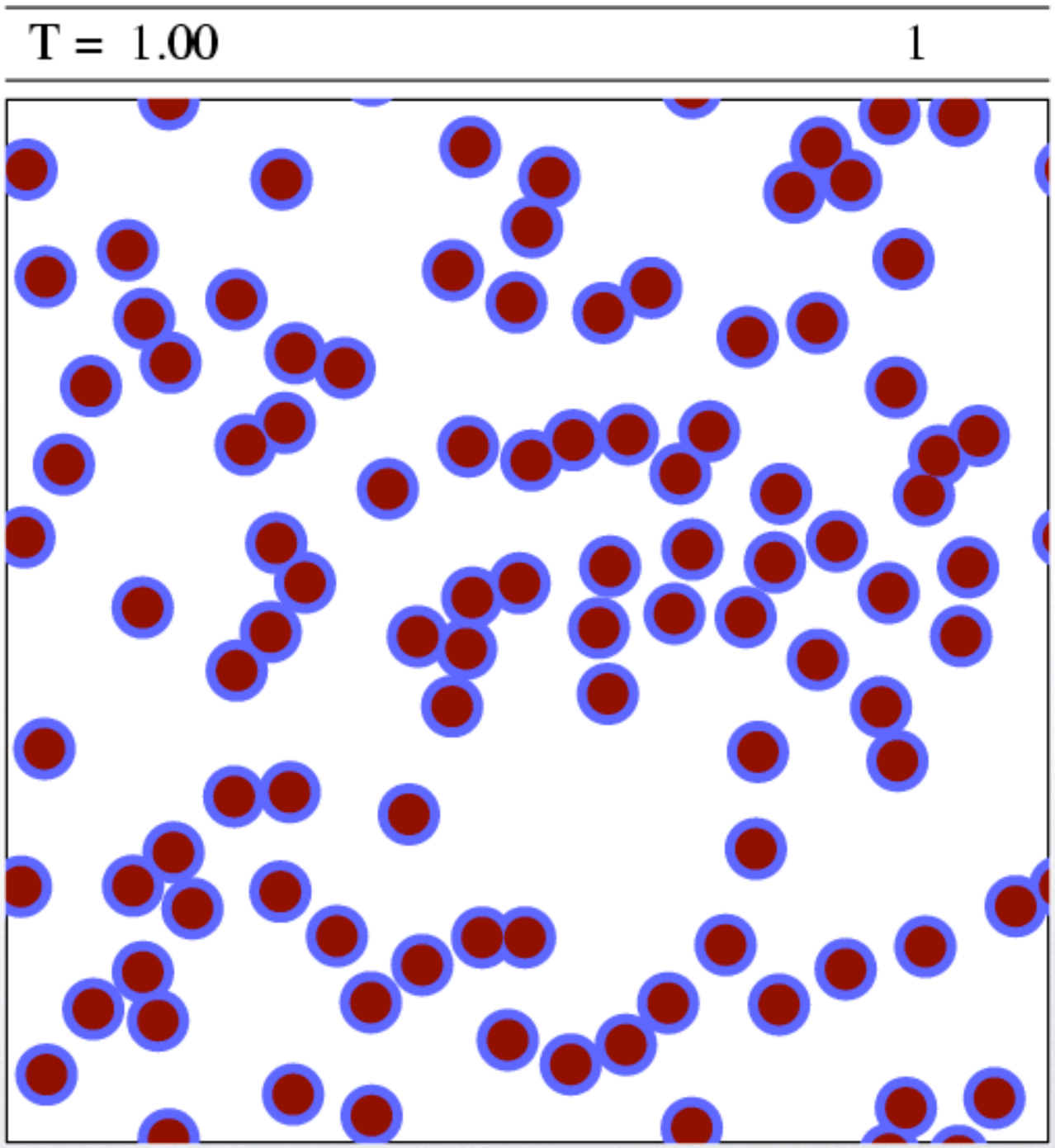
Monte Carlo Simulations

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

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

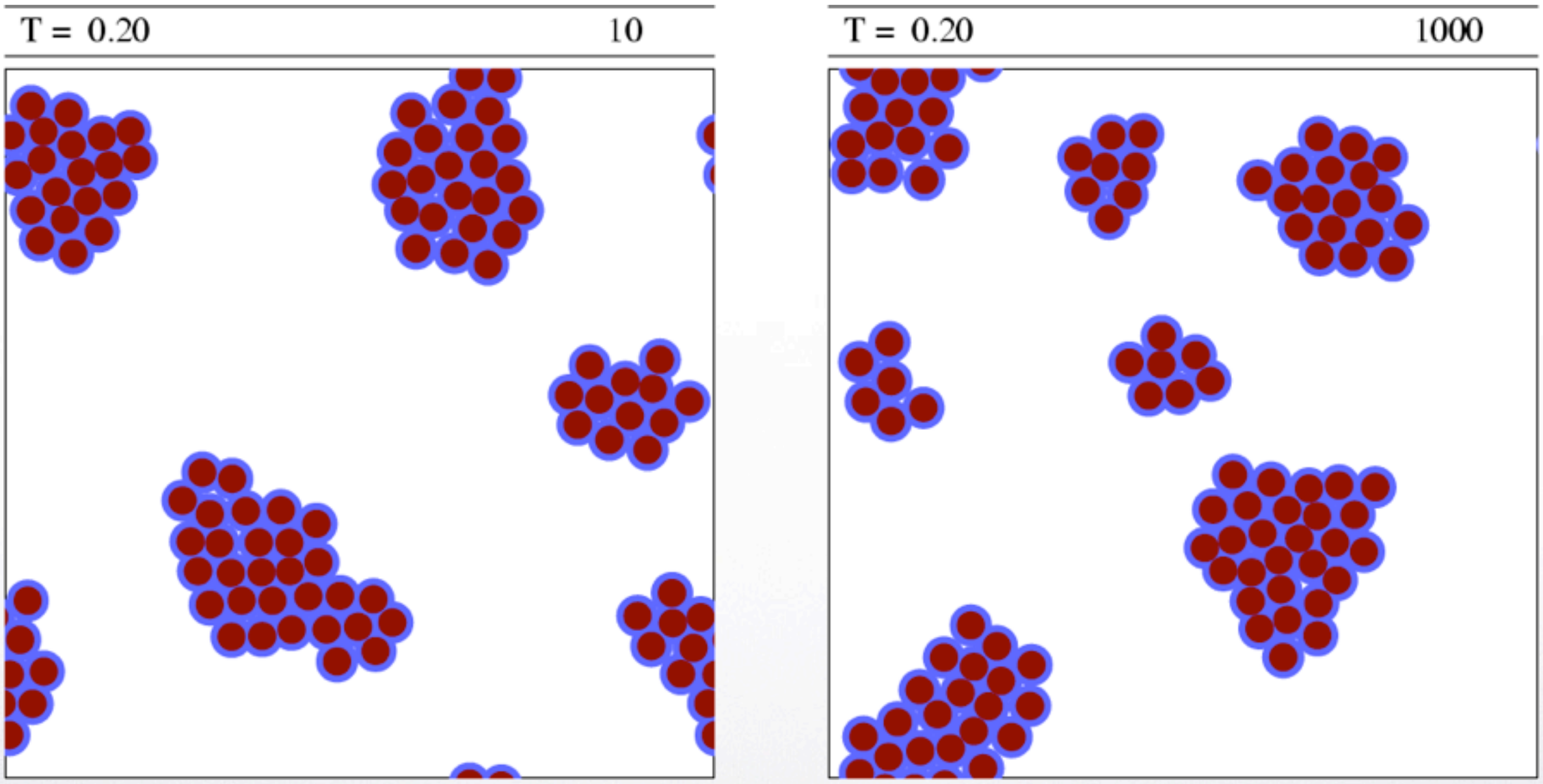


$$P(\{r_i\}) \propto e^{-E/T}, \quad E = \sum_{r_1, r_2} V(r_i - r_j)$$



What happens when the temperature is lowered ?

Monte Carlo Simulations



Transition into liquid state has taken place

Slow movement & growth of droplets

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

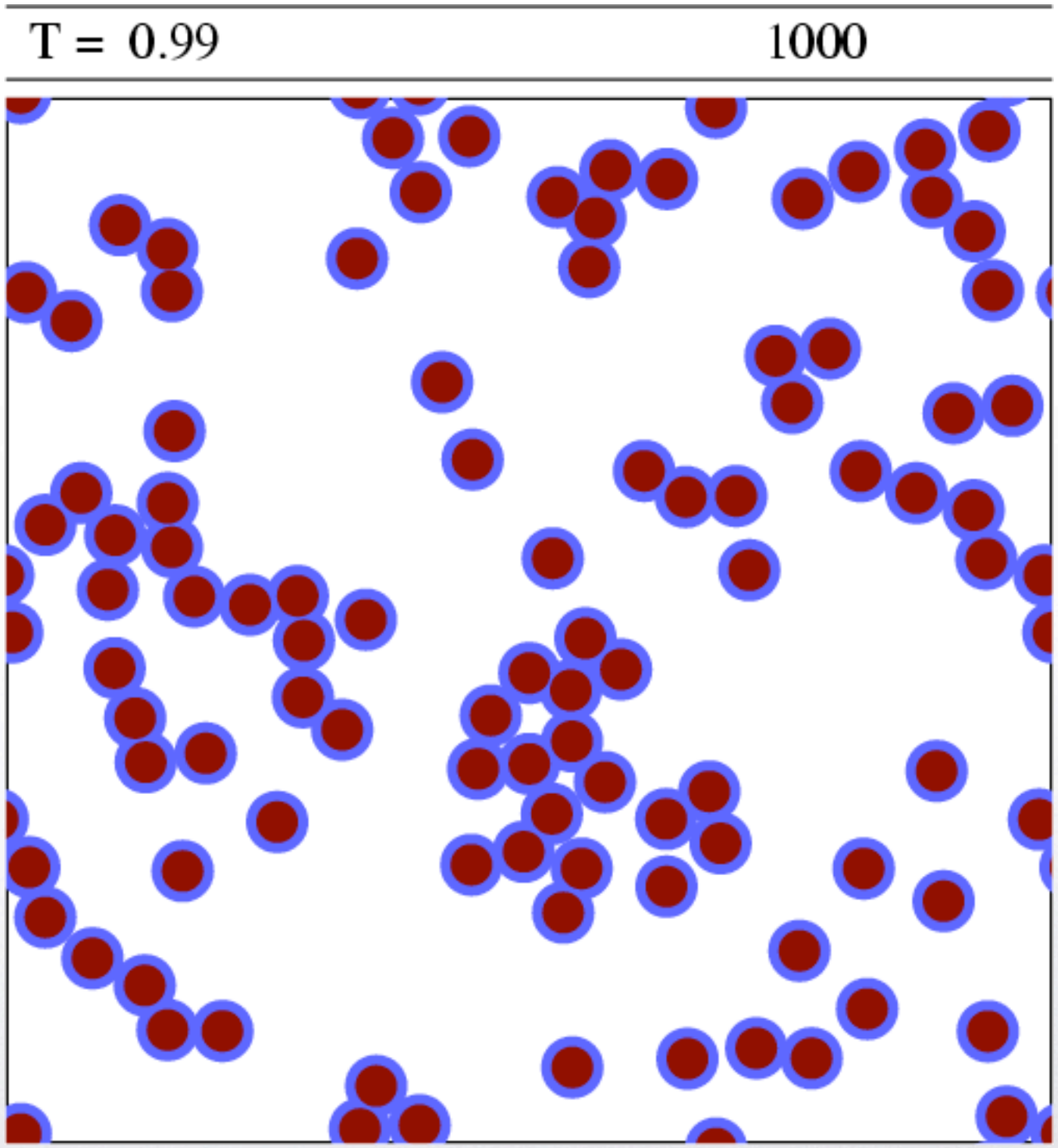
Simulated Annealing

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?

Quantum Annealing

Reduce quantum fluctuations as a function of time

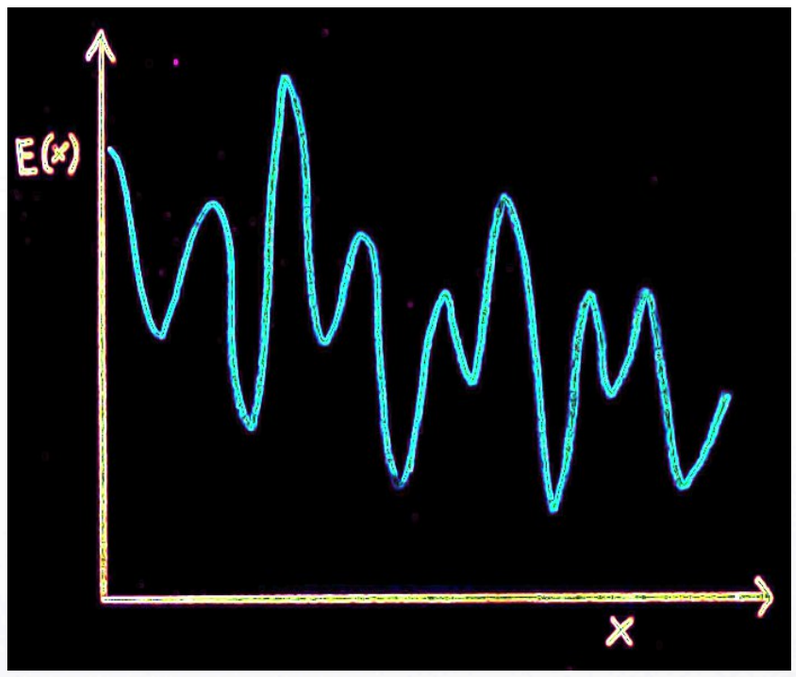
- start with a simple quantum Hamiltonian (s=0)

- end with a complicated classical potential (s=1)

$$H(s) = sH_{\text{classical}} + (1-s)H_{\text{quantum}}$$

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

$$H_{\text{classical}} = V(x) \quad H_{\text{quantum}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$



Adiabatic Theorem:

If the velocity v is small enough the system stays in the ground state of H[s(t)] at all times

At $t=t_{max}$ we then know the minimum of V(x): $\Psi(x) = \delta(x - x_0)$

Can quantum annealing be more efficient than thermal annealing?

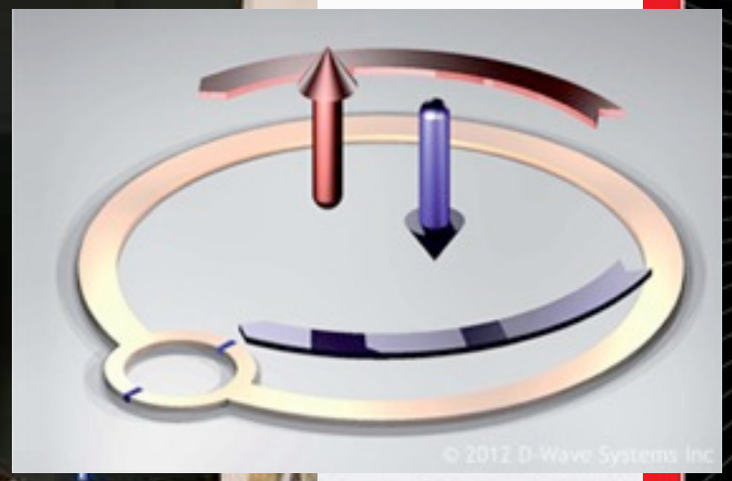
Ray, Chakrabarty,Chakrabarty (PRB 1989), Kadowaki, Nishimory (PRE 1998),...

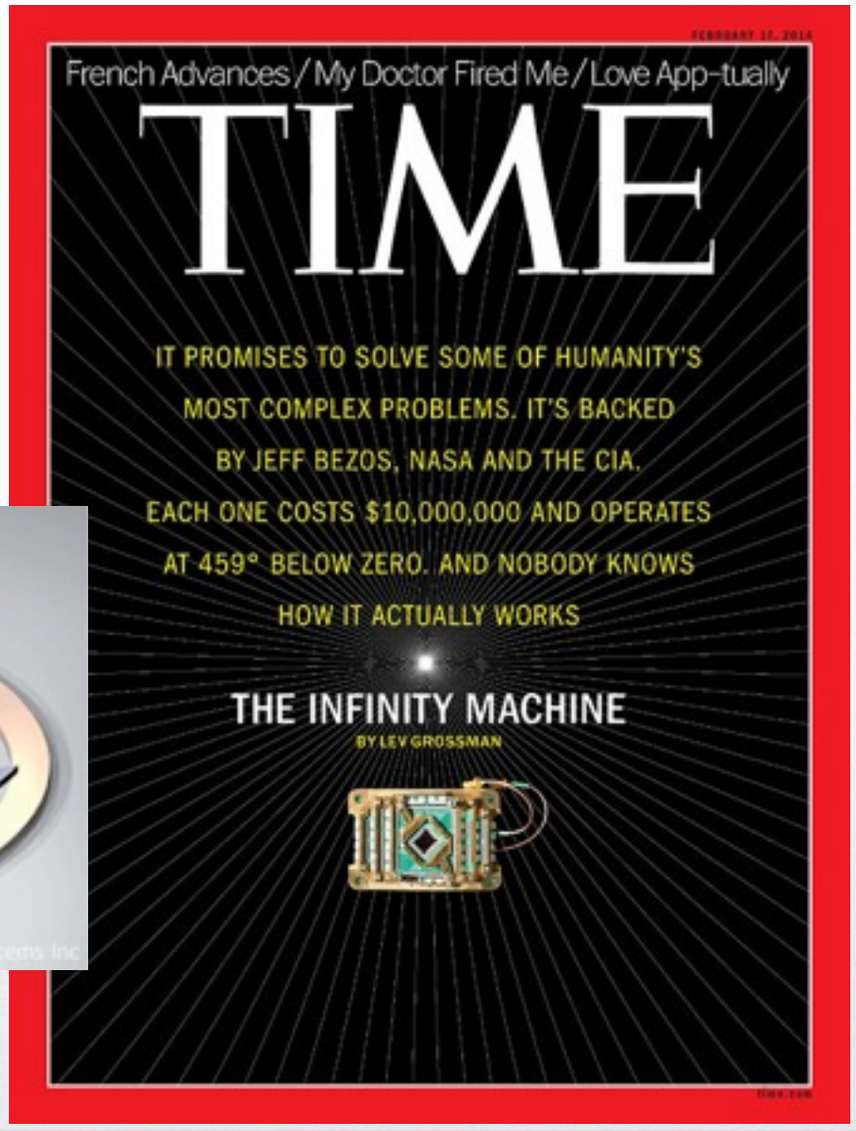
Useful paradigm for quantum computing?

Quantum Annealing & Quantum Computing

D-wave "quantum annealer"; 512 flux q-bits

- **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)?**



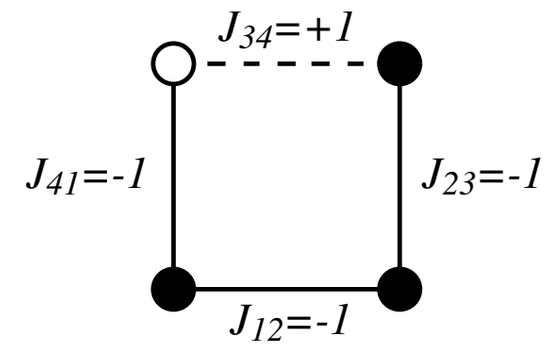


Hamiltonian implemented in D-wave quantum annealer....

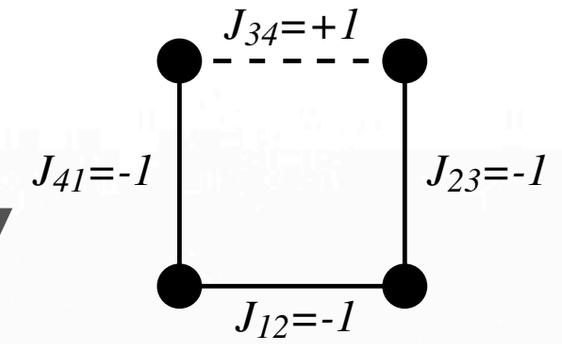
Spin Glasses

Ising models with frustrated interactions

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



Hard to find ground states if the interactions are highly frustrated (spin glass phase)
- many states with same or almost same energy



Many (almost all) optimization problems can be mapped onto some general model
- hard problems correspond to spin glass physics

Quantum fluctuations (quantum spin glasses)
- add transversal field Ising (H → H + $H_{quantum}$)

$$H_{\text{quantum}} = -h \sum_{i=1}^{N} \sigma_i^x = -h \sum_{i=1}^{N} (\sigma_i^+ + \sigma_i^-)$$

The D-wave machine is based on this model on a special lattice

Nature of ground states of H depends on h and $\{J_{ij}\}$

Quantum Phase Transition

There must be a quantum phase transition in the system

$$H(s) = sH_{\text{classical}} + (1-s)H_{\text{quantum}}$$

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 $s=s_c$

<u>Simple example:</u> 1D transverse-field Ising ferromagnet

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

- trivial x-oriented ferromagnet at s=0 (→→→)

- z-oriented (↑↑↑ or ↓↓↓, symmetry broken) at s=1

- s_c=1/2 (exact solution, mapping to free fermions)

Have to pass through s_c and beyond adiabatically

- how long does it take? $s = s(t) = vt, \quad v = 1/t_{\max}$

Let's look at a simpler problem first...

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

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

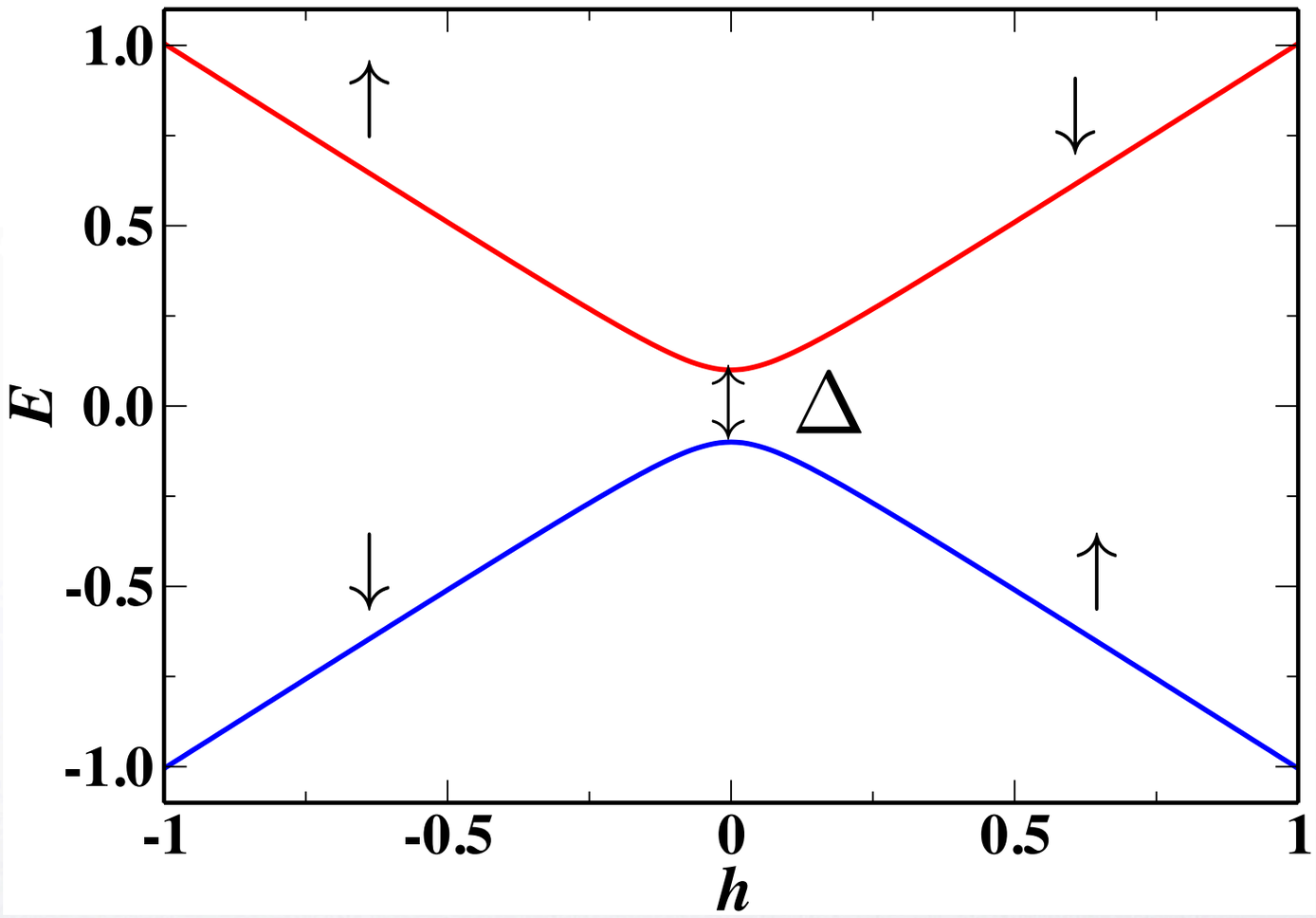
Smallest gap: Δ=2ε

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

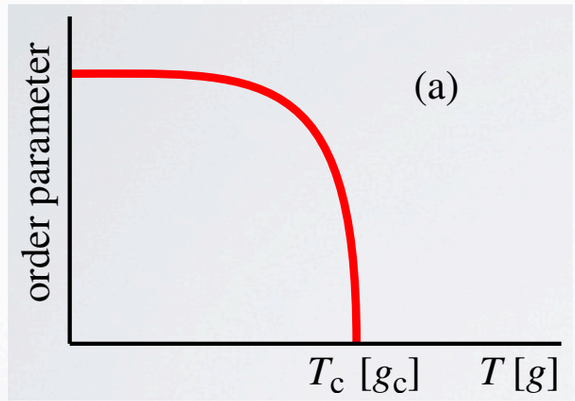
$$\xi_r \sim |\delta|^{-\nu}, \qquad \xi_t \sim \xi_r^z \sim |\delta|^{-\nu z}$$

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

Continuous quantum phase transition

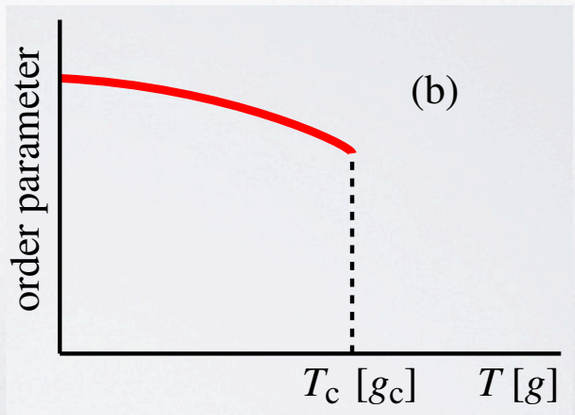
- excitation gap at the transition depends on the system size and z as

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



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 more than z

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

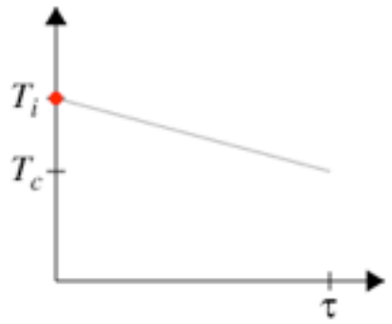
$$A(\delta, v, L) = L^{-\kappa/\nu} g(\delta L^{1/\nu}, v L^{z+1/\nu})$$

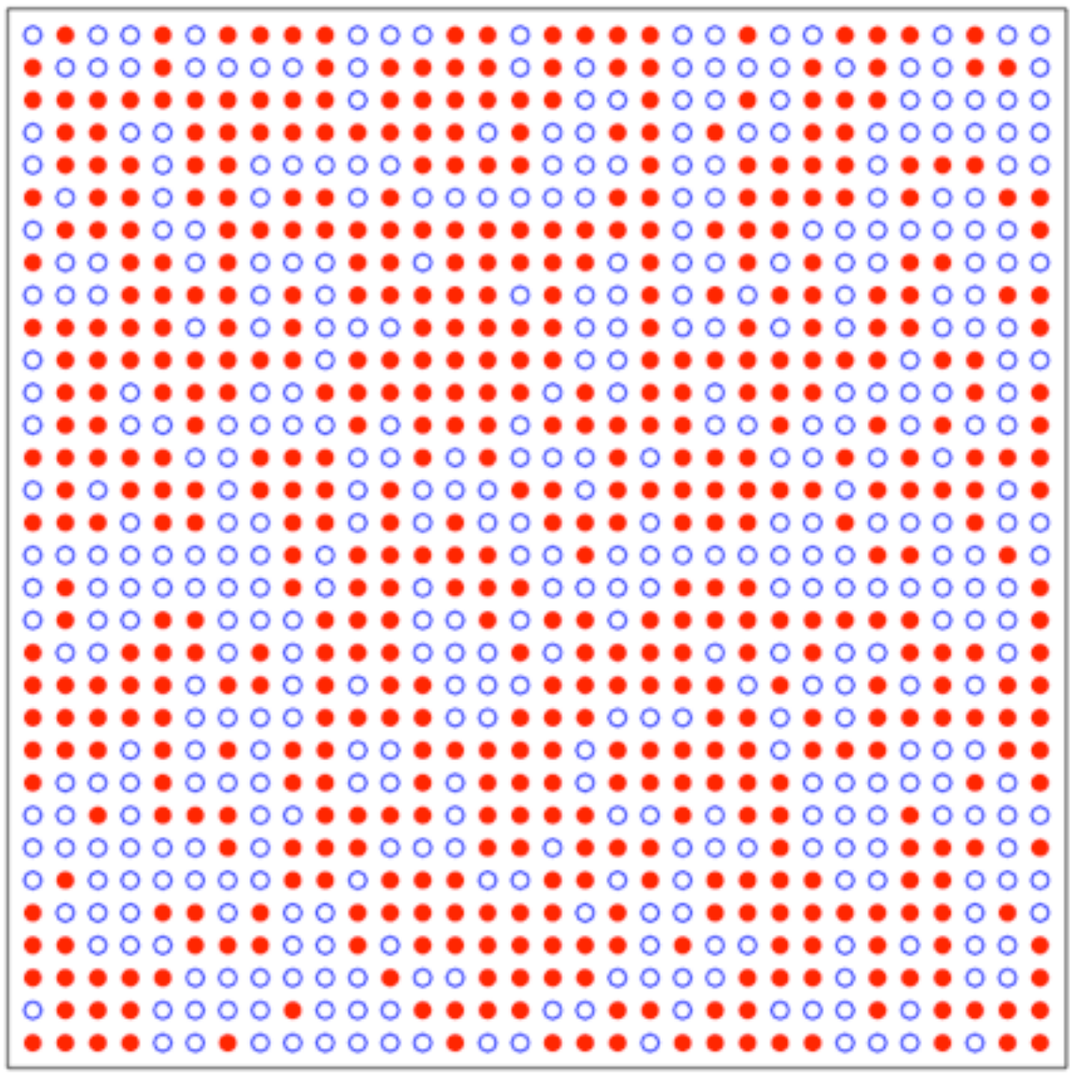
$$A(\delta, v, N) = N^{-\kappa/\nu'} g(\delta N^{1/\nu'}, v N^{z'+1/\nu'}), \quad \nu' = d\nu, \; z = z/d$$

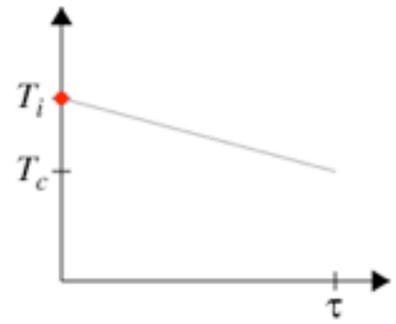
Will use for spin glasses of interest in quantum computing

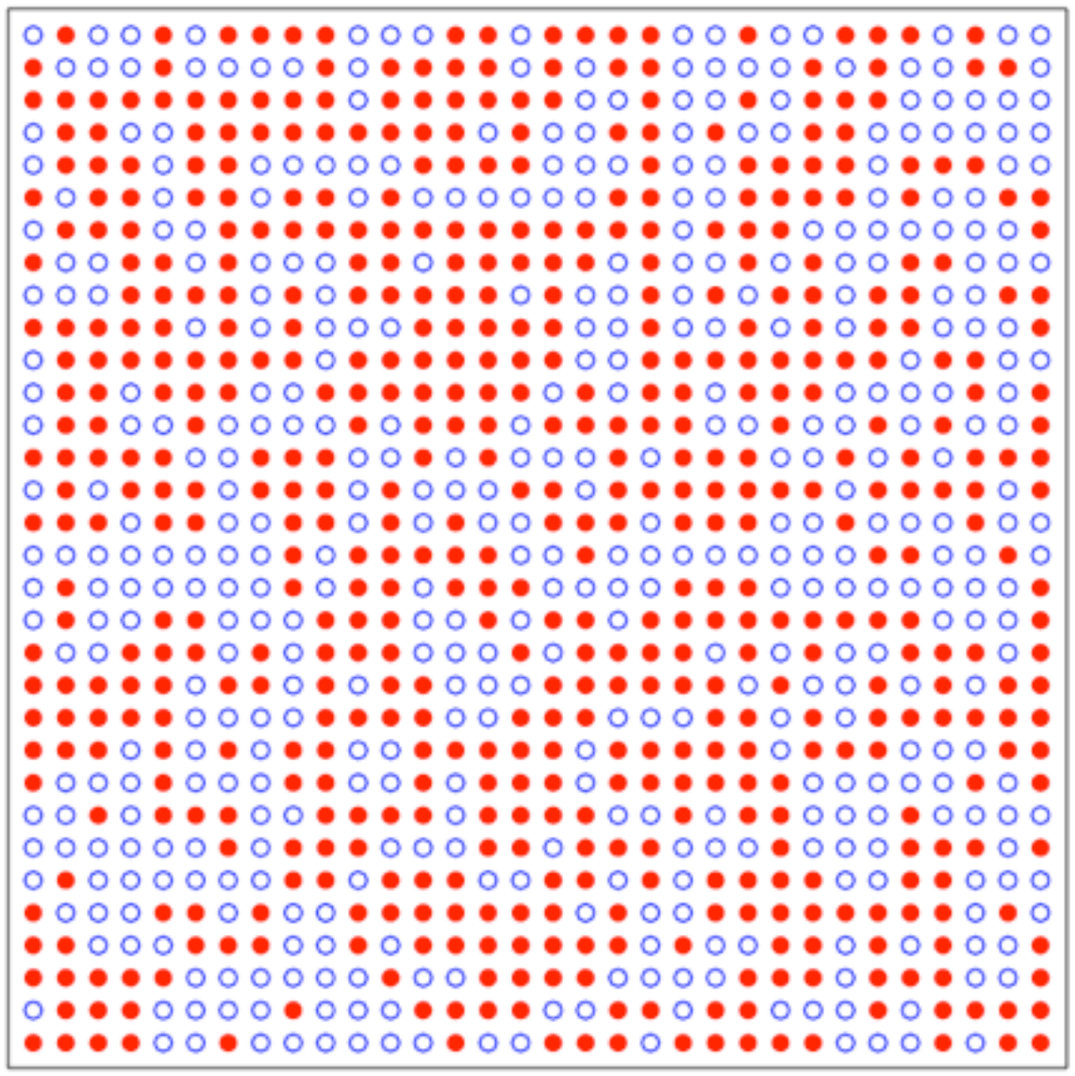
Apply to well-understood clean system first...

Fast and Slow Classical Ising Dynamics







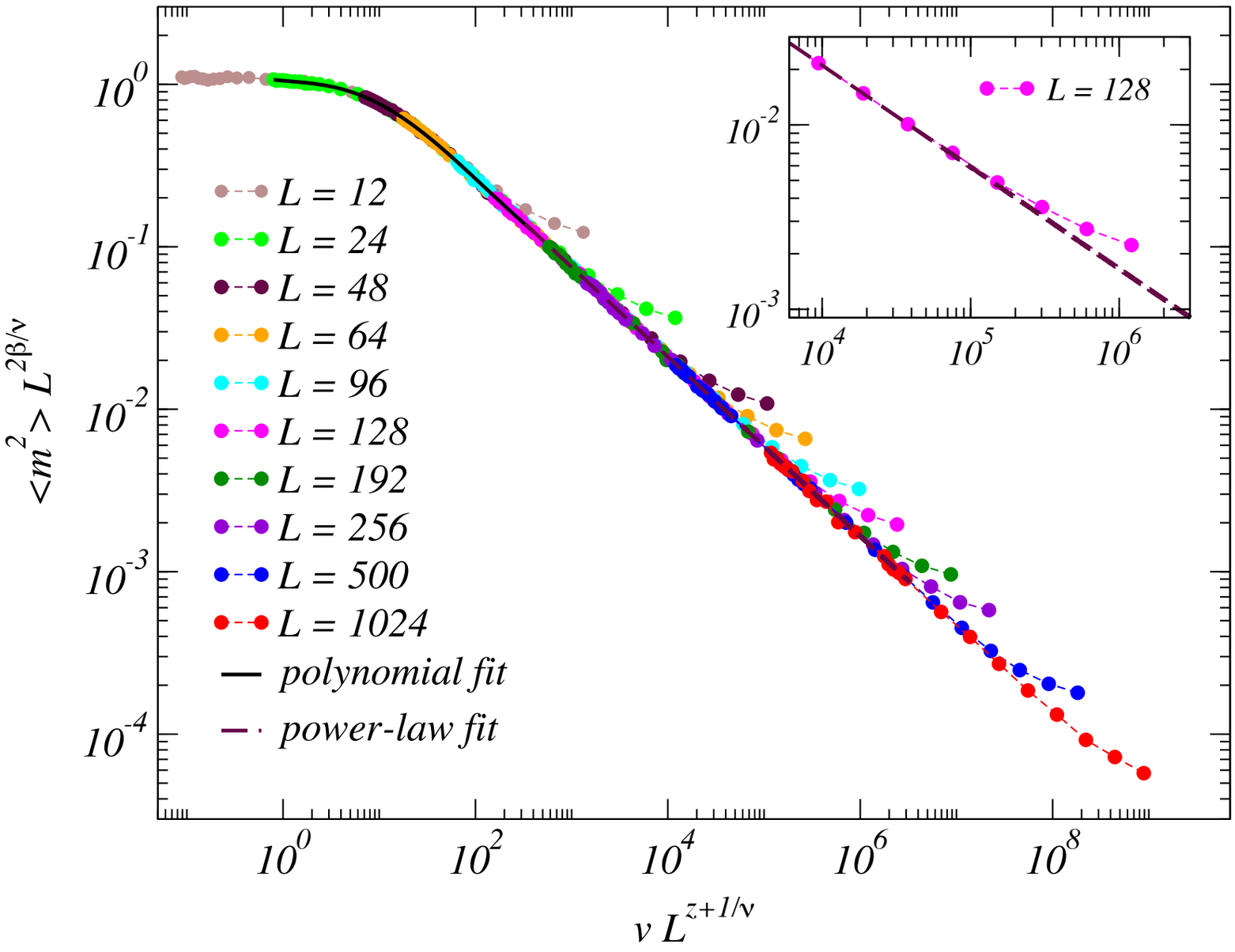


Repeat many times, collect averages, analyze,....

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

Result: z ≈2.17 consistent with values obtained in other ways

Liu, Polkovnikov, Sandvik, PRB 2014

Can we do something like this for quantum models?

Quantum Evolution in Imaginary Time

Schrödinger dynamic at imaginary time t=-iτ

$$|\Psi(\tau)\rangle = U(\tau,\tau_0)|\Psi(\tau_0)\rangle$$

Time evolution operator

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

Dynamical exponent z same as in real time!

(DeGrandi, Polkovnikov, Sandvik, PRB2011)

- **Can be implemented in quantum Monte Carlo**

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

Simpler scheme: evolve with just a H-product

(Liu, Polkovnikov, Sandvik, PRB2013)

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

How does this method work?

QMC Algorithm Illustration

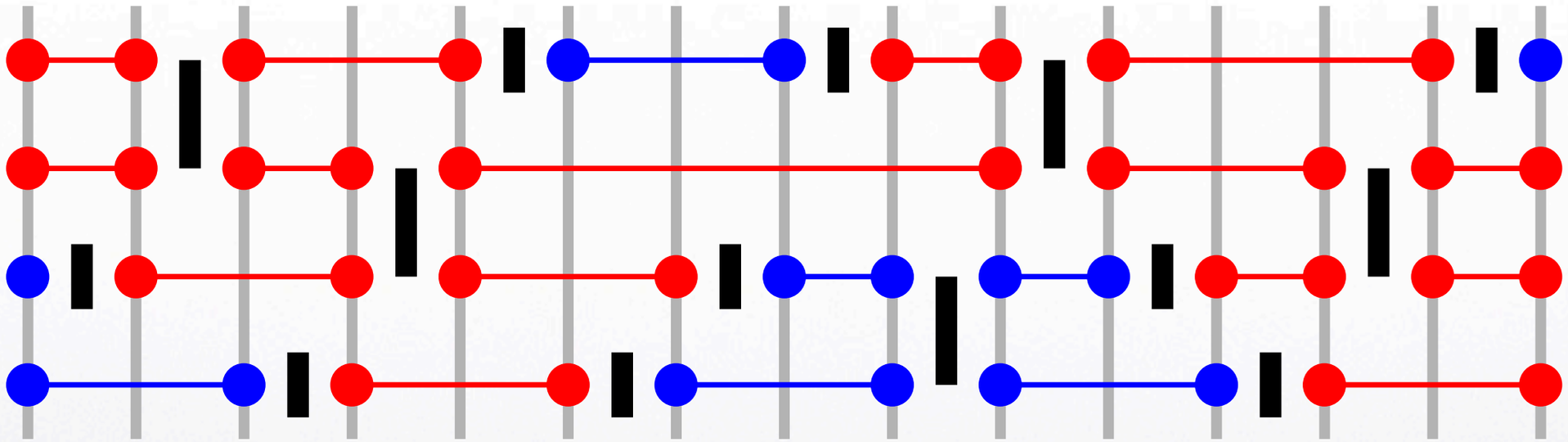
Transverse-field Ising model: 2 types of operators:

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

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

Represented as "vertices"

MC sampling of networks of vertices



Similar to ground-state projector QMC

How to define (imaginary) time in this method?

Time and velocity Definitions

The parameter in H changes as

$$s_i = i\Delta_s, \quad \Delta_s = \frac{s_M}{M}$$

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

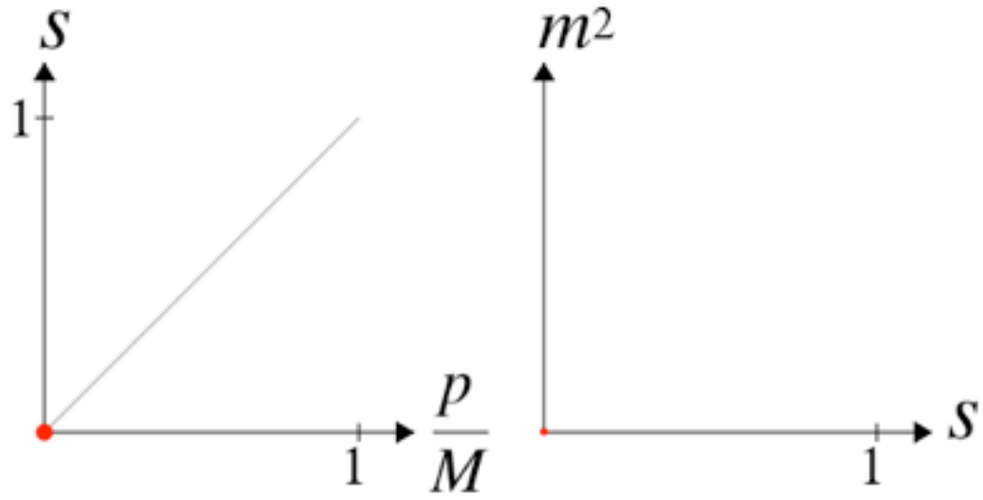
$$v \propto N\Delta_s$$

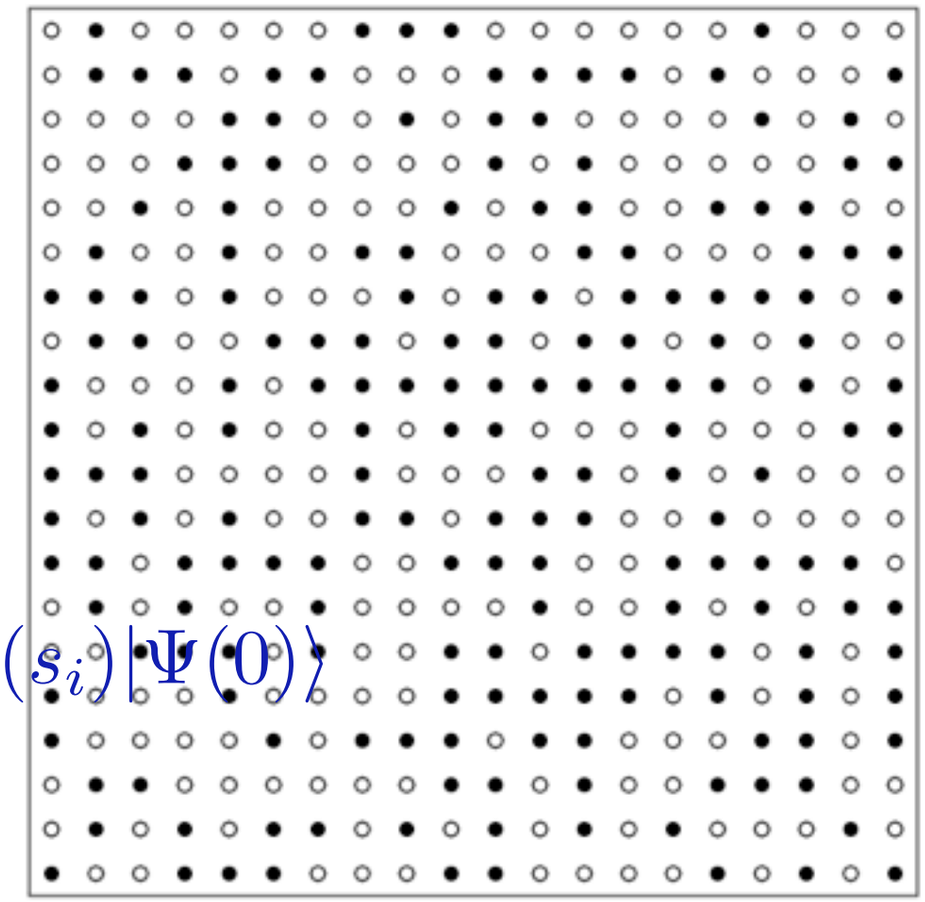
Def reproduces v-dependence in imag-time Schrödinger dynamics to order v (enough for scaling)

To this order we can use "asymmetric" expectation values

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

All s in one simulation!





Collect data, do scaling analysis...

2D Transverse-Ising, Scaling Example

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

If z, ν known, s_c not: use

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

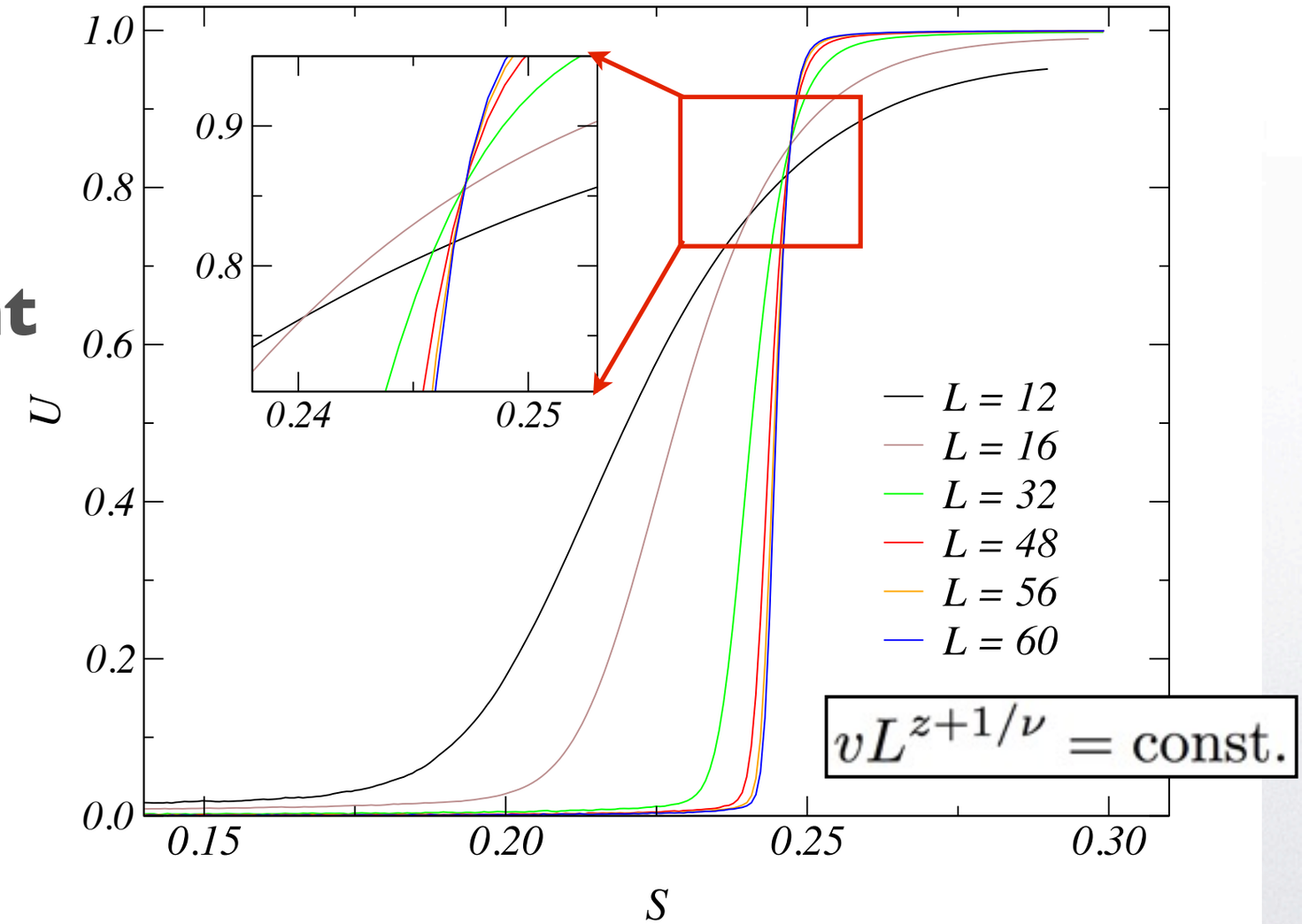
for 1-parameter scaling

Example: Binder cumulant

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

Should have step from U=0 to U=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

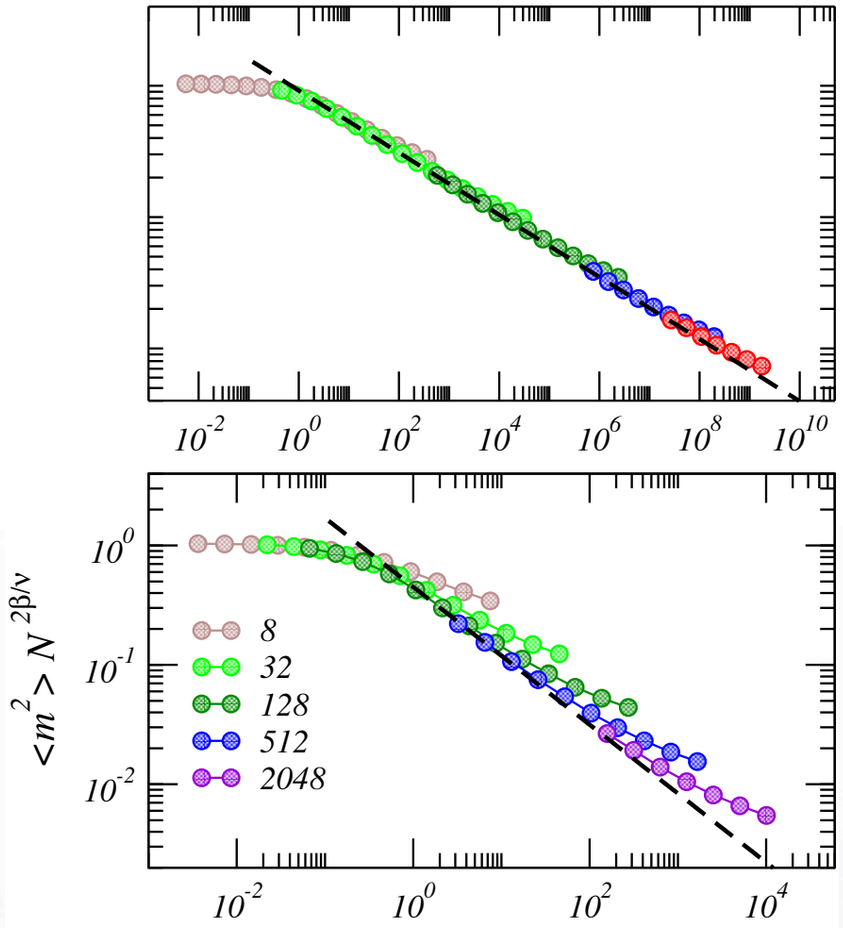
Note on QMC Simulation Dynamics

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

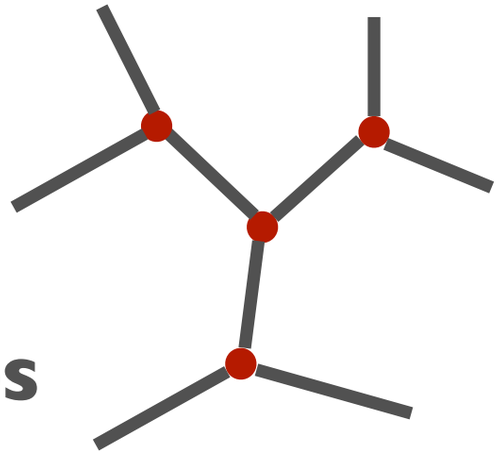
Is this the same as Hamiltonian quantum dynamics?

NO! Only accesses the dynamics of the QMC method

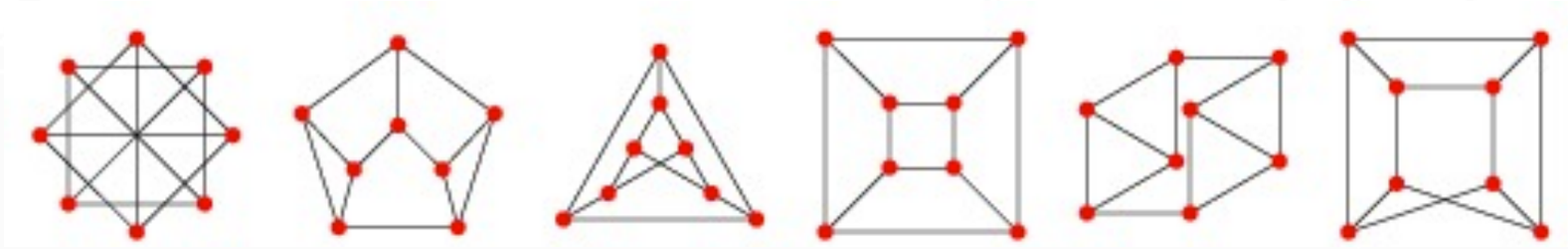


3-regular graphs

Ising spin glass with coordination-number 3
- N spins, randomly connected to each other
- all antiferromagnetic couplings
- frustration because of closed odd-length loops



N=8



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...

Spin-Glass order Parameter

Spin glasses are massively-degenerate
- many "frozen" states
- replica symmetry breaking (going into one state)

Cannot use a standard order parameter such as $\langle m^2 \rangle$
- nor any Fourier mode
- since no periodic ordering pattern

Edwards-Anderson order parameter

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

(1) and (2) are from independent simulations (replicas)
- with same random interactions
- |q| large if the two replicas are in similar states

$\langle q^2 \rangle > 0$ for N $\to \infty$ in spin-glass phase (disorder average)

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

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

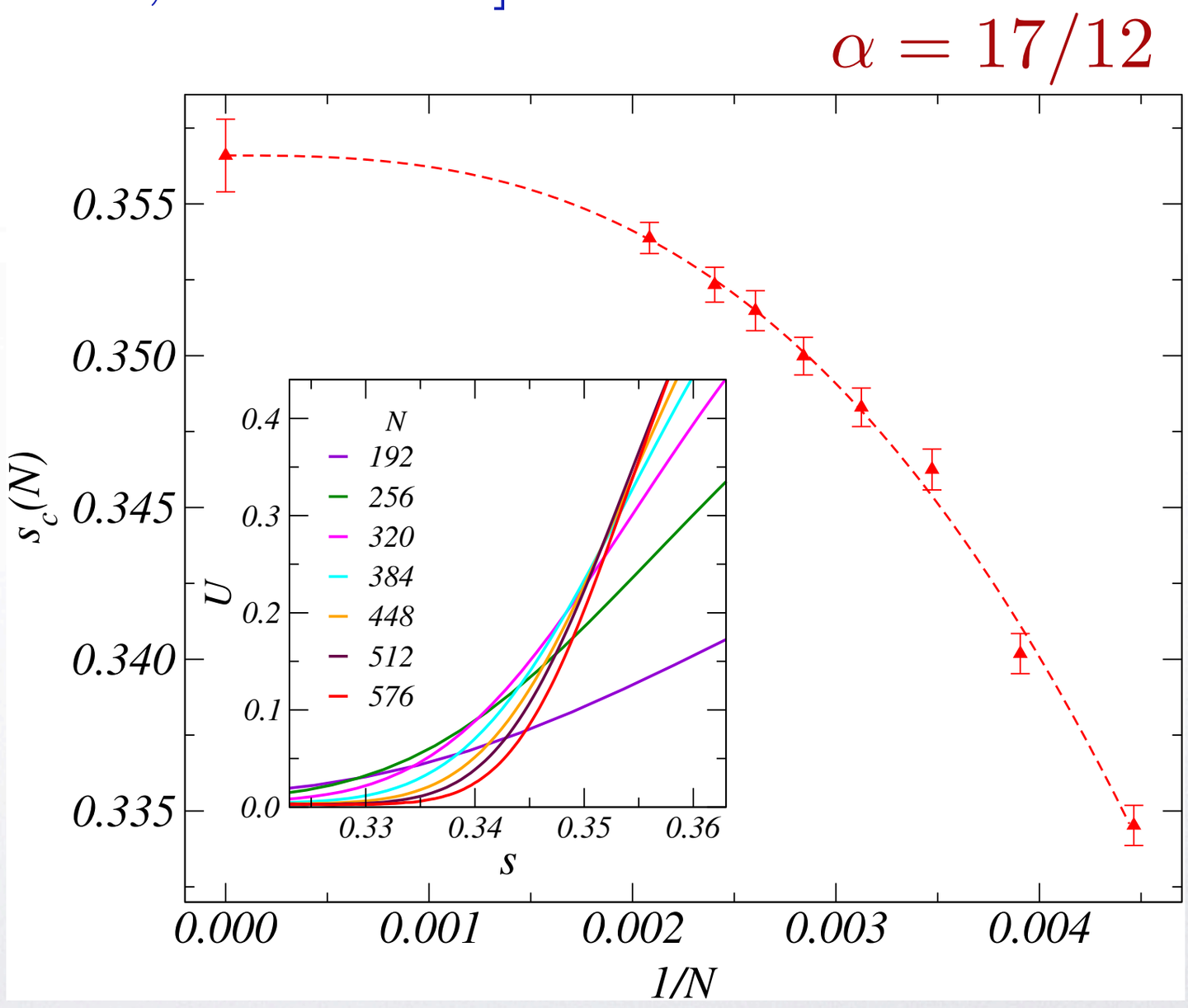
- do several α

- 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**

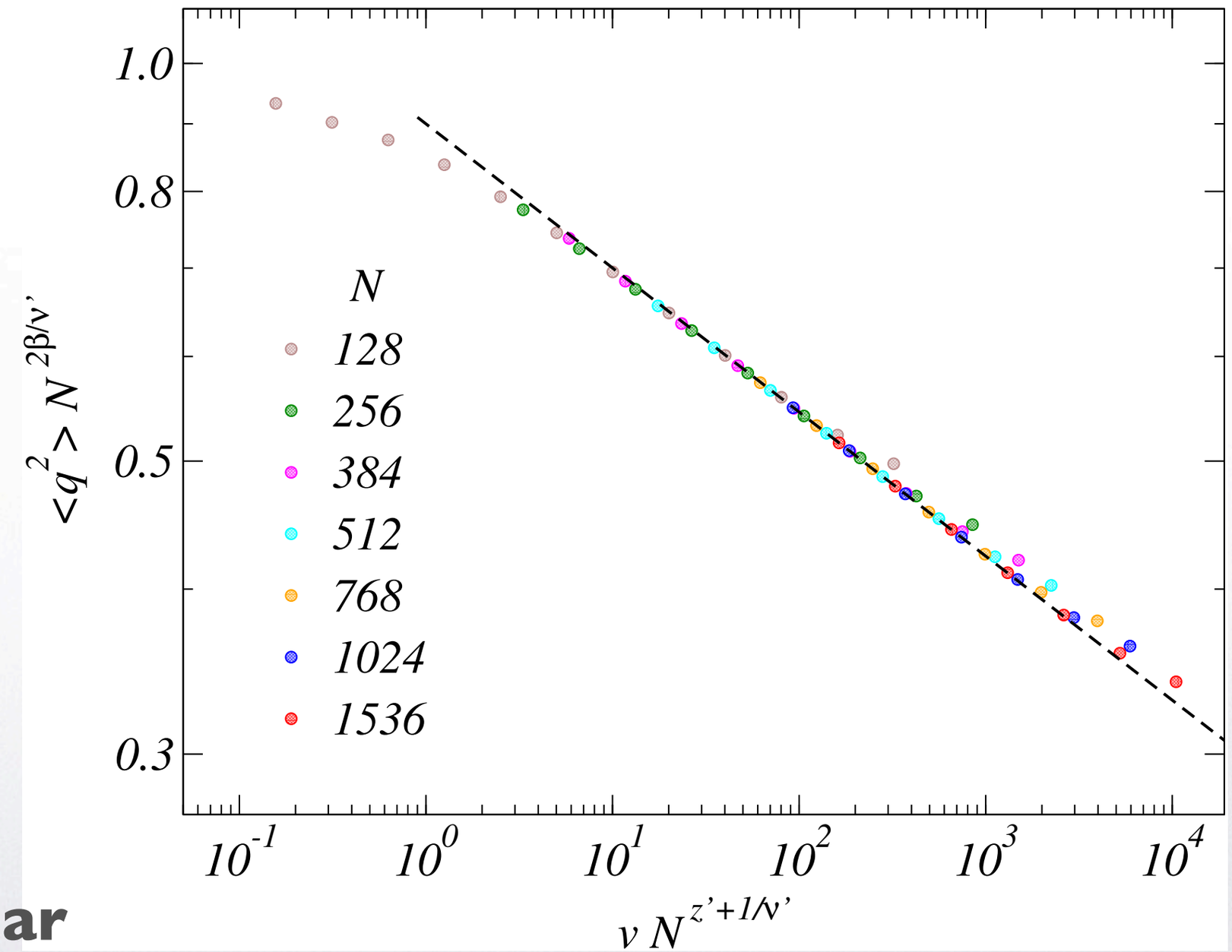
$$\langle q^2(s_c)\rangle \propto N^{-2\beta/\nu'} f(vN^{z'+1/\nu'})$$

$2\beta/\nu' \approx 0.86$
$z'+1/\nu' \approx 1.3$

These values differ from the values expected for d=∞:

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

Reason unclear. Fully-connected model gives same exponents as 3-regular



Do the exponents have any significance?

Relevance to Quantum Computing

The time needed to stay adiabatic up to s_c scales as

$$t \sim N^{z'+1/\nu} \qquad z' + 1/\nu' \approx 1.31$$

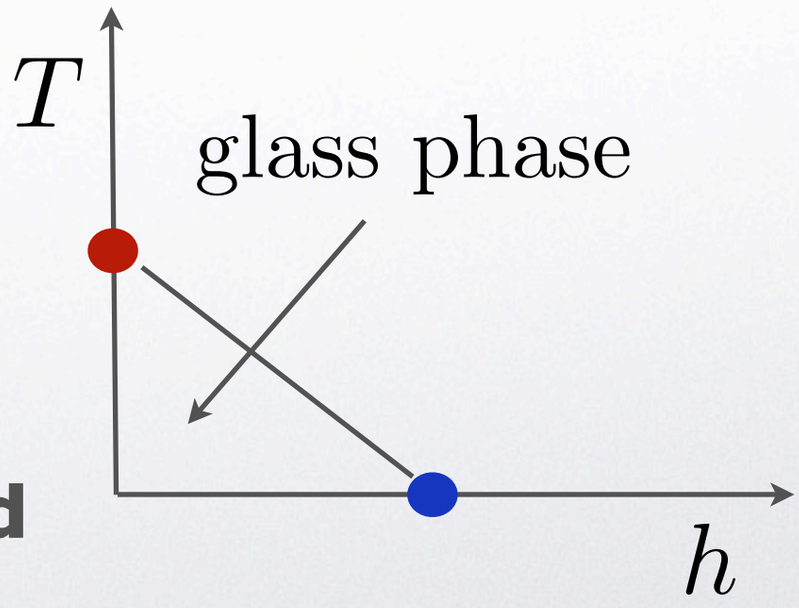
Reaching s_c, the degree of ordering scales as

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

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!