Spin correlations in the Heisenberg chain

$$H = J \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

Let's look at the (staggered) spin correlation function

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle (-1)^r$$

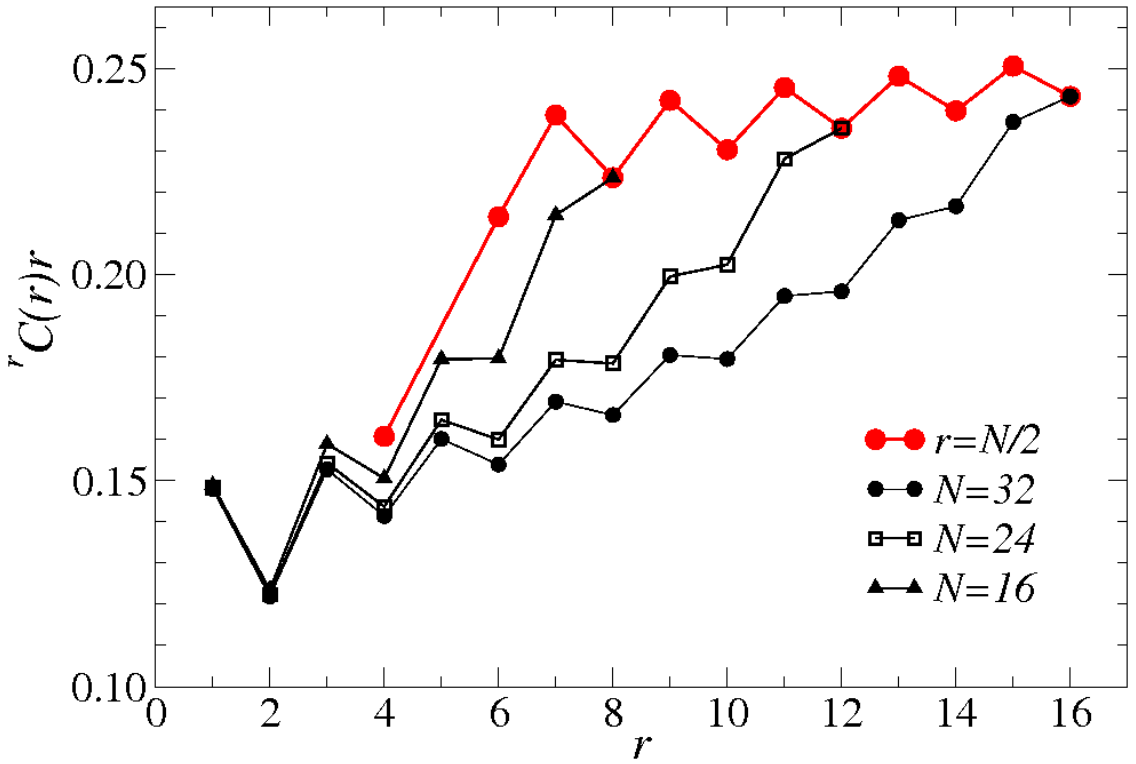
versus the distance r and at r=N/2 versus system size N

Theory (bosonization conformal field theory) predicts (for large r, N)

$$C(r) \propto \frac{\ln^{1/2}(r/r_0)}{r}$$

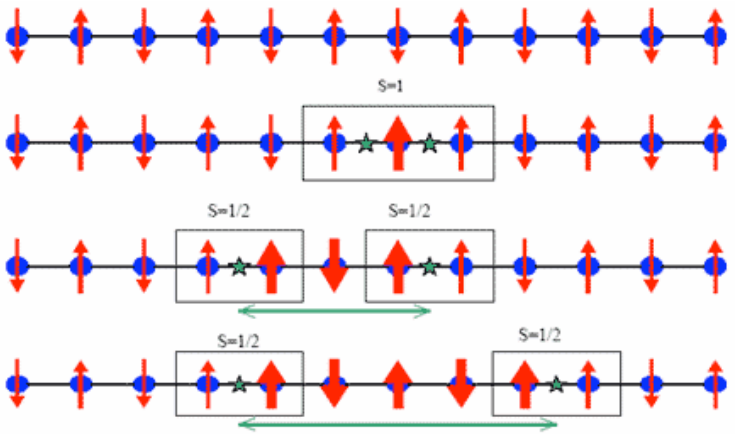
Plausible based on N up to 32
- other methods for larger N

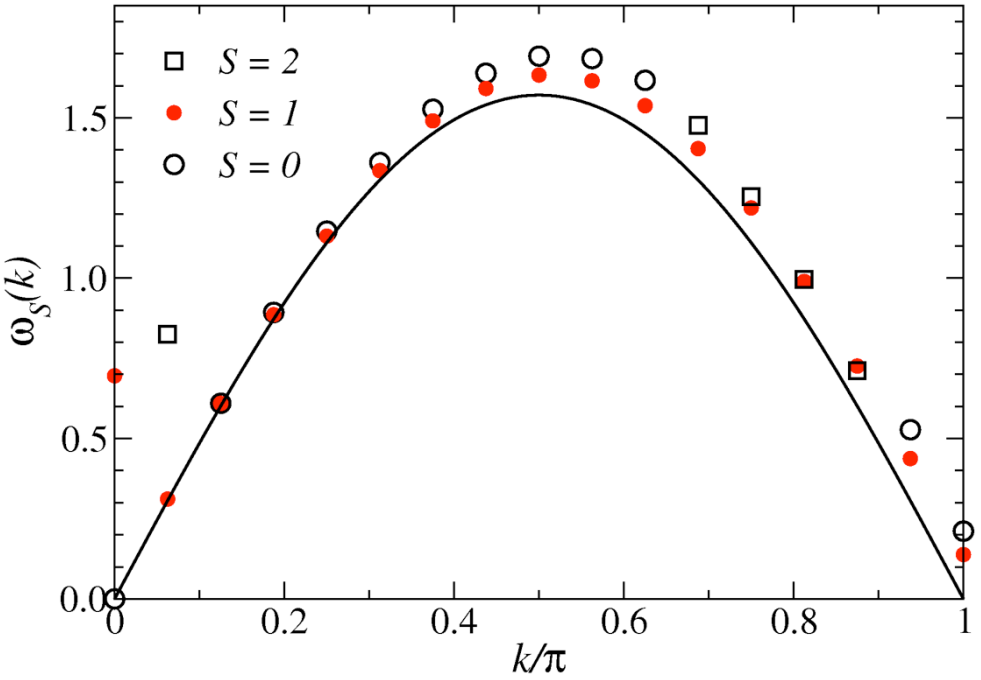
log correction caused by marginally irrelevant operator in CFT



Excitations of the Heisenberg chain

- the ground state is a singlet (S=0) for even N
- the first excited state is a triplet (S=1)
- can be understood as pair of “spinons”

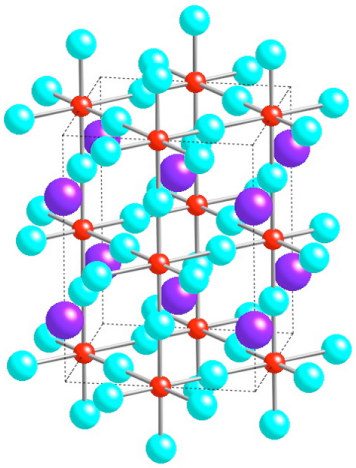


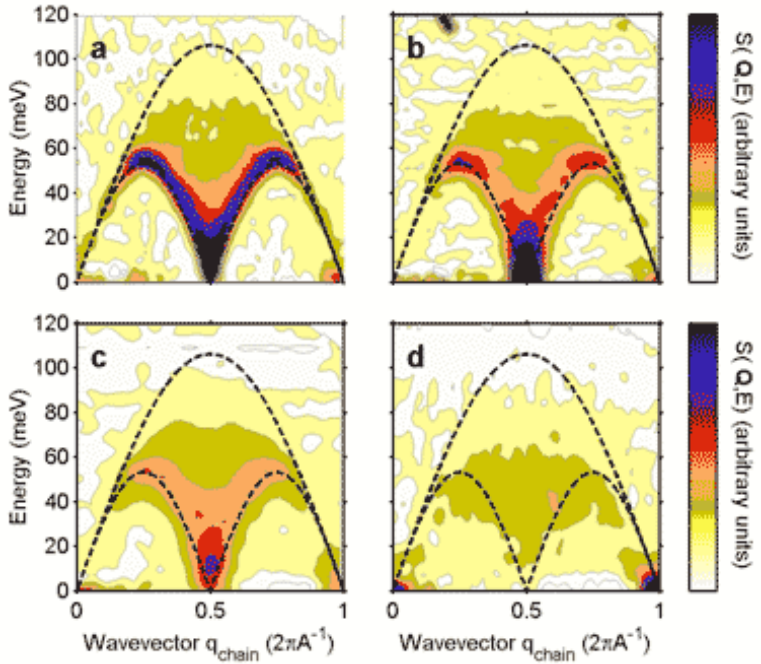


Neutron scattering experiments

- quasi-one-dimensional $KCuF_3$

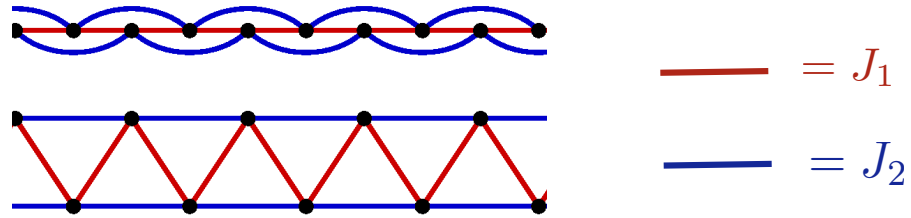
B. Lake et al., Nature Materials 4 329-334 (2005)





Heisenberg chain with frustrated interactions

$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$

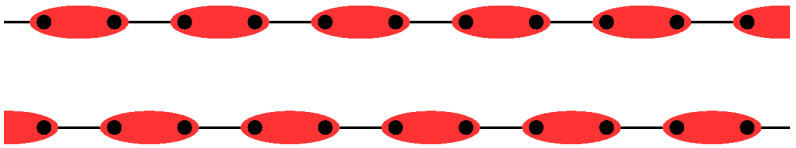


For the special point $J_2/J_1=0.5$, this model has an exact solution (Majumdar & Ghosh)

Singlet-product states $(a,b) = (\uparrow_a \downarrow_b - \downarrow_a \uparrow_b)/\sqrt{2}$

$$|\Psi_A\rangle = |(1,2)(3,4)(5,6)\cdots\rangle$$

$$|\Psi_B\rangle = |(1,N)(3,2)(5,4)\cdots\rangle$$



It is not hard to show that these are eigenstates of H

The system has this kind of order (with fluctuations, no exact solution) for all $J_2/J_1>0.2411$..... This is a **quantum phase transition** between

- a critical state
- a valence-bond-solid (VBS) state

The system at $(J_2/J_1)_c$ is described by a CFT (k=1 WZW theory)

- marginal operator goes to zero at this point
- log corrections to scaling in the critical phase, leads to VBS order above

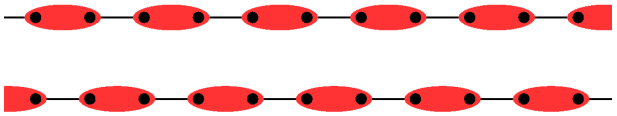
Translational symmetry of the VBS state is not broken for finite N

- the ground state is a superposition of the two ordered states

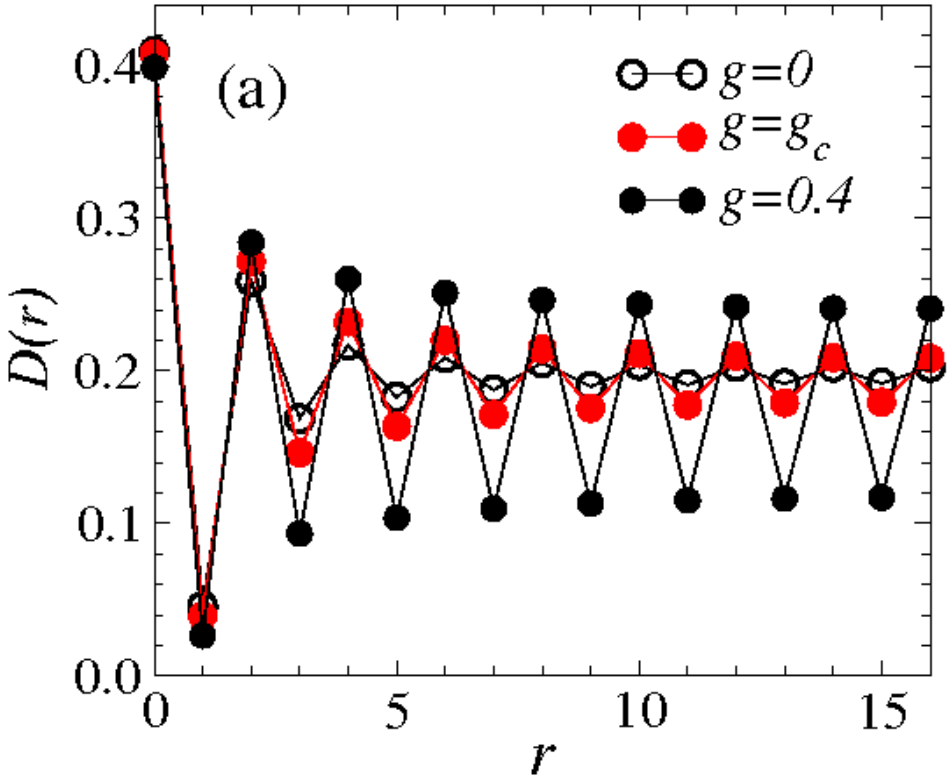
$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle, \qquad |\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$

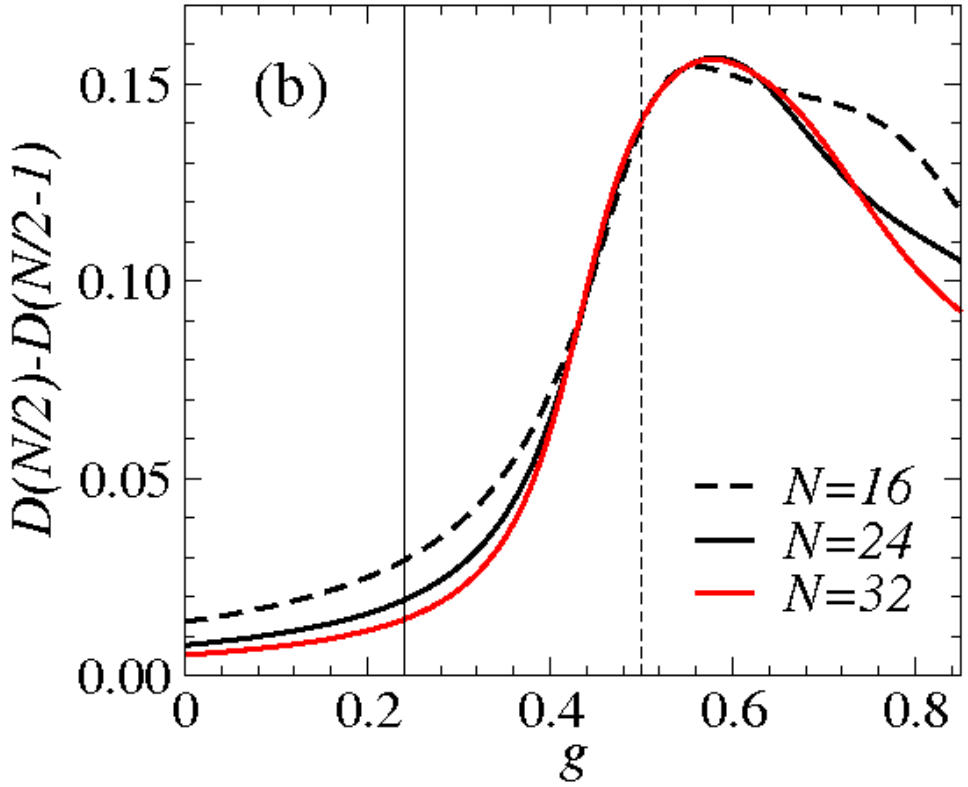
The VBS state can be detected in finite systems using “dimer” correlations

$$D(r) = \langle B_i B_{i+r} \rangle = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+1+r}) \rangle$$



Results from Lanczos diagonalization; different coupling ratios ***g=J₂/J₁***

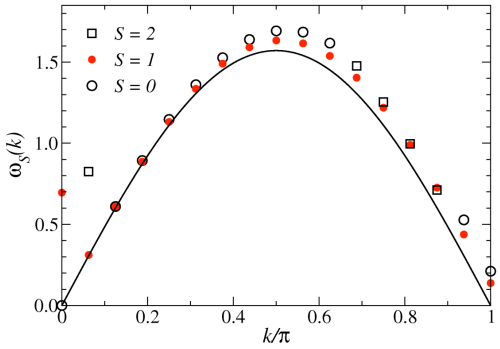




It is not easy to detect the transition this way

- much larger systems are needed for observing a sharp transition
- other properties can be used to accurately determine the critical point g_c
  - level crossings [K. Okamoto and K. Nomura, Phys. Lett. A 169, 443 (1992)]

Determining the transition point using level crossings



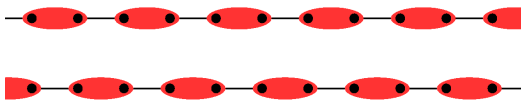
Lowest excitation for the g=0 Heisenberg chain is a triplet

- this can be expected for all $g<g_c$

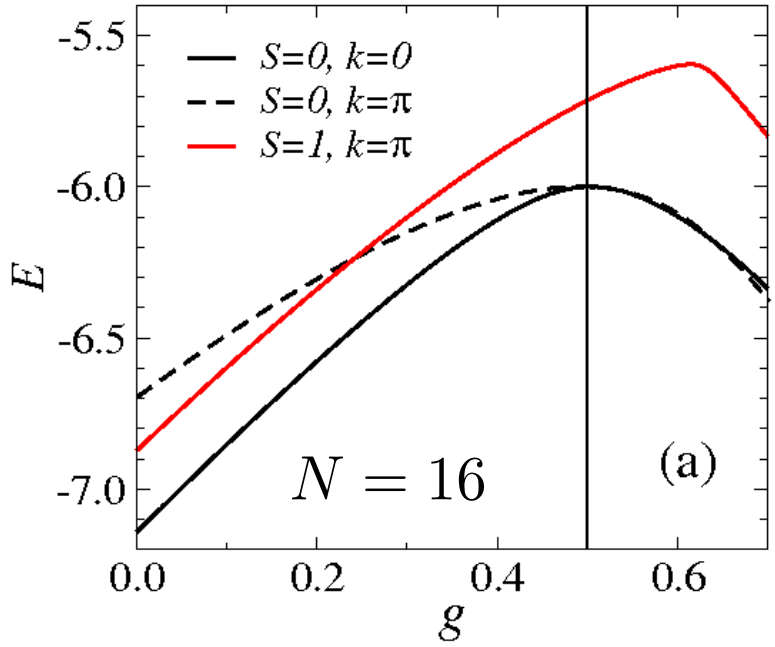
The VBS state is 2-fold degenerate for infinite N

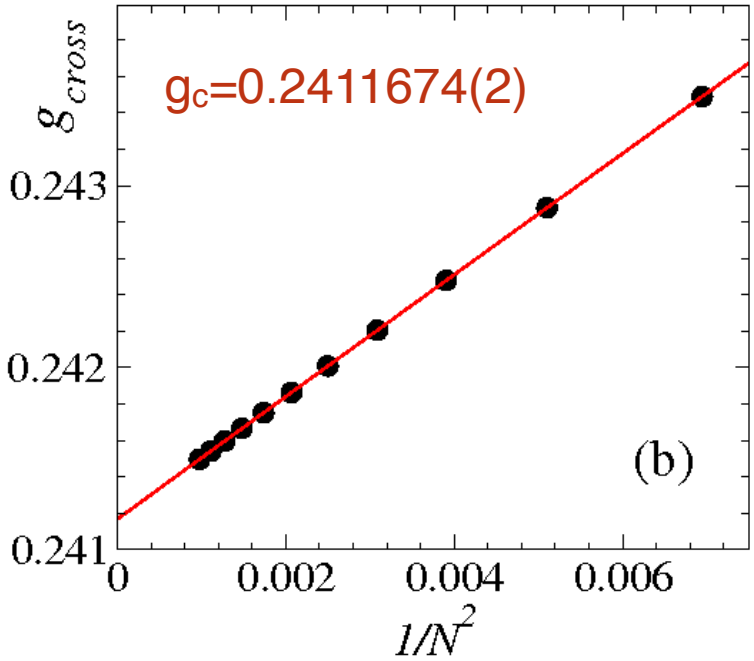
- and for any N at g=1/2
- these two states are singlets
- gap between them closes exponentially as $N\to\infty$
- the lowest excitation is the second singlet

$$|\Psi_0\rangle \sim |\Psi_A\rangle + |\Psi_B\rangle$$
$$|\Psi_1\rangle \sim |\Psi_A\rangle - |\Psi_B\rangle$$



The two lowest excited states should cross at g_c



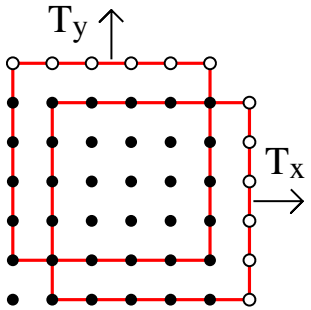


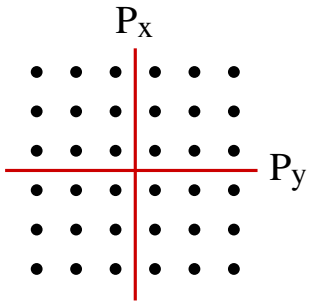
1/N² shift can be explained by CFT (k=1 WZW)

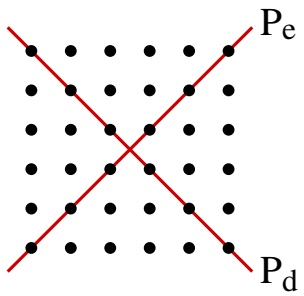
- same transition in many other systems; 1D J-Q, Heisenberg chains with phonons,…
- QMC study of emergent O(4) symmetry: Patil, Katz, Sandvik, PRB (2018)

2D square lattice

Use translation symmetry
- momentum states







$$|a(\mathbf{k})\rangle = |a(k_x,k_y)\rangle = \frac{1}{\sqrt{N_a}} \sum_{x=0}^{L_x-1} \sum_{y=0}^{L_y-1} \mathrm{e}^{-i(k_x x + k_y y)} T_y^y T_x^x |a\rangle \qquad k_\gamma = \frac{2\pi}{L_\gamma} m_\gamma, \quad m_\gamma = 0,1,\ldots,L_\gamma - 1$$

At high-symmetry (k_x,k_y) one can also use one or more reflection symmetry

Block sizes for

L=4, L=6
(k_x,k_y) = (0,0)
m_z = 0

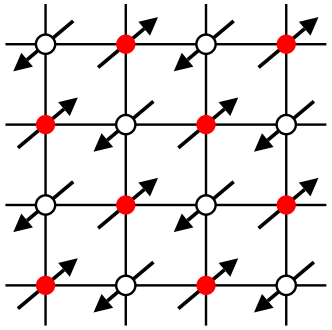
p_x	p_y	p_d	z	$M(L=4)$	$M(L=6)$
+1	+1	+1	+1	107	15,804,956
+1	+1	+1	−1	46	15,761,166
+1	+1	−1	+1	92	15,796,390
+1	+1	−1	−1	38	15,752,772
−1	−1	+1	+1	50	15,749,947
−1	−1	+1	−1	45	15,739,069
−1	−1	−1	+1	42	15,741,544
−1	−1	−1	−1	36	15,730,582
+1	−1		+1	75	31,481,894
+1	−1		−1	108	31,525,574

Quantum rotor states (Anderson tower) in 2D Heisenberg model

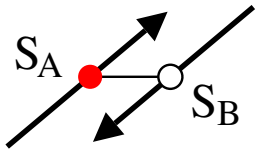
- see details in AIP Conf Proc. 1297, 135 (2010)

Lowest excitations (finite N): two large sublattice spins (S_A, $S_B \sim N$)

$$H = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$



$$\longrightarrow \quad H_{\rm eff} = J_{\rm eff}\, \vec{S}_{\rm A} \cdot \vec{S}_{\rm B}$$



Gap and susceptibility for the effective system →

$$\Delta_S = \frac{S(S+1)}{3\chi N} \qquad \chi = d\langle m(h)\rangle/dh, \qquad H(h) = H(0) - hS^z$$

→ Susceptibility of full model

$$\frac{1}{\chi(S,N)} = \frac{3N_S(E_S - E_0)}{S(S+1)}$$

$(0,0)_4$

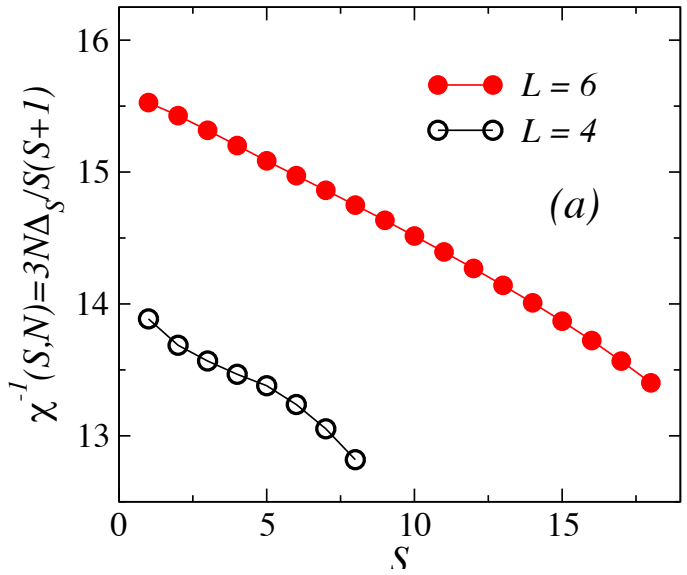
$(\pi,\pi)_3$

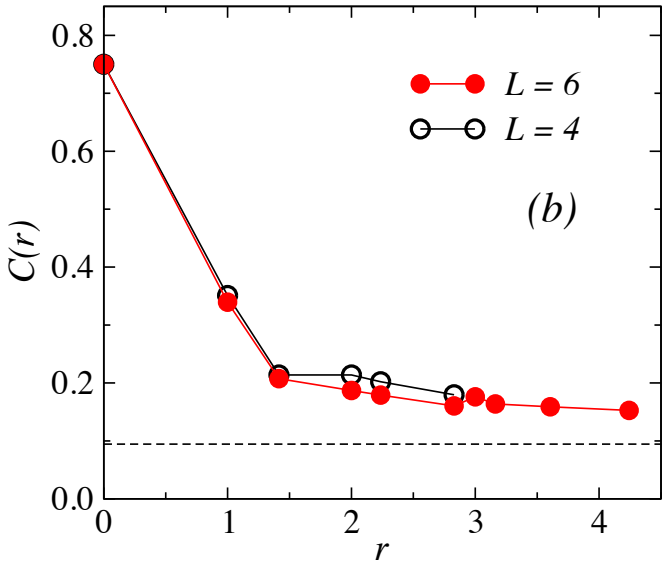
$(0,0)_2$

$(\pi,\pi)_1$

$(0,0)_0$

$(k_x,k_y)_S$





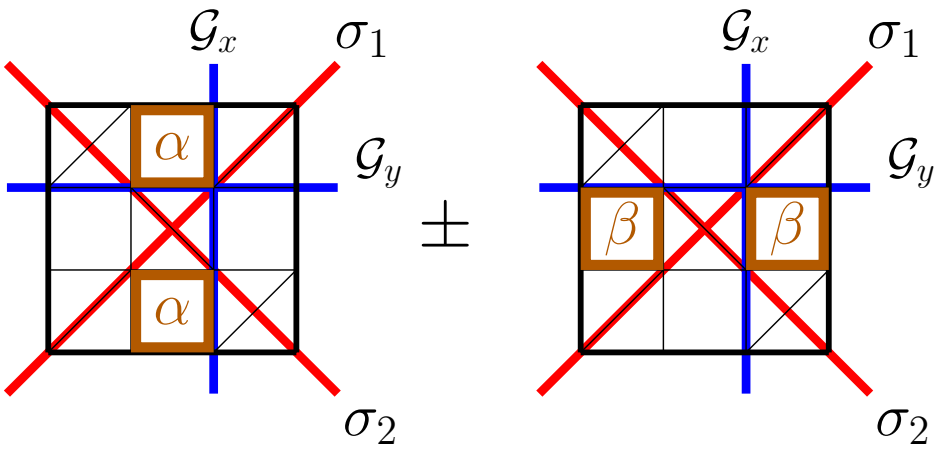
Long-range Néel AFM order seems plausible from on spin-spin correlation function

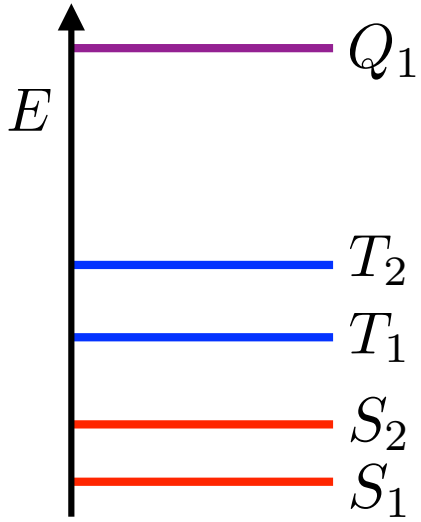
- can be confirmed with QMC

Level crossings in the SS model

Wang, Zhang, Sandvik,
CPL 2022 (arXiv:2205.02476)

quasi-degenerate singlet ground state
of the plaquette-singlet-solid (PSS)





Singlets S_1, S_2
Triplets T_1, T_2
Quintuplet Q

Gaps: $\Delta(S_2) = E(S_2) - E(S_1) \quad \Delta(T_1) = E(T_1) - E(S_1)$

Composite gaps: $\delta_T = E(T_2) - E(S_2) \quad \delta_Q = E(Q_1) - E(T_1)$

Gap criteria for PSS and AFM ordered phases

PSS: $\Delta(S_2) < \Delta(T_1)$ doubly-degenerate ground state, triplet gapped

AFM: $\Delta(Q_1) < \Delta(S_2), \quad \delta_T < \Delta(S_2)$

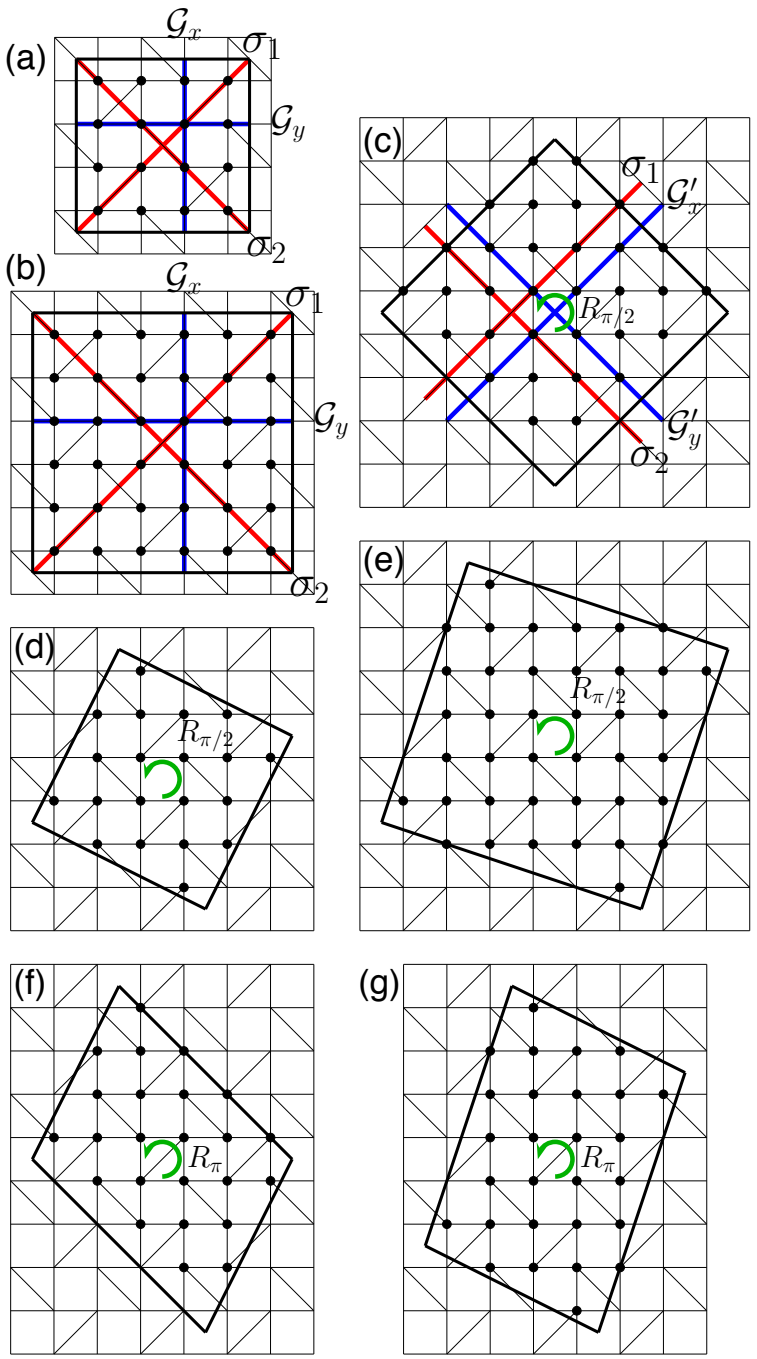
$E_S \propto S(S+1)/N$

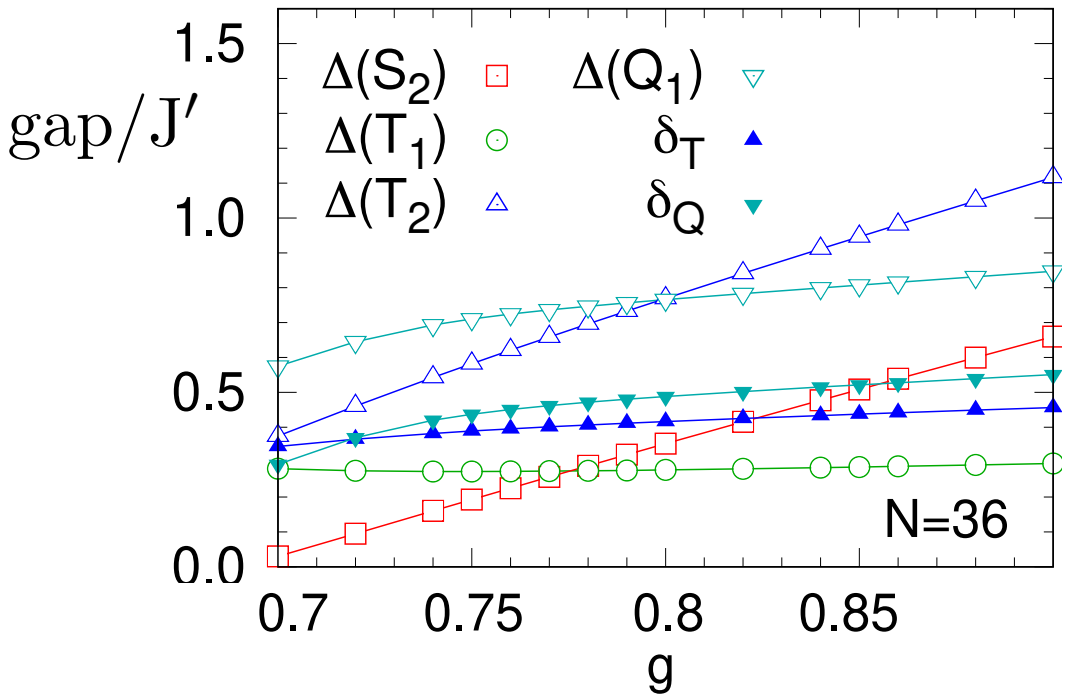
S_2 gapped; amplitude mode

Gap crossings vs g to detect quantum phase transitions

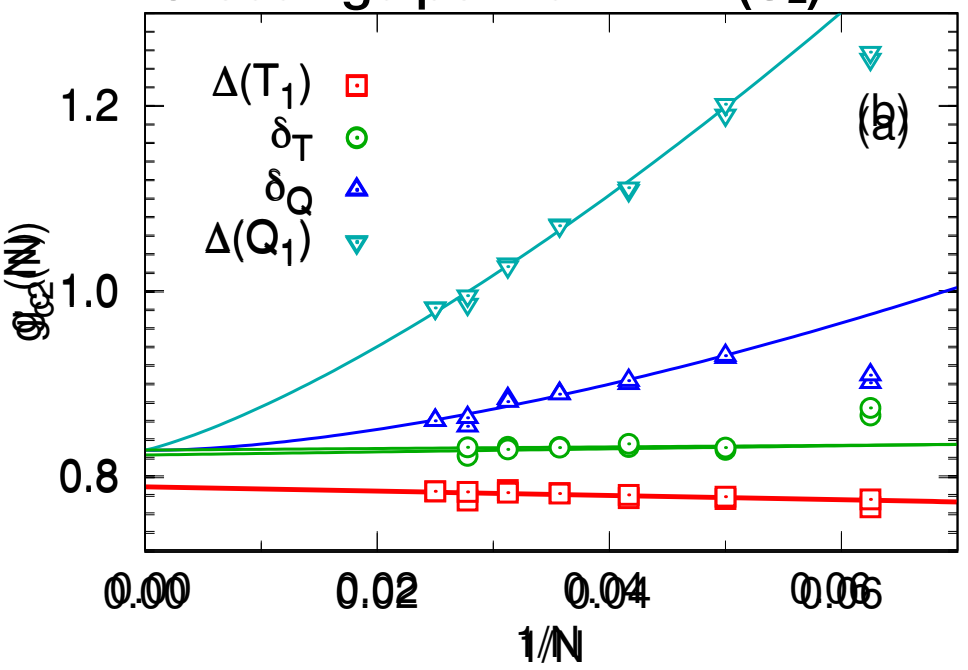
Lanczos calculations for N up to 36

Clusters and symmetries





Crossings points with $\Delta(S_2)$



Gapless spin liquid phase for g ∈ (0.79,0.83)?

Open-source program QuSpin (by Phillip Weinberg and Marin Bukov)

- Many functionalities for exact solution of small systems

QuSpin: a Python Package for Dynamics and Exact Diagonalisation of Quantum Many Body Systems.

Part I: spin chains

arXiv : 1610.03042

QuSpin: a Python Package for Dynamics and Exact Diagonalisation of Quantum Many Body Systems.

Part II: bosons, fermions and higher spins

arXiv : 1804.06782

http://weinbe58.github.io/QuSpin/index.html

Comment: Even though exact methods are limited to small system sizes, they are very useful for

- learning quantum many-body concepts
- extracting initial features for models
- testing other methods

Bootstrapping Nature: Non-perturbative Approaches to Critical Phenomena, Training Week
Galileo Galilei Institute, Florence, Italy, October 3-7, 2022

Anders Sandvik, Boston University

Monte Carlo Simulations

1) Classical Monte Carlo

2) Quantum Monte Carlo

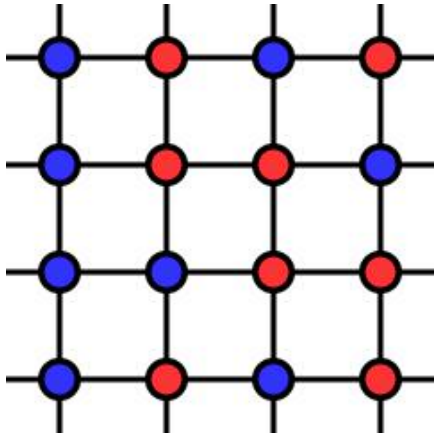
Ising model

Two states on each lattice site $\text{spin} \uparrow, \downarrow$

Can arise for quantum mechanical S=1/2: $S_i^z = \pm 1/2$

Strong anisotropies; z-interactions can dominate

$$E = \sum_{i,j} J_{ij} S_i^z S_j^z$$



This is the Ising model

- important in the theory of phase transitions
- effective model for many stat mech problems ("lattice gases", binary alloys, atom adsorption on surfaces,...)

With only nearest-neighbor interactions (J), the Ising model can be solved analytically in 1D and 2D

- Numerical simulations important in most other cases

Phase transition

Spontaneous ordering (symmetry breaking) at critical temperature

magnetization (ferromagnet, J<0)

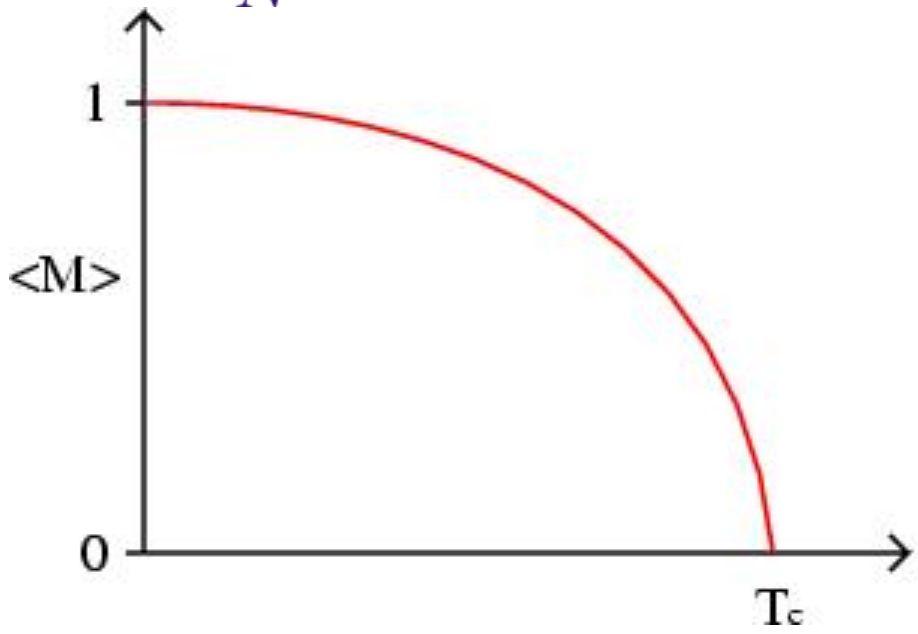
$$T_c/J = 2/\ln(1+\sqrt{2})$$

$$T_c/J \approx 2.269$$

$$M = \frac{1}{N}\sum_{i=1}^{N}\sigma_i$$

sublattice (staggered) magnetization (antiferromagnet, J>0)

$$M = \frac{1}{N}\sum_{}^{N}(-1)^{x_i+y_i}\sigma_i$$



Broken symmetry
only in infinite system

<M>=0 for finite N

<M^2> or <|M|> can be used

Monte Carlo simulations of the 2D Ising model

Stochastic sampling of spin configurations to estimate

$$\langle A \rangle = \frac{1}{Z} \sum_S A(S) \mathrm{e}^{-E(S)/T}, \quad Z = \sum_S \mathrm{e}^{-E(S)/T}$$

Spin configurations $S = (\sigma_1, \sigma_2, \ldots, \sigma_N)$

2^N configurations; can sample very small fraction for large N

Trivial (uniform) sampling of S fails at low T, because the sum is then dominated by configurations with large ordered domains, which are very unlikely to be generated in random sampling

Extreme case: T=0. Only two configurations contribute, but the probability to generate them is $1/2^{N-1}$

Solution: **Importance sampling:**

- Generate configurations according to Boltzmann distribution

Importance sampling

First, rewrite expectation value as

$$\langle A \rangle = \sum_S P(S)A(S), \quad P(S) = \frac{1}{Z} \mathrm{e}^{-E(S)/T}$$

P(S) can be interpreted as the probability of configuration S

Uniform sampling of N configurations

$$\langle A \rangle \approx \frac{1}{N} \sum_{i=1}^{N} A(S_i)P(S_i)$$

Importance sampling: The probability to pick S is P(S)

$$\langle A \rangle \approx \frac{1}{N} \sum_{i=1}^{N} A(S_i)$$

This sampling selects exactly the important configurations, and hence the statistical errors will be much smaller at low T.

But how do we accomplish importance sampling in practice?

Imagine **ensemble** of huge number of states in equilibrium

Number of states A is $N_0(A)$, proportional to P(A)

We now make some random change in each state (e.g., flip spins)

Possible transitions: $A \to B, C, \ldots$

Number of states A after the "update"

$$N_1(A) = N_0(A) + \sum_{B \neq A} N_0(B)P(B \to A) - N_0(A)P(A \to B)$$

This is the **master equation** for the stochastic process

If we want the distribution to remain P(A) after the update

$$\sum_{B \neq A} N_0(B)P(B \to A) - N_0(A)P(A \to B) = 0$$

$$\sum_{B \neq A} P(B)P(B \to A) - P(A)P(A \to B) = 0$$

Many possible solutions; an obvious solution, called the **detailed-balance** solution (condition): For every A, B

$$P(B)P(B \to A) = P(A)P(A \to B)$$

Time evolution of a single configuration; **Markov process**

Time average of a Markov process same as ensemble average

If we make random updates on a single configuration, and satisfy detailed balance, $P(B)P(B \to A) = P(A)P(A \to B)$, and if the updates are such that any configuration can be reached in a series of updates (ergodicity).

Then, the **time distribution of configurations A will approach the distribution P(A) independently of the initial configuration**

Alternative form of the detailed-balance condition

With $P(A) = \exp[-E(A)/T]/Z = W(A)/Z$

$$\frac{P(B \to A)}{P(A \to B)} = \frac{W(A)}{W(B)}$$

We have to construct transition probabilities satisfying this

The transition probability can typically be written as

$$P(A \to B) = P^A_{\text{attempt}}(B) P^A_{\text{accept}}(B)$$

where the two factors have the following meaning:

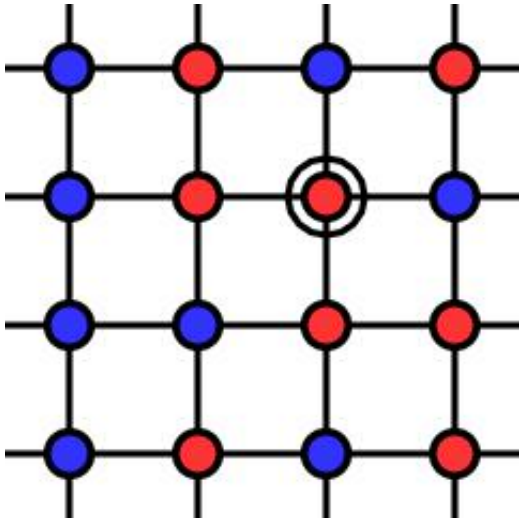
$P^A_{\text{attempt}}(B)$ - The probability of selecting B as a candidate among a number of possible new configurations

$P^A_{\text{accept}}(B)$ - The probability of actually making the transition to B after the selection of B has been done

If B has been selected but is not accepted (rejected); stay with A

For an Ising model

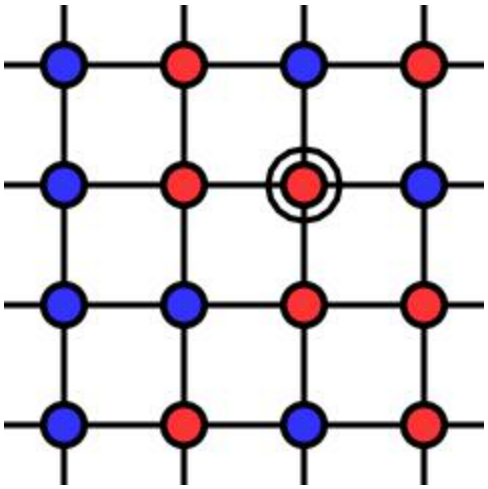
- Select a spin at random as a candidate to be flipped (attempt)
- Actually flip the spin with a probability to be determined (accept)
- Stay in the old configuration if the flip is not done (reject)



$P^A_{\text{attempt}}(B) = 1/N_{\text{spin}}$ uniform, independent of A, B

$P^A_{\text{accept}}(B)$ constructed to satisfy detailed balance condition

$$\frac{P^A_{\text{accept}}(B)}{P^B_{\text{accept}}(A)} = \frac{W(B)}{W(A)}$$



Two commonly used acceptance probabilities

Metropolis: $P^A_{\text{accept}}(B) = \min\left[\frac{W(B)}{W(A)}, 1\right]$

Heat bath: $P^A_{\text{accept}}(B) = \frac{W(B)}{W(A) + W(B)}$

Easy to see that these satisfy detailed balance

The ratios involve the change in energy when a spin has been flipped (or, more generally, when the state has been updated in some way)

Metropolis algorithm for the Ising model

Spin update

- Select a spin at random
- Calculate the change in energy if the spin is flipped
- Use the energy change to calculate the acceptance probability P
- Flip the spin with probability P; stay in old state with 1-P
- Repat from spin selection

Current configuration: S

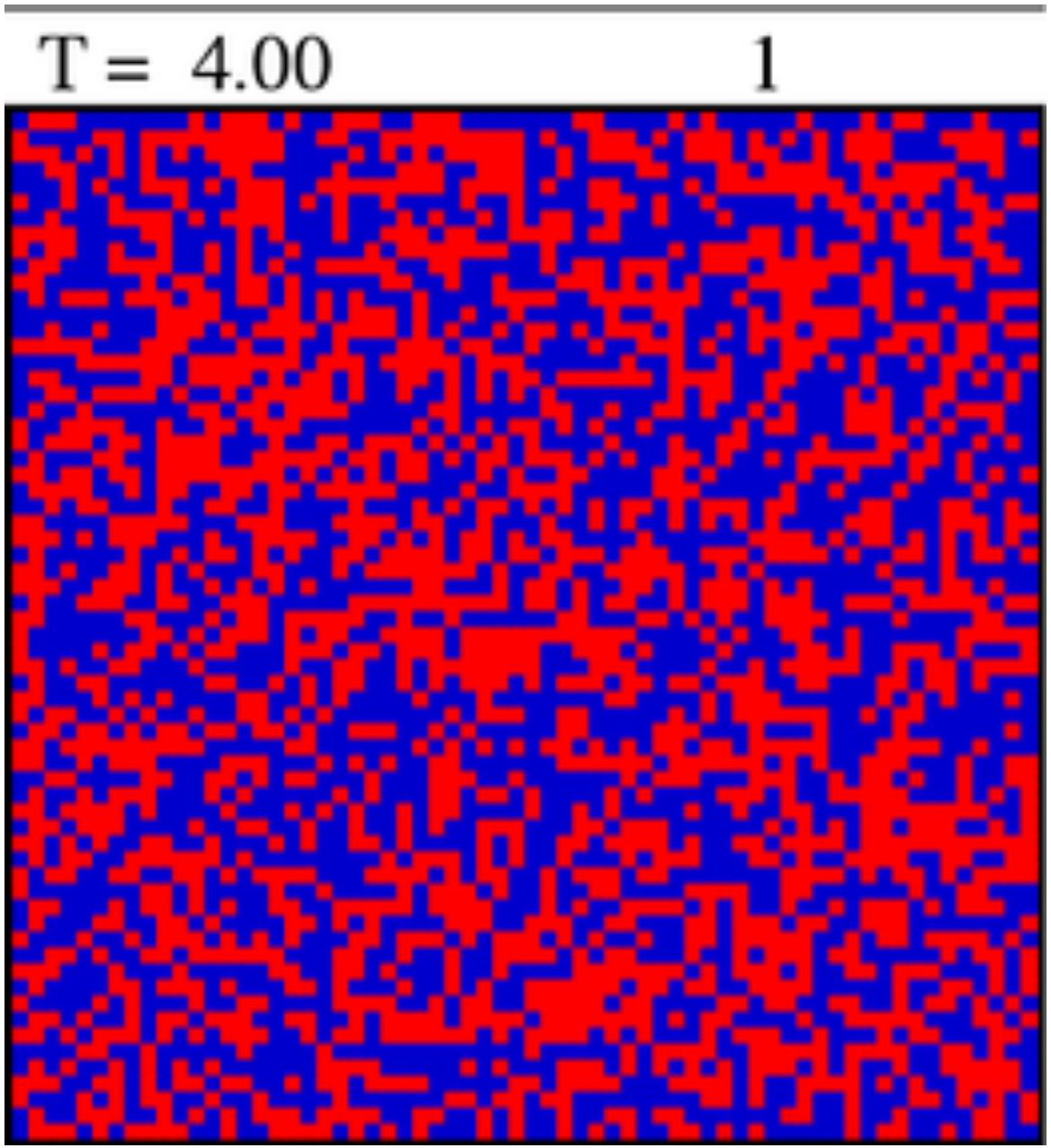
Configuration after flipping spin j: $\tilde{S}_j$

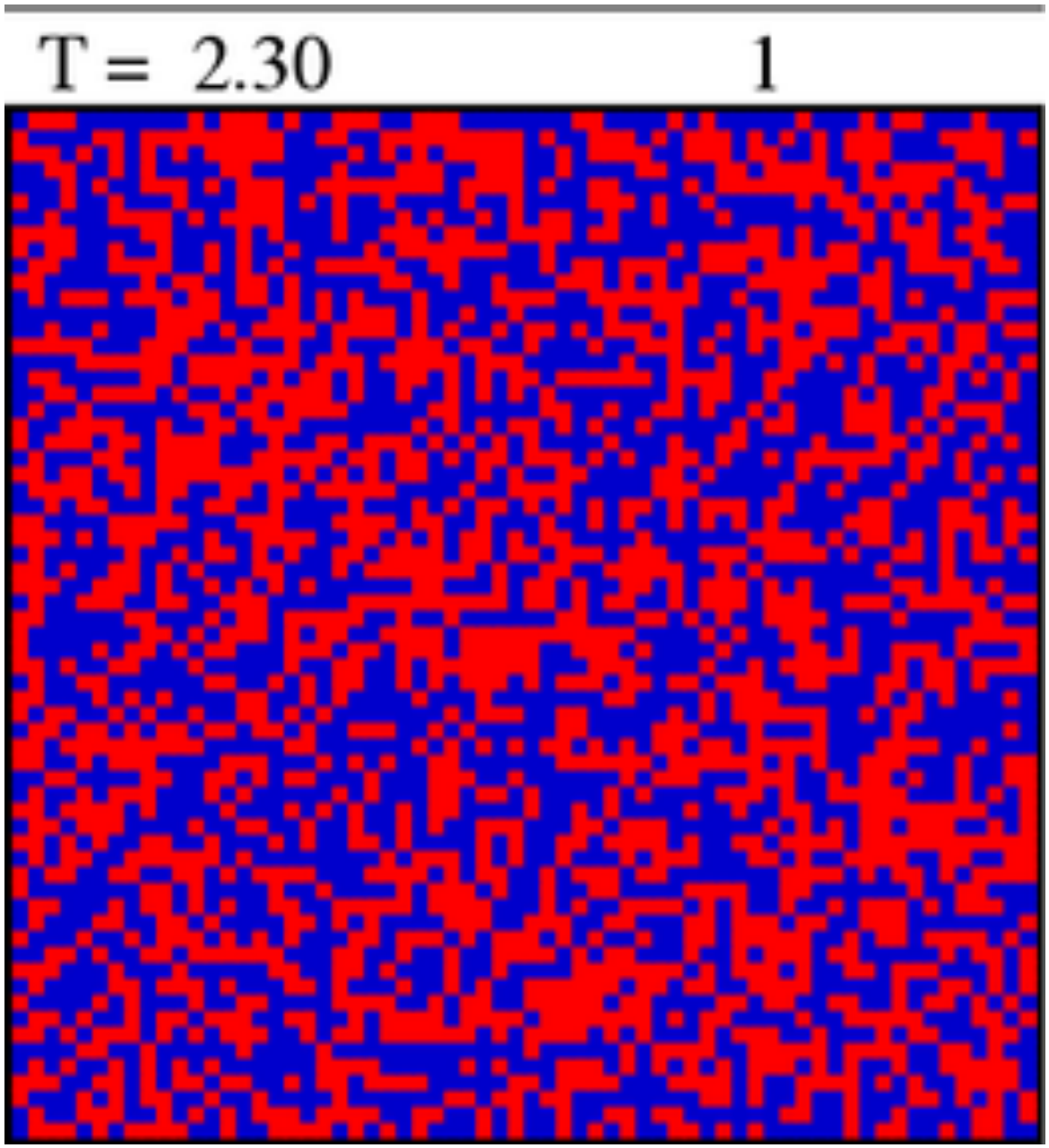
Acceptance probability: $P(S \to \tilde{S}_j) = \min\left[\frac{W(\tilde{S}_j)}{W(S)}, 1\right]$

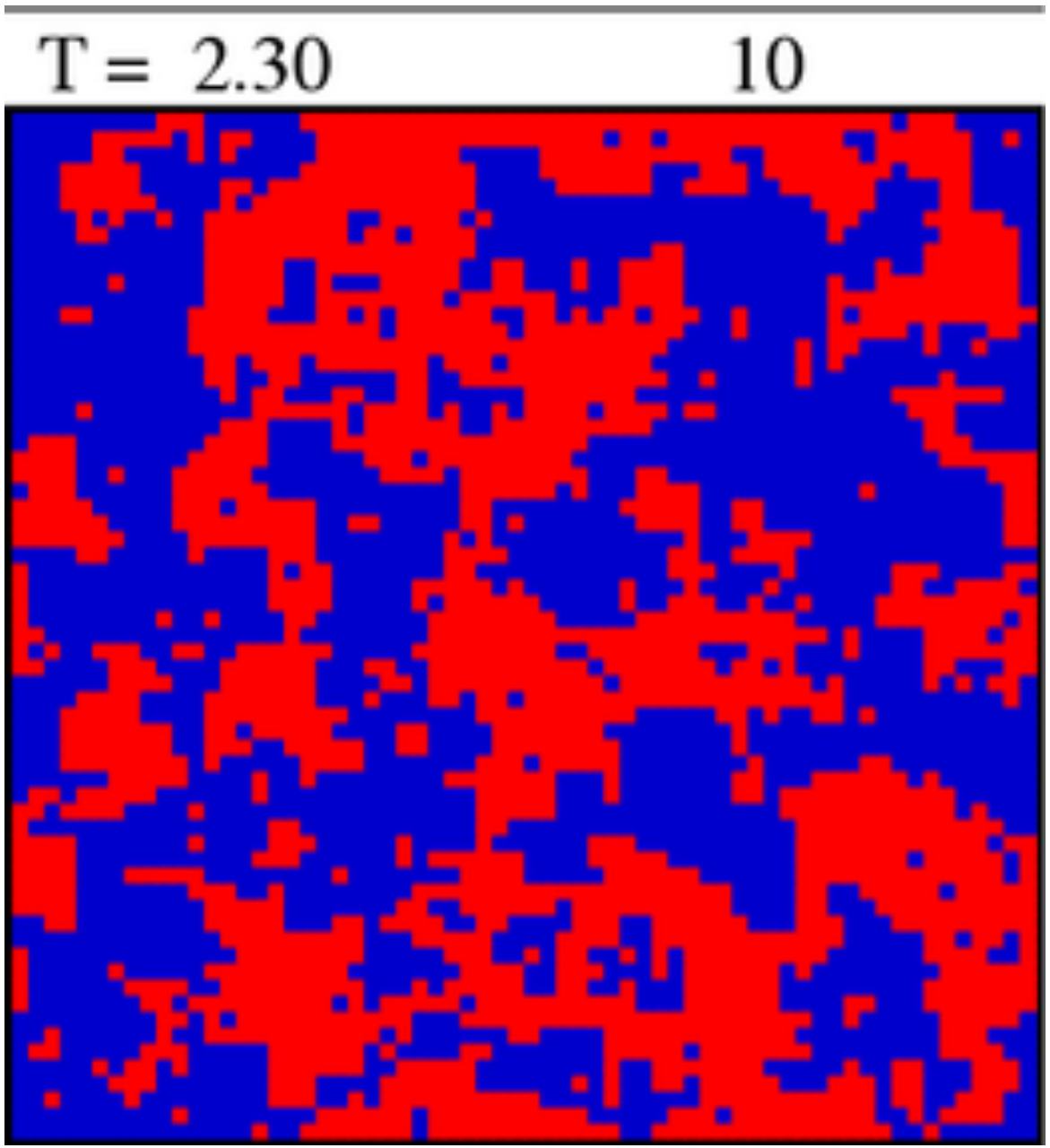
$$W(S) = \mathrm{e}^{-E(S)/T} = \mathrm{e}^{-\frac{J}{T}\sum \sigma_i \sigma_j} = \prod \mathrm{e}^{-\frac{J}{T}\sigma_i \sigma_j}$$

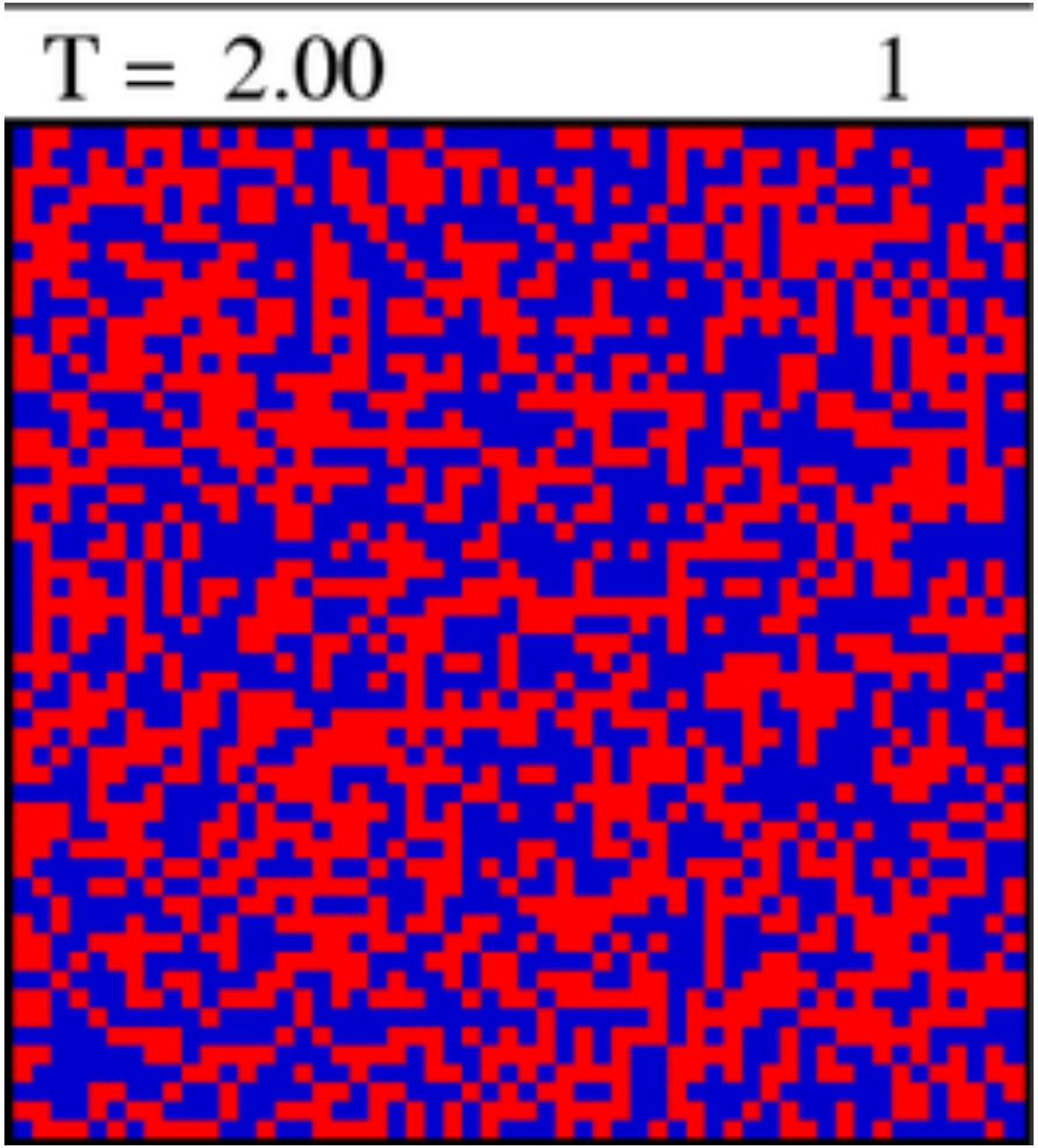
Only factors containing spin j survive in W-ratio

$$\frac{W(\tilde{S}_j)}{W(S)} = \exp\left[-\frac{2J}{T}\sigma_j \sum_{\delta(j)} \sigma_{\delta(j)}\right], \quad \delta(j) = \text{neighbor of } j$$


T = 4.00
1


T = 2.30
1


T = 2.30
10


T = 2.00
1

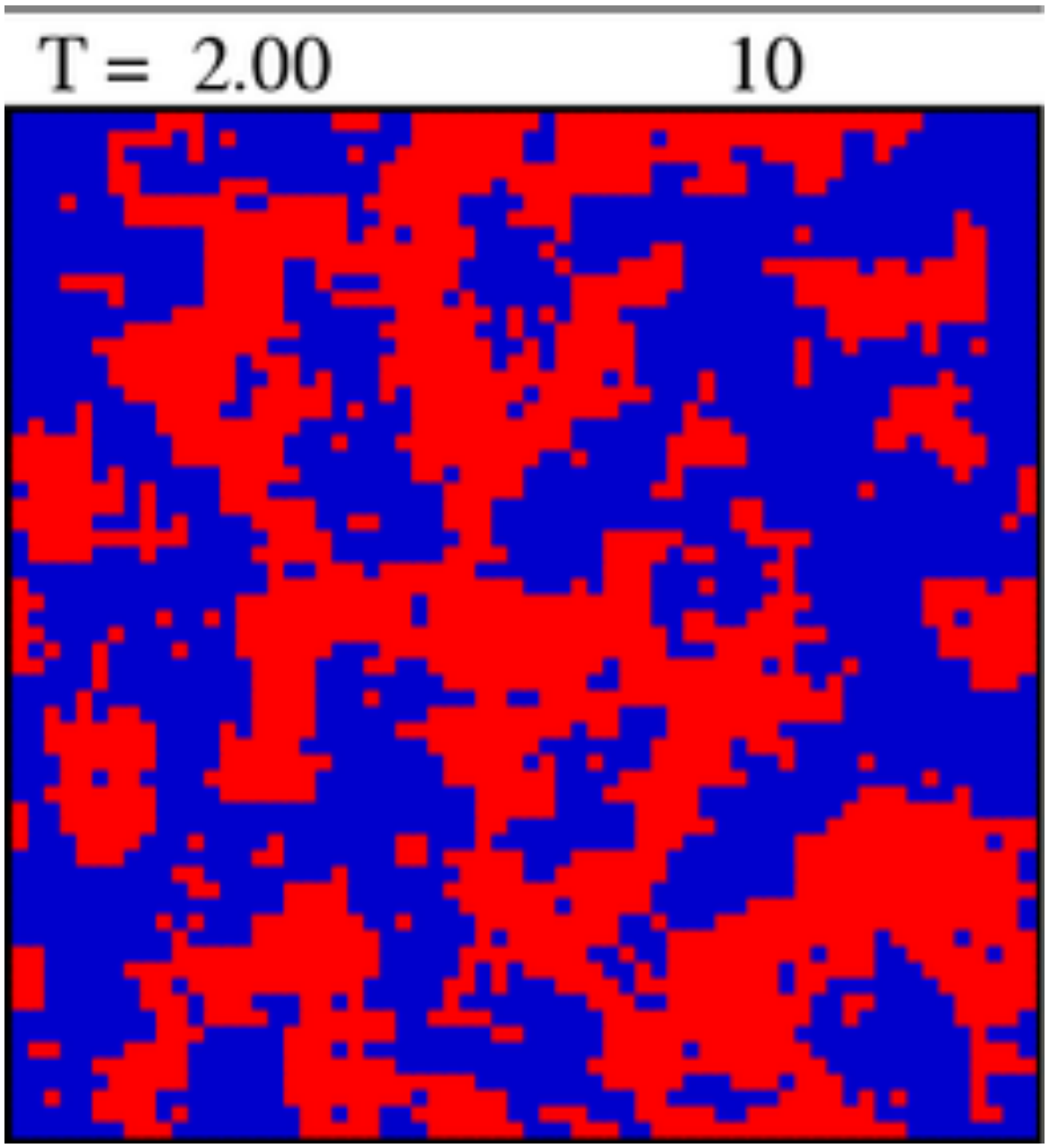
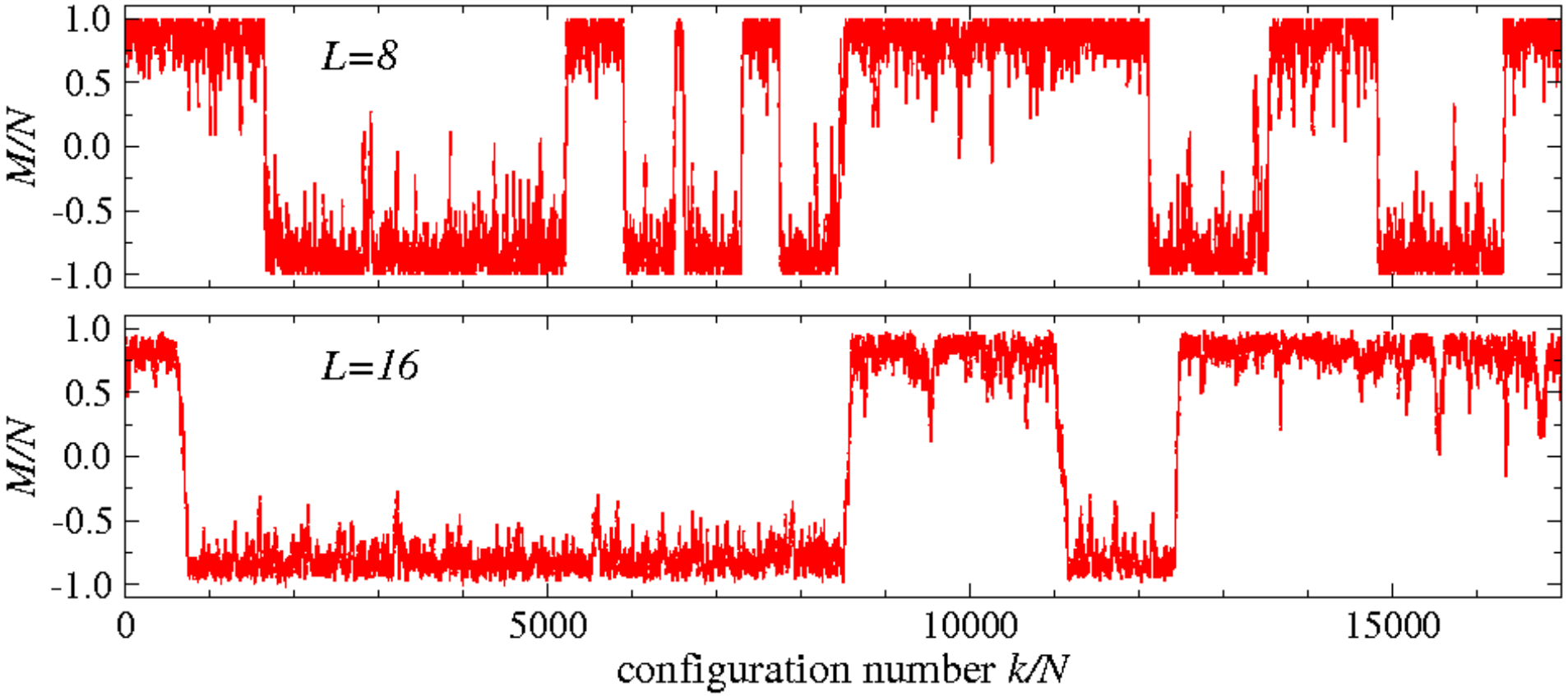

T = 2.00
10

Illustration of simulation

Evolution of the magnetization, 2D Ising model, T/J=2.2 (below Tc)

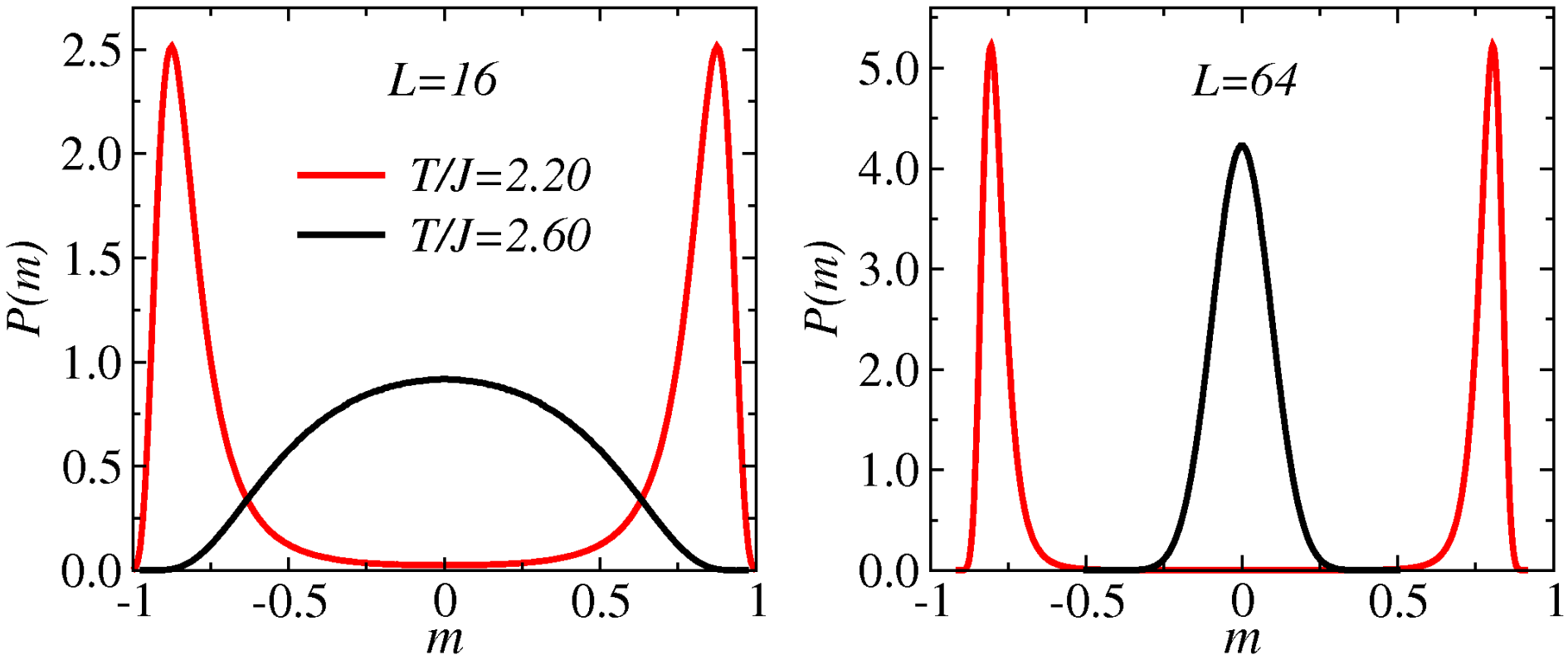
- <M>=0, but time scale for M-reversal increases with L
- Symmetry-breaking occurs in practice for large L



The magnetization distribution depends on T and L

- single peak around m=0 for T>Tc
- double peak around +<m> and-<m> for T<Tc

$$P(m) \propto e^{-F(m)/T}$$



Symmetry breaking (sampling of only m>0 or m<0 states) occurs in practice for large L

- Because extremely small probability to go between them

"Measuring" physical observables

Order parameter of ferromagnetic transition: Magnetization

$$M = \sum_{i=1}^{N} \sigma_i, \qquad m = \frac{M}{N}$$

Expectation vanishes for finite system; calculate $\langle |m| \rangle, \ \langle m^2 \rangle$

Susceptibility: Linear response of <m> to external field

$$E = E_0 - hM, \quad E_0 = J \sum_{i,j} \sigma_i \sigma_j$$

$$\chi = \left. \frac{d\langle m \rangle}{dh} \right|_{h=0}$$

Deriving Monte Carlo estimator

$$\langle m \rangle = \frac{1}{Z} \sum_S m \mathrm{e}^{-(E_0 - hM)/T}, \quad Z = \sum_S \mathrm{e}^{-(E_0 - hM)/T}$$

$$\chi = -\frac{dZ/dh}{Z^2} \sum_S m \mathrm{e}^{-(E_0 - hM)/T} + \frac{1}{Z} \frac{1}{T} \sum_S m M \mathrm{e}^{-(E_0 - hM)/T}$$

$$\frac{dZ}{dh} = \frac{1}{T} \sum_S M \mathrm{e}^{-(E_0 - hM)/T}$$

$$\chi = \frac{1}{N}\frac{1}{T}\left(\langle M^2\rangle - \langle M\rangle^2\right) = \frac{1}{N}\frac{1}{T}\langle M^2\rangle, \quad (h=0)$$

Extrapolating to infinite size, this gives the correct result only in the disordered phase when extrapolating N to infinity.

We can also define the susceptibility estimator as

$$\chi = \frac{1}{N}\frac{1}{T}\left(\langle M^2\rangle - \langle |M|\rangle^2\right)$$

Gives correct infinite-size extrapolation for any T

Specific heat

$$C = \frac{1}{N}\frac{dE}{dT} = \frac{1}{N}\frac{d}{dT}\sum_C E(C)\mathrm{e}^{-E(C)/T} = \frac{1}{N}\frac{1}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$$

Correlation function

$$C(\vec{r}) = \langle \sigma_i \sigma_{j(\vec{r},i)}\rangle \rightarrow \langle M^2\rangle/N \text{ when } r, N \rightarrow \infty$$

Average over all spins i

$$C(\vec{r}) = \frac{1}{N}\sum_{i=1}^{N}\langle \sigma_i \sigma_{j(\vec{r},i)}\rangle$$

Squared magnetization for different system sizes:
- development of phase transition (singularity)