

Classical Monte Carlo Simulation

Monte Carlo for Statistical Physics

Magnetism

The Ising Model & MC Simulation

Monte Carlo for Statistical Physics

- ⊕ Canonical distribution

$$P_s = \frac{1}{Z} e^{-\beta E_s}, \quad \beta = 1/k_B T.$$

- ⊕ Partition function

$$Z = \sum_{s=1}^M e^{-\beta E_s}$$

- ⊕ Thermal average

$$\langle E \rangle = \sum_{s=1}^M E_s P_s = \frac{1}{Z} \sum_{s=1}^M E_s e^{-\beta E_s}$$

- ⊕ Simulation

$$\langle A \rangle = \sum_{s=1}^M A_s P_s \approx A_m = \sum_{s=1}^m E_s P_s, \quad m \ll M.$$

Simulate probability with m samples

What is Monte Carlo Simulation?

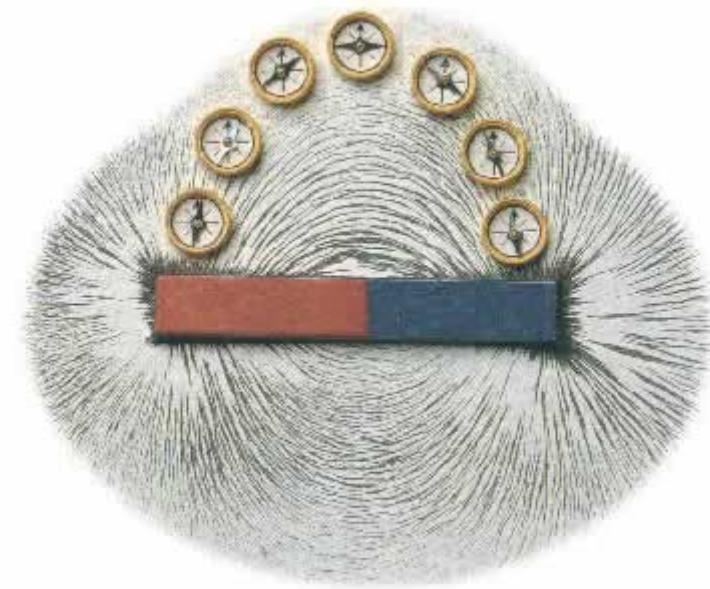
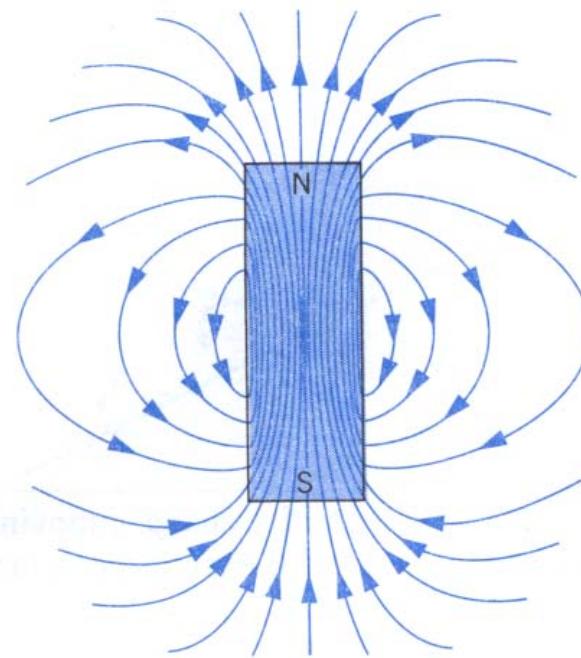
A way to perform summations.

Solving problems by random process.

Application in statistical physics are very
successful, especially for classical systems

Example: **magnetism**

Magnet and Magnetic Field



The Earth's Magnetic Field

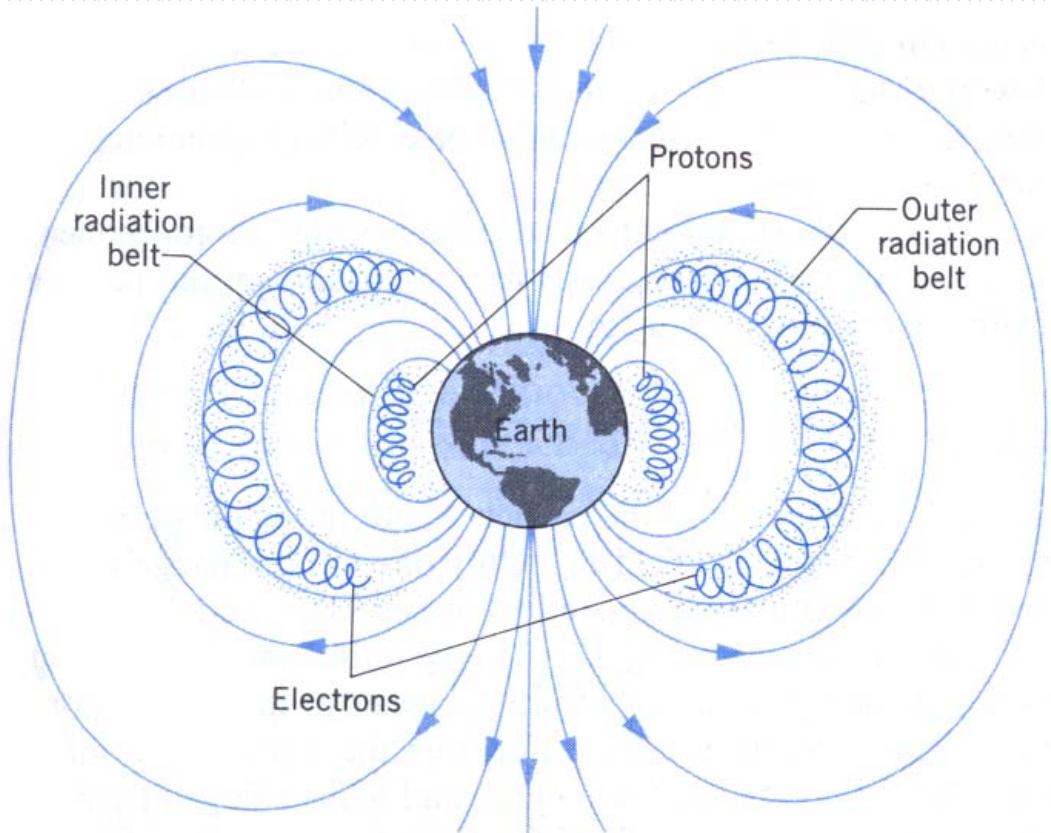


Figure 15 The Earth's magnetic field, showing protons and electrons trapped in the Van Allen radiation belts.

Introduction to Magnetic Systems

- ⊕ Compass, Earth, E&M waves (Radio), CDs, video, computer, etc.

- ⊕ Magnetic monopole

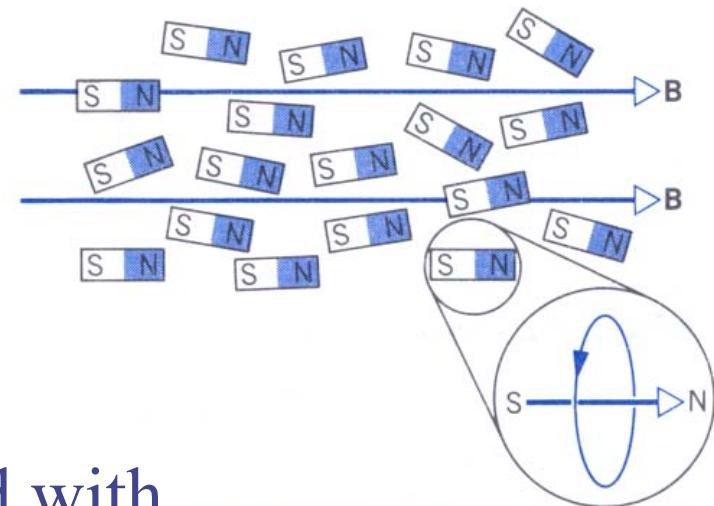
- ⊕ Magnetic dipole moments

- ⊕ Magnetic moment associated with the orbital motion of electrons in atoms

$$\mu_L = - (e/2m) \mathbf{L}.$$

- ⊕ Bohr magneton:

$$\mu_B = (e/2m)(h/2\pi) = 9.27 \times 10^{-24} \text{ J/T.}$$



Intrinsic Magnetic Moments of Electrons

$$\mu_s = - (e/m) \mathbf{S}.$$

- \mathbf{S} is called *Spin*, with unit of $h/2\pi$.
- Electron: $S = 1/2, \mu_s = - 1.0012 \mu_B$;
- Proton: $S = 1/2, \mu_s = + 0.0015 \mu_B$;
- Neutron: $S = 1/2, \mu_s = - 0.0010 \mu_B$;

Magnetic Properties

- ⊕ The magnetic properties of a material are determined by the total magnetic dipole moment of its atoms,

$L (= \sum_i l_i)$ *classical*

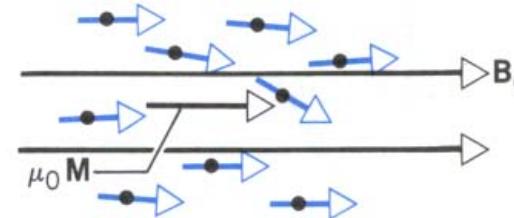
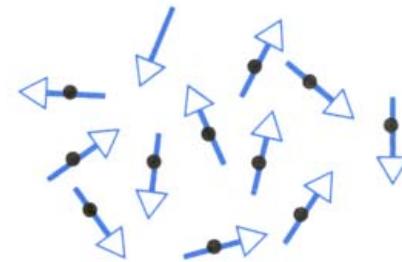
+

$S (= \sum_i s_i)$ *quantum mechanical*

- ⊕ *The Spin part is more important.*

Magnetic Materials

- ⊕ Magnetization, $M = (1/V) \sum_i \mu_i$
- ⊕ Paramagnet/Diamagnet: become magnetized when an external magnetic field is applied.
 - Paramagnetic materials are attracted by a magnet.
 - Diamagnetic materials are repelled by a magnet.



- ⊕ Ferromagnet: permanently magnetized (or after external field is removed). Examples: iron, cobalt, nickel, some rare earth elements, some compounds and alloys

Types of Magnetic Ordering



Linear arrays of spins illustrate
ferromagnetic ordering:

All (almost) moments parallel to each other

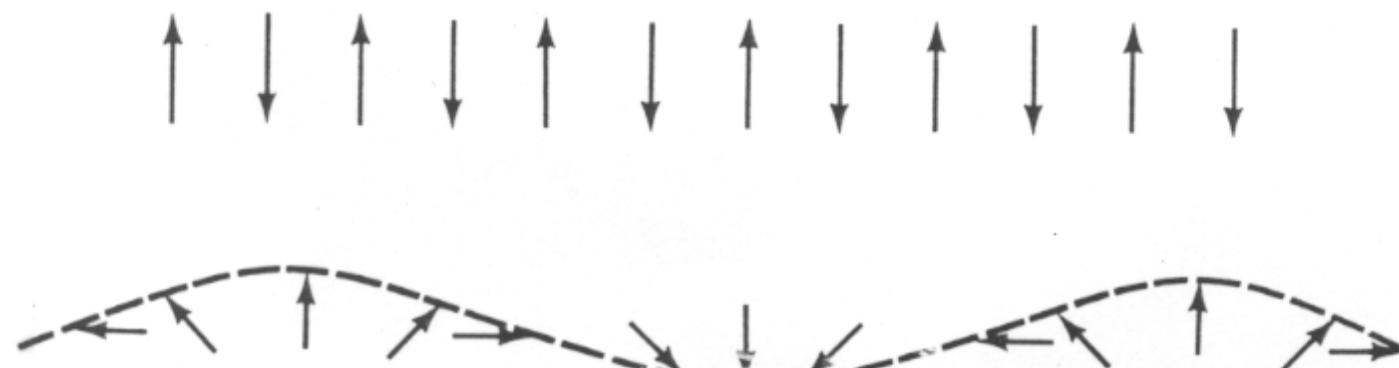


Types of Magnetic Ordering



Linear arrays of spins illustrate
anti-ferromagnetic ordering:

FM on sublattices, but with net moment zero



Types of Magnetic Ordering

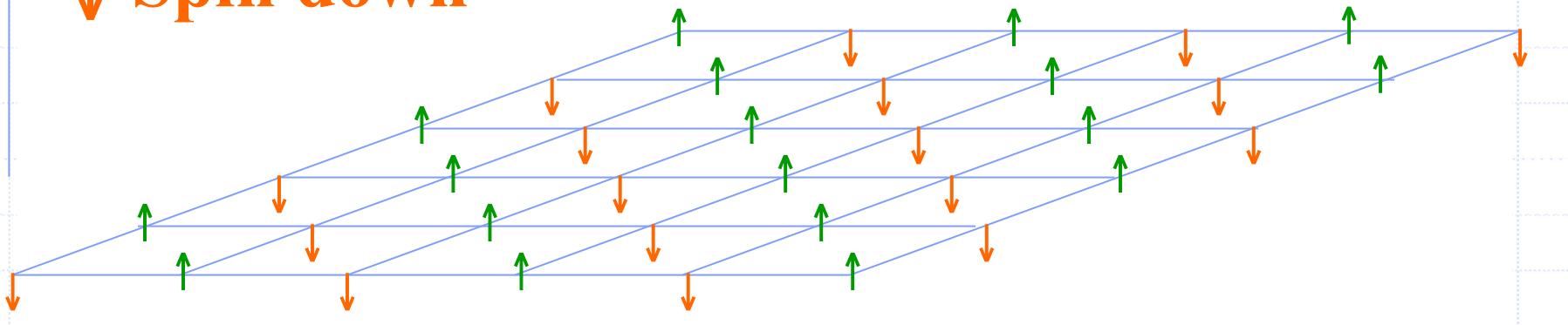


Linear arrays of spins illustrate
ferrimagnetic ordering: $M_A > M_B$



Neél Ordering in two-dimension $m_s = 1/2$

↑ Spin up
↓ Spin down



1970, Nobel Prize. Louis Eugene Félix Neél
"for fundamental work and discoveries concerning
antiferromagnetism and ferrimagnetism which have led
to important applications in solid state physics"

Physical Issues

- There are many
- Why/how the nature creates these ordered structures? (quantum mechanical, microscopic)
- Order \leftrightarrow Disorder Transition
(thermodynamic properties, macroscopic)

The Ising Model

- ⊕ The most popular model in statistical physics
- ⊕ Proposed by Lenz (1920) and investigated by his graduate student, Ising (1900-1998), to study the phase transition from a paramagnet to ferromagnet (1925).
- ⊕ Consider a lattice containing N sites and assume that each lattice site i has associated with it a number s_i (spin)

$$s_i = +1 \Leftrightarrow \text{“up”} (\uparrow), \quad s_i = -1 \Leftrightarrow \text{“down”} (\downarrow)$$

The Ising Model

- ⊕ A microstate of the lattice is specified by a set of variables $\{s_1, s_2, \dots, s_N\}$ for all lattice sites.
(binary representation?)
- ⊕ The total energy E of the Ising model

$$E(\{S_i\}) = -J \sum_{i,j=nn(i)}^N S_i S_j - h \sum_{i=1}^N S_i$$

J : exchange constant (integral)

h : external magnetic field

- ⊕ $J > 0$, $\uparrow\uparrow$ or $\downarrow\downarrow$ win, *ferromagnetic*
 $J < 0$, $\uparrow\downarrow$ or $\downarrow\uparrow$ win, *antiferromagnetic*

Modified Ising Model

$$E(\{S_i\}) = - \sum_{\langle i,j \rangle}^N J_{ij} S_i S_j - \sum_{i=1}^N h_i S_i$$

$$J_{ij} = \begin{cases} J \\ \text{Random } [-J, J] \\ J(\text{most bond}), -J(\text{a few bond}) \end{cases}$$

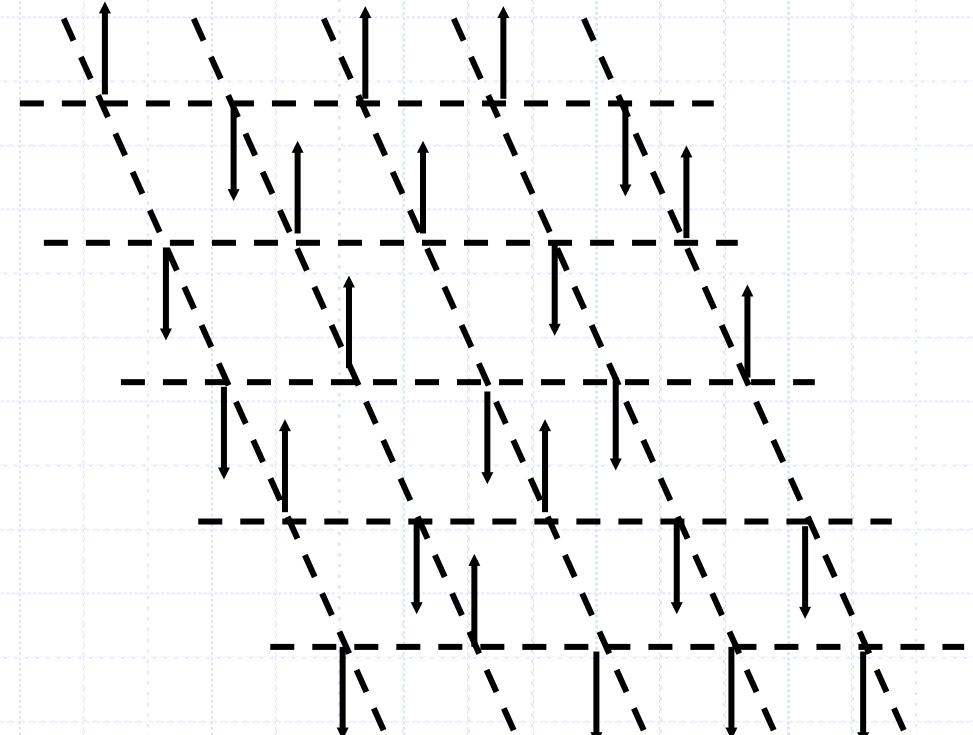
- Introduce defects
- Order \leftrightarrow disorder transition

Square-lattice Ising Model

Zero external
magnetic field

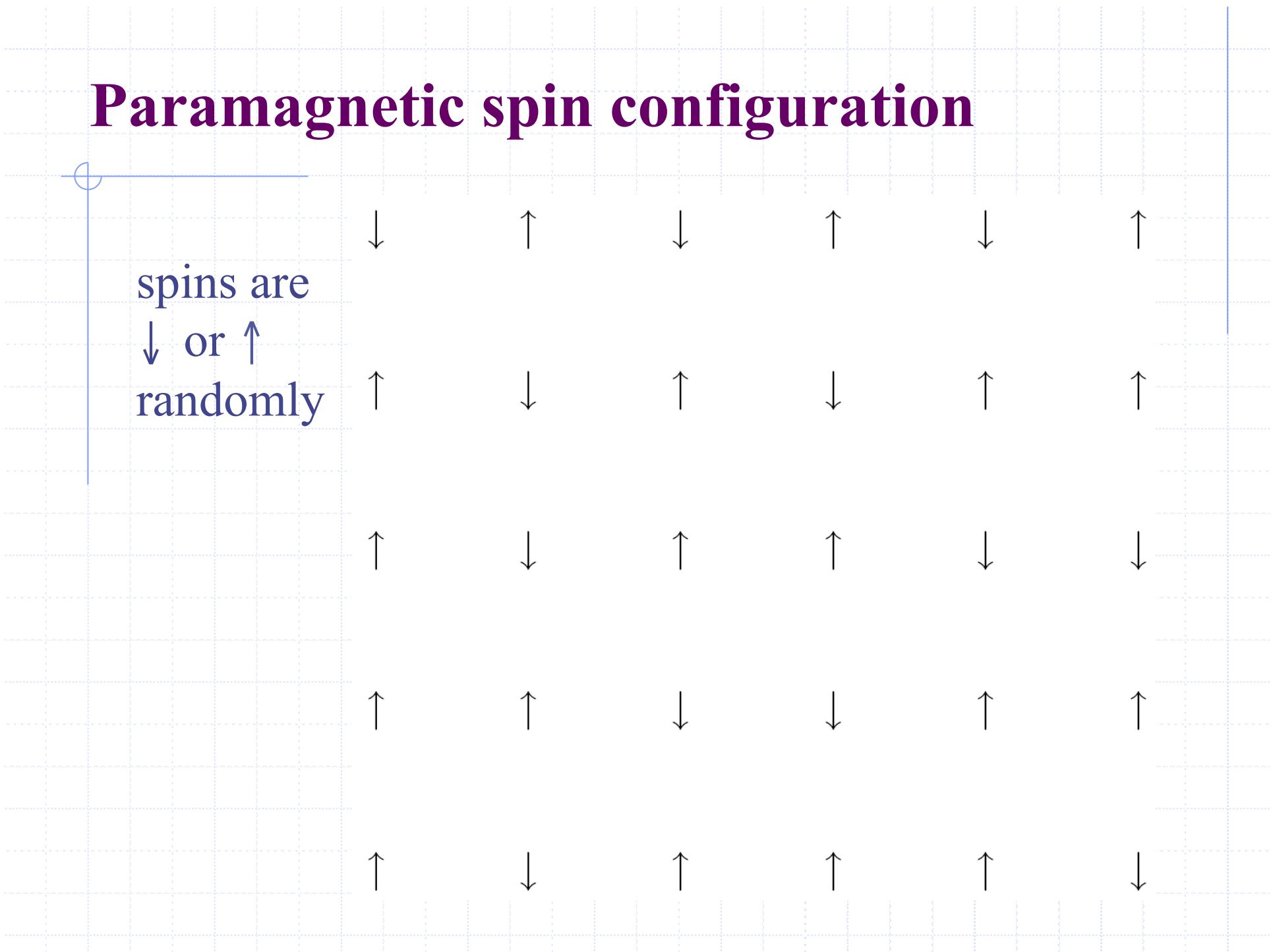
$$\rightarrow H = 0$$

$$E = -J \sum_{i,j=nn(i)}^N S_i S_j$$



Paramagnetic spin configuration

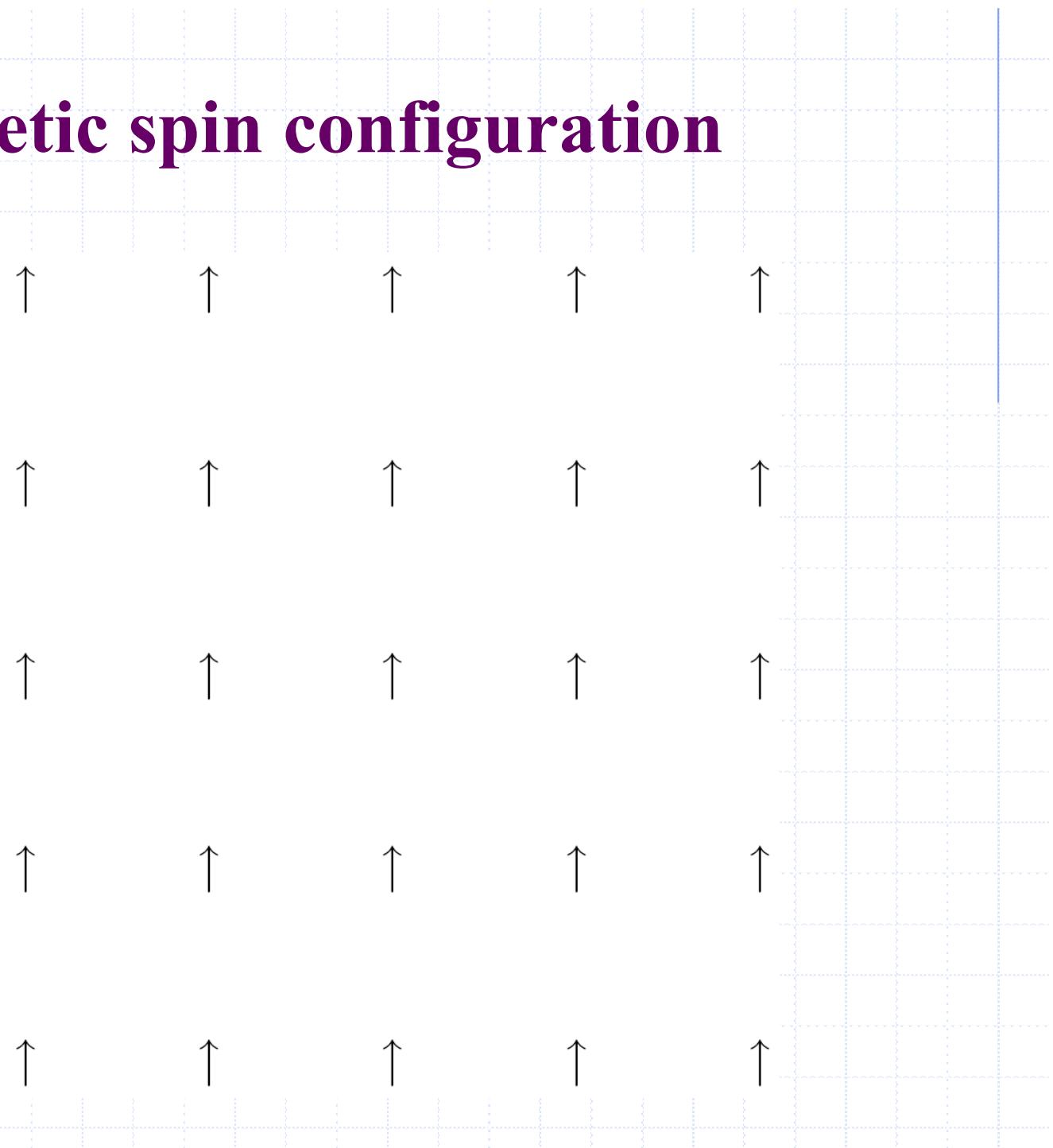
spins are
↓ or ↑
randomly



Ferromagnetic spin configuration



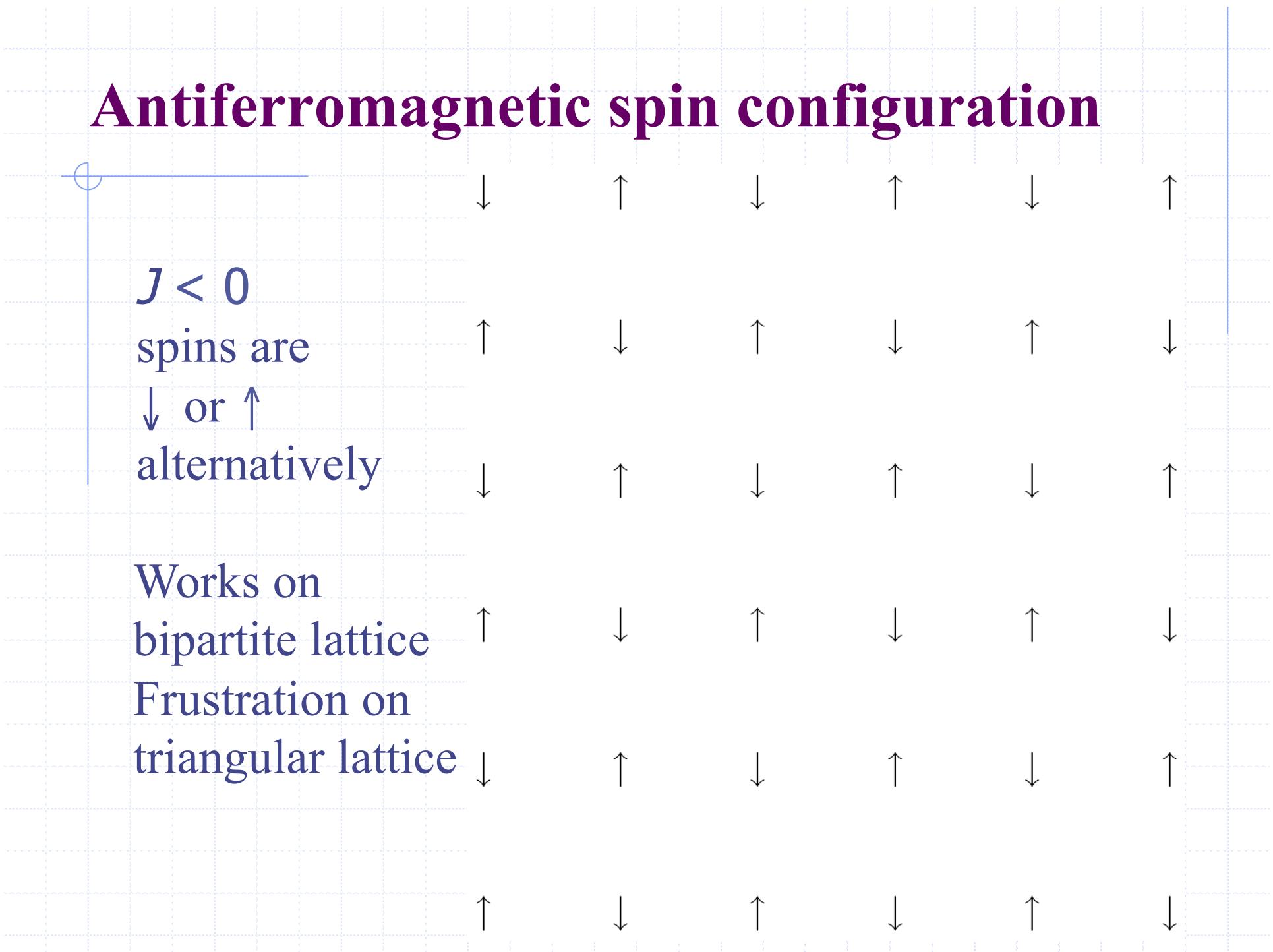
$J > 0$
All spins are
 \downarrow or \uparrow
together



Antiferromagnetic spin configuration

$J < 0$
spins are
 \downarrow or \uparrow
alternatively

Works on
bipartite lattice
Frustration on
triangular lattice



Thermal Fluctuation

- ⊕ Temperature $T \neq 0$
=> Participation of
Excited States

with probability

$$p_i = \exp(-\Delta E/k_B T),$$

$$\Delta E = E_i - E_0$$

- ⊕ Spin flip
configurations:

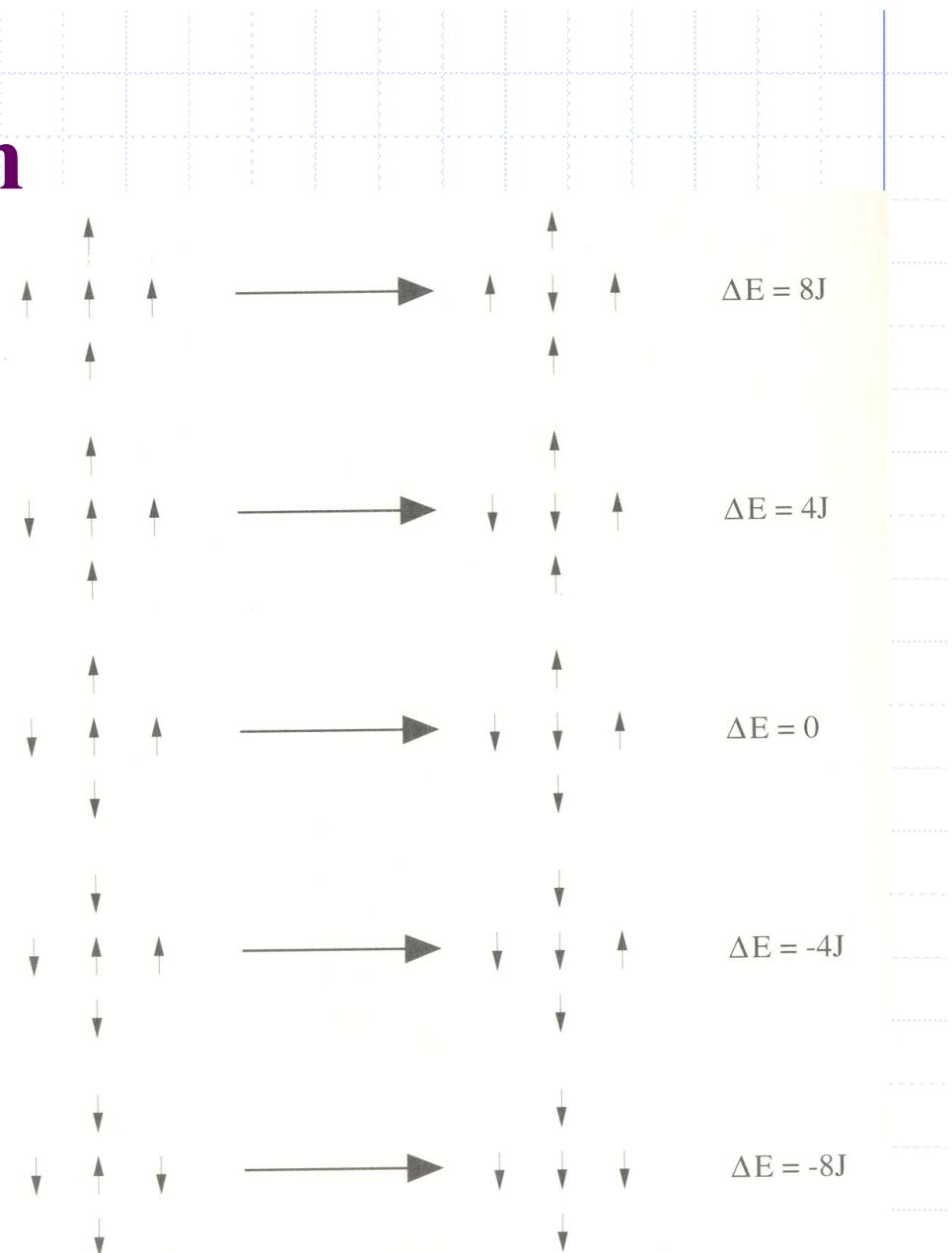


Fig. 16.3 The five possible transitions of the Ising model on the square lattice with spin flip dynamics.

Magnetic Phase Transition



Induced by temperature (thermal fluctuation)

Magnetization



Paramagnetic

Ising Model,
 $T_c=?$

Ferromagnetic

1 / Temperature

1 / T_c

(Critical Temperature)

Magnetic Phase Transition

$T < T_c$ Low temperature	order alignment nonzero magnetization
$T > T_c$ High temperature	disorder (thermal fluctuations) random alignment spins and fields cancel zero magnetization
$T = T_c$ Critical temperature	magnetization divergent (for an infinite system)

History of the Ising Model



- Proposed by **Wilhelm Lenz**
- 1D model solved by
Lenz's student Ernst Ising
 - No phase transition
- 2D (square lattice) model solved by
Lars Onsager (Nobel Prize in Chemistry)
 - Has a phase transition
- 3D model investigated by computer simulation

The Famous Onsager Paper



PHYSICAL REVIEW

VOLUME 65, NUMBERS 3 AND 4

FEBRUARY 1 AND 15, 1944

Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition

LARS ONSAGER

Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut

(Received October 4, 1943)

The partition function of a two-dimensional "ferromagnetic" with scalar "spins" (Ising model) is computed rigorously for the case of vanishing field. The eigenwert problem involved in the corresponding computation for a long strip crystal of finite width (n atoms), joined straight to itself around a cylinder, is solved by direct product decomposition; in the special case $n = \infty$ an integral replaces a sum. The choice of different interaction energies ($\pm J$, $\pm J'$) in the (0 1) and (1 0) directions does not complicate the problem. The two-way infinite crystal has an order-disorder transition at a temperature $T = T_c$ given by the condition

$$\sinh(2J/kT_c) \sinh(2J'/kT_c) = 1.$$

The energy is a continuous function of T ; but the specific heat becomes infinite as $-\log |T - T_c|$. For strips of finite width, the maximum of the specific heat increases linearly with $\log n$. The order-converting dual transformation invented by Kramers and Wannier effects a simple automorphism of the basis of the quaternion algebra which is natural to the problem in hand. In addition to the thermodynamic properties of the massive crystal, the free energy of a (0 1) boundary between areas of opposite order is computed; on this basis the mean ordered length of a strip crystal is

$$(\exp(2J/kT) \tanh(2J'/kT))^n.$$

Solving the Ising Model

- ⊕ Cited about 600 times, but title search of “Ising model” is about 800 times per year.
- ⊕ People are still working on different approach to the Ising model, in the hope of solving the 3D version. Baxter once wrote “the 399th solution of the Ising model”.
- ⊕ Luttinger wrote to Onsager, saying that he wants to try solving the 3D Ising model, Onsager replied that the probability is almost zero.
- ⊕ Many people tried, but no prevail.
- ⊕ For 2D, Onsager solved $\alpha=0$, and wrote down $\beta=1/8$, but never explained how. It was CN Yang who solved in 1952. Wu found $\gamma=7/4$.
- ⊕ How did Onsager find the solution?

Thermodynamic Quantities

We are going to use the 2D Ising model with periodic boundary conditions as an illustration

1. Mean energy:

$$\langle E \rangle (T) = \frac{\sum_{i=0} E_i p_i}{\sum_{i=0} p_i}$$

$$\langle E \rangle (T = \infty) = 0$$

$$\langle E \rangle (T = 0) = E_0 = -2JN$$

Spin configuration depends on the sign of J

Thermodynamic Quantities

2. Heat capacity:

$$C_V(T) = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{kT^2} (\langle E^2 \rangle - \langle E \rangle^2)$$

$$C_V(T = 0) = 0$$

$$C_V(T = \infty) = 0$$

$$C_V(T) \sim |T - T_c|^{-\alpha}$$

α : critical exponent.

Experimentally measurable

Heat Capacity Cv

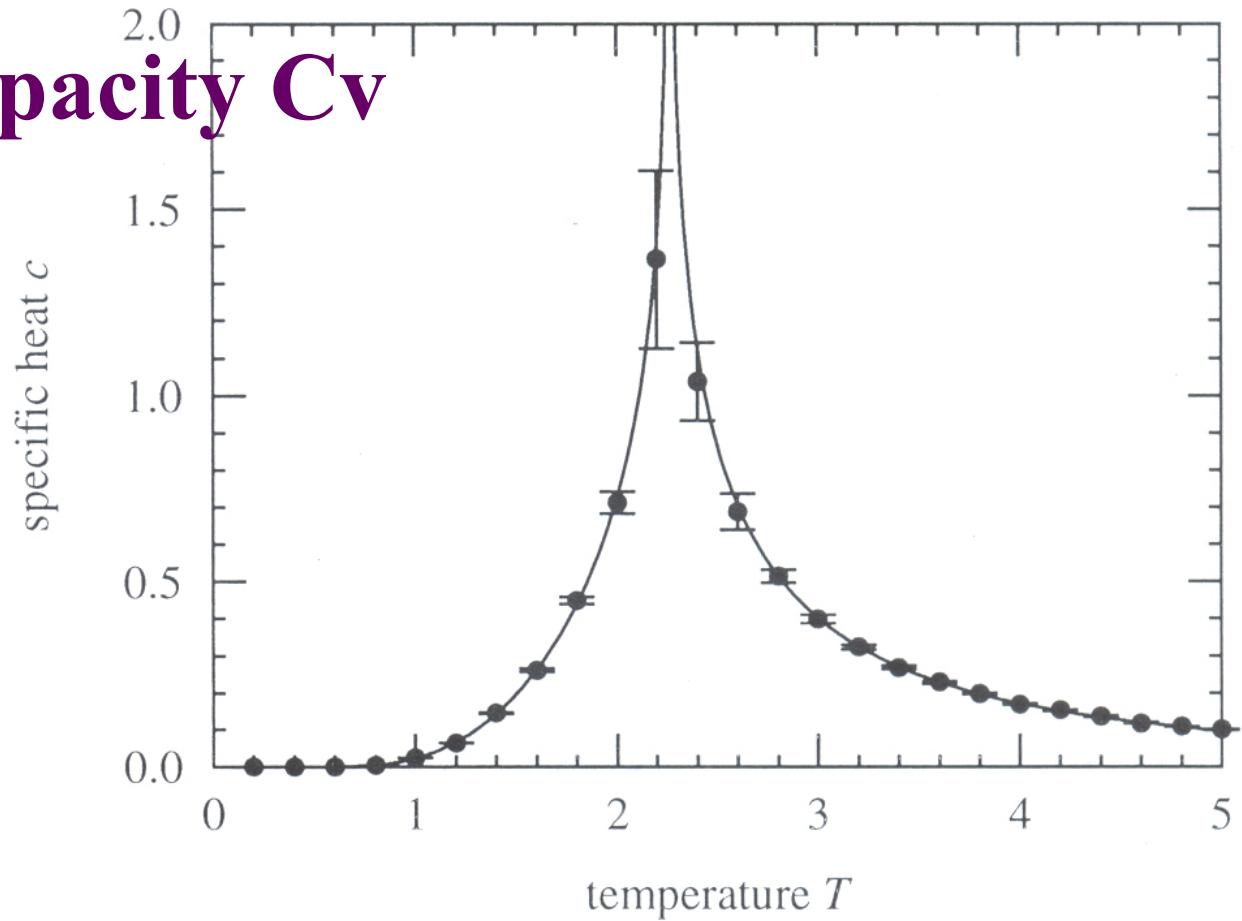
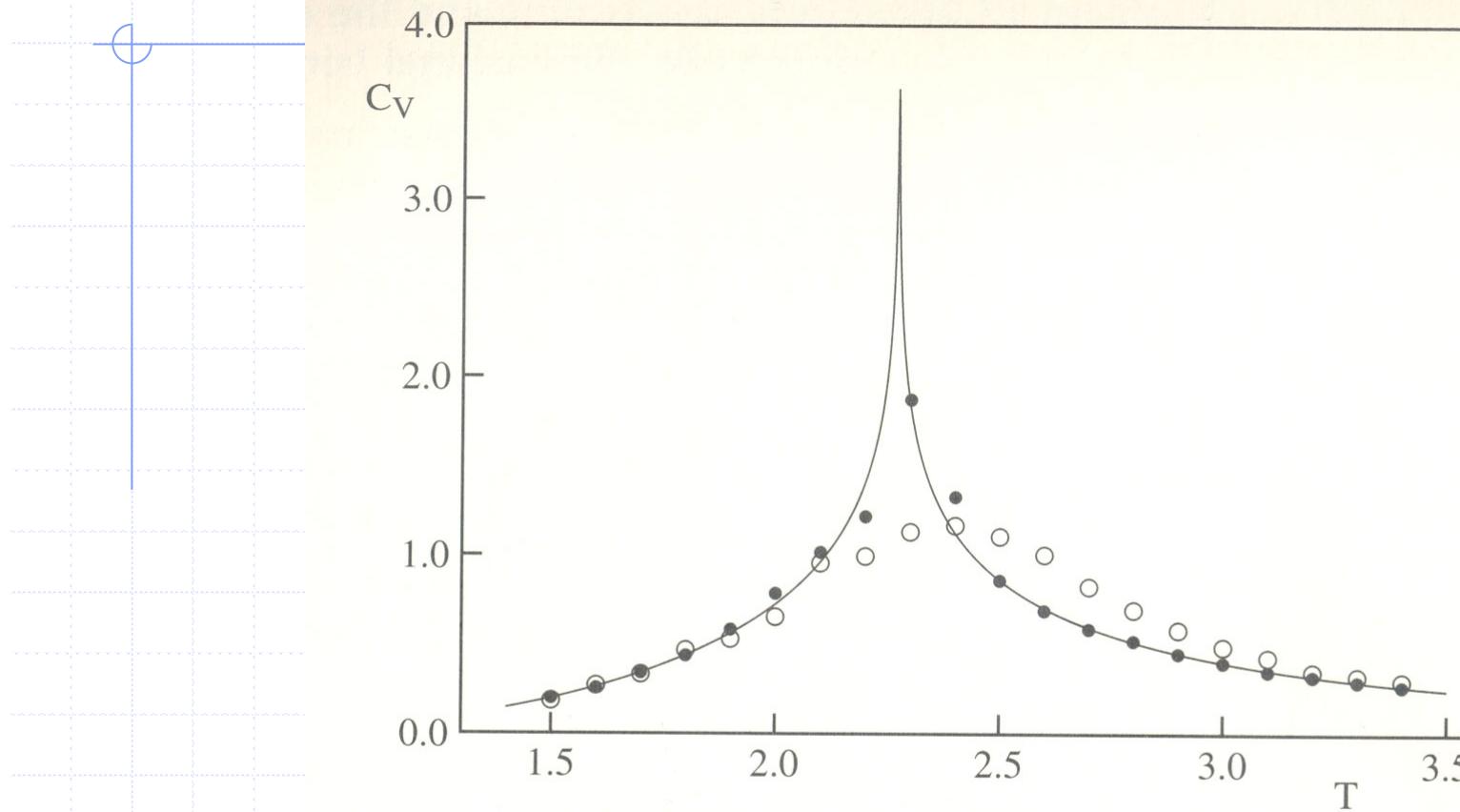


FIGURE 3.10 The specific heat per spin of the two-dimensional Ising model calculated by Monte Carlo simulation (points with error bars) and the exact solution for the same quantity (solid line). Note how the error bars get bigger close to the peak in the specific heat. This phenomenon is discussed in detail in the next section.

Heat Capacity C_V



$L=8, 16$

Fig. 17.2 The temperature dependence of the specific heat C (per spin) of the Ising model on a $L = 8$ and $L = 16$ square lattice with periodic boundary conditions. One thousand Monte Carlo steps per spin were used for each value of the temperature. The continuous line represents the temperature dependence of C in the limit of an infinite lattice. (Note that C is infinite at $T = T_c$ for an infinite lattice.)

Thermodynamic Quantities

3. Magnetization M :

$$m(T) = \langle \frac{M}{N} \rangle = \langle \frac{1}{N} \sum_{i=1}^N s_i \rangle$$

$$m(T = 0) = 1$$

$$m(T = \infty) = 0$$

$$m(T) \sim |T - T_c|^\beta$$

β : critical exponent. Experimentally measurable

Magnetization

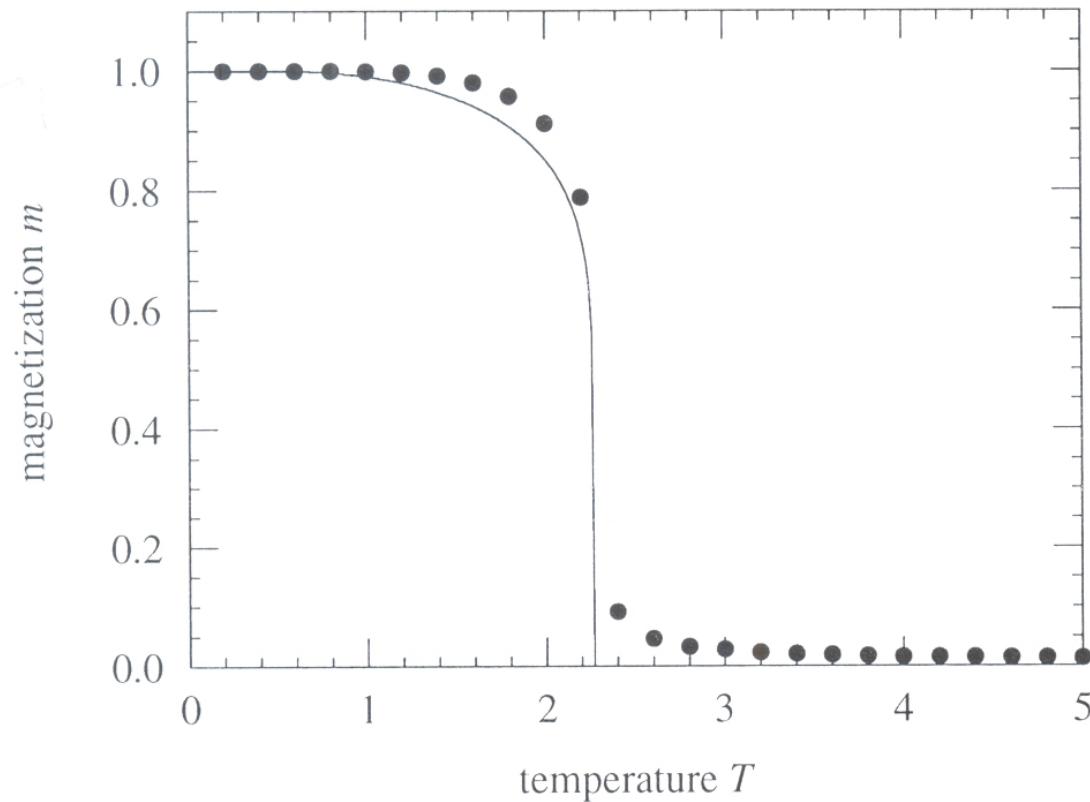


FIGURE 3.9 The magnetization per spin of the two-dimensional Ising model. The points are the results from our Monte Carlo simulation using the Metropolis algorithm. The errors are actually smaller than the points in this figure because the calculation is so accurate. The solid line is the known exact solution for the Ising model on an infinite two-dimensional square lattice.

Thermodynamic Quantities

4. Magnetic susceptibility χ :

$$\chi = \lim_{B \rightarrow 0} \frac{\partial \langle M \rangle}{\partial B} = \frac{1}{kT} (\langle M^2 \rangle - \langle M \rangle^2)$$

$$\chi(T) \sim |T - T_c|^{-\gamma}$$

γ : critical exponent
Experimentally measurable

Thermodynamic Quantities

Energy

$$E = -J \sum_{i,j=nn(i)}^N S_i S_j$$

Magnetization

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

Heat Capacity

$$C = \frac{\partial \langle E \rangle}{\partial T} = \frac{1}{kT^2} [\langle E^2 \rangle - \langle E \rangle^2]$$

Susceptibility

$$\chi = \lim_{H \rightarrow 0} \frac{\partial \langle M \rangle}{\partial H} = \frac{1}{kT} [\langle M^2 \rangle - \langle M \rangle^2]$$

Solving the Ising Model

- ⊕ Analytical solution: 1D & 2D square lattice
 - 1D: Ernst Ising; Graduate student work; $T_c=0$
 - 2D: Lars Onsager; Very difficult to understand;
 $\sinh(2J/k_B T_c) \sinh(2J'/k_B T_c) = 1$
- ⊕ Numerical solution
 - Exact enumeration
 - Monte Carlo simulation
 - ...
- ⊕ Approximation approach: many

Exact Enumeration

- ⊕ Find out all 2^N possible configurations and sum up.
(Binary representation could be used).
- ⊕ Calculate thermodynamic quantities

2×2 square lattice : $2^4 = 16$ 4-bit binary number.

3×3 square lattice : $2^9 = 512$ 9-bit binary number.

...

...

$L \times L$ square lattice: 2^N N-bit binary number.

($N = L \times L$, No. of spin in lattice)

Exact Enumeration

As the number of spins increases, so are

- binary number needed
- computer memory needed
- runtime

For large lattice (e.g., $L > 6$),

Numerical simulation is needed !!!

It is always useful to have a program (or data)
of exact enumeration for bench mark.

MC Simulation Program

- ⊕ Set up parameters: J/T , B , lattice, BC, etc.
- ⊕ MC updating spin configurations
- ⊕ To reach equilibrium
- ⊕ Measurement: energy, heat capacity, magnetization and susceptibility, correlation functions, etc.
- ⊕ Data analysis
- ⊕ ...

MC Simulation of the Ising Model

- ⊕ Metropolis algorithm & Simulation
- ⊕ Magnetic phase transition
- ⊕ Symmetry breaking
- ⊕ Finite size effects
- ⊕ Critical slowing down and other algorithms

Simulation Steps

- ⊕ Set up lattice, L_x, L_y, J_{ij}, T , other parameters.
- ⊕ Randomly pick up any configuration
 $S = \{s_i; i=1,2, \dots, N\}$.
- ⊕ Update: change spin configuration based on a selected algorithm, e.g., Metropolis.
- ⊕ Repeat “Update” for many times
- ⊕ Calculate thermodynamic quantities, correlation, etc., as simulation goes on.

Metropolis Algorithm

- ⊕ It is based on the following transition

$$W(A \rightarrow B) = \begin{cases} e^{-\Delta E / kT} & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0 \end{cases}$$

- ⊕ Choose a site j , flip its spin $s_j \Rightarrow -s_j$, and calculate corresponding energy difference ΔE .
- ⊕ If $\Delta E < 0$, save the new configuration
If $\Delta E > 0$, get $r = \text{RAND}[0,1]$. If $W > r$, save the new configuration. Otherwise, keep the old one.

Heat-bath Algorithm

- ⊕ Choose a spin s_j at random from the lattice
- ⊕ The probability for the spin $s_j = \sigma$ is

$$P(s_j = \sigma) = e^{-\beta E(\sigma)} / \sum_{\sigma} e^{-\beta E(\sigma)}$$

The probability does not depend on the initial state.

For the Ising model,

$$P(\sigma = \pm 1) = \frac{e^{-\beta E(\sigma=\pm 1)}}{e^{-\beta E(\sigma=1)} + e^{-\beta E(\sigma=-1)}}$$

- ⊕ Acceptance Rate is

$$A = \frac{e^{-\beta \Delta E/2}}{e^{-\beta \Delta E/2} + e^{\beta \Delta E/2}}$$

Measurements

- ⊕ Energy E
- ⊕ Magnetization m (symmetry broken issue)
- ⊕ Specific heat C_v (fluctuation theorem,
derivatives)
- ⊕ Magnetic susceptibility χ
- ⊕ Correlation functions

⊕ ...

Measuring Correlation Functions

- ⊕ The most frequently measured quantity
- ⊕ Example, spin-spin correlation

$$G_c(i,j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle = \langle s_i s_j \rangle - m^2$$

- ⊕ For system of translational invariant, one has

$$G_c(r_i, r_i + r) = G_c(r)$$

- ⊕ Thus we can improve our estimation of $G_c(r)$ by averaging its value over the whole lattice

$$G_c(r) = (1/N) \sum [\langle s_i s_j \rangle - m^2] \text{ over } r_i - r_j = r$$

Measuring Correlation Functions

- To evaluate $G_c(r)$ for all r directly requires N^2 calculations.
- One may use Fourier transform to reduce the computation time. Procedures are

$$\begin{aligned} G_c(k) &= \sum G_c(r) \exp(ik \cdot r) \\ &= (1/N) \sum \sum e^{ik \cdot r} [\langle s_i s_j \rangle - m^2] \\ &= (1/N) \langle \sum e^{ik \cdot r_i} (s_i - m) \sum e^{-ik \cdot r_j} (s_j - m) \rangle \\ &= (1/N) \langle |s(k)|^2 \rangle \end{aligned}$$

Data Analysis

- Consider m sets measurements each with N samples

$$\bar{A} = \frac{1}{M} \sum_{m=1}^M A_m = \frac{1}{MN} \sum_{m=1}^M \sum_{j=1}^N x_{m,j}$$

different from the expectation value $A_m \equiv \langle A \rangle$.

- Average Variance (uncorrelated)

$$\sigma^2 = \frac{1}{MN} \sum_{m=1}^M \sum_{j=1}^N (x_{m,j} - \bar{A})^2$$

Variance of individual

$$\sigma_A^2 = \frac{1}{M} \sum_{m=1}^M (A_m - \bar{A})^2 = \frac{1}{MN^2} \sum_{m=1}^M \left(\sum_{j=1}^N x_{m,j} - \bar{A} \right) \left(\sum_{j=1}^N x_{m,j} - \bar{A} \right)$$

$$\sigma_A^2 = \sigma^2 / N$$

Variance of the mean

Data Analysis

- Variance (correlated)

$$\sigma_{\bar{A}}^2 = \frac{\sigma^2}{N} \times 2\tau_{\bar{A},\text{int}}$$

the integrated autocorrelation time

$$\tau_{\bar{A},\text{int}} = \frac{1}{2} + \sum_{j=1}^N C(j)\left(1 - \frac{j}{N}\right)$$

$$C(j) = \frac{\langle A_i A_{i+j} \rangle - \langle A_i \rangle^2}{\langle A_i^2 \rangle - \langle A_i \rangle^2}$$

σ is interpreted as the error in the original n measurements.

Data Analysis

- ⊕ Binning technique: divide data $\{A_i, i=1, 2, \dots, N\}$ into L groups, $K=N/L$, and let

$$B_l = \frac{1}{K} \sum_{k=(l-1)*K+1}^{l*K} A_k$$

now we work on the data set $\{B_l, l=1, 2, \dots, L\}$ instead.

- ⊕ Random binning: select data randomly from each group.
- ⊕ Check if data follow Gaussian distribution

Data Binning

Correlated → Uncorrelated

A set of N correlated data



$$N_p = N / P$$

The Bootstrap Method

- ⊕ This is a reliable re-sampling method used for error estimation.
- ⊕ Take specific heat as an example
- ⊕ The procedure:
 - pick out n number of energy measurements at random
 - calculate the specific heat c from these n numbers just as we would normally do
 - repeat the process

The Bootstrap Method

- ⊕ The procedure: (continue)
 - after we have repeated this calculations several times, the standard derivation of the distribution in the results for c is a measure of the error in the value of c , i.e., $\sigma_c = \sqrt{\bar{c}^2 - \bar{c}^2}$
(no extra factor of $1/(n-1)$ as before.)
 - duplication is about $1 - 1/e = 63\%$
 - whether these n data are independent of each other is not important.

Systematic Errors

- ⊕ Systematic errors are much harder to gauge than statistical ones. They could be
 - equilibration time is long
 - measurements are too correlated
 - ...
- ⊕ Try different algorithms

Critical Exponents

- Define a dimensionless parameter, t ,

$$t = (T - T_c)/T_c$$

The **reduced temperature**

- Divergence of the correlation length

$$\xi \sim |t|^{-\nu}$$

ν is called the **Critical Exponent**

- Universality:** the value of ν is independent of details of the model, such as the coupling J , or the type of lattices we are studying.

Critical Exponents

- ⊕ Other universal critical exponents

magnetic moment $m \sim |t|^\beta$

magnetic susceptibility $\chi \sim |t|^{-\gamma}$

heat capacity $c \sim |t|^{-\alpha}$

correlation time $\tau \sim |t|^{-z\nu}$

- ⊕ Measuring critical exponents is the most important part of the simulation, and it is far from being a trivial exercise.
- ⊕ They are not totally independent.

Calculate Critical Exponents

- Consider the exponent ν , $\xi \sim |t|^{-\nu}$

- Since $\xi = b \xi' \sim |t'|^{-\nu}$

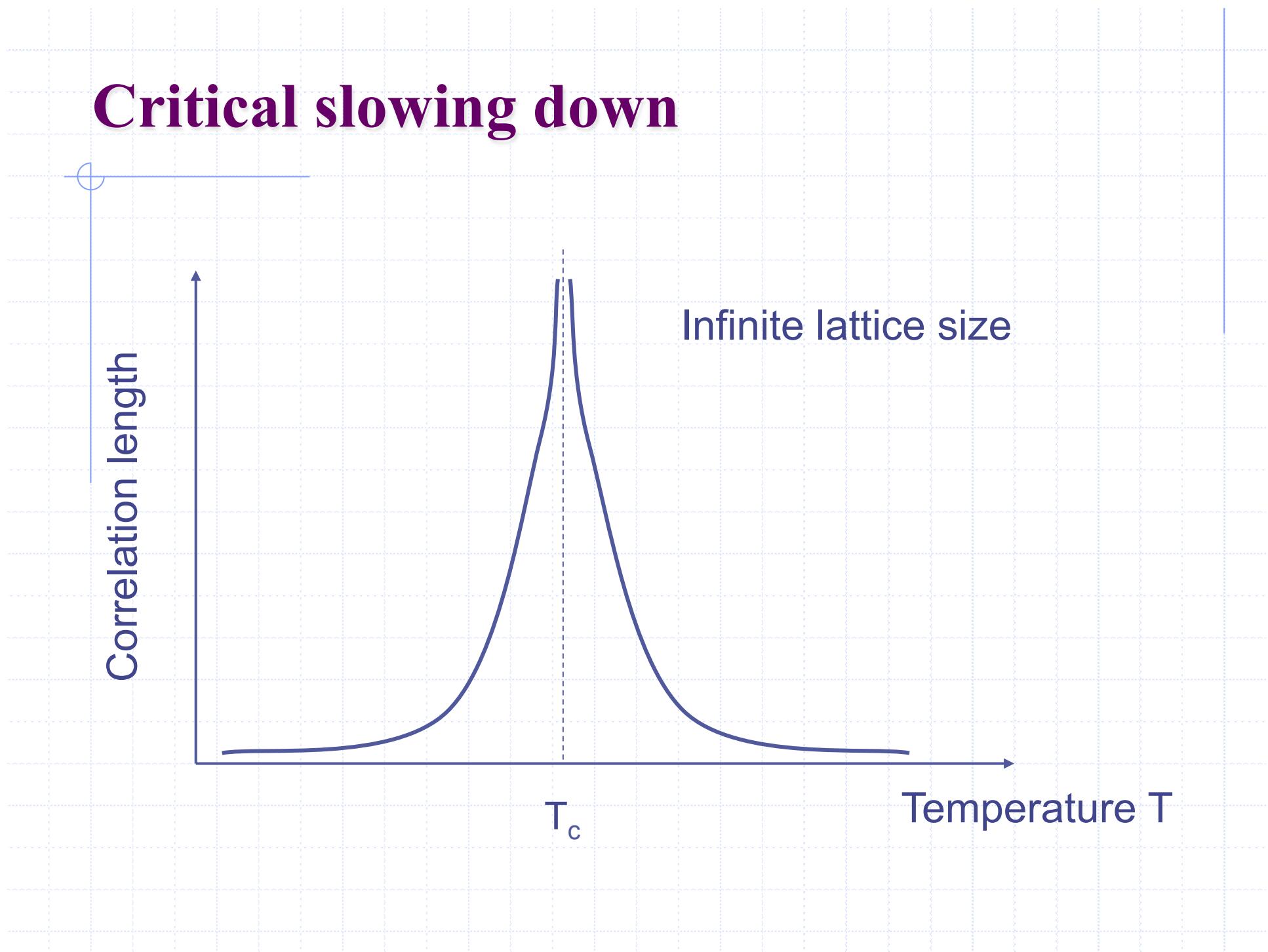
we obtain the renormalization transformation equation

$$|t/t'|^{-\nu} = b.$$

- These equations are valid only close to T_c , the standard way of solving this equation is linearize it by the Taylor expansion to the leading order:

$$T' - T_c = (T - T_c) \frac{dT'}{dT}|_{T_c} \Rightarrow \nu = \frac{\log b}{\log \frac{dT'}{dT}|_{T_c}}.$$

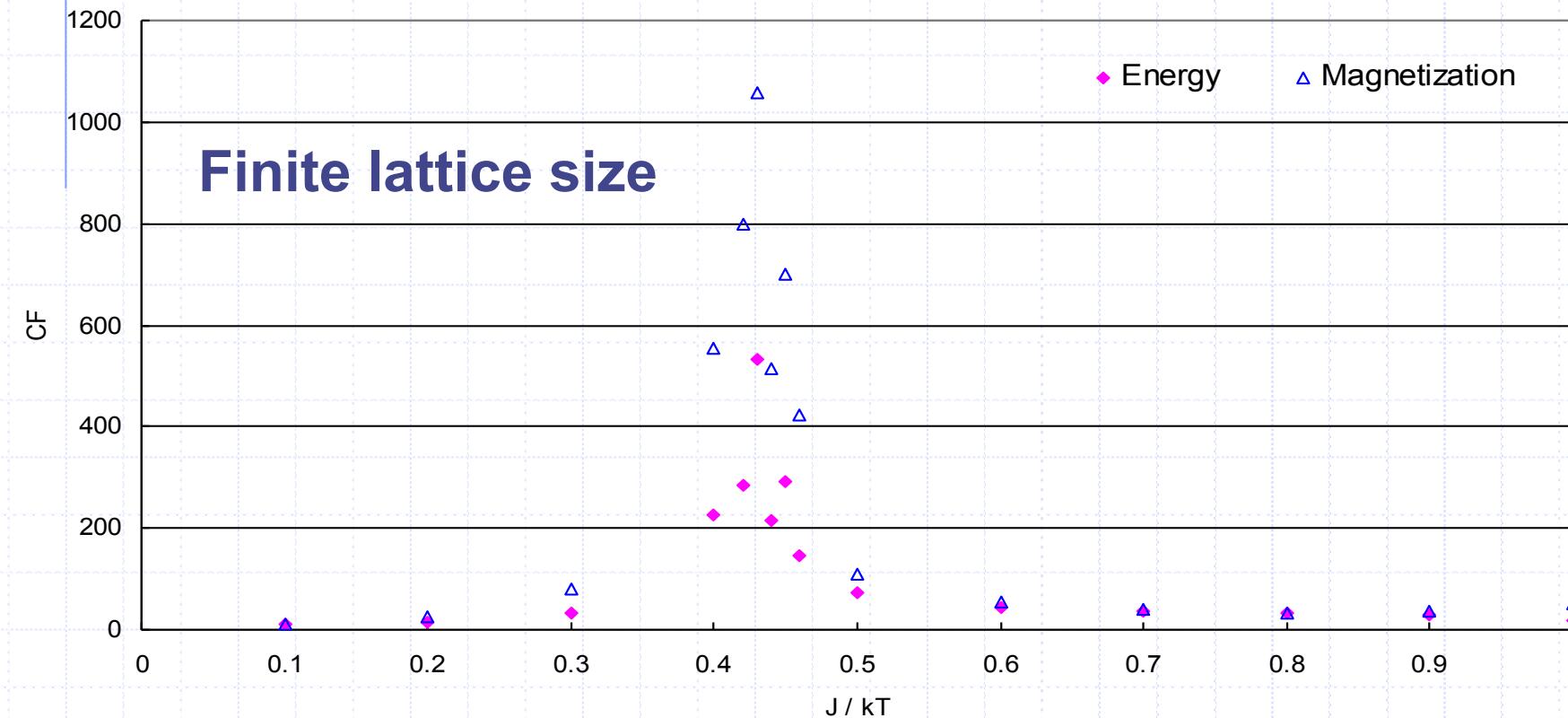
Critical slowing down



Critical slowing down

AutoCorrelation of Energy and Magnetization vs betaJ

Lattice = 16 x 16



Other Algorithms

- ⊕ The Wolff algorithm
- ⊕ The Swendsen-Wang algorithm
- ⊕ Niedermayer's algorithm
- ⊕ Multigrid methods
- ⊕ Renormalization Group
- ⊕ ...
- ⊕ Parallel computing

Monte Carlo Renormalization Group

- ⊕ An alternative way to estimate critical exponents.
- ⊕ Start from an $L \times L$ lattice and shrink it by a rescaling factor b (say, 2) in each direction.
- ⊕ Then represent each block by just one block spin, the value of the block spin is assigned by certain rules, e.g., the “**majority rule**”.

(Other procedures: such as summation.)

Real-Space Renormalization

- ⊕ **Basic assumption:** the series of blocked states generated also appear with their correct Boltzmann probabilities, if we perform calculation using the same Ising Hamiltonian as for the original system.
(Correct?)
- ⊕ Correlation length is rescaled, $\xi' = \xi/b$, i.e., we are doing simulation at different temperature, except if we are at the critical temperature!

A Simple RG Scheme

- ⊕ We perform an MC simulation at temperature T and calculate the internal energy $\langle E \rangle$.
- ⊕ We take each of the states generated by our simulation and block them, using a selected blocking scheme (e.g., the majority rule).
- ⊕ We calculated the internal energy $\langle E' \rangle$ for the blocked system.
- ⊕ Vary temperature until we find the point at which $\langle E' \rangle = \langle E \rangle$. This is the critical temperature T_c of the system.

Problems with Simple RG Scheme

- ⊕ There is no method to estimate error. For some models, the approximation (basic RG assumption) is an uncontrolled one.
- ⊕ There still exists finite size effects, even though the RG methods aims at reducing finite size effects. Sometimes one has to perform simulation with the size of the rescaled system directly!
- ⊕ The assumption that after blocking the system is still governed **same Hamiltonian** could be a very poor one.

Brief Review

- ⊕ MC for statistical physics: summation!
- ⊕ Types of magnetic ordering: issues, e.g.,
order \Leftrightarrow disorder transition, critic T, etc.
- ⊕ The Ising Model: Hamiltonian (energy form)
and quantities to calculate.
- ⊕ Solution: 1D (and 2D), enumeration, basic
concepts, etc.
- ⊕ Related models: similarity & applications.

Monte Carlo Simulation

- ⊕ Program structure: set up, MC, measure, data, etc.
- ⊕ Metropolis algorithms and others, detail balance.
- ⊕ Simulation Issues:
 - How to identify phase transition?
 - Symmetry breaking: measurement
 - data analysis: error estimation
 - correlation functions: FFT, etc.
 - finite size effects: scaling function, etc.
 - critical exponents: universality, experiments, etc.
 - critical slowing down & some useful algorithms: global versus local, computer time, etc.

Histogram Method

Use information at T to estimate properties of $(T \pm \Delta T)$

$$P(E, \beta_0) = \frac{H_0(E)}{\sum_E H_0(E)}$$

E is the measurement of Energy after MC (not average)

$$\therefore P(E, \beta) = \frac{W(E)e^{-\beta E}}{\sum_E W(E)e^{-\beta E}}$$

$$W(E) = a_0(\beta_0)H_0(E)e^{\beta_0 E}$$

$W(E) = \#$ of microstate with energy E (DOS).

It is independent of T .

Histogram Method

- ⊕ Let $\beta = \beta_0$ in $P(E, \beta)$ and compare with $P(E, \beta_0)$

$$P(E, \beta) = \frac{H_0(E)e^{-(\beta-\beta_0)E}}{\sum_E H_0(E)e^{-(\beta-\beta_0)E}}$$

- ⊕ Then

$$\langle A(\beta) \rangle = \sum_E A(E)P(E, \beta)$$

or

$$\langle A(\beta) \rangle = \sum_{E,M} A(E, M)P(E, M, \beta)$$

$$= \frac{\sum_{E,M} A(E, M)H_0(E, M)e^{-(\beta-\beta_0)E}}{\sum_{E,M} H_0(E, M)e^{-(\beta-\beta_0)E}}$$

- ⊕ This is useful only $H_0(E)$ represents similar physics!

Lee-Kosterlitz Method

$$F(E) = -k_B T \ln W(E) e^{-\beta E}$$

- ⊕ For systems with a 1st-order phase transitions, $F(E)$ has two local minima (low T , high T). At transition T , two minima have the same value of $F(E)$.
- ⊕ For system with no transition in the thermodynamic limit, $F(E)$ has only one minimum for all T .
- ⊕ Varying system sizes,
 - $\Delta F \uparrow$ as $L \uparrow$ (1st order)
 - $\Delta F \sim$ as $L \uparrow$ (continuous)
 - $\Delta F \downarrow$ as $L \uparrow$ (no transition)

Lee-Kosterlitz Method

1. Do a simulation at a temperature close to the suspected transition temperature, and compute $H(E)$. Usually, the temperature at which the peak in the specific heat occurs is chosen as the simulation temperature.
2. Use the histogram method to compute $-\ln H_0(E) + (\beta - \beta_0)E \propto F(E)$ at neighboring values of T . If there are two minima in $F(E)$, vary β until the values of $F(E)$ at the two minima are equal. This temperature is an estimate of the possible transition temperature T_c .
3. Measure the difference ΔF at T_c between $F(E)$ at the minima and $F(E)$ at the maximum between the two minima.
4. Repeat steps (1) - (3) for larger systems. If ΔF increases with size, the transition is first-order. If ΔF remains the same, the transition is continuous. If ΔF decreases with size, there is no thermodynamic transition.

Lee-Kosterlitz Method

The above procedure is applicable when the phase transition occurs by varying the temperature. Transitions also can occur by varying the pressure or the magnetic field. These *field-driven transitions* can be tested by a similar method. For example, consider the Ising model in a magnetic field at low temperatures below T_c . As we vary the magnetic field from positive to negative, there is a transition from a phase with magnetization $M > 0$ to a phase with $M < 0$. Is this transition first-order or continuous? To answer this question, we can use the Lee-Kosterlitz method with a histogram $H(E,M)$ generated at zero magnetic field, and calculate $F(M)$ instead of $F(E)$. The quantity $F(M)$ is proportional to $-\ln \sum_E H(E,M) e^{-(\beta - \beta_0)E}$. Because the states with positive and negative magnetization are equally likely to occur for zero magnetic, we should see a double minima structure for $F(M)$ with equal minima. As we increase the size of the system, ΔF should increase for a first-order transition and remain the same for continuous transition.

Other Applications of the Ising Model

- ⊕ Hysteresis loop: $m(B)$ with external field B
- ⊕ Lattice gas (2-state system):

molecule occupies site (1)

molecule NOT occupies site (0)

Gas-liquid transition ($\mu \leftrightarrow B$)

- ⊕ Glass:
(many metastable states)

- ⊕ The Potts Model
For $q = 2 \rightarrow$ Ising

$$\sum J_{ij} \sigma_i \sigma_j$$

$$H = -J \sum_{\langle ij \rangle} \delta_{S_i, S_j} \quad S_i = 1, 2, \dots, q$$

Other Applications of the Ising Model

- ⊕ Classical Heisenberg Model

$$H = \sum J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

\mathbf{S} classical vector

- ⊕ XY Model

$$H = -\sum J_{ij} \cos(\phi_i - \phi_j) - B \sum \cos \phi_i$$

- ⊕ Lennard-Jones

$$\phi(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right]$$