Ising Model of a ferromagnetic spin system

Assume an array of N ferromagnetic spin, $s_i = \pm 1$, i=1,2,…, N, immersed in an external magnetic field, **B**.

Spin here is synonym to microscopic magnetic moment. It is constrained to point only in the up or down directions, with respect to the external magnetic field, **B**.

To be specific, we will consider N spins arranged in a 2-D surface, so that now we have a 2-D Ising model. In Figure, there are N=9 spins, and each spin has z =4 nearest neighbours.

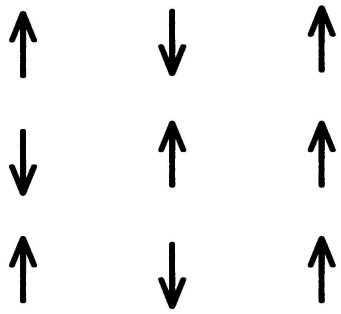


Figure 8.1: Schematic spin model for a ferromagnet.

First, assume zero spin-spin interactions.

The total interaction energy due to the interactions between the spins and the **B** field are given by

$$E_M = -\mu \sum \mathbf{s}_i \cdot \mathbf{B} = -\mu B \sum s_i$$

where μ is the microscopic magnetic moment (Bohr magneton).

If a spin $\boldsymbol{s}_i$ is parallel to the external magnetic field **B**, $\boldsymbol{s}_i$ //**B**, the interaction energy is $\varepsilon_i = -\mu \mathbf{s}_i \cdot \mathbf{B} = -\mu B s_i = -\mu B$. Likewise, $\varepsilon_i = -\mu \mathbf{s}_i \cdot \mathbf{B} = -\mu B s_i = +\mu B$ if $\boldsymbol{s}_i$ is anti-parallel to **B**.

The system is said to be ferromagnetic since the configuration with the spins **s** parallel to **B** is favorable. Such configuration favors a state with negative E_M.

In statistical mechanics, a single spin **s** in an external magnetic field **B** has both possibilities to point in the up as well as down directions. The respective probabilities are

$$P_+ = \frac{1}{Z}\exp\left(-\frac{\varepsilon_+}{kT}\right) = \frac{1}{Z}\exp\left(-\frac{\mu B}{kT}\right); P_- = \frac{1}{Z}\exp\left(-\frac{\varepsilon_-}{kT}\right) = \frac{1}{Z}\exp\left(+\frac{\mu B}{kT}\right),$$

where T is the temperature at which the spin is in thermal equilibrium with.

$$Z = \exp\left(+\frac{\mu B}{kT}\right) + \exp\left(-\frac{\mu B}{kT}\right)$$

is the so-called partition function, obtained by requiring that the total probability is normalized, i.e., $P_+ + P_- = 1$.

According to statistical mechanics, the observed value of a spin in a magnetic field is an averaged value of the microscopic configuration, given by

$$\langle s \rangle = P_+ s_+ + P_- s_- = \frac{1}{Z}\exp\left(-\frac{\mu B}{kT}\right) - \frac{1}{Z}\exp\left(+\frac{\mu B}{kT}\right) = \tanh\left(\frac{\mu B}{kT}\right)$$

In the presence of spin-spin interaction, the “pure” magnetic field interaction energy μB will have to be replaced by an “effective magnetic field” interaction μH_{eff} that contains the spin-spin interaction in addition to the magnetic field interaction energy,

$$\langle s\rangle = \tanh\left(\frac{\mu H_{\text{eff}}}{kT}\right).\ \text{Eq. (1)}$$

We will derive H_{eff} in the next part with mean field approximation.

Ising model in the presence of spin-spin interactions

Now we will add in spin-spin interaction to the picture. We assume the simplest Ising model: (i) 1-D, and (ii) a spin only interacts with it nearest neighbour (nn) in the form of

$$E_I = -J\sum_{\langle i,j\rangle} s_i s_j\ ,$$

J is called the exchange energy, or coupling energy between adjacent spins. For ferromagnet, $J > 0$. For the special case of a 1-D spin-chain with N=5 spins, for example,

$$\frac{E_I}{-J} = \sum_{\langle i,j\rangle} s_i s_j = \sum_{i=1}^{i=5} s_i\left(\sum_{\langle i,j\rangle} s_j\right) = s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_5;$$

$$\sum_{\langle i,j\rangle} s_i s_j = \sum_{i=1}^{i=5} s_i\left(\sum_{\langle i,j\rangle} s_j\right) = \frac{1}{2}\left[s_1(s_0+s_2)+s_2(s_1+s_3)+s_3(s_2+s_4)+s_4(s_3+s_5)+s_5(s_4+s_6)\right] = \frac{1}{2}\sum_{i=1}^{i=5} s_i(s_{i-1}+s_{i+1});\ s_0 = s_6 = 0$$

Note that $\sum_{\langle i,j\rangle} s_i s_j$ expressed in the form of $\frac{1}{2}\sum_{i=1}^{i=5} s_i(s_{i-1}+s_{i+1})$ will be useful for coding of MC simulation latter.

The total energy of N spins in the simplest 1-D Ising model in the presence of both nn interaction and external magnetic field is

$$E = E_M + E_I = -\mu B\sum_{i=1}^{i=N} s_i - J\sum_{\langle i,j\rangle} s_i s_j$$

We rewrite it as

$$E = -\mu B\sum_{i=1}^{i=N}\left[s_i - J\left(\sum_{\langle i,j\rangle} s_j\right)s_i\right] = -\mu\sum_{i=1}^{i=N}\left(B + \frac{J}{\mu}\sum_{\langle i,j\rangle} s_j\right)s_i\ .$$

Mean field approximation (MFA)

Now we would like to evoke the mean field approximation to solve for E. In mean field approximation, the effect of the spin-spin interaction is assumed to be described by an effective magnetic field energy. We would now attempt to derive the form of the effective magnetic field, H_{eff}, which is kind of similar to E_M but with the spin-spin interaction effects in it.

By construct, for a single spin, the effect of H_{eff} is $\varepsilon_i = -\mu H_{\text{eff}} s_i$.

For a collection of N spins,

$$E = \sum_i \varepsilon_i = -\mu H_{\text{eff}}\sum_{i=1}^{i=N} s_i = -\mu\sum_{i=1}^{i=N} H_{\text{eff}} s_i$$

Since $E = -\mu\sum_{i=1}^{i=N}\left(B + \frac{J}{\mu}\sum_{\langle i,j\rangle} s_j\right)s_i$

$$\Rightarrow H_{\text{eff}} = B + \frac{J}{\mu}\sum_{\langle i,j\rangle} s_j = B + \frac{J}{\mu}\times(\text{Sum of the spins of nearest neighbours to a generic spin})$$

Next, we make another approximation, that the value of any individual spin is replaced by its thermal average, $s_i \to \langle s_i\rangle = \langle s\rangle$. As a result,

$$\begin{aligned}\mu H_{\text{eff}} &= B + \frac{J}{\mu}\times(\text{Sum of the spins of nearest neighbours to a generic spin})\\ &= B + \frac{J}{\mu}\times\left(s(\text{left nn}) + s(\text{right nn})\right)\\ &\downarrow s(\text{left nn}) \to \langle s\rangle, s(\text{right nn}) \to \langle s\rangle\\ \mu H_{\text{eff}} &= \mu B + J\sum 2\langle s\rangle = \mu B + Jz\langle s\rangle\end{aligned} \qquad \text{Eq. (2)}$$

where $z = 2$ is the number of nn for any spin i. Essentially, in the mean field approximation,

$$\begin{aligned}H_{\text{eff}} &= B + \frac{J}{\mu}\sum_{\langle i,j\rangle} s_j = B + \frac{J}{\mu}\times(\text{Sum of the spins of nearest neighbours to a generic spin})\\ &= B + \frac{J}{\mu}\times\left(s(\text{left nn}) + s(\text{right nn})\right) \approx B + \frac{J}{\mu}\times z\langle s\rangle\end{aligned}$$

It is straight forward to show that Eq. (2) also holds for Ising model in 2-D and 3-D by replacing z with the corresponding value. For 2-D case, $z = 4$; for 3-D, $z = 6$.

The average spin $\langle s\rangle$ as described in Eq. (1) is derived from statistical mechanics. Its value can now be solved for in the mean field approximation of Eq. (2):

$$\langle s\rangle = \tanh\left(\frac{\mu H_{\text{eff}}}{kT}\right) = \tanh\left(\frac{\mu B + Jz\langle s\rangle}{kT}\right)$$

Given kT, z, J and B, we can solve for $\langle s\rangle$ numerically, as follows:

Let $f(\langle s\rangle) = \langle s\rangle - \tanh\left(\frac{\mu B + Jz\langle s\rangle}{kT}\right)$. We wish to find the value of $\langle s\rangle$. This can be obtained at the zeros of the function $f(\langle s\rangle)$, i.e, $f(\langle s\rangle) = 0$. Now the problem of finding the numerical value of $\langle s\rangle$ is simple to find the roots of $f(\langle s\rangle) = 0$.

Newton-Raphson method for root finding

Use Newton-Raphson (NR) method to solve for the root of an equation of the form $f(x) = 0$. Choose a point on the x-axis as the zero approximation to the equation $f(x) = 0$.

Taking the derivative of $f(x)$ at $x=x_0$ gives $f'(x_0)$.

$f'(x_0)$ is the slope at the point $(x_0, f(x_0))$ on the curve $y=f(x)$. The slope $f'(x_0)$ cut through the y-axis at x_1. The triangle defined by the points $(x_0, f(x_0))$, $(0, x_0)$, $(0, x_1)$ are related by Pythogorus theorem, $f'(x_0) = \frac{f(x_0)}{x_0 - x_1} \Rightarrow x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$. Once x_1 is obtained, we can proceed to obtain x_2 using the same procedure, where now x_0 is replaced by x_1. We can keep repeating the same procedure to approximate closer the true root x_{true} from $x_0 \to x_1 \to x_2 \to \ldots x_n \to \ldots$, where $x_n = x_{n-1} - \frac{f(x_n)}{f'(x_n)}$

The procedure is repeated until N where $\Delta x_N = |x_N - x_{N-1}|$ is sufficiently small. If this happens, we say x_N converges. x_N is then taken as a good approximation to x_{true}.

See sample code 8.1 where the NR method is used to solve $f(\langle s\rangle)=0$ at a fixed kT. Code 8.2 modifies sample code 8.1 to find the root for $f(\langle s\rangle)=0$ as a function of kT.

Spontaneous magnetisation

The magnetisation of a system with N spins as measured in experiment, according to statistical mechanics, is given by

$$M = N\mu\langle s\rangle .$$

Hence, the average megenetisation per spin, m, is $m = M/N = \mu\langle s\rangle$. M is directly proportional to $\langle s\rangle$.

If is found that for the case where B=0, $\langle s\rangle$ tends towards 0 as $T >> zJ/k$. For $T < zJ/k$, $\langle s\rangle \to \pm 1$ as $T \to 0$. We interpret this as: Below $T = zJ/k$, the spin system is in a ferroelectric phase, with non-zero magnetization. Above $T = zJ/k$, the spin system enters paramagnetic phase with an average of zero magnetization.

Critical temperature

In the mean field approximation, assuming **B** = 0, once the temperature is larger than $T=zJ/k$ the spin system losses its magnetization and entered the paramagnetic phase.

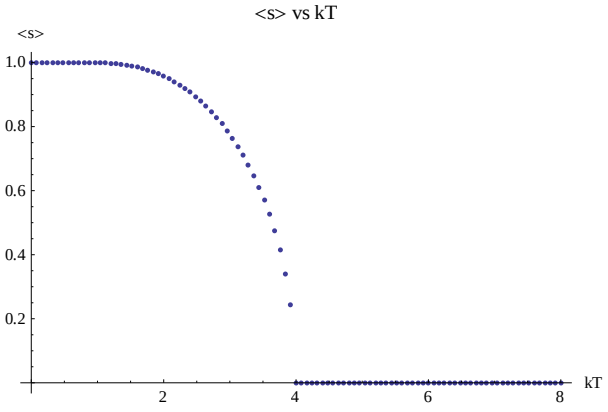
The **critical temperature** as obtained in the mean field approximation for zero magnetic field, is given by

$$T_c = zJ/k.$$

We shall see that the true value for the critical temperature of a 2-dimensional Ising system deviates from the above expression due to the fact that MFA fails to capture the physics near the critical point where phase transition is taking place.

Second order phase transition, induced thermally.

In other words, a spontaneous magnetization occurs at $T = T_c$ when temperature is reduced from above. The system losses its magnetization above T_c because thermal fluctuation, kT, dominates over the spin-spin interactions. This is an example of **phase transition** in which the magnetization spontaneously appear from a paramagnetic phase when temperature crosses a critical value. The phase transition we see here is induced by temperature at a fixed external magnetic field.



Numerical solution of mean field equation for <s> as a function of temperature, where J/k =1, z = 4. Note that for $T \geq T_c = zJ/k$, magnetization vanishes.

The abrupt transition of magnetization at $T = T_c$ as predicted by the mean field approximation is an example of a second order phase transition. Phase transition is known as critical behavior. It is characterized by an abrupt change of an *order parameter* (of which the magnetization is) at some critical temperature. The critical behaviour at the vicinity at the critical temperature is usually given some power laws, with universal value of critical exponent. In the case there, the power law has the form

$$\langle s \rangle \sim (T - T_c)^{\beta},$$

β is a universal critical exponent. The value of β for any other systems undergoing 2nd order phase transition is known to be the same. This is an amazing fact.

The critical behavior of magnetization in the Ising model is a result of the (i) interaction between the Ising spins with the environment (the heat bath at temperature *T*), and (ii) the spin-spin interactions. These interactions play the role to mediate energy exchange among the spins so that the system can be brought to thermalisation with the heat bath. To certain extent the behavior of a system also may be influenced by the geometry of the system (e.g., finite size effect, the way how the spins are arranged in 3D, the degree of freedoms of a spin, boundary conditions etc.).

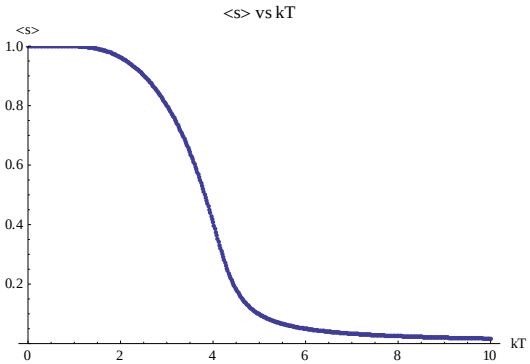
In mean field approximation, we can expand $\langle s \rangle$ about the critical temperature to find that β =1/2. This is the value predicted by mean field approximation. β can also be calculated using exact method, i.e., without approximation. In this way it is shown that the mean field β deviates from the exact value given by

$$\beta = 1/8.$$

This discrepancy illustrates the limitation of mean field approximation. A more detailed way to calculate β is called for. We will use Monte Carlo method for such purpose.

Magnetization with a non-zero **B**

Also note that once *B* field is switched on, the critical behavior is modified. The critical transition now appears to become smoother.



Numerical solution of mean field equation for <*s*> as a function of temperature, where *J*/*k* =1, *z* = 4, *B*=0.1.

Monte Carlo Simulation of 2D Ising model

We will use MC to simulate the values of average magnetization $M = N\langle s \rangle$, as well as the average energy of the 2D Ising model. Say the spin system comprise of $N = L \times L$ spins in a square lattice. The sites are index by a pair of number $\{i,j\}$. *N* is the total number of spins in the simulation square = number of grid points.

Essentially we will simulate how the Ising spin system interacts with the environment. MC is a stochastic method similar to the simulation of random walk. But here the temperature (heat bath)

and energy (a.k.a. interaction) is taken into account. The heat bath exchanges energy with the spin system to bring it into equilibrium at some temperature T.

In MC, we simulate the microscopic states of the spin system, and then take averages of these states. The experimentally measured physical quantities (e.g., heat capacity, magnetization, magnetic susceptibility) are, in the language of statistical physics, the averages of these microscopic states.

The MC scheme we will be using is the simplest and historically the earliest: Metropolis algorithm. First, we fix a temperature for which the simulation is to be done. Then we choose an initial configuration for the spin system (e.g. all up/down or random). The energy of the system is calculated, and we call it E_0. We randomly choose a spin and flip it. The total energy of the flipped states is evaluated at $E_{\text{trial}} = E_0 + E_{\text{flip}}$. If $E_{\text{flip}} < 0$, we accept the move and replace the current configuration by the trial configuration, and also $E_1 = E_{\text{trial}}$. If $E_{\text{trial}} > 0$, the trial state is accepted if the Boltzmann factor $\exp(-E_{\text{flip}}/kT) > q$, a random number uniformly distributed on [0,1]. If $\exp(-E_{\text{flip}}/kT) < q$, the trial move is rejected. The current state then remains as it is, and $E_1 = E_0$. The procedure is repeated for a sufficiently long step. At time step n in the MC simulation, the current magnetization and the corresponding energy can be calculated via

$$\begin{aligned} M_n &= \sum_{i,j}^{N} s(i,j) = \sum_{i}^{N}\left(\sum_{j}^{N} s(i,j)\right) \\ &= \left[s(1,1)+s(1,2)+\ldots+s(1,L)\right] \\ &\quad +\left[s(2,1)+s(2,2)+\ldots+s(2,L)\right] \\ &\quad +\ldots \\ &\quad +\left[s(L,1)+s(L,2)+\ldots+s(L,L)\right] \end{aligned}$$

$$E_n = -J \sum_{\{i,i',j,j'\}} s(i,j)s(i',j') - \mu B \sum_{i,j} s(i,j)\,.$$

$s(i,j)$ is the value of the spin (either +1 or -1) at site $\{i,j\}$. The sum runs over all nearest neighboring spins. For the special case where external magnetic field is switched off, the total energy is only contributed by the spin-spin interaction term:

$$E_n = -J \sum_{\{i,i',j,j'\}} s(i,j)s(i',j')$$

Periodic boundary condition is adopted to minimize the finite size effect due to the termination of the sample at its edges.

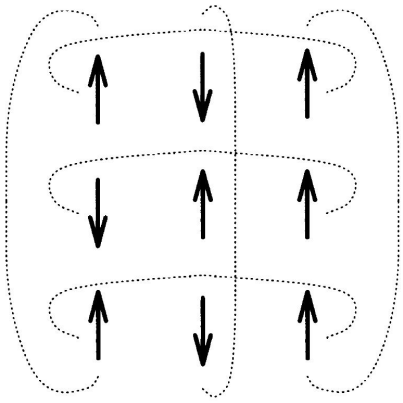


Figure 8.6: Ising model with periodic boundary conditions. Spins that are connected by the dotted lines that wrap around the lattice are considered to be nearest neighbors and thus to interact with exchange energy J.

This simply means:

$$s(0,j) = s(L,j); s(L+1,j) = s(0,j);$$
$$s(i,0) = s(i,L); s(i,L+1) = s(i,0);$$

EXAMPLE 8.1 Monte Carlo algorithm for the Ising model on an $L \times L$ square lattice

- Set the desired T and H.
- Initialize all spins s_i $(i = 1, 2, ..., L^2)$. (We can take $s_i = 1$ for all i, for example.)
- Perform the desired number of Monte Carlo sweeps through the lattice.
  - ▷ For a given sweep, loop through the L rows (or columns) of the lattice. On each row (or column), consider each spin for updating.
    - Calculate E_{flip}, the energy required to flip the selected spin. For nearest-neighbor interactions, E_{flip} only depends on the nearest neighbors. For spins on an edge, apply the chosen boundary condition (see below) to determine which spins are the neighbors.
    - If $E_{\text{flip}} \leq 0$, flip the spin.
    - If $E_{\text{flip}} > 0$, generate a uniform random number r between 0 and 1, and compare it with $\exp(-E_{\text{flip}}/k_B T)$.
      - ▷ If $r \leq \exp(-E_{\text{flip}}/k_B T)$, flip the spin.
      - ▷ If $r > \exp(-E_{\text{flip}}/k_B T)$, leave it undisturbed.
  - ▷ After each sweep is completed, record the new energy, magnetization, and any other quantities of interest.
- Store (and/or plot) the recorded thermodynamic quantities.

In the simulation, *T* is in unit of J/*k*, *B* in unit of J/μ.

A MC run is done by fixing the number of fixed step say *nlast*. The first quantity we wish to monitor is the magnetization per spin, $m = M/N$, as a function of time step *n*.

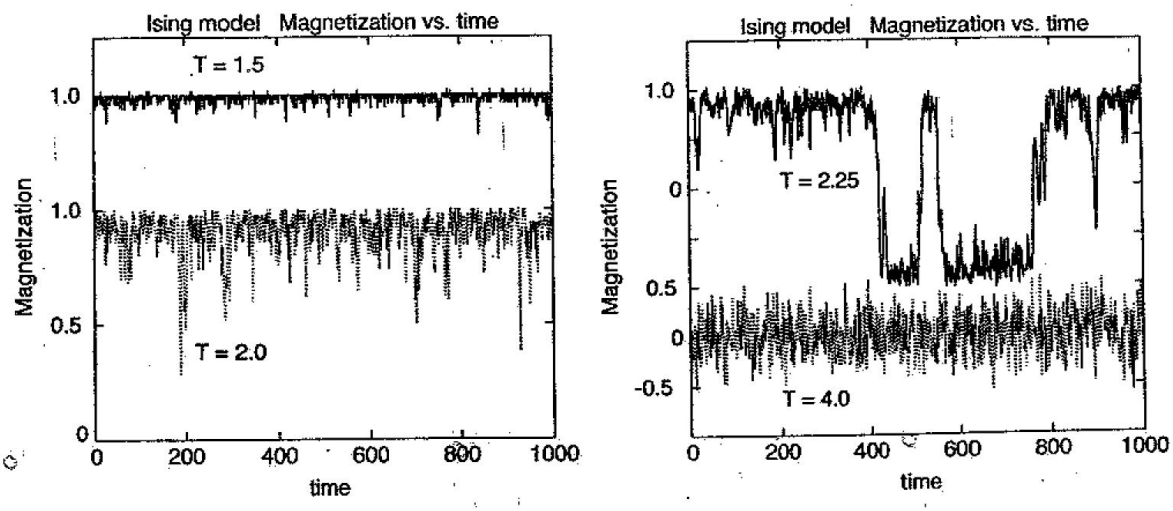


FIGURE 8.6: Magnetization versus time for the Ising model on a 10×10 square lattice at several different temperatures. Note that we have normalized the magnetization so that $M = 1$ corresponds to complete alignment of all of the spins. Left: at relatively low temperatures compared to T_c, with the results for $T = 1.5$ offset upwards for clarity; right: at temperatures near and above T_c (the two results are again offset for clarity).

The MC code of sample code 8.3 implements the above described procedure to simulate the microscopic states M_n and the corresponding energy E_n as a function of time step. For the same of simplicity, we set off the magnetic field contribution to the total energy.

Second order phase transition induced by thermal effect at zero magnetic field.

We should find the following behavior of the magnetization at fixed temperature T (with $B = 0$):

1) If T is lower than a value of $T_c = 1/\ln(2 + \sqrt{2}) = 2.27$, fluctuation in m is small.
2) When we set T closer to 2.27, say, $T = 2.0$, we find that the fluctuation becomes larger.
3) When we set T at very close to 2.27, fluctuation in m becomes very large. It infers that the all the spins of the entire system change direction, as at close to the critical point, the system is extremely sensitive to small perturbation. A small perturbation in the temperature can already cause strong response.
4) When T is much larger than T_c, we see that the average magnetization fluctuates around $m = 0$. The size of the fluctuation is larger than that at temperature $T << T_c$. The magnetization is zero now and the system is in the paramagnetisation phase. This is attributed to the fact that now the thermal fluctuation, originated from the temperature term kT as appear in the Boltzmann factor $\exp(-E_{flip}/kT)$ dominates over the spin-spin interaction which is responsible for the development of ferromagnetic phase.

The critical temperature $T_c = 1/\ln(2 + \sqrt{2}) = 2.27$ is obtained from analytical solution. The MC simulation confirms quite comfortably that indeed when the temperature of the system approach $T_c = 2.27$, a phase transition happens.

In addition, the following behavior in the simulated energy E_n is also be observed:

(i) When B = 0, $T \rightarrow 0$, $E/N \rightarrow -2J$, $m \rightarrow \pm 1$
(ii) When B = 0, $T > T_c$, $E/N \rightarrow 0$, $m \rightarrow 0$

Next, the average of interested quantity such as the average energy and average energy squared at step *n*,

$$<E_n>=\sum_{n-n_0}^{ilast}\frac{E_n}{n-n_0},\ \left\langle E_n^2\right\rangle=\sum_{n-n_0}^{ilast}\frac{E_n^2}{n-n_0},$$

are also monitored as a function of time step *n*. n_0 is the initial time step we need to wait before the averages are taken so that the average values are that belongs to the states that are already entered thermal equilibrium.

These averages are important because from them we can evaluate the variance of the energy, $(\Delta E)^2=\left\langle E^2\right\rangle-\langle E\rangle^2$ at each time step *n*. The square root of the variance, $\sqrt{(\Delta E)^2}$, is the standard deviation that measures how much the energy deviate from its average value $\langle E\rangle$.

According to fluctuation dissipation theorem, we can obtain the heat capacity of the spin system from the variance in energy via

$$C=\frac{(\Delta E)^2}{kT^2}$$

Heat capacity per spin is defined as $c=C/N=\frac{(\Delta E)^2}{NkT^2}$ is a normalized quantity. We should find from the MC simulation that *c* display large peak at *T* close to T_c. This is direct consequence of the fact that fluctuation in energy becomes large (in fact diverges in the analytical limit) at T_c. Sample code 8.4 implements a MC code that calculates $\langle E\rangle, \left\langle E^2\right\rangle$ and the heat capacity at fixed temperature. Sample code 8.5 is obtained by modifying sample code 8.4 to calculate specific heat, magnetisation *m* as a function of temperature *T*. Basically, to do so we simply put the sample code 8.4 into a loop to vary for temperature.

From sample code 8.5, we see that the phase of magnetisation changes continuously. However, the heat capacity, which is a second order derivative of the free energy *F* of the spin system change discontinuously at T_c. This is a phase transition termed second order phase transition, in which the second order derivative of the free energy changes discontinuously.

First order phase transition induced by external magnetic field at fixed temperature.

In the previous case we assume that the external magnetic field contribution to be switched off. The phase transition was induced by thermal effect. Now, in sample code 8.6, we include the magnetic field into the MC code to calculate magnetisation as a function of magnetic field at fixed temperature. The magnetic field comes into the picture through the definition of the total energy TE = TE (spin - spin) + TE (magnetic):

$$E_n=-J\sum_{\{i,i',j,j'\}}s(i,j)s(i',j')-\mu B\sum_{i,j}s(i,j)$$

Below T_c we will find from the MC simulation that found that magnetisation *m* undergoes a first order phase transition. First, we let B to increase according to the trend: $B<0 \rightarrow B=0 \rightarrow B>0$. The entire spin states of the system flips simultaneously when B passes through some critical value $B=B_c\neq 0$.

In this kind of phase transition, the magnetisation changes discontinuously. Since the magnetisation is a first derivative of the free energy *F* of the spin system, the phase transition in which the phase of *m* changes abruptly is termed first order transition.