

Handout 12. Ising Model

February 25, 2011

Contents

| | | |
|----------|---|-----------|
| 1 | Definition of Ising model | 2 |
| 2 | Solving the 1D Ising model | 4 |
| 2.1 | Non-interacting model ($J = 0$) | 4 |
| 2.2 | Ising model at zero field ($h = 0$) | 5 |
| 2.3 | The general case ($J \neq 0, h \neq 0$) | 7 |
| 3 | Generalized 1D Ising model | 11 |
| 3.1 | Spins with more than two states | 11 |
| 3.2 | More than one row of spins | 12 |
| 4 | 2D Ising model | 13 |
| 4.1 | Analytic solution | 13 |
| 4.2 | Monte Carlo simulation | 14 |
| 4.3 | Qualitative behavior | 17 |
| 4.4 | Sketch of derivations of partition function in 2D | 20 |

A major topic of interest in statistical mechanics (and in physics in general) is the understanding of phase transitions (e.g. freezing of water to form ice), which requires the study of interacting models.

The 2-dimensional (2D) Ising model (see front page image on coursework) is one of the few interacting models that have been solved analytically (by Onsager, who found the expression of its partition function). It turns out that the 2D Ising model exhibits a phase transition. The analytic and numerical solutions of the Ising model are important landmarks in the field of statistical mechanics. They have significantly influenced our understanding of phase transitions.

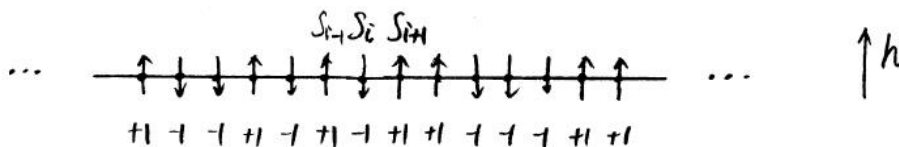
We will first discuss the simpler 1-dimensional (1D) Ising model, whose analytic solution is

easier to obtain. This will pave the road to the discussion of the 2D Ising model which comes next.

Reading assignment: Sethna p.163-165. Reif Chapter 10.

1 Definition of Ising model

Ising (Z. Physik, 31, 253, 1925) introduced a model consisting of a lattice of “spin” variables s_i , which can only take the values $+1$ (\uparrow) and -1 (\downarrow). Every spin interacts with its nearest neighbors (2 in 1D) as well as with an external magnetic field h .



The Hamiltonian¹ of the Ising model is

$$H(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \quad (1)$$

The sum $\langle i, j \rangle$ is over nearest neighbors ($j = i \pm 1$ in 1D).

J is a constant specifying the strength of interaction. The Ising model is usually studied in the canonical ensemble. (It would be a nightmare to do it in the microcanonical ensemble.)

In the canonical ensemble, the probability of finding a particular spin configuration $\{s_i\}$ is,

$$p(\{s_i\}) = \frac{1}{Z} \exp(-\beta H(\{s_i\})), \quad \beta \equiv \frac{1}{k_B T} \quad (2)$$

where $Z = \sum_{\{s_i\}} \exp(-\beta H(\{s_i\}))$ is the partition function. Due to the Boltzmann factor, $e^{-\beta H}$, spin configurations with lower energies will be favored.

We can now discuss the effect of J and h on the behavior of the spins.

- when $h > 0$, $s_i = +1$ is favored.
- when $h < 0$, $s_i = -1$ is favored.

This means that the spins want to align with the direction of h .

¹Here the Hamiltonian is no longer a function of coordinate q_i and momentum p_i , as in the case of classical mechanics. We still call H the Hamiltonian because it represents the total energy of the Ising model.

- when $J > 0$, neighboring spins prefer to be parallel, e.g. $s_i = +1$ and $s_{i+1} = +1$, or $s_i = -1$ and $s_{i+1} = -1$. (This is called the *ferromagnetic model*.)
- when $J < 0$, neighboring spins prefer to be anti-parallel, e.g. $s_i = +1$ and $s_{i+1} = -1$, or $s_i = -1$ and $s_{i+1} = +1$. (This is called the *anti-ferromagnetic model*.)

At low enough temperature, all spins in the 2D Ising model will “cooperate” and spontaneously align themselves (e.g. most spins become $+1$) even in the absence of the external field ($h = 0$). This phenomenon is called *spontaneous magnetization*.

At high enough temperatures, the spontaneous magnetization is destroyed by thermal fluctuation. Hence the 2D Ising model has a critical temperature T_c , below which there is spontaneous magnetization and above which there isn’t. In other words, there is a phase transition at T_c .

Unfortunately this doesn’t occur in the 1D Ising model. The 1D Ising model *does not* have a phase transition. We are discussing it here just to “warm up” for the discussion of the 2D Ising model.

The term “spin” and “magnetic field” in the Ising model originate from its initial application to the phenomenon of *spontaneous magnetization* in ferromagnetic materials such as iron. Each iron atom has a unpaired electron and hence a net spin (or magnetic moment). At low temperature, the spins spontaneously align giving rise to a non-zero macroscopic magnetic moment. The macroscopic magnetic moment disappears when the temperature exceeds the Curie temperature (1043 K for iron). (See <http://en.wikipedia.org/wiki/Ferromagnetic> for more details.) As we will see later, the Ising model can be applied to many other problems beyond magnetism, such as phase separation in binary alloys and crystal growth.

2 Solving the 1D Ising model

Q: What do we mean by solving the Ising model?

A: We are really after the partition function Z , as a function of J and h . If we have the analytic expression for Z , we can easily obtain all thermodynamic properties of the Ising model.

2.1 Non-interacting model ($J = 0$)

Let us first consider the simpler case of $J = 0$ ($h \neq 0$). This is a non-interacting model. It is the same as the two-level systems we have considered in the canonical ensemble section!

$$\begin{aligned} Z &= \sum_{\{s_i\}} e^{\beta h \sum_i s_i} = \sum_{\{s_i\}} \prod_{i=1}^N e^{\beta h s_i} = \prod_{i=1}^N \sum_{\{s_i=\pm 1\}} e^{\beta h s_i} \\ &= (e^{\beta h} + e^{-\beta h})^N = (2 \cosh \beta h)^N \end{aligned} \quad (3)$$

Q: What thermodynamic quantities are we interested in?

A: Helmholtz free energy $A(N, T, h)$, energy E , entropy S , and average magnetization $M(N, T, h) \equiv \left\langle \sum_{i=1}^N s_i \right\rangle$.

Hyperbolic functions

$$\begin{aligned} \cosh x &= \frac{e^x + e^{-x}}{2} \\ \sinh x &= \frac{e^x - e^{-x}}{2} \\ \frac{d}{dx} \cosh x &= \sinh x \\ \frac{d}{dx} \sinh x &= \cosh x \\ \tanh x &= \frac{\sinh x}{\cosh x} \\ \frac{d}{dx} \tanh x &= 1 - (\tanh x)^2 \end{aligned}$$

(See http://en.wikipedia.org/wiki/Hyperbolic_function for more details.)

$$A = -k_B T \ln Z = -N k_B T \ln(2 \cosh \beta h) \quad (4)$$

$$E = -\frac{\partial}{\partial \beta} \ln Z = -N h \tanh \beta h \quad (5)$$

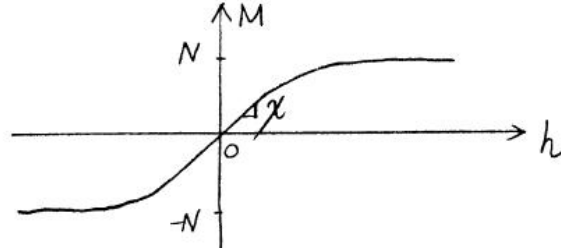
In this special case ($J = 0$), $H = -h \sum_i s_i$. Therefore,

$$E \equiv \langle H \rangle = -h \cdot M \quad (6)$$

$$M = -\frac{E}{h} = N \tanh \beta h \quad (7)$$

The *magnetic susceptibility*² is

$$\chi \equiv \frac{1}{N} \left(\frac{\partial M}{\partial h} \right)_T = (1 - \tanh^2 \beta h) \beta \quad (8)$$



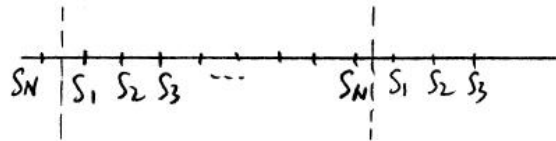
2.2 Ising model at zero field ($h = 0$)

For the first time, we are discussing an interacting model.

$$H(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j = -J \sum_i s_i s_{i+1} \quad (9)$$

The interaction makes the derivation of the partition function more difficult. It is not surprising that we will try some coordinate transformations to turn it into an equivalent non-interacting model. After all, that's all we know how to solve at this point!

Before we proceed, we need to be more specific about the the boundary conditions (B.C.). A widely used B.C. is the periodic boundary condition (PBC). The advantage is that no spin is different from the others.



²The magnetic susceptibility is a response function of the material. It describes how much does the magnetization M changes when the external field h is changed. It is analogous to the specific heat, $c_V \equiv \frac{1}{N} \left(\frac{\partial E}{\partial T} \right)_h$, which describes how much heat the system absorbs when the temperature T is changed.

PBC states that $s_{N+1} = s_1$. Therefore the Hamiltonian can be written as,

$$H = -J(s_1s_2 + s_2s_3 + \cdots + s_{N-1}s_N + s_Ns_1) \quad (10)$$

Alternatively, we can use the “free-end” B.C.

$$H = -J \sum_{i=1}^{N-1} s_i s_{i+1} = -J(s_1s_2 + s_2s_3 + \cdots + s_{N-1}s_N) \quad (11)$$

The difference between different B.C. should vanish in the thermodynamic limit ($N \rightarrow \infty$).

Under free-end B.C., the partition function can be easily evaluated through a coordinate transformation.

$$\{s_1, s_2, \cdots, s_N\} \rightarrow \{s_1, p_2, \cdots, p_N\} \quad (12)$$

where $p_2 = s_1s_2$, $p_3 = s_2s_3$, \cdots , $p_N = s_{N-1}s_N$.

Since $s_i = \pm 1$, $p_i = \pm 1$, p_i describes whether the spin flips from i to $i + 1$.

The inverse transform can be written as

$$s_2 = s_1p_2, \quad s_3 = s_1p_2p_3, \quad s_N = s_1p_1 \cdots p_N \quad (13)$$

Hence there is a one to one correspondence between

$$\{s_1, s_2, \cdots, s_N\} \quad \text{and} \quad \{s_1, p_2, \cdots, p_N\} \quad (14)$$

- For free-end B.C., $H = -J(p_2 + p_3 + \cdots + p_N)$. Hence the partition function is

$$\begin{aligned} Z &= \sum_{\{s_1, p_2, \cdots, p_N\}} e^{\beta J(p_2 + p_3 + \cdots + p_N)} \\ &= 2 \prod_{i=2}^N \sum_{p_i = \pm 1} e^{\beta J p_i} \\ Z &= 2 (2 \cosh \beta J)^{N-1} \end{aligned} \quad (15)$$

- One can show that under PBC

$$Z = (2 \cosh \beta J)^N \cdot [1 + (\tanh \beta J)^N] \quad (16)$$

We see that here J is taking the place of h in the previous section.

Given the partition function Z , we can easily obtain A , E , S , M , as well as specific heat c_V .

2.3 The general case ($J \neq 0, h \neq 0$)

To obtain the magnetic susceptibility χ at non-zero J , we need to consider the case of $J \neq 0, h \neq 0$, which is a true interacting model.

The partition function is usually expressed in terms of the trace of a matrix.

The trace is the sum of the diagonal elements of a matrix

$$\text{Tr}(B) = B_{11} + B_{22} + \cdots + B_{nn} \quad (17)$$

$$\text{where } B = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1n} \\ B_{21} & B_{22} & \cdots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{nn} \end{pmatrix} \quad (18)$$

For example, for an Ising model with one spin, $H = -h s_1$, the partition function is

$$Z = \text{Tr} \begin{pmatrix} e^{\beta h} & 0 \\ 0 & e^{-\beta h} \end{pmatrix} = e^{\beta h} + e^{-\beta h} \quad (19)$$

Now consider two spins, under periodic B.C.,

$$H(s_1, s_2) = -J s_1 s_2 - J s_2 s_1 - h s_1 - h s_2 \quad (20)$$

Define matrix

$$P \equiv \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix} \quad (21)$$

then,

$$Z = \sum_{\{s_1 s_2\}} e^{-\beta H} = \text{Tr}(P \cdot P) \quad (22)$$

Q: Why?

A: Notice that P is a 2×2 matrix.

Let the 1st row (column) correspond to $s = +1$, and let the 2nd row(column) correspond to $s = -1$, e.g.,

$$\begin{aligned} P_{+1,+1} &= e^{\beta(J+h)}, & P_{+1,-1} &= e^{-\beta J}, \\ P_{-1,+1} &= e^{-\beta J}, & P_{-1,-1} &= e^{\beta(J-h)}, \end{aligned}$$

$$P_{s_1 s_2} = e^{\beta(J s_1 s_2 + \frac{h}{2} s_1 + \frac{h}{2} s_2)} \quad (23)$$

$$\text{Tr}(P \cdot P) = \sum_{s_1} (P \cdot P)_{s_1, s_1} = \sum_{s_1, s_2} P_{s_1, s_2} P_{s_2, s_1} \quad (24)$$

$$\begin{aligned}
\therefore \quad \text{Tr}(P \cdot P) &= \sum_{s_1, s_2} e^{\beta(Js_1s_2 + \frac{h}{2}s_1 + \frac{h}{2}s_2)} \cdot e^{\beta(Js_2s_1 + \frac{h}{2}s_2 + \frac{h}{2}s_1)} \\
&= \sum_{s_1, s_2} e^{-\beta H(s_1, s_2)} \\
&= Z
\end{aligned} \tag{25}$$

In general, for N spins forming a linear chain under PBC, the partition function is

$$\begin{aligned}
Z &= \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \\
&= \sum_{\{s_i\}} e^{\beta(Js_1s_2 + \frac{h}{2}s_1 + \frac{h}{2}s_2)} \cdot e^{\beta(Js_2s_3 + \frac{h}{2}s_2 + \frac{h}{2}s_3)} \dots \\
&\quad e^{\beta(Js_{N-1}s_N + \frac{h}{2}s_{N-1} + \frac{h}{2}s_N)} \cdot e^{\beta(Js_Ns_1 + \frac{h}{2}s_N + \frac{h}{2}s_1)} \\
&= \text{Tr}(P^N)
\end{aligned} \tag{26}$$

Now we have obtained a concise formal expression for the partition function. But to compute matrix P^N , it requires a lot of calculations. Fortunately, we don't need P^N . we just need $\text{Tr}(P^N)$. This is the time we need to introduce a little more matrix theory, concerning the properties of the trace.

1. Every symmetric (real) matrix can be diagonalized,

$$P = U \cdot D \cdot U^T \tag{27}$$

where U is a unitary matrix ($U \cdot U^T = I$), and D is a diagonal matrix. For 2×2 matrices, define $\lambda_+ \equiv D_{11}$, $\lambda_- \equiv D_{22}$ ($D_{12} = D_{21} = 0$). λ_{\pm} are the eigenvalues of matrix P .

2. Trace is unchanged after diagonalization

$$\text{Tr}(P) = \text{Tr}(D) = \lambda_+ + \lambda_- \tag{28}$$

Hence the trace equals the sum of the eigenvalues.

3. The same matrix U that diagonalizes P also diagonalizes P^N , because

$$P^N = (U \cdot D \cdot U^T) \cdot (U \cdot D \cdot U^T) \dots (U \cdot D \cdot U^T) = U \cdot D^N \cdot U^T \tag{29}$$

4. Notice that

$$D^N = \begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \tag{30}$$

We have

$$\text{Tr}(P^N) = \text{Tr}(D^N) = \lambda_+^N + \lambda_-^N \tag{31}$$

Thus, all we need to do is to diagonalize P . We can do this using Matlab (or Maple, Mathematica, etc). The result is

$$\lambda_{\pm} = e^{\beta J} \left[\cosh \beta h \pm \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right] \quad (32)$$

$$U = \begin{bmatrix} -e^{\beta J} (e^{\beta(J-h)-\lambda_+}) & 1 \\ 1 & -e^{\beta J} (e^{\beta(J+h)-\lambda_-}) \end{bmatrix} \quad (33)$$

$$\text{Tr}(P) = \lambda_+ + \lambda_- = 2e^{\beta J} \cosh \beta h \quad (34)$$

$$\begin{aligned} Z &= \text{Tr}(P^N) = \lambda_+^N + \lambda_-^N \\ &= e^{N\beta J} \left\{ \left[\cosh \beta h + \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right]^N \right. \\ &\quad \left. + \left[\cosh \beta h - \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right]^N \right\} \end{aligned} \quad (35)$$

In the special case of $h = 0$,

$$\begin{aligned} Z &= \text{Tr}(P^N) \\ &= e^{N\beta J} \left[(1 + e^{-2\beta J})^N + (1 - e^{-2\beta J})^N \right] \\ &= (e^{\beta J} + e^{-\beta J})^N + (e^{\beta J} - e^{-\beta J})^N \\ &= (2 \cosh \beta J)^N + (2 \sinh \beta J)^N \\ Z &= (2 \cosh \beta J)^N [1 + (\tanh \beta J)^N] \end{aligned} \quad (36)$$

Given the general expression for $Z(N, T, J, h)$, we can obtain analytic expressions for

- Magnetization

$$M(N, T, h) = \left\langle \sum_{i=1}^N s_i \right\rangle = k_B T \frac{1}{Z} \frac{\partial Z}{\partial h} = k_B T \frac{\partial \ln Z}{\partial h} = -\frac{\partial A}{\partial h} \quad (37)$$

- Magnetic susceptibility

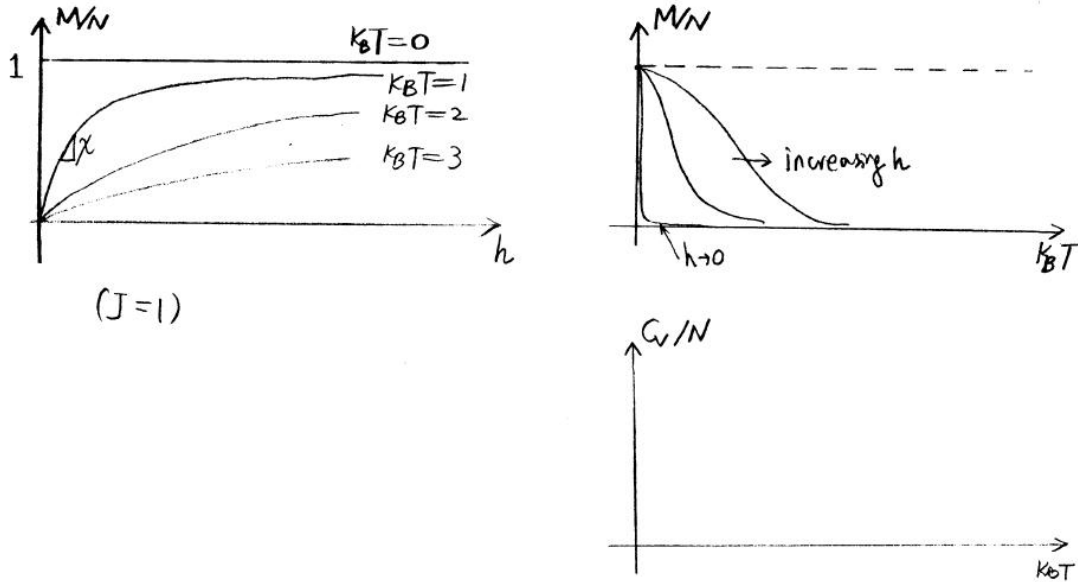
$$\chi \equiv \frac{1}{N} \left(\frac{\partial M}{\partial h} \right)_T = \frac{k_B T}{N} \frac{\partial^2 \ln Z}{\partial h^2} \quad (38)$$

In the thermodynamic limit ($N \rightarrow \infty$), notice that $\lambda_+ > \lambda_-$, we have,

$$\begin{aligned}\ln Z \approx N \ln \lambda_+ &= N \ln \left\{ e^{\beta J} \cdot \left[\cosh \beta h + (\sinh^2 \beta h + e^{-4\beta J})^{1/2} \right] \right\} \\ &= N\beta J + N \ln \left[\cosh \beta h + (\sinh^2 \beta h + e^{-4\beta J})^{1/2} \right]\end{aligned}\quad (39)$$

$$\begin{aligned}A &= -k_B T \ln Z \\ &= -NJ - N k_B T \ln \left[\cosh \beta h + (\sinh^2 \beta h + e^{-4\beta J})^{1/2} \right]\end{aligned}\quad (40)$$

$$\begin{aligned}E &= \dots \\ C_V &= \frac{\partial E}{\partial T} = \dots \\ M &= k_B T \frac{\partial \ln Z}{\partial h} = -\frac{\partial A}{\partial h} = \dots \\ \chi &= \frac{1}{N} \frac{\partial M}{\partial h} = -\frac{1}{N} \frac{\partial^2 A}{\partial h^2} = \dots\end{aligned}\quad (41)$$



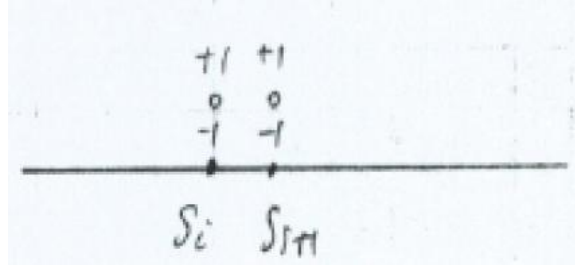
3 Generalized 1D Ising model

3.1 Spins with more than two states

The **transfer matrix method** can be applied to generalized Ising models. For example, we can consider a Hamiltonian similar to the one considered above,

$$H(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \quad (42)$$

except that each spin can take three possible values, $s_i = -1, 0, +1$.³



The partition function can be written as

$$Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} = \text{Tr}(P^N) \quad (43)$$

where P is now a 3×3 matrix,

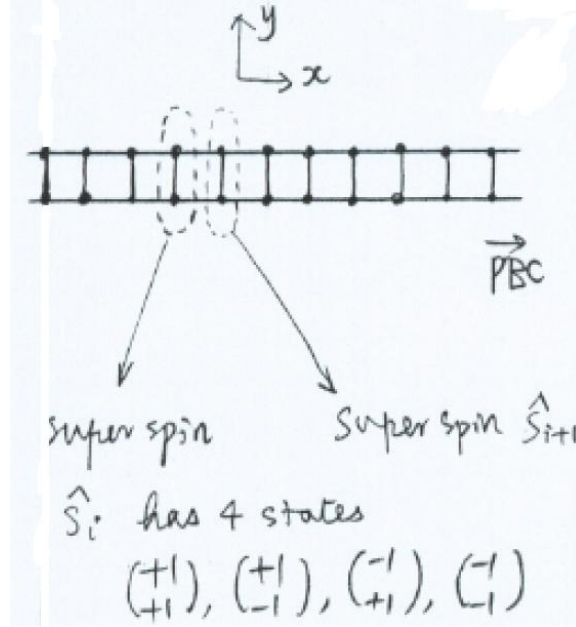
$$P = \begin{matrix} & \begin{matrix} s_j = 1 & s_j = 0 & s_j = -1 \end{matrix} \\ \begin{matrix} s_i = 1 \\ s_i = 0 \\ s_i = -1 \end{matrix} & \begin{pmatrix} e^{\beta J + h} & e^{\frac{\beta}{2}h} & e^{-\beta J} \\ e^{\frac{\beta}{2}h} & 1 & e^{-\frac{\beta}{2}h} \\ e^{-\beta J} & e^{-\frac{\beta}{2}h} & e^{\beta J - h} \end{pmatrix} \end{matrix}$$

$$\begin{aligned} Z &= \lambda_+^N + \lambda_0^N + \lambda_-^N \\ &\approx \lambda_+^N \quad (N \rightarrow \infty) \end{aligned} \quad (44)$$

³This is similar to the Potts model (http://en.wikipedia.org/wiki/Potts_model).

3.2 More than one row of spins

Another generalization of the 1D Ising model is to consider two rows of spins interacting with their nearest neighbors.⁴



Apply periodic boundary condition in x -direction and free-end boundary condition in y -direction. In this case, each spin has 3 nearest neighbors. The Hamiltonian and partition function can still be written in the same way as before,

$$H(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$

$$Z = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} = \text{Tr} (P^N)$$

To apply the transfer matrix method, let us consider the two rows of spins as one row of "super-spins", \hat{s}_i . Each "super-spin" represents the 2 spins in each column, and hence has 4 different states: $(+, +)$, $(+, -)$, $(-, +)$, $(-, -)$. Hence we can still write,

$$Z = \text{Tr} (P^N) \quad (45)$$

where P is a 4×4 matrix, N is the size of the Ising model in the x -direction.

Handwritten expression for the transfer matrix P . It shows $P = \hat{s}_i = \begin{pmatrix} +,+ & +,- & -,+ & -,- \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$ with a grid of dashed lines representing the states.

Let $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ be the four eigenvalues of matrix P ($\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4$). Then,

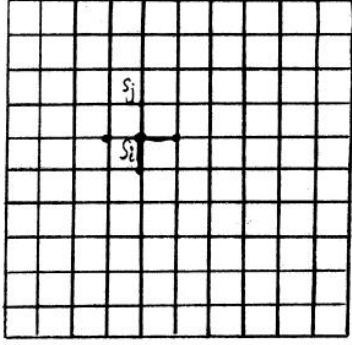
$$Z = \lambda_1^N + \lambda_2^N + \lambda_3^N + \lambda_4^N \approx \lambda_1^N \quad (N \rightarrow \infty) \quad (46)$$

⁴We can consider this as a baby 2D model. As the number of rows increases, we gradually go to the 2D Ising model.

4 2D Ising model

4.1 Analytic solution

Consider the 2D Ising model defined over a square lattice of N spins under periodic boundary conditions. Again, the Hamiltonian can be written as



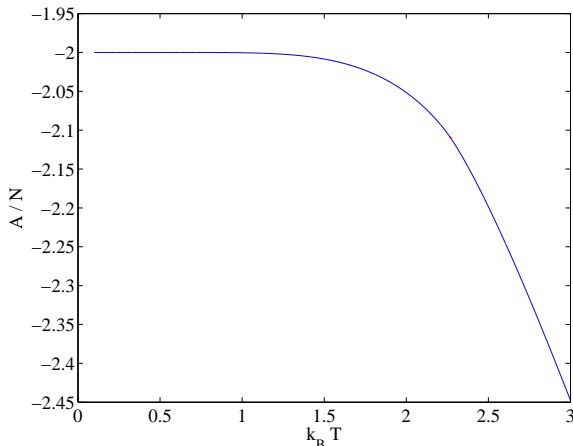
$$H(\{s_i\}) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \quad (47)$$

J describes the strength of interaction, h is external magnetic field, and the sum $\sum_{\langle i,j \rangle}$ is over all nearest neighbor pairs. Each spin has 4 nearest neighbors.

Onsager's solution in the absence of magnetic field $h = 0$ in the thermodynamic limit is [4]

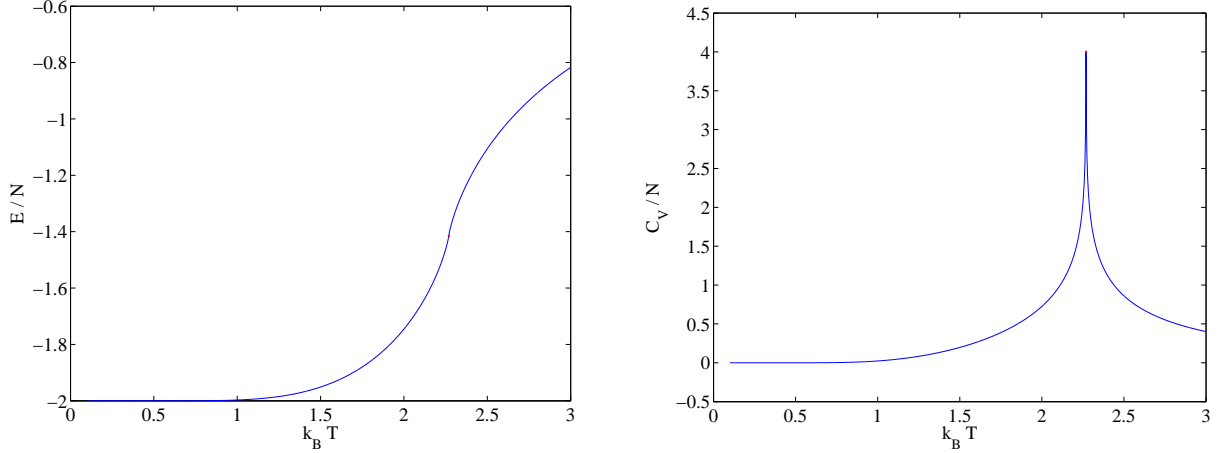
$$\begin{aligned} A &= -k_B T \ln Z \\ Z &= \lambda^N \\ \ln \lambda &= \ln(2 \cosh 2\beta J) + \frac{1}{\pi} \int_0^{\pi/2} dw \ln \left[\frac{1}{2} \{1 + (1 - K^2 \sin^2 w)^{1/2}\} \right] \\ K &= \frac{2 \sinh 2\beta J}{(\cosh 2\beta J)^2} \end{aligned} \quad (48)$$

Onsager's original solution used the transfer matrix method, and was very complicated (Phys. Rev. 65, 117, 1943). Nine years later, Kac and Ward (Phys. Rev. 88, 1332, 1952) re-derived the result using a much simpler graphical/combinatorial approach. The combinatorial approach was also explained in Feynman's book on Statistical Mechanics (Ref. 2). While Onsager was well known for his exact solution of the 2D Ising model, he won the 1968 Nobel Prize in Chemistry (not in Physics) for his reciprocal relations in non-equilibrium thermodynamics.



$$k_B T_c = \frac{2J}{\ln(1 + \sqrt{2})} = 2.269 \dots J \quad (49)$$

Onsager's solution predicts a phase transition at $T = T_c$. From Monte Carlo simulation (below), we will see that $T < T_c$ is the ordered phase; $T > T_c$ is the disordered phase. T_c of Ising model is analogous to the Curie Temperature of magnetic materials (e.g. Fe). The spontaneous magnetization disappears if $T > T_c$.



From Eq. (48) we can obtain the energy E of the 2D Ising model and its heat capacity.

$$E = -\frac{\partial \ln Z}{\partial \beta} = -N \frac{\partial \ln \lambda}{\partial \beta} \quad (50)$$

$$C_V = \frac{\partial E}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial E}{\partial \beta} = \frac{N}{k_B T^2} \frac{\partial^2 \ln \lambda}{\partial \beta^2} \quad (51)$$

In the above, we plot A , E and C_V for the 2D Ising model as a function of $k_B T$ (with $J = 1$). (Download `plot_Onsager_solution.m` and try it yourself.) We see that C_V becomes singular as $T \rightarrow T_c$. (It has been shown that $C_V \propto \ln|T - T_c|$ as $T \rightarrow T_c$.) This means that the slope of the $E(T)$ curve becomes infinite as $T \rightarrow T_c$. The second derivative of the $\ln \lambda(\beta)$ curve becomes infinite as $T \rightarrow T_c$. In other words, the second derivative of the integral with respect to β in Eq. (48) becomes infinite at $T = T_c$ ($K = 1$). The integral itself and its first derivative with respect to β remain finite at $T = T_c$ ($K = 1$).

4.2 Monte Carlo simulation

The Metropolis algorithm is a simple and widely used approach to generate the canonical ensemble. It is especially convenient to explain (and to implement) for an Ising model. The algorithm has the following steps.

0. Start with some spin configuration $\{s_i\}$.
1. Randomly choose a spin s_i
2. Attempt to flip it, i.e. $s_i := -s_i$ (trial).
3. Compute the energy change ΔE due to this flip.
4. If $\Delta E < 0$, accept the trial.
5. If $\Delta E > 0$, accept the trial with probability $p^{\text{acc}} = e^{-\beta \Delta E}$.

- * More details about this algorithm will be discussed later.

| $k_B T = 0.5$ | $k_B T = 2.269$ | $k_B T = 3$ |
|---------------|-----------------|-------------|
| | | |

To simplify the notation, let A, B represent arbitrary spin configurations $\{s_i\}$. Our goal is to prove that when the MC simulation has reached equilibrium, the probability of sampling state A is

where

— the sum is over all possible (2^N) spin configurations.

For an Ising model with N spins, there are 2^N spin configurations (states). So π_{AB} is a $2^N \times 2^N$ matrix. However, most entries in π_{AB} are zeros.

$$\begin{array}{ll} \text{if } A = \{+1, +1, +1, +1, +1, +1\} & \text{then} \\ \text{for } B = \{+1, -1, +1, +1, +1, +1\}, & \pi_{AB} > 0 \\ \text{but for } B = \{-1, -1, +1, +1, +1, +1\}, & \pi_{AB} = 0 \end{array}$$

To prove the Metropolis algorithm generates the canonical ensemble:

(1) transition matrix can be written as

$$\pi_{AB} = \alpha_{AB} \cdot p_{AB}^{\text{acc}}, \quad \text{for } B \neq A \quad (54)$$

$$\pi_{AA} = 1 - \sum_{B \neq A} \pi_{AB} \quad (55)$$

where α_{AB} is the trial probability that satisfies

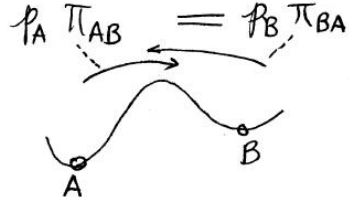
$$\alpha_{AB} = \alpha_{BA} \quad (56)$$

and p_{AB}^{acc} is the acceptance probability.

without loss of generality, let's assume $E_B > E_A$, then

$$\begin{cases} p_{AB}^{\text{acc}} = \exp\left(-\frac{E_B - E_A}{k_B T}\right) \\ p_{BA}^{\text{acc}} = 1 \end{cases} \implies \frac{\pi_{AB}}{\pi_{BA}} = \frac{\alpha_{AB} p_{AB}^{\text{acc}}}{\alpha_{BA} p_{BA}^{\text{acc}}} = \exp\left(-\frac{E_B - E_A}{k_B T}\right) \quad (57)$$

(2) If the equilibrium distribution is reached, with p_A being the probability of sampling state A , then we expect the following balance of fluxes.



$\therefore p_A \pi_{AB} = p_B \pi_{BA}$
 $\frac{p_A}{p_B} = \frac{\pi_{BA}}{\pi_{AB}} = e^{\frac{E_B - E_A}{k_B T}}$
 $\implies p_A = \text{const} \cdot e^{-\frac{E_A}{k_B T}} \quad \text{for all } A$

(58)

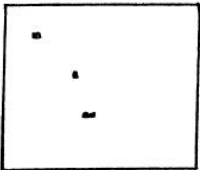


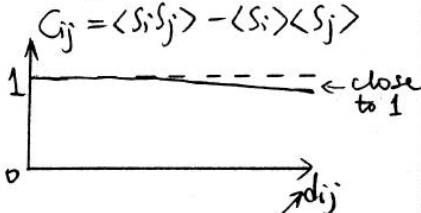
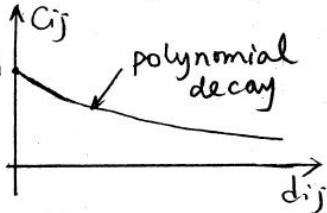
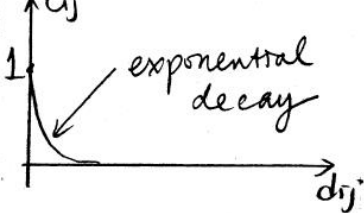
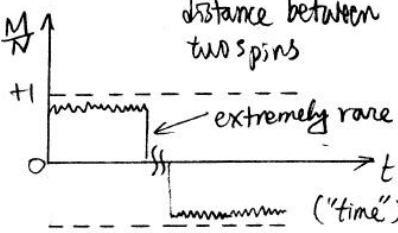
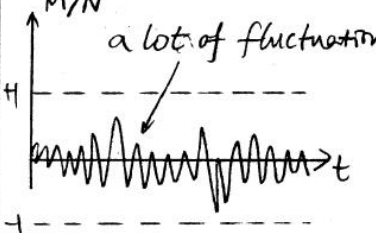
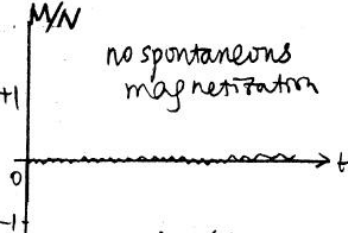
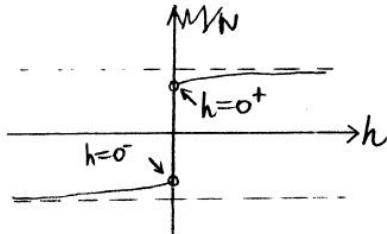
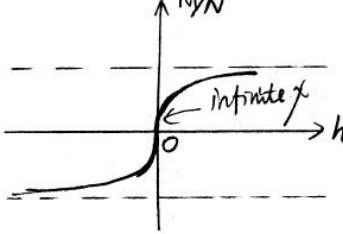
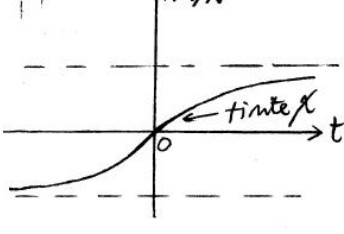
The normalization of p_A , $\sum_A p_A = 1$, requires that

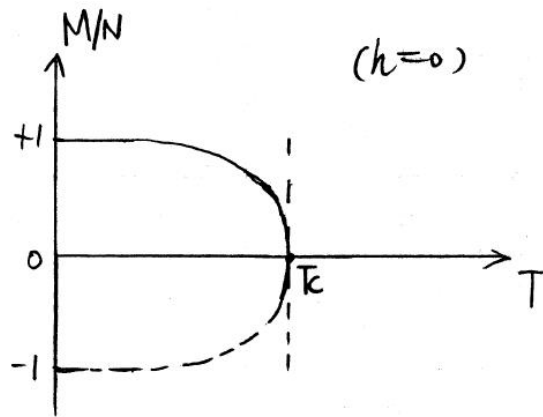
$$p_A = \frac{1}{Z} e^{-\frac{E_A}{k_B T}}, \quad Z = \sum_A e^{-\frac{E_A}{k_B T}} \quad (59)$$

(end of proof)

4.3 Qualitative behavior

Observations from MC simulation at $h=0$

| $T < T_c$ | $T = T_c$ | $T > T_c$ |
|--|--|--|
| low temperature phase | critical temperature | high temperature phase |
|  |  |  |
| <ol style="list-style-type: none"> 1. Dominance of one spin (e.g. $S_i = +1$) with fluctuations of the other spin (e.g. $S_i = -1$) as isolated clusters 2. Number & size of clusters increase as $T \uparrow$ 3. Long range correlation $C_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$  | <ol style="list-style-type: none"> 1. fluctuation at all scales 2. no clear dominance of one spin 3. Long range correlation C_{ij} vs d_{ij}  | <ol style="list-style-type: none"> 1. no dominance of either spin 2. no obvious patterns 3. Short range correlation C_{ij} vs d_{ij}  |
|  |  |  |
|  |  |  |

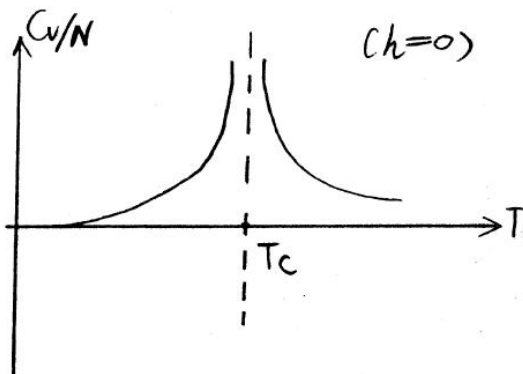


$$\frac{M}{N} \propto (T_c - T)^\beta \quad T < T_c$$

$$\text{critical exponent } \beta = \frac{1}{8} \quad (2D)$$

$$\beta \approx 0.313 \quad (3D)$$

(not to be confused with reciprocal temperature $\beta \equiv \frac{1}{k_B T}$)



$$\frac{C_v}{N} \propto \frac{8k_B}{\pi} \left(\frac{J}{k_B T} \right)^2 \ln \left| \frac{1}{T - T_c} \right| \quad (2D)$$

$$\frac{C_v}{N} \propto |T - T_c|^{-\alpha} \quad \alpha \approx 0.125 \quad (3D)$$

There is a problem with the top plot M/N vs T .

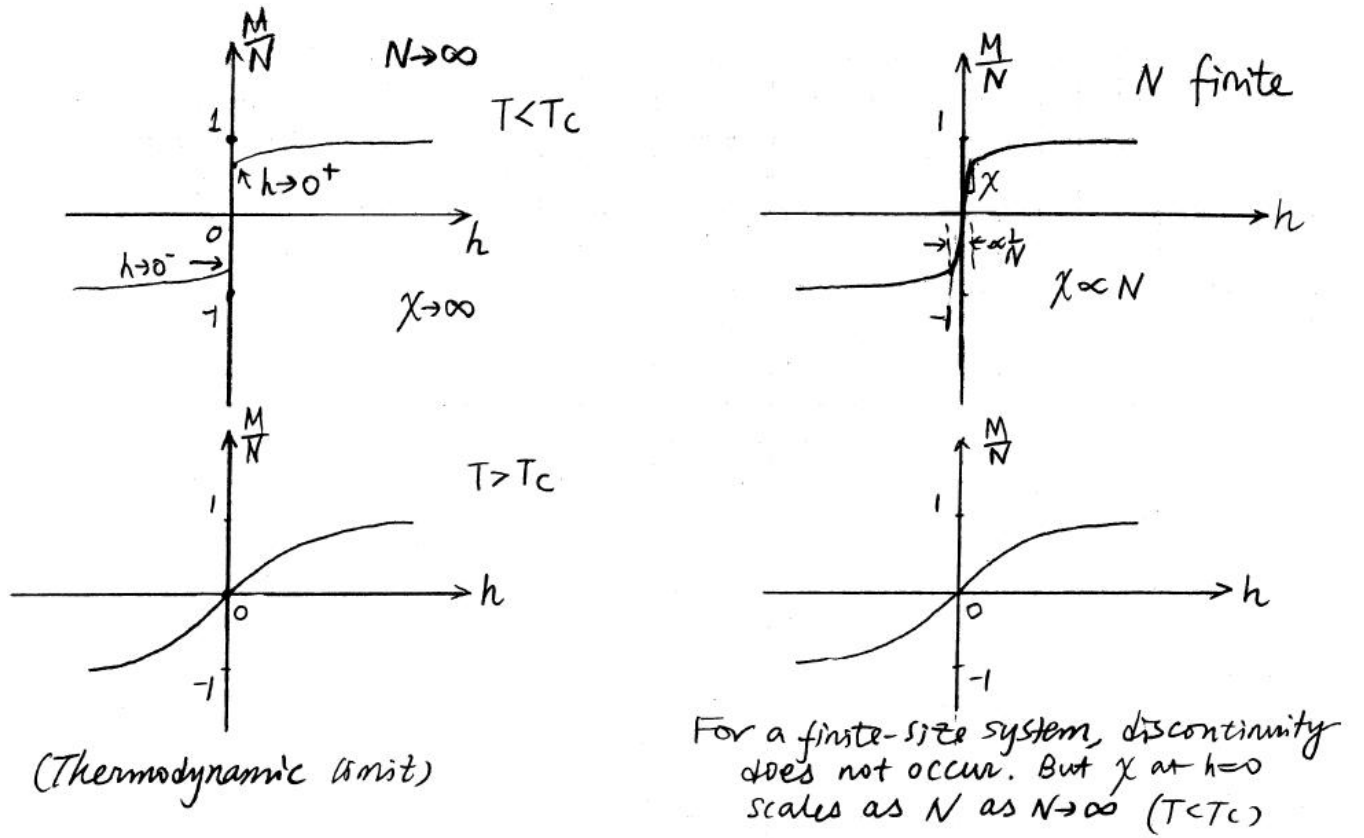
If we define $M \equiv \left\langle \sum_{i=1}^N s_i \right\rangle$, then if $h = 0$, we should always have $M = 0$ by symmetry.

Why do we claim that there is a difference between low temperature regime ($T < T_c$) and high temperature regime ($T > T_c$)?

To reduce this paradox, we need to imagine the magnetic field h is a very small but positive number. $h \rightarrow 0^+$.

In this case, only the upper branch of the $\frac{M}{N}(T)$ curve will be selected, when $T < T_c$. The value remains positive as $h \rightarrow 0^+$ when $T > T_c$. The magnetization $\frac{M}{N} \rightarrow 0^+$ as $h \rightarrow 0^+$.

This is too complicated to do in a numerical simulation. So we need a different way to compute magnetic susceptibility χ , especially near $h \rightarrow 0$.



We expect the susceptibility $\chi \equiv \frac{1}{N} \frac{\partial M}{\partial h}$ to diverge if $T < T_c$ and $N \rightarrow \infty$.

Fluctuation-Dissipation Theorem

$$\chi = \frac{1}{N} \frac{\partial M}{\partial h} = \frac{1}{N k_B T} \left(\langle \tilde{M}^2 \rangle - \langle \tilde{M} \rangle^2 \right) \quad (60)$$

where $\tilde{M} \equiv \sum_{i=1}^N s_i$

$$\begin{aligned} M &\equiv \langle \tilde{M} \rangle = \left\langle \sum_{i=1}^N s_i \right\rangle, & \langle \tilde{M}^2 \rangle &= \left\langle \left(\sum_{i=1}^N s_i \right)^2 \right\rangle. \\ \chi &= \frac{1}{N k_B T} \sum_{i,j=1}^N \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \end{aligned} \quad (61)$$

Therefore, we arrived at another of fluctuation-dissipation theorem (FDT),

$$\chi = \frac{1}{k_B T} \sum_{j=1}^N C_{ij} \quad (\text{the right hand side does not depend on } i) \quad (62)$$

where

$$C_{ij} \equiv \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \quad (63)$$

is the correlation function between spins i and j . When $T < T_c$, $\chi \rightarrow \infty$, corresponding to long range correlation, $\sum_{j=1}^N C_{ij} \propto N$. (unbounded as $N \rightarrow \infty$).

Proof of Eq. (60)

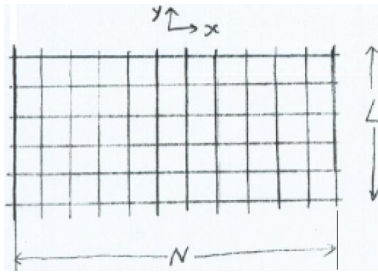
$$\begin{aligned} Z &= \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} = \sum_{\{s_i\}} \exp \left[\beta J \sum_{\langle i,j \rangle} s_i s_j + \beta h \sum_i s_i \right] \\ \frac{\partial Z}{\partial h} &= \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \beta \tilde{M} \end{aligned} \quad (64)$$

$$M = k_B T \frac{1}{Z} \frac{\partial Z}{\partial h} \quad (65)$$

$$\begin{aligned} \frac{\partial M}{\partial h} &= k_B T \left[\frac{1}{Z} \frac{\partial^2 Z}{\partial h^2} - \frac{1}{Z^2} \left(\frac{\partial Z}{\partial h} \right)^2 \right] \\ &= k_B T \left[\beta^2 \langle \tilde{M}^2 \rangle - \beta^2 \langle \tilde{M} \rangle^2 \right] \\ &= \frac{1}{k_B T} \left[\langle \tilde{M}^2 \rangle - \langle \tilde{M} \rangle^2 \right] \end{aligned} \quad (66)$$

4.4 Sketch of derivations of partition function in 2D

Consider a 2D array of spins with dimension $N \times L$ under periodic boundary conditions in both directions.



We can follow the approach in Section 3.2 and define “super-spins” for each column of spins. The system then becomes a linear chain of N “super-spins”. But each “super-spin” has 2^L states. This means the transfer matrix P is a $2^L \times 2^L$ matrix. Let λ_1 be the largest eigenvalue of matrix P . Then,

$$Z = \text{Tr}(P^N) \approx \lambda_1^N \quad (N \rightarrow \infty) \quad (67)$$

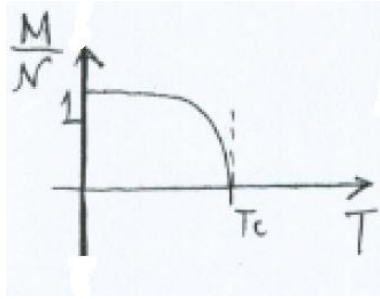
If L is not too large, this problem can be solved numerically using Matlab.

This is the approach Onsager took (1943) to find the analytic solution for Z in the limit of $N \rightarrow \infty$, $L \rightarrow \infty$.⁵

Onsager used some very advanced mathematical techniques to solve this problem. His solution predicts a critical temperature of $k_B T_c = \frac{2J}{\ln(1+\sqrt{2})} = 2.269 J$. Onsager also stated the zero-field magnetization should be

$$\frac{M}{\mathcal{N}} = [1 - \sinh^{-4}(2\beta J)]^{1/8} \quad (68)$$

for $T < T_c$, but **did not give a proof** (Onsager 1943)! Finally, C. N. Yang (1952) was able to proof this (again) using a very difficult derivation.



In 1952, Kac and Ward found a much simpler approach to re-derive Onsager's result, using a graphical/combinatorial approach, which is what we will describe below.

The new idea is to rewrite the partition function as a multiplication and expand all the terms.

$$\begin{aligned} Z &= \sum_{\{s_i\}} e^{\beta J \sum_{\langle i,j \rangle} s_i s_j} \\ &= \sum_{\{s_i\}} \prod_{\langle i,j \rangle} e^{\beta J s_i s_j} \end{aligned} \quad (69)$$

Notice that $s_i s_j = \pm 1$, hence

$$\begin{aligned} e^{\beta J s_i s_j} &= \frac{e^{\beta J} + e^{-\beta J}}{2} + \frac{e^{\beta J} - e^{-\beta J}}{2} s_i s_j \\ &= (\cosh \beta J) + (\sinh \beta J) s_i s_j \\ &= \cosh \beta J (1 + t \cdot s_i s_j) \end{aligned} \quad (70)$$

where $t \equiv \tanh \beta J$. Therefore,

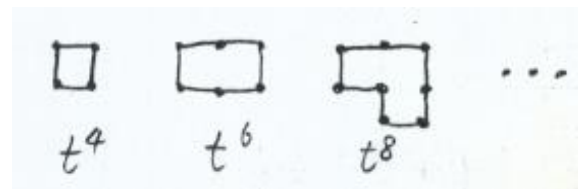
$$Z = (\cosh \beta J)^N \sum_{\{s_i\}} \prod_{\langle i,j \rangle} (1 + t \cdot s_i s_j) \quad (71)$$

The key is to find the term following $(\cosh \beta J)^N$.

⁵Onsager obtained the solution for the case of $h = 0$. No analytic solution has been found for $h \neq 0$.

$$\begin{aligned}
Z' &= \sum_{\{S_i\}} \prod_{\langle ij \rangle} (1 + t S_i S_j) \\
&= \sum_{\{S_i\}} \underbrace{(1 + t S_1 S_2) \cdot (1 + t S_1 S_3) \cdot (1 + t S_1 S_4) \cdot \dots}_{\# \text{ of terms} = \# \text{ of bonds.}} \\
&= \sum_{\{S_i\}} \underbrace{1 + t S_1 S_2 + t^2 S_1 S_2 S_1 S_3 + \dots}_{\text{contribute 0}} \\
&\quad + t^4 \underbrace{S_1 S_2 S_2 S_6 S_6 S_3 S_3 S_1}_{\text{contribute non-zero}} + \dots
\end{aligned}$$

It turns out that Z' can be obtained by summing over all polygons that can be drawn on a square lattice, each one contributes t^n , where n is the number of lattice points on the polygon. For example,



It also turns out that there is a “simple” way to sum over all the graphs (need to use Fourier transform).

The entire derivation was explained by Richard Feynman [2] in 14 pages. So it is not so “easy”. But all we need to do is to “count carefully”. There is no need to master the theory of Group and Group Representations, which are used in Onsager’s original proof.

References

1. B. M. McCoy and T. T. Wu, “The Two-Dimensional Ising Model”, Harvard University Press (1973).
2. R. P. Feynman, “Statistical Mechanics: A Set of Lectures”, W. A. Benjamin, Inc. (1972).
3. L. Onsager, “Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition”, Physical Review, 65, 117 (1944).
4. C. K. Majumdar, “Analytic Properties of the Onsager Solution of the Ising Model”, Physical Review, 145, 158 (1966).