8.08 Statistical Physics II — Spring 2019
Recitation Note 5

Huitao Shen
huitao@mit.edu

Mar 11, 2019

Contents

1 Ising Model in 1D: Exact Solution

The Ising model is the simplest microscopic model for ferromagnet-paramagnet transition. Its Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i, \tag{1}$$

where the spin $S_i = \pm 1$ and the summation $\langle ij \rangle$ is restricted to nearest-neighbor pairs. Computing the partition function of this Hamiltonian exactly is easy only in 1D.

In 1D, the Hamiltonian can be written as

$$H = -\sum_{i=1}^{N} \left[J S_i S_{i+1} + \frac{B}{2} (S_i + S_{i+1}) \right]. \tag{2}$$

We impose the periodic boundary condition as $S_1 = S_{N+1}$.

The partition function is

$$\begin{aligned} Z &= \sum_{S_1, S_2, \ldots, S_N} \exp \left[\sum_{i=1}^{N} \beta \left(J S_i S_{i+1} + \frac{B}{2} (S_i + S_{i+1}) \right) \right] && (3) \\ &= \sum_{S_1, S_2, \ldots, S_N} \prod_{i=1}^{N} \exp \left[\beta \left(J S_i S_{i+1} + \frac{B}{2} (S_i + S_{i+1}) \right) \right]. && (4) \end{aligned}$$

The trick is to convert the summation to the matrix multiplication. Define the 2×2 transfer matrix T as

$$\langle S | T | S' \rangle = \exp \left[\beta \left(J S S' + \frac{B}{2} (S + S') \right) \right]. \tag{5}$$

In other words,

$$T = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix}. \tag{6}$$

It follows

$$\begin{aligned} Z &= \sum_{S_1, S_2, \ldots, S_N} \prod_{i=1}^{N} \exp \left[\beta \left(J S_i S_{i+1} + \frac{B}{2} (S_i + S_{i+1}) \right) \right] && (7) \\ &= \sum_{S_1, S_2, \ldots, S_N} \prod_{i=1}^{N} \langle S_i | \exp \left[\beta \left(J S_i S_{i+1} + \frac{B}{2} (S_i + S_{i+1}) \right) \right] | S_{i+1} \rangle && (8) \\ &= \sum_{S_1} \langle S_1 | T^N | S_1 \rangle && (9) \\ &= \mathrm{tr}(T^N) = \mathrm{tr} \left[\left(Q \Lambda Q^{-1} \right)^N \right] = \mathrm{tr}(Q^{-1} Q \Lambda^N) = \mathrm{tr}(\Lambda^N) && (10) \\ &= \lambda_+^N + \lambda_-^N, && (11) \end{aligned}$$

where we have used the eigenvalue decomposition $T = Q \Lambda Q^{-1}$. Q is the orthogonal matrix and $\Lambda = \mathrm{diag}(\lambda_+, \lambda_-)$. We have also used the cyclic property of trace $\mathrm{tr}(AB) = \mathrm{tr}(BA)$.

$$\lambda_\pm = e^{\beta J} \left[\cosh(\beta B) \pm \sqrt{\sinh^2(\beta B) + e^{-4\beta J}} \right]. \tag{12}$$

Since $\lambda_+ > \lambda_-$, in the limit when $N \to \infty$, the partition function simplifies to $Z = \lambda_+^N$. The free energy is

$$F = -k_B T \ln Z = -k_B T N \ln \lambda_+. \tag{13}$$

The magnetization is

$$M = -\frac{\partial F}{\partial B} = -\frac{k_B T N}{\lambda_+}\frac{\partial \lambda_+}{\partial B} = N\frac{\sinh(\beta B) + \frac{\sinh(\beta B)\cosh(\beta B)}{\sqrt{\sinh^2(\beta B)+e^{-4\beta J}}}}{\cosh(\beta B) + \sqrt{\sinh^2(\beta B) + e^{-4\beta J}}}. \tag{14}$$

For any finite β (i.e. nonzero temperature), when $B \to 0$, $\sinh(\beta B) \to 0$ and $\cosh(\beta B) \to 1$, it is not hard to see the magnetization $M \to 0$. Therefore, there is no ferromagnet-paramagnet phase transition at finite temperature in 1D.

2 Ising Model in 4D and Higher: Mean-field Theory

It is extremely difficult to solve Ising model exactly in 2D and is impossible in 3D. In order to obtain nontrivial results, we need to resort to certain approximation methods. The approximation we are going to use is called the mean-field approximation. It is a very general method and is extremely useful. Furthermore, it can be proved that in dimensions higher than four, the result given by mean-field theory is exact at thermodynamic limit.

2.1 Homogeneous Case

Recall the order parameter

$$M = \frac{1}{N}\sum_{i=1}^{N}\langle S_i \rangle, \tag{15}$$

we rewrite the spin as $S_i = M + (S_i - M)$ and assume $(S_i - M)$ is small such that all high order terms (greater than one) can be ignored. In this way,

$$\begin{aligned} H = & - J\sum_{\langle ij \rangle}\left[M + (S_i - M)\right]\left[M + (S_j - M)\right] - B\sum_i S_i & (16)\\ \approx & - J\sum_{\langle ij \rangle}\left(S_i M + S_j M - M^2\right) + B\sum_i S_i & (17)\\ = & - \underbrace{(JMz + B)}_{B_{\text{eff}}}\sum_i S_i - \frac{1}{2}JNzM^2. & (18) \end{aligned}$$

The interaction between the nearest-neighbor spins are replaced by an effective magnetic field, whose strength depends on the order parameter and is going to be determined self-consistently.

The problem is now reduced to the familiar single spin in the magnetic field. The partition function is straightforward to compute:

$$Z = e^{-\beta JNzM^2/2}\left(e^{-\beta B_{\text{eff}}} + e^{\beta B_{\text{eff}}}\right)^N. \tag{19}$$

The free energy is then

$$F = -k_B T\ln Z = \frac{1}{2}JNzM^2 - k_B TN\ln\left(e^{-\frac{B_{\text{eff}}}{k_B T}} + e^{\frac{B_{\text{eff}}}{k_B T}}\right). \tag{20}$$

One can plot F as a function of M, which is in great agreement with the Ginzburg-Landau theory.

To determine M, the self-consistency relation is

$$M = -\frac{\partial F}{\partial B} = \frac{\sum_{S=\pm 1} Se^{-\beta B_{\text{eff}} S}}{\sum_{S=\pm 1} e^{-\beta B_{\text{eff}} S}} = \tanh\left(\beta B_{\text{eff}}\right). \tag{21}$$

One can also minimize the free energy directly as a function of the magnetization, as what we did in the Ginzburg-Landau theory. This will also lead to Eq. (21). In this way we confirm the consistency of the mean-field approximation.

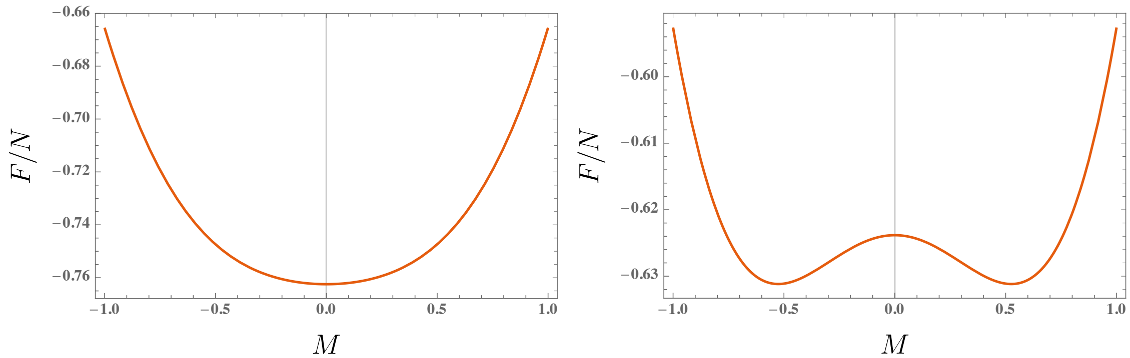

Figure 1: Free energy as a function of magnetization according to Eq. (20). Here we set $B = 0$ and $Jz = 1$. Left: $T/T_c = 1.1$; Right: $T/T_c = 0.9$.

Note that in the energy minimization approach, it is important to keep the $JNzM^2/2$ term in the free energy, although this term can be safely neglected in the self-consistency approach.

As an example, we consider the zero field limit $B = 0$. The self-consistency equation becomes

$$M = \tanh(\beta JMz). \tag{22}$$

It is not hard to see nonzero solution of M exists only when $\beta Jz > 1$. Therefore, the critical temperature is

$$T_c = \frac{Jz}{k_B}. \tag{23}$$

The reader is encouraged to work with the general case when $B \neq 0$ and compare thermodynamic properties of the model with those from the Ginzburh-Landau theory.

2.2 Nonhomogeneous Case

Instead of imposing a homogeneous magnetic field, we apply a spatially periodic magnetic field $B(\mathbf{r}) = B_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$. The magnetization is also expected to be periodic $M = M_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$. The homogeneous case can be seen as the $B_{\mathbf{k}} = \delta(\mathbf{k})$ limit.

Under the mean-field framework, the deviation of the magnetization around the homogeneous solution at point $\mathbf{r}$ can be expressed as

$$M(\mathbf{r}) = \chi_0 B_{\text{eff}}(\mathbf{r}) = \chi_0 B(\mathbf{r}) + \chi_0 J \sum_{\boldsymbol{\delta}\in\text{NN}} M(\mathbf{r}+\boldsymbol{\delta}). \tag{24}$$

Here $\chi_0 = \partial M/\partial B|_{B\to 0}$ is the susceptibility of a single spin in the magnetic field. The above expression is accurate in the weak magnetic field limit.

After Fourier transform,

$$M_{\mathbf{k}} = \chi_0 B_{\mathbf{k}} + \chi_0 J M_{\mathbf{k}}(z - ak^2), \tag{25}$$

where z is the coordination number and $a > 0$ is some constant. To see how the last term appears:

$$\begin{aligned}
\sum_{\mathbf{r}}\sum_{\boldsymbol{\delta}\in\text{NN}} M(\mathbf{r}+\boldsymbol{\delta})e^{i\mathbf{k}\cdot\mathbf{r}} =& \sum_{\mathbf{r}} M(\mathbf{r}) \sum_{\boldsymbol{\delta}\in\text{NN}} e^{i\mathbf{k}\cdot(\mathbf{r}-\boldsymbol{\delta})} && (26)\\
=& \sum_{\mathbf{r}} M(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\boldsymbol{\delta}\in\text{NN}} e^{-i\mathbf{k}\cdot\boldsymbol{\delta}} && (27)\\
=& M_{\mathbf{k}} \sum_{\boldsymbol{\delta}\in\text{NN}} \cos(\mathbf{k}\cdot\boldsymbol{\delta}) && (28)\\
\approx& M_{\mathbf{k}}(z + ak^2). && (29)
\end{aligned}$$

Here we assumed the lattice has inversion symmetry such that whenever $\boldsymbol{\delta}$ is a nearest-neighbor vector, so does $-\boldsymbol{\delta}$. Therefore, the resulting integral is even in k and the lowest k-dependent term is quadratic.

In this way, the momentum dependent susceptibility of the Ising model is

$$\chi_{\mathbf{k}} = \left.\frac{\partial M_{\mathbf{k}}}{\partial B_{\mathbf{k}}}\right|_{B_{\mathbf{k}}\to 0} = \frac{\chi_0}{1 - Jz + aJ\chi_0 k^2} = \frac{1}{\chi_0^{-1} - Jz + aJk^2}. \tag{30}$$

When the temperature is high enough, $\chi \sim T^{-1}$. Also note $T_c = Jz/k_B$. We can rewrite the above expression as

$$\chi_{\mathbf{k}} = \frac{A}{B(T - T_c) + k^2}, \tag{31}$$

where A and B are some temperature independent constants. When $k = 0$, we have $\chi \sim (T - T_c)^{-1}$, which is consistent with the results computed from the homogeneous susceptibility.

On the other hand, the correlation length ξ is defined as

$$\chi_{\mathbf{k}} \sim \frac{1}{\xi^{-2} + k^2}. \tag{32}$$

By comparing the above two results, $\xi \sim |t|^{-1/2}$, where $t = 1 - T/T_c$. It is find that the correlation length also diverges at the critical point.

Based on this result, we can argue why mean-field result is exact at dimensions higher than four. Physically, mean-field approximation neglects the fluctuation effect. The approximation is valid if near the critical point

$$\langle(\delta M)^2\rangle \ll \langle M\rangle^2. \tag{33}$$

This condition is called the "Ginzburg criterion".

From Ginzburg-Landau theory or mean-field calculation, we already know that $\langle M\rangle^2 \sim t$ near the critical point, independent of the dimension. In order to estimate$\langle(\delta M)^2\rangle$, we need to work out the spatial dependent susceptibility.

$$\chi(\mathbf{r}) \sim \int d\mathbf{k} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2 + \chi^{-2}} \sim \frac{e^{-r/\xi}}{r^{d-2}}. \tag{34}$$

Therefore $\langle(\delta M)^2\rangle \sim \chi(\xi) \sim \chi^{2-d} \sim t^{(d-2)/2}$.

It follows

$$\frac{\langle(\delta M)^2\rangle}{\langle M\rangle^2} \sim \frac{t^{(d-2)/2}}{t} \sim t^{d/2-2}, \tag{35}$$

which does not diverge at $t = 0$ only when $d > 4$.