MATH 505 Project: Ising model – Phase transition

Xin-Zeng Wu Di Li Zheng Dai

1 Introduction

Ising model is a mathematical model of ferromagnetism in statistical mechanics, which was invented by Wilhelm Lenz (1920). Wilhelm Lenz gave the model as a problem to his student Ernst Ising. Ising solved this problem in one-dimension in his PHD thesis (1924)[1], which worked on linear chains of coupled magnetic moments. Rudolf Peierls named this model by Ising model in his 1936 publication "On Ising's model of ferromagnetism". However, this model was ignored by most scientists for many years and even Ising himself gave up due to the difficulty of solving two-dimensional Ising model. Almost twenty years later, Lars Onsager, winner of the 1968 Nobel Prize in Chemistry, solved two dimensional Ising model in 1944 and exhibited phase transition. And then Ising model enjoyed increased popularity and took its place as the preferred basic theory of all cooperative phenomena. In that time, Ising model is the only one which offers much hope of an accurate study of mechanism. More and more people involved in solving high dimensional Ising model. They modeled phase transition in higher dimensions.

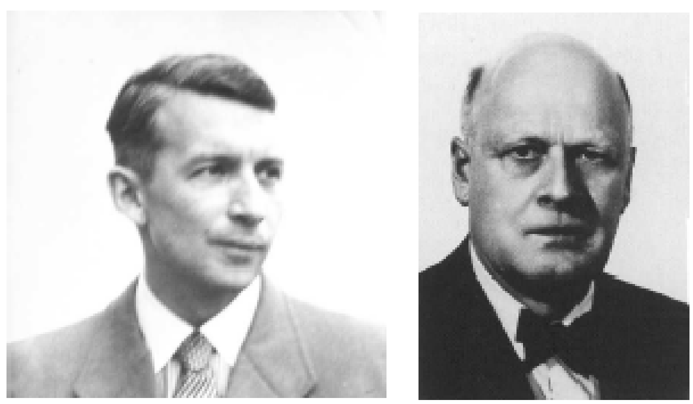

Figure 1: Left: Ernst Ising, Right:Lars Onsager

The Ising model is concerned with the physical phase transitions. When a small change in a parameter such as temperature or pressure causes a large-scale, qualitative change in the state of a system, it is called phase transitions, which are common in physics and familiar in everyday life. For example, whenever the temperature drops below 0C or it is above 100C, we will see phase transitions of water. Moreover, the original purpose of Ising's doctoral dissertation is to show an understanding of ferromagnetism and especially "spontaneous magnetization", which is also a good example of phase transition.In spite of their familiarity, phase transition are not well understood. One purpose of the Ising model is to explain how short-range interactions between molecules in a crystal give rise to long-range, correlative behavior and predict in some sense the potential for a phase transition. Since Ising model can be formulated as a mathematical problem, it has been also applied to problems in chemistry, molecular biology, and other areas where "cooperative" behavior of large systems is studied. [3]

2 One dimensional solution

The one dimensional Ising model used the Hamiltonian function as

$$\mathscr{H} = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i \quad \Rightarrow \quad \mathscr{H} = -J\sum_{\langle ij \rangle} \sigma_i\sigma_j - h\sum_i \sigma_i$$

In the case we are interested in, we only care about constant J_{ij} and constant ε_i. Moreover, we can rewrite our Hamiltonian in an interactive way as following:

$$\mathscr{H} = -J\sum_{\langle ij \rangle} \sigma_i\sigma_j - \frac{\varepsilon}{2}\sum_i\sum_j(\sigma_i + \sigma_j)$$

where the first sum is over $\langle ij \rangle$ which describes the closest neighbors of a single site.

This was solved by Ising himself. Although there are not so many interesting properties in the result, the mathematical method employed still a simpler sketch of the higher dimensional models.

2.1 General model

In order to solve the one dimensional Ising model, we first need to calculate the partition function of the system. Consider the string with N sites of spins, each my with value ± 1. Then the ith site has interaction with the external field and the spins of $i+1$ and $i-1$.

$$\mathscr{Z} = \sum_{s\in S} e^{-\beta E(s)} = \sum_{s\in S} e^{\beta\sum_{\langle ij \rangle}[\frac{\varepsilon}{2}(\sigma_i+\sigma_j)+J\sigma_i\sigma_j]} = \sum_{s\in S}\prod_{\langle ij \rangle} e^{\beta[\frac{\varepsilon}{2}(\sigma_i+\sigma_j)+J\sigma_i\sigma_j]}$$

Now we can define *transfer matrix* and its eigenvalues can be written as

$$\mathscr{P} = \begin{bmatrix} e^{\beta(J+h)} & e^{\beta J} \\ e^{\beta J} & e^{\beta(J-h)} \end{bmatrix} \qquad \lambda_{\pm} = e^{\beta J}\left(\cosh\beta h \pm \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right)$$

Now, in terms of the partition function, we observe that it is just matrix mulplications of $\mathscr{P}$, and if we take the boundary condition into account which is that the first spin should be equal to the last spin (we can also think it as a periodic boundary condition), then it is straightforward to think that the partition function $\mathscr{Z}$ is just the trace of matrix product of $\mathscr{P}$. So the partition function can be rewritten as:

$$\mathscr{Z} = \mathrm{Tr}(\mathscr{P}^N) = e^{N\beta J}\left[\left(\cosh\beta h + \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right)^N + \left(\cosh\beta h - \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right)^N\right]$$

If we take $N \to \infty$, we get $\mathscr{Z} = \lambda_+^N + \lambda_-^N \approx \lambda_+^N$, the free energy can be shown as

$$\frac{F}{N} = -\frac{1}{N\beta}\ln\mathscr{Z} = -J - \frac{1}{\beta}\ln\left(\cosh\beta h + \sqrt{\sinh^2\beta h + e^{-4\beta J}}\right)$$

other properties of the system can be calculated directly by the formulas, e.g.

- Energy $\dfrac{E}{N} = -\dfrac{1}{N}\dfrac{\partial}{\partial\beta}\ln\mathscr{Z}$, Specific heat $\dfrac{C(T)}{Nk} = \dfrac{1}{Nk}\dfrac{\partial E}{\partial T} = \dfrac{\beta^2}{N}\dfrac{\partial^2}{\partial\beta^2}\ln\mathscr{Z}$
- Magnetization $\dfrac{\mathbf{M}}{N} = \dfrac{1}{N\beta}\dfrac{\partial}{\partial h}\ln\mathscr{Z}$, Magnetic susceptibility $\dfrac{\chi}{N} = \dfrac{1}{N}\dfrac{\partial\mathbf{M}}{\partial h} = \dfrac{1}{N\beta}\dfrac{\partial^2}{\partial h^2}\ln\mathscr{Z}$

2.2 Absence of external field

In the special case of no external field ($h = 0$), the partition function becomes

$$\mathscr{Z} = (2\cosh\beta J)^N + (2\sinh\beta J)^N = (2\cosh\beta J)^N\left[1 + (\tanh\beta J)^N\right]$$

For the case $N \to \infty$, we can eliminate the second term and calculate the free energy and the internal energy per spin site

$$\frac{F}{N} = -\frac{1}{N\beta}\ln\mathscr{Z} = -\frac{1}{\beta}\ln\left[2\cosh(\beta J)\right] \qquad \frac{E}{N} = -\frac{1}{N}\frac{\partial}{\partial\beta}\ln\mathscr{Z} = -J\tanh(\beta J)$$

The specific heat is thus

$$\frac{C(T)}{Nk} = \frac{1}{Nk}\frac{\partial E}{\partial T} = \frac{\beta^2}{N}\frac{\partial^2}{\partial\beta^2}\ln\mathscr{Z} = (\beta J)^2\mathrm{sech}^2(\beta J) = \left(\frac{J}{kT}\right)^2\mathrm{sech}^2\left(\frac{J}{kT}\right)$$

the specific heat is a smooth function at $T \in [0, \infty)$, there is no phase transition in one dimensional Ising model.

3 Two dimensional solution

In solving the one dimensional Ising model, one should notice that there are only two terms in the partition function $\mathscr{Z}$. To explain this, we can expand the partition function in cluster of interactions. That is

$$\begin{aligned}\mathscr{Z} &= \sum_{\{\sigma_i\}}\prod_{\langle ij\rangle} e^{\beta J\sigma_i\sigma_j} = \sum_{\{\sigma_i\}}\prod_{\langle ij\rangle}\left[\cosh(\beta J) + \sigma_i\sigma_j\sinh(\beta J)\right] = \sum_{\{\sigma_i\}}\prod_{\langle ij\rangle}\cosh(\beta J)\left[1 + \sigma_i\sigma_j\tanh(\beta J)\right] \\ &= \left[\cosh(\beta J)\right]^N\sum_{\{\sigma_i=\pm1\}}\left[1 + \tanh(\beta J)\sum_{\langle ij\rangle}\sigma_i\sigma_j + \tanh^2(\beta J)\sum_{\langle ij\rangle\neq\langle kl\rangle}\sigma_i\sigma_j\sigma_k\sigma_l + \cdots\right]\end{aligned}$$

where $\langle ij\rangle$ is sum over the neighbors j of a single i. In the cluster expansion, most of the terms will canceled after the summation, since we need to sum over each spin for $\sigma_i = \pm1$. However, when the clustered interactions form a close loop, each spin site in it will be multiplied twice in each term, thus will always has value 1. In one dimensional case, the only way to form such loop is to go through the whole one dimensional Ising string, this term is in the power N cluster. When sum over all N spin sites there are 2^N possible ways to order the spins. We can write this partition function as

$$\mathscr{Z} = (\cosh\beta J)^N\,2^N\left[1 + (\tanh\beta J)^N \times 1\right]$$

which gives the same result as the previous section. In higher dimensional cases, however, there are many more ways to form a closed loop in the cluster expansion. As we said before, there will be a term:

$$\sum_{s\in S}\left(\prod_{\langle ij\rangle}(1+\sigma_i\sigma_j T)\right)$$

showing up in the partition function, and we have only a polynomial depending on $\tanh(\beta J)$ left:

$$P(T)=\sum_{k=1}^{dN}c_d(k)T^k$$

It is pretty straightforward to see that the coefficients $c_d(k)$ count the number of loops with even lengths k's. It follows that this is exactly the number of loops with length k whose components consist of closed paths. So the work to do now is to calculate the number of diagrams for each orders in the cluster expansion. In 1944, Onsager [2] developed a way to calculate it through *quaternion algebra*. In the following years, may similar ways were developed by scientists.

The partition function of the two dimensional Ising model is

$$\frac{1}{N}\ln\mathscr{Z}=\ln\left[\sqrt{2}\cosh(2\beta J)\right]+\frac{1}{\pi}\int_0^{\pi/2}\ln\left[1+\sqrt{1-\kappa^2\sin^2\phi}\right]d\phi\ \ ,\ \ \kappa=\frac{2\sinh(2\beta J)}{\cosh^2(2\beta J)}$$

It is not hard to figure that the first term has the similar form as the one dimensional result. However, the second term contains interesting properties that make the result significantly different from one dimensional case.

4 Phase transition in 2-D Model

As stated in the previous section, the most different properties in the two dimensional Ising model is the phase transition phenomena. People concern on the phase transition of two values in the two dimensional Ising model: the specific heat $C(T)$ and the spontaneous magnetization M. Intuitively, the two desired functions can be easily derived from the partition function if we have the exact form as the previous section. Before Onsager published his work on the exact solution of the two dimensional problem, some scientists had developed some theories to achieve those critical exponents. The critical temperature of the specific heat $C(T)$ was obtained by Kramers and Wannier [6] in 1941, before the discovery of the exact solution. The critical phenomenon of the magnetization M was first derived by Yang [7] in 1952 by using similar mathematical tools. The exact partition function of two dimensional Ising model under external field remains an open question until now (2014).

To illustrate the implicit argument without writting down the partition function. We can consider the following question: What is the probability that we find a spin down deep inside the lattice afterwards, if we put all spins up on the lattice boundary? Since the spins of the boundary sites of the lattice are all +1, so if finally we have at least one spin down inside, it is clear that we obtain groups of spin (-1) sites. These groups have boundaries and its main body. Now to find the probability that $\sigma_0=-1$ where 0 is a lattice site deep inside, we have to sum over all possible configurations that contain $\sigma_0 = -1$. We denote this domain as Ω_0. In the first step, we take a certain boundary surrounding 0 and give the probability of a certain configuration with that boundary, which will be the sum over $\Omega_S \subseteq \Omega_0$. Then we can try to change the signs in configuration $\sigma \in \Omega_S$ of all sites inside the boundary to be +1, we obtain the following:

$$\sum_{\langle ij \rangle \notin S} \sigma_i \sigma_j = \sum_{\langle ij \rangle} \sigma'_i \sigma'_j - n(S)$$

Where $n(s)$ is the length of the boundary S. The $-n(S)$ results from the fact that each cross-segment of the boundary is associated with a pair of lattice sites of opposite spin, in which the inner one is -1 while the outer one is $+1$. It follows as of the probability that

$$\begin{aligned}
P(\omega_S) &= e^{-\beta J n(S)} \frac{1}{Z} \sum_{\sigma \in \Omega_S} e^{\beta J \sum_{\langle ij \rangle \notin S} \sigma_i \sigma_j} \\
&< e^{-\beta J n(S)} \frac{1}{Z} \sum_{\sigma' \in \Omega'_S} e^{-\beta E(\sigma')} \\
&< e^{-\beta J n(S)} \frac{1}{Z} \sum_{\sigma \in \Omega} e^{-\beta E(\sigma)} = e^{-\beta J n(S)}
\end{aligned}$$

So we have $P(\sigma_0 = -1) = \sum_{n \geq 4} s(n) e^{-\beta J n(S)}$, where $s(n)$ is the number of boundaries surrounding 0 with length n. One can estimate this number by $s(n) < n4^n$ and plug it in and get:

$$\begin{aligned}
P(\sigma_0 = -1) &< \sum_{n \geq 4} n 4^n e^{-\beta J n} = \sum_{n \geq 4} n \left(4e^{-\beta J}\right)^n \xrightarrow{def\ x = 4e^{-\beta J}} \\
&= \sum_{n \geq 4} n x^n = x \frac{d}{dx} \sum_{n \geq 4} x^n \leq x \frac{d}{dx} \frac{1}{1-x} = \frac{x}{(1-x)^2}
\end{aligned}$$

Thus we obtain a geometric series for the probability which finally gives:

$$P(\sigma_0 = -1) < \left(\frac{4e^{-\beta J}}{(1 - 4e^{-\beta J})^2} \right)$$

which becomes infinitesimal for the temperature sufficiently low. So we have proved theoretically a spontaneous magnetization for low temperatures.

We then discuss the critical temperature and the specific heat from the partition function. From the partition function we have got in the previous paragraph, we can further implement the formulas in statistical mechanics to achieve the properties of the two dimensional Ising model.

$$E = -\frac{\partial}{\partial \beta} \ln \mathscr{Z} \qquad C(T) = \frac{\partial E}{\partial T} = k\beta^2 \frac{\partial^2}{\partial \beta^2} \ln \mathscr{Z}$$

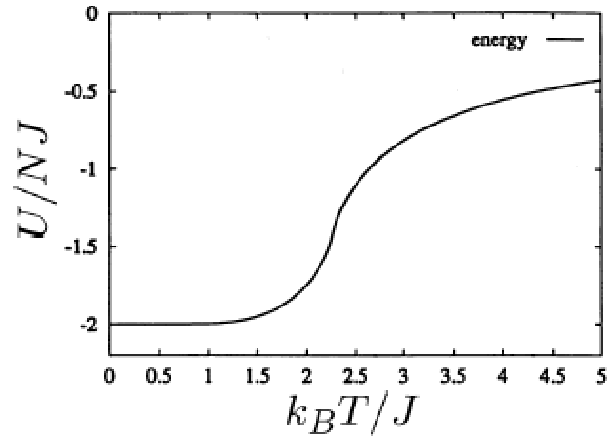

Figure 2: Internal energy of 2D Ising model vs. scaled temperature

The elliptic integral in the partition function will produce many tedious calculation. After the derivation, we can approximate the elliptic integral as a logarithmic function. Finally, we write down the specific heat verses temperature as

$$\frac{C(T)}{Nk} \approx -\frac{8}{\pi}\left(\frac{J}{kT_c}\right)^2 \ln\left|1-\frac{T}{T_c}\right| + \text{const} = -0.4945 \ln\left|1-\frac{T}{T_c}\right| + \text{const}$$

it is obvious that there is a logarithmic divergence at $T = T_c$ where the phase transition occurs. As $\mathscr{N} \to \infty$, the critical temperature T_c is calculated as

$$\tanh\frac{2J}{kT_c} = \frac{1}{\sqrt{2}} \quad \Rightarrow \quad \frac{kT_c}{J} = \frac{2}{\log\left(1+\sqrt{2}\right)} = 2.269$$

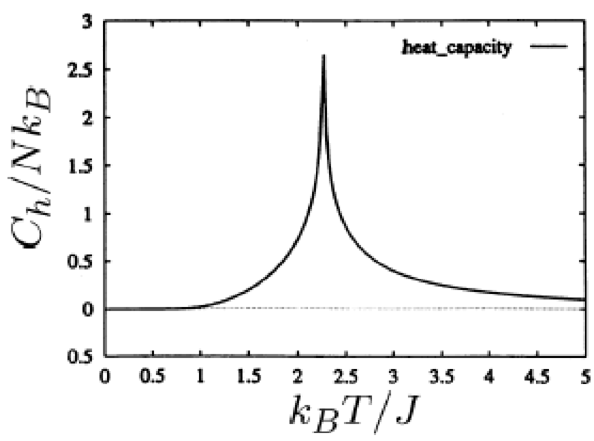

Figure 3: Specific heat of 2D Ising model vs. scaled temperature

Actually this value was discovered first by Kramers before the exact partition function is written down. Kramers used the method of *duality transformation* to achieve this value.

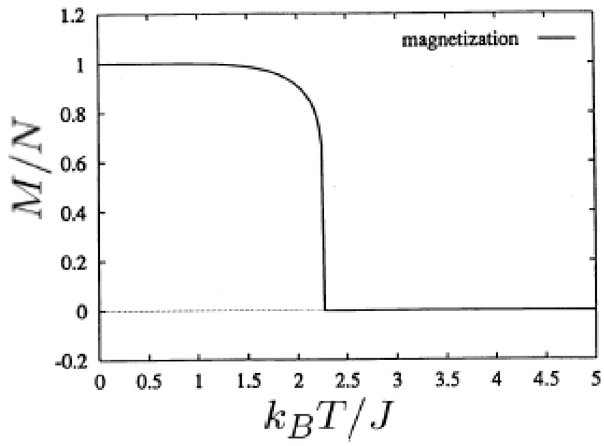

Figure 4: Spontaneous magnetization of 2D Ising model vs. scaled temperature

Following the dual lattice method, the behavior of the magnetization M at the region $T < T_c$ is calculated as

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

the most important result is the critical exponent 1/8 which describes the property of the phase transition.

5 Demonstrations on three dimensional solution

Onsager's approach made a significant breakthrough in the condensed matter study. Some mathematical equivalent arguments were also developed by the scientists.

The most intuitive way to do the three dimensional Ising model problem is to extend the method which is used in two dimensional case. However, one will get stock during the implementation. From the combinatorial approach in the two dimensional Ising model, we need to count the number of closed loops in the crystal. The most important issue of that method is to eliminate the overlap of the closed loops which may lead to form a non-closed loop. In the combinatorial approach of the two dimensional model, we introduce the phase (or weight) to each turn in our diagram. This makes the contribution of the non-closed loops cancels each other in the summation. Thus we can easily get our desired value to form the partition function. Then we made a Fourier transform to work this problem in k-space, and discovered that there is only one four by four matrix problem. The partition function is actually the inverse Fourier transform of the solution to the matrix problem.

However, this no longer works in three dimensional case. Almost all the approaches based on Onsager's work failed in this point. Thus the eigenvalues of the transfer matrix cannot be determined.[8] Scientists and mathematicians now focus their works on finding a new geometrical structure in three dimensional Ising model.

6 Conclusion

Ising model is the simplest model in the spin lattice. The problem has existed for 90 years. The exact solution of the two dimensional model inspired people to discover the geometrical structure of systems in condensed matter physics. Although the three dimensional model still cannot be solved, the mathematical tools developed by the scientists and mathematicians for Ising model enlighten the research of spin glass and spin liquid systems. Which are very important branches of physics study in recent 50 years.

References

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