Statistical Mechanics Notes

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1 Motivation and Plan

In this lecture, we discuss the topic of duality in the 2D Ising model. In this case, duality refers not to the linear algebra concept of duality, but rather the duality of two lattices, which we will discuss later. The goal of this lecture is to work with the 2D Ising model and derive a relationship between partition functions in a low-temperature phase, and partition functions in a high-temperature phase, first for the square lattice, and then, if time permits, for the triangle and hexagonal lattices.

The 2D Ising model considers a lattice of points rather than a line or circle of them, and values at each point are still $+$ or $-$ (up or down), and Hamiltonians still only consider the energy of first-neighbor pairs.

2 Square Lattices

A man by the name of Peierls argued that the 2D Ising model has a high temperature phase which is generally disordered, and a low temperature phase which is generally ordered. This argument is linked below. We will separately find the series expansion for the partition function under both high/low temperatures, and then discuss how these two relate (which is called self-duality).

2.1 High Temperature Series Expansion

Consider a square lattice $\mathcal{L}$ with M horizontal (first-neighbor) links and M vertical (first-neighbor) links. If there are N lattice points, then note that $\frac{M}{N} \to 1$ as $N \to \infty$. Recall that the partition function is defined as

$$Z(N, \beta) = \sum_{\mathcal{C}} \exp(-\beta E(\mathcal{C}))$$

Fix $\beta = \frac{1}{kT}$, and take the energy of a configuration $\{\sigma\}$ to be

$$E(\{\sigma\}) = \mathcal{J} \sum_{(i,j)} \sigma_i \sigma_j + \mathcal{J}' \sum_{(i,k)} \sigma_i \sigma_k$$

where the first term describes energy from all horizontal links, multiplied by a constant factor $\mathcal{J}$ and the second term describes energy from all vertical links, multiplied by a potentially different $\mathcal{J}'$. The partition function is given by

$$Z_N = \sum_{\{\sigma\}} \exp\left[K \sum_{(i,j)} \sigma_i\sigma_j + L \sum_{(i,k)} \sigma_i\sigma_k\right]$$

$$K = \beta\mathcal{J},\ L = \beta\mathcal{J}'$$

The identity

$$\exp(x\sigma_i\sigma_j) = \cosh(x)(1 + \sigma_i\sigma_j \tanh(x))$$

gives

$$Z_N = (\cosh(K)\cosh(L))^M \sum_{\{\sigma\}} \left[\prod_{(i,j)} (1 + v\sigma_i\sigma_j) \prod_{(i,k)} (1 + w\sigma_i\sigma_k)\right]$$

$$v = \tanh(K),\ w = \tanh(L)$$

Note that for high temperatures, $0 < v, w << 1$. When we expand out the products, we have 2^{2M} terms. For a given configuration, we can express each term as the product along the edges of a given (potentially disconnected path) on the lattice, where each horizontal edge (i, j) has weight $v\sigma_i\sigma_j$ if it is filled in, and 1 otherwise, and each vertical edge (i, k) has weight $w\sigma_i\sigma_k$ if it is filled in and 1 otherwise. It is not difficult to see that this is a bijective mapping, and that all terms are of the form

$$v^r w^s \sigma_1^{n_1} \dots \sigma_N^{n_N}$$

where r is the number of horizontal edges and s is the number of vertical ones. We can then rewrite Z_N as a constant multiplied by the sum of these terms over all configurations and all possible edge arrangements. We can then switch this summation, and fix a path. Summing over all possible $\{\sigma\}$ configurations, gives a sum of 0 for all edge arrangements where the n_i is odd for some i. For the edge arrangements with only even powers $n_1, \dots, n_N$, we have a sum of $2^N v^r w^s$. We call these edge arrangements "closed polygonal lines" (P in summations). We can then write

$$Z_N = 2^N (\cosh(K)\cosh(L))^M \sum_P v^r w^s$$

Define the geometric quantity

$$\Phi(v, w) = \sum_P v^r w^s$$

Note that the first few terms are given approximately by

$$\Phi(v, w) = 1 + N(vw)^2 + N(v^2w^4 + v^4w^2) + \dots$$

In order, these values are the number of 0-edged polgons, squares, and 1 by 2 rectangles. We don't need to understand all of the terms, though, just the geometric nature of the sum.

2.2 Low-temperature Series Expansion

In this case, the spins tend to align with each other, so fix a configuration and let r be the number of anti-aligned vertical links and s the respective value for horizontal links. The contribution to the partition function of this configuration is

$$\exp[K(M-2s)+L(M-2r)]$$

Define the dual lattice $\mathcal{L}_D$ by connecting the circumcenters of each unit square in the lattice, as follows:

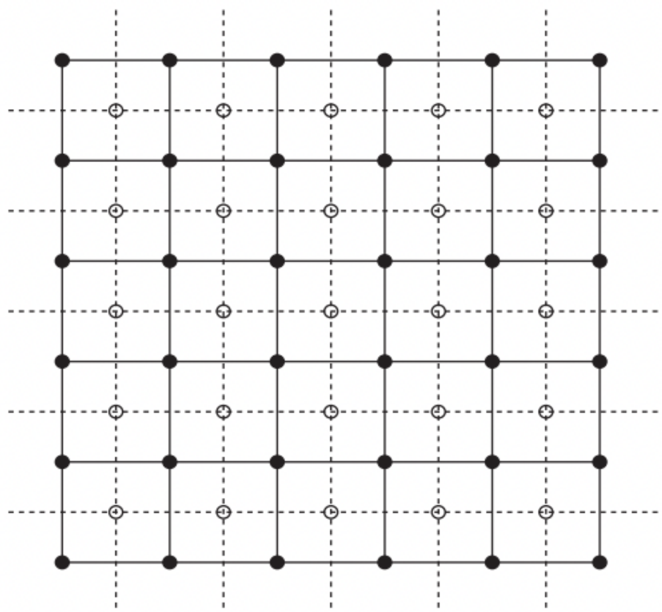

Fig. 4.4 *Dual square lattices.*

Now, for the configuration on $\mathcal{L}$, construct an edge arrangement of the dual lattice by selecting all edges which cross through an anti-aligned link. There are now r horizontal edges and s vertical ones. It is easy to see that there are an even number of edges connected to each dual lattice point, and so we end up with a closed polygonal line on the dual lattice. It is also clear that this closed polygonal line separates positive domains from negative domains. For each close polygon, there are 2 corresponding configurations (attained by flipping all signs), so we end up with

$$Z_N = 2\exp[M(K+L)]\sum_{\tilde{P}}\exp(-(2Lr+2Ks)$$

over all closed polygons on the dual lattice $\mathcal{L}_D$.

Similar to the high-temperature case, we end up with Z_N depending on a few constants multiplied by

$$\tilde{\Phi}(e^{-2L}, e^{-2K}) = \sum_{\tilde{P}} \exp(-2Lr - 2Ls)$$

This is the low temperature case, since when $T \to 0$, K, L are large and the dominant terms of the expansion are given by low values of r, s.

Again, the first few terms are given by when no edges are chosen on the dual lattice (all spins same on original lattice), 4 edges on dual lattice (all spins same except one), and 6 edges on dual lattice (2 neighboring spins differ from all others), which gives us the terms

$$\tilde{\Phi}(e^{-2L}, e^{-2K}) = 1 + Ne^{-4K-4L} + N(e^{-4K-8L} + e^{-8K-4L})$$

We can pretty easily see the connection between the high temperature case and the low temperature case.

2.3 Self-duality

Our constructions for the high temperature and low temperature equations suggest some sort of equality. However, the sums differ for finite lattices due to odd behavior at the boundaries of the lattice. However, these disappear as $N \to \infty$ (recall $\frac{M}{N} \to 1$).

If we define

$$v = \tanh(K) = e^{-2\tilde{L}}, \ w = \tanh(L) = e^{-2\tilde{K}}$$

we can write

$$\tilde{\Phi}(e^{-2\tilde{K}}, e^{-2\tilde{L}}) = \Phi(v, w)$$

$$\implies \frac{Z_N(K, L)}{2^N \cosh(L)^N \cosh(K)^N} = \frac{Z_N(\tilde{K}, \tilde{L})}{2 \exp(N(\tilde{K} + \tilde{L}))}$$

Or, symmetrically, our definitions can be rewritten as follows using the identities $\cosh^2(x) - \sinh^2(x) = 1$, $\sinh(2x) = 2\sinh(x)\cosh(x)$

$$\sinh(2\tilde{K})\sinh(2L) = 1 = \sinh(2K)\sinh(2\tilde{L})$$

$$\implies \frac{Z_N(K, L)}{(\sinh(L)\sinh(K))^{N/4}} = \frac{Z_N(\tilde{K}, \tilde{L})}{(\sinh(\tilde{L})\sinh(\tilde{K}))^{N/4}}$$

There is a sort of symmetry between high and low temperature phases, where small values of K, L correspond to large values of $\tilde{K}, \tilde{L}$ and vice versa.

The calculation of the critical point is fairly simple for the isotropic case ($K = L$). We must then have $\tilde{K} = \tilde{L}$ and the above equations, assuming that there is only one critical point (which is suggested empirically), the 4 constants are all the same (K_c), giving us

$$\sinh(2K_c) = 1 \implies T_c^{square} = \ln(1 + \sqrt{2}) \approx 2.26922\mathcal{J}/k$$

When the coupling constants are different vertically and horizontally, we can derive the equation

$$\sinh(2K)\sinh(2L) = \frac{1}{\sinh(2\tilde{K})\sinh(2\tilde{L})}$$

which fixes all pairs (K, L) with

$$\sinh(2K)\sinh(2L) = 1$$

Assuming there is only one fixed line, the constraint ensures criticality of the 2D Ising model with a square lattice.

3 Duality Relation: Hexagonal and Triangular Lattices

Note that the dual lattice of a triangular lattice is a hexagonal one, and vice versa.

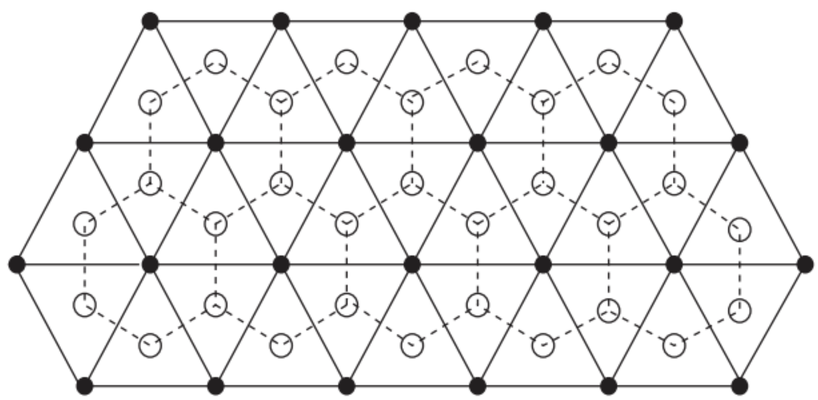

Fig. 4.7 *Dual lattices: hexagonal and triangle lattices.*

If we define the coupling constants K_i, L_i for $i = 1, 2, 3$ relative to the triangular and hexagonal lattices, respectively, then the partition function of a hexagonal lattice is

$$Z_N^H(\mathcal{L}) = \sum_{\{\sigma\}} \exp\left[\mathcal{L}_1 \sum \sigma_i\sigma_j + \mathcal{L}_2 \sum \sigma_i\sigma_k + \mathcal{L}_3\sigma_i\sigma_l\right]$$

where the summations are across all first-neighbor links in directions 1, 2, and 3 and $\mathcal{L}_i = \beta L_i$.

Similarly, the partition function of a triangle lattice is

$$Z_N^T(\mathcal{K}) = \sum_{\{\sigma\}} \exp\left[\mathcal{K}_1 \sum \sigma_i\sigma_j + \mathcal{K}_2 \sum \sigma_i\sigma_k + \mathcal{K}_3\sigma_i\sigma_l\right]$$

where the summations are across all first-neighbor links in directions 1, 2, and 3 and $\mathcal{K}_i = \beta K_i$.

Mimicking the process from the previous section, take the high-temperature expansion of the partition function on the triangle lattice:

$$Z_N^T(\mathcal{K}) = (2\cosh\mathcal{K}_1 \cosh\mathcal{K}_2 \cosh\mathcal{K}_3)^M \sum_P v_1^{r_1} v_2^{r_2} v_3^{r_3}$$

where the sum is over all closed polygons on the triangle lattice, and with $v_i = \tanh(\mathcal{K}_i)$.

The low-temperature expansion of the partition function on the hexagonal lattice can be given by (hexagonal lattice as $2N$ points):

$$Z_{2N}^H(\mathcal{L}) = e^{N(\mathcal{L}_1+\mathcal{L}_2+\mathcal{L}_3)} \sum_P \exp[-2(\mathcal{L}_1 r_1 + \mathcal{L}_2 r_2 + \mathcal{L}_3 r_3)]$$

Like before, we define $\tanh(\mathcal{K}_i^*) = \exp[-2\mathcal{L}_i]$, and (left as an exercise up to the reader) we can relate the partition functions by

$$Z_{2N}^H(\mathcal{L}) = (2a_1a_2a_3)^{N/2} Z_N^T(\mathcal{K}^*)$$

where

$$a_i = \sinh(2\mathcal{L}_i) = \frac{1}{\sinh(2\mathcal{K}_i^*)}$$

The critical relation becomes

$$\sinh(2\mathcal{L}_i)\sinh(2\mathcal{K}_i^*) = 1$$

but we cannot solve for the critical temperature since we do not have self-duality. The next section covers the star-triangle identity, which is needed to solve for the critical temperature.