

Advanced Statistical Mechanics

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Week 3

6 2D Ising Model: Peierls Argument

2D Ising model is defined on a 2D lattice.

$$Z = \sum_{\sigma_i = \pm 1} e^{\beta H}, \quad H = \sum_{i, \mu} \sigma_i \sigma_{i+\mu}, \quad (6.1)$$

where i is the position of the spin and $i + \mu$ denotes either vertical or horizontal neighbor of i .

Peierls argument in this case says that at large β the spins will order. Indeed, a droplet of negative spins in the sea of positive spins has relative energy $2\beta L$ and relative contribution to Z as $e^{-2\beta L}$, where L is the length of the droplet's boundary. On the other hand, there are c^L ways to position a droplet. This produces a contribution to Z of the order of $e^{L \log c - 2\beta L}$ which, at large β , will always be small. In other words, the free energy of the droplet is

$$F = E - TS = 2\beta L - L \log c \quad (6.2)$$

and its minimum at large beta is achieved at small L .

At critical β there's a phase transition between ordered and disordered spins.

7 Transfer Matrix and the Hamiltonian

We designate one direction as space, the other as time. We will also allow for the bond strengths β to be different along these two directions. We write the partition function as

$$Z = T^N \quad (7.3)$$

where T is a 2^N by 2^N matrix. Its explicit form is

$$T_{\tilde{\sigma}, \sigma} = a^N \sum_{\{\sigma'\} = \pm 1} \prod_i \left[e^{\gamma \tau_i^1} \right]_{\tilde{\sigma}_i \sigma'_i} \left[\prod_i e^{\beta \tau_i^3 \tau_{i+1}^3} \right]_{\{\sigma'\} \{\sigma\}}, \quad (7.4)$$

where τ_i^1, τ_i^3 are the appropriate Pauli matrix which act on the i -th Ising spin, and $\sinh \gamma = \exp(-\beta) / \sqrt{2 \sinh(2\beta)}$, just as in 1D.

We would like to write this down as $T = \exp(-NH)$. In general it's not easy to find H , but at least in one regime this is very easy. Take $\gamma \ll 1$, $\beta \ll 1$. Since $\gamma \propto \exp(-2\beta)$, this is only possible if the bond strengths are different along space and time direction. Then

$$H = -\gamma \sum_i \tau_i^1 - \beta \sum_i \tau_i^3 \tau_{i+1}^3. \quad (7.5)$$

This Hamiltonian is called the 1D transfer field Ising model. The reason for it is simple: this is a 1D chain of quantum spins in the magnetic field perpendicular to them.

8 Ordered and Disordered Regimes

If $\gamma \ll \beta$, then as a first approximation the ground state is

$$|0\rangle = \prod_i \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i, \text{ or } |0\rangle = \prod_i \begin{pmatrix} 0 \\ 1 \end{pmatrix}_i. \quad (8.6)$$

The first excited state is the one where spins to the left of a certain point point up and the one to the right point down.

$$|y\rangle = \prod_{i < y} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i \prod_{i \geq y} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_i. \quad (8.7)$$

Now let us add the γ term as a small perturbation. Its matrix elements are

$$\langle y | \gamma \sum_i \tau_i^1 |y'\rangle = -\gamma \delta_{y,y'+1} - \gamma \delta_{y,y'-1} \quad (8.8)$$

Diagonalizing this gives the spectrum

$$E(k) - E(0) = 2\beta - 2\gamma \cos(k) = 2\beta - 2\gamma + 4\gamma \sin^2\left(\frac{k}{2}\right). \quad (8.9)$$

This gives a gap of $2\beta - 2\gamma$, so the spins are ordered (assuming it survives at higher order, which it does as the exact solution will show).

Analogous calculation at $\gamma \gg \beta$ gives a gap as well, $2\gamma - 2\beta$, but the spins are disordered.

9 Jordan-Wigner transformation

Now we will solve the Hamiltonian (7.5) exactly. First of all we do a unitary transformation so that

$$H = -\gamma \sum_i \tau_i^3 - \beta \sum_i \tau_i^1 \tau_{i+1}^1. \quad (9.10)$$

Corresponding transformation is given by $U = \frac{1}{\sqrt{2}}(1 + i\tau^2)$, and

$$U^\dagger \tau^3 U = -\tau^1, \quad U^\dagger \tau^1 U = \tau^3. \quad (9.11)$$

It is convenient to introduce

$$b = \frac{1}{2}(\tau^1 + i\tau^2), \quad b^\dagger = \frac{1}{2}(\tau^1 - i\tau^2) \quad (9.12)$$

They satisfy

$$b^2 = b^{\dagger 2} = 0, \quad b^\dagger b + b b^\dagger = 1 \quad (9.13)$$

In this way they look like creation and annihilation operators.

Now we introduce the Jordan-Wigner string

$$a_j = e^{i\pi \sum_{k<j} b_k^\dagger b_k} b_j, \quad a_j^\dagger = e^{-i\pi \sum_{k<j} b_k^\dagger b_k} b_j^\dagger. \quad (9.14)$$

Then not only a_i obey creation and annihilation relations on a given site, but also

$$a_i^\dagger a_j + a_j a_i^\dagger = 0, \quad i \neq j, \quad (9.15)$$

and so do a_i , a_j and a_i^\dagger , a_j^\dagger . Therefore, these are now fermions, called Jordan-Wigner fermions. Therefore, the Hamiltonian becomes (taking into account the Jordan-Wigner string)

$$H = \gamma \sum_i (a_i^\dagger a_i - a_i a_i^\dagger) - \beta \sum_i (a_i^\dagger - a_i) (a_{i+1}^\dagger + a_{i+1}) \quad (9.16)$$

This is the so-called Bogoliubov Hamiltonian, studied in superconductivity. To diagonalize it, we employ the Bogoliubov transformations,

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = U \begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}. \quad (9.17)$$

Here U has to be unitary, $U^\dagger U = 1$ as a consequence of the anticommutation relations.

In this basis,

$$H = \begin{pmatrix} \gamma + \frac{\beta}{2}\Delta & \frac{\beta}{2}\Gamma \\ -\frac{\beta}{2}\Gamma & -\gamma - \frac{\beta}{2}\Delta \end{pmatrix} = \left(\gamma + \frac{\beta}{2}\Delta \right) \Sigma_3 + i \frac{\beta}{2} \Gamma \Sigma_2, \quad (9.18)$$

where Δ and Γ are matrices such that

$$\Delta_{ij} = \delta_{i,j+1} + \delta_{i,j-1}, \quad \Gamma_{ij} = \delta_{i,j-1} - \delta_{i,j+1}, \quad (9.19)$$

and Σ_3 , Σ_2 are Pauli matrices. Our task is to diagonalize H , after which it can be written as

$$H = \sum_i \left[h_i c_i^\dagger c_i - h_i c_i c_i^\dagger \right], \quad (9.20)$$

where h_i are eigenvalues of H (more precisely, the absolute value of the eigenvalues).

To find h_i , we will use a series of unitary transformations.

We first rotate Σ_3 into Σ_1 by employing $U = \frac{1}{\sqrt{2}} (1 + i\Sigma_2)$ and $H' = U^\dagger H U$. We find

$$H = \left(\gamma + \frac{\beta}{2}\Delta \right) \Sigma_1 + i \frac{\beta}{2} \Gamma \Sigma_2. \quad (9.21)$$

The eigenvalue equations become

$$hs_i = \gamma t_i + \beta t_{i+1}, \quad (9.22)$$

$$ht_i = \gamma s_i + \beta t_{i-1}. \quad (9.23)$$

These can be solved in terms of plane waves, to get

$$h(k) = \pm \sqrt{(\gamma - \beta)^2 + 4\gamma\beta \sin^2\left(\frac{k}{2}\right)}. \quad (9.24)$$

We fill all the negative $h(k)$ states with fermions to lower the total energy as much as we can. Then the excitations are either filling the states with negative $h(k)$ or vacating the states with positive k . The excitation spectrum is then $2h(k)$. It is easy to check that in the limit $\gamma \ll \beta$ it crosses over to (8.9).

Interesting to note that at small k it has a relativistic form,

$$h^2(k) = (\gamma - \beta)^2 + \gamma\beta k^2. \quad (9.25)$$

This is the spectrum of particles of mass $m = |\gamma - \beta|$.

Finally, the correlation length is the gap and is given by

$$\xi \propto \frac{1}{|\gamma - \beta|} \propto \frac{1}{m}. \quad (9.26)$$

It diverges at $\gamma = \beta$. It is customary, if the correlation function is divergent at some critical T_c , to denote the power of its divergence as ν :

$$\xi \propto \frac{1}{(T - T_c)^\nu}. \quad (9.27)$$

We see that for the 2D Ising model $\nu = 1$. This is one of Onsager's exact results. Another result for the free energy easily follows as well. The free energy is given by

$$F = -T \log Z. \quad (9.28)$$

Since Z is proportional to $\exp(-NE_0)$ where E_0 is the ground state energy and N is the length of the Ising model in the "time" direction, that gives

$$F = TNE_0 \quad (9.29)$$

In other words, the ground state energy in quantum mechanics is the same as the free energy in statistical mechanics. In this problem

$$E_0 \propto - \int dk \sqrt{(\gamma - \beta)^2 + 4\gamma\beta \sin^2 \left(\frac{k}{2} \right)} \quad (9.30)$$

An interesting quantity is the specific heat.

$$c = -T \frac{\partial^2 F}{\partial T^2} \quad (9.31)$$

To find it we need to differentiate E_0 with respect to T , remembering that γ and β are both temperature dependent. Differentiating E_0 with respect to them we find

$$c \propto \log \left(\frac{1}{|\gamma - \beta|} \right). \quad (9.32)$$

This is another of Onsager's famous results. A standard notation in statistical mechanics is

$$c \propto \frac{1}{|T - T_c|^\alpha} \quad (9.33)$$

From here it follows that $\alpha = 0$.