Statistical Mechanics - Class Exercise 7

December 20, 2022

Exercise 5651 - Ising spins with interaction that is mediated by atoms

Consider a one dimensional Ising model of spins $\sigma_i = \pm 1$ labeled $i = 1, 2, 3, ..., M$. Between each two spins there is a site $n_i = 0, 1$ that can be occupied by an atom. If the atom is present the feromagnetic coupling is decreased from J to $(1 - \lambda)J$.

1. Evaluate the partition sum assuming that there are N atoms in the M sites with open boundary condition. Allow all configurations of spins and of atoms. Calculate the free energy F.
2. Repeat (1) with periodic boundary condition. in which limit we get a different result?
3. If the atoms are stationary impurities one needs to evaluate the free energy F for some random configuration of the atoms. What is the entropy difference between the results?

Answer

1. If we have open chain the partition function is:

$$Z = \sum_{\{n\}} \sum_{\{\sigma\}} e^{-\beta\left(-J\sum_{i=1}^{M-1}(1-\lambda n_i)\sigma_i\sigma_{i+1}\right)}$$

We can define

$$s_i = \sigma_i \sigma_{i+1} = \pm 1$$

So the partition function can be written as:

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\{n\}} \sum_{\{s\}} e^{\beta J\sum_{i=1}^{M-1}(1-\lambda n_i)s_i} = 2\sum_{\{n\}} \prod_{i=1}^{M-1} \sum_{\{s\}} e^{\beta J(1-\lambda n_i)s_i} = 2\sum_{\{n\}} \prod_{i=1}^{M-1} 2\cosh\left(\beta J\left(1-\lambda n_i\right)\right)$$

We know that we have N atoms in the M sites, so

$$Z = \frac{M!}{N!\left(M-N\right)!} 2^M \cosh^{M-1-N}\left(\beta J\right)\cosh^N\left(\beta J\left(1-\lambda\right)\right)$$

The free energy is therefore $(M - 1 \approx M)$:

$$F = -T\ln Z = -T\ln\left(M!\right) + T\ln\left(N!\right) + T\ln\left(\left(M-N\right)!\right) - T\left(M-N\right)\ln\left(2\cosh\left(\beta J\right)\right) - TN\ln\left(2\cosh\left(\beta J\left(1-\lambda\right)\right)\right)$$

2. If we have closed chain we need to use Transfer matrices formalism:

$$T^{(n_i)} = \begin{pmatrix} e^{\beta J(1-\lambda n_i)} & e^{-\beta J(1-\lambda n_i)} \\ e^{-\beta J(1-\lambda n_i)} & e^{\beta J(1-\lambda n_i)} \end{pmatrix}$$

where

$$T^{(n_i)}_{\sigma_i \sigma_{i+1}} = e^{\beta J(1-\lambda n_i)\sigma_i \sigma_{i+1}} = \left\langle \sigma_i \left| T^{(n_i)} \right| \sigma_{i+1} \right\rangle, \quad \sigma_i = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{aligned} Z =& \sum_{\{n\}} \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \cdots \sum_{\sigma_n=\pm 1} \left\langle \sigma_1 \left| T^{(n_1)} \right| \sigma_2 \right\rangle \left\langle \sigma_2 \left| T^{(n_2)} \right| \sigma_3 \right\rangle \ldots \left\langle \sigma_M \left| T^{(n_M)} \right| \sigma_1 \right\rangle = \\ =& \sum_{\{n\}} \sum_{\{\sigma\}} T^{(n_1)}_{\sigma_1\sigma_2} T^{(n_2)}_{\sigma_2\sigma_3} \ldots T^{(n_M)}_{\sigma_M\sigma_1} = \sum_{\{n\}} \text{trace} \left(T^{(n_1)} T^{(n_2)} \ldots T^{(n_M)} \right) \end{aligned}$$

We have two kinds of matrices

$$T^{(0)} = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}, \; T^{(1)} = \begin{pmatrix} e^{\beta J(1-\lambda)} & e^{-\beta J(1-\lambda)} \\ e^{-\beta J(1-\lambda)} & e^{\beta J(1-\lambda)} \end{pmatrix}$$

But both matrices commute So the multiplication order does not matter:

$$\left[T^{(0)}, T^{(1)} \right] = 0$$

In addition, the two matrices have the same Modal matrix

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} e^{\beta J(1-\lambda n_i)} & e^{-\beta J(1-\lambda n_i)} \\ e^{-\beta J(1-\lambda n_i)} & e^{\beta J(1-\lambda n_i)} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \left[e^{\beta J(1-\lambda n_i)} + e^{-\beta J(1-\lambda n_i)} \right] & 0 \\ 0 & \left[e^{\beta J(1-\lambda n_i)} - e^{-\beta J(1-\lambda n_i)} \right] \end{pmatrix}$$

So

$$\begin{aligned} Z =& \frac{M!}{N!\,(M-N)!} \text{trace} \left(T^{(0)M-N} T^{(1)N} \right) \\ =& \frac{M!}{N!\,(M-N)!} \text{trace} \left(\begin{pmatrix} 2^{M-N} \cosh^{M-N}(\beta J) & 0 \\ 0 & 2^{M-N} \sinh^{M-N}(\beta J) \end{pmatrix} \begin{pmatrix} 2^N \cosh^N(\beta J(1-\lambda)) & 0 \\ 0 & 2^N \sinh^N(\beta J(1-\lambda)) \end{pmatrix} \right) \\ =& \frac{M!}{N!\,(M-N)!} 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda)) \left(1 + \tanh^{M-N}(\beta J) \tanh^N(\beta J(1-\lambda)) \right) \end{aligned}$$

For $M \to \infty$ because $-1 \le \tanh(x) \le 1$

$$Z = \frac{M!}{N!\,(M-N)!} 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda))$$

3. For any configuration with exactly N impurities, the partition function is:

$$Z = 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda))$$

As the impurities are fixed, the combinatorial factor is not needed.

The free energy for any configuration with N impurities is:

$$F = -T\ln Z = -T\left(M-N\right)\ln\left(2\cosh\left(\beta J\right)\right) - TN\ln\left(2\cosh\left(\beta J\left(1-\lambda\right)\right)\right)$$

The average free energy for a given N is:

$$\langle F\rangle = \frac{\sum_{configurations} F}{\sum_{configurations}} = \frac{\frac{M!}{N!(M-N)!}\left(-T\left(M-N\right)\ln\left(2\cosh\left(\beta J\right)\right) - TN\ln\left(2\cosh\left(\beta J\left(1-\lambda\right)\right)\right)\right)}{\frac{M!}{N!(M-N)!}}$$

$$\langle F\rangle = -T\left(M-N\right)\ln\left(2\cosh\left(\beta J\right)\right) - TN\ln\left(2\cosh\left(\beta J\left(1-\lambda\right)\right)\right)$$

The entropy difference between the two calculations:

$$\triangle S = -\frac{\partial F}{\partial T} + \frac{\partial\langle F\rangle}{\partial T} = \ln\left(\frac{M!}{N!\left(M-N\right)!}\right)$$