Statistical Mechanics - Class Exercise 7

May 24, 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 $i = 1, 2, 3, ..., M$, with periodic boundary condition. 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. Allow all configurations of spins and of atoms. Calculate the free energy F.
2. 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. The partition function is:

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

If we have open chain 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

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

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

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

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

$$T_{\sigma_i\sigma_{i+1}} = \begin{pmatrix} e^{\beta J(1-\lambda n_i)} & e^{-\beta J(1-\lambda n_i)} \\ e^{-\beta J(1-\lambda n_i)} & e^{\beta J(1-\lambda n_i)} \end{pmatrix}$$

where

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

$$Z = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_n=\pm 1} \langle \sigma_1 | T_{\sigma_1\sigma_2} | \sigma_2 \rangle \langle \sigma_2 | T_{\sigma_2\sigma_3} | \sigma_3 \rangle \dots \langle \sigma_M | T_{\sigma_M\sigma_1} | \sigma_1 \rangle =$$
$$= \sum_{\{\sigma\}} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \dots T_{\sigma_M\sigma_1} = \text{trace}\left(T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \dots T_{\sigma_M\sigma_1}\right)$$

We have two kinds of matrices

$$T = \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix}, \; T^{'} = \begin{pmatrix} e^{\beta J(1-\lambda)} & e^{-\beta J(1-\lambda)} \\ e^{-\beta J(1-\lambda)} & e^{\beta J(1-\lambda)} \end{pmatrix}$$

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

$$\left[T, T^{'}\right] = 0$$

So

$$Z = \frac{M!}{N!\,(M-N)!}\text{trace}\left(T^{M-N} T^{'N}\right)$$
$$= \frac{M!}{N!\,(M-N)!}\text{trace}\left(\begin{pmatrix} 2^{M-N}\cosh^{M-N}(\beta J) & 0 \\ 0 & 2^{M-N}\sinh^{M-N}(\beta J) \end{pmatrix}\begin{pmatrix} 2^{N}\cosh^{N}(\beta J(1-\lambda)) & 0 \\ 0 & 2^{N}\sinh^{N}(\beta J(1-\lambda)) \end{pmatrix}\right)$$
$$= \frac{M!}{N!\,(M-N)!} 2^M \cosh^{M-N}(\beta J) \cosh^N(\beta J(1-\lambda)) \left(1 + \tanh^{M-N}(\beta J) \tanh^N(\beta J(1-\lambda))\right)$$

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

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

2. For any configuration with exactly M impurities, the partition function is:

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

As the number of impurities is fixed, the combinatorial factor is not needed.
The free energy for any configuration with M impurities is:

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

The average free energy for a given M is:

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

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

The entropy difference between the two calculations:

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