FK7058: Handin2

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Consider Ising model, with the following Hamiltonian:

$$-\mathcal{H} = H(S_1 + S_2) + JS_1S_2,$$

where $J > 0$ and $S_i = \pm 1 \forall i$.

1)

Enumerate all the microstates of the system as well as the probabilities of these microstates.

Answer: All the possible states are the combination of the two spins S_1 and S_2.

1. $S_1 = 1$ and $S_2 = 1$.
2. $S_1 = 1$ and $S_2 = -1$.
3. $S_1 = -1$ and $S_2 = 1$.
4. $S_1 = -1$ and $S_2 = -1$.

There is an equal probability for each state and since there are four microstates, the probability of each state is 1/4.

2)

Calculate the partition function.

Answer: The partition function is given as:

$$\begin{aligned} Z = \sum_i e^{-\beta E_i} &= e^{\beta(2H+J)} + 2e^{\beta J} + e^{\beta(-2H+J)} \\ &= e^{\beta J}\left[2 + e^{2\beta H} + e^{-2\beta H}\right] \\ &= e^{\beta J}\left[2 + 2\cosh(2\beta H)\right] \end{aligned}$$

3)

How does the partition function (and hence the free energy) change if we replace H by $-H$?

Answer: If instead H is replaced by $-H$ the partition function becomes:

$$\begin{aligned} Z &= \sum_i e^{-\beta E_i} \\ &= e^{-\beta E_1} + e^{-\beta E_2} + e^{-\beta E_3} + e^{-\beta E_4} \\ &= e^{-\beta(-2H+J)} + 2e^{\beta(J)} + e^{-\beta(2H+J)} \\ &= e^{\beta J}\left[2 + 2\cosh(2\beta H)\right]. \end{aligned}$$

The partition function does not change, and thus, neither does the free energy.

4)

Calculate the average energy of this system.

Answer: The average energy of the system is given by:

$$\begin{aligned}
\langle E \rangle &= \frac{1}{Z}\frac{\partial Z}{\partial \beta} \\
&= -\frac{1}{Z}\frac{\partial}{\partial \beta}\left[e^{\beta J}\left[2 + 2\cosh(2\beta H)\right]\right] \\
&= -\frac{1}{Z}\left[e^{\beta J} J\left[2 + 2\cosh(2\beta H)\right] + e^{\beta J}\left[4H\sinh(2\beta H)\right]\right] \\
&= -\frac{1}{Z}e^{\beta J}\left[J\left[2 + 2\cosh(2\beta H)\right] + \left[4H\sinh(2\beta H)\right]\right] \\
&= -\frac{J\left(2 + 2\cosh(2\beta H)\right) + 4H\sinh(2\beta H)}{2 + 2\cosh(2\beta H)} \\
&= -\left[J + 2H\tanh(\beta H)\right]
\end{aligned}$$

5)

Calculate the magnetization per unit spin $M = \langle\frac{M_1+M_2}{2}\rangle$. How is M related to the free energy of the system? What is M at $H = 0$?

Answer:

6)

What is M in the limit $T \to 0$?

Answer:

7)

Calculate $\langle S_1 \cdot S_2\rangle - \langle S_1\rangle\langle S_2\rangle$ the connected correlation function.

Answer: We begin by computing the average of S_1 and S_2:

$$\langle S_1 \rangle = \sum_i S_1^{(i)} \cdot p_i = \frac{1}{4} - \frac{1}{4} = 0,$$
$$\langle S_2 \rangle = \sum_i S_2^{(i)} \cdot p_i = \frac{1}{4} - \frac{1}{4} = 0.$$

Hence, we can write the connected correlation function as:

$$\begin{aligned}
\langle S_1 \cdot S_2 \rangle &= \frac{1}{Z} \sum_{S_1} \sum_{S_2} \exp\left[\beta\left(H(S_1 + S_2) + K(S_1 \cdot S_2)\right)\right] \\
&= \frac{1}{Z} \left[\sum_{S_1} \exp\left(H(S_1 + 1) + J(S_1 \cdot 1)\right) + \exp\left(H(S_1 - 1) + J(S_1 \cdot 1)\right)\right] \\
&= \frac{1}{Z} \left[\sum_{S_1} \exp\left(\beta(H(2) + J(1))\right) + \exp\left(\beta(H(-2) + J(1))\right) + 2e^{\beta J}\right] \\
&= \frac{e^{\beta J}}{Z} \left[e^{2\beta H} + 2 + e^{-2\beta H}\right] \\
&= \frac{e^{\beta J}(2 + 2\cosh(2\beta H)))}{e^{\beta J}\left[2 + 2\cosh(2\beta H)\right]} = 1.
\end{aligned}$$

8)

Show that, if we change the Hamiltonian of the system so that:

$$-\mathcal{H} = H_1 S_1 + H_2 S_2 + J S_1 S_2,$$

the connected correlation function can be written as the second derivative of the free energy.

Answer: We first define the partition function:

$$Z = \sum_i e^{-\beta \mathcal{H}_i}.$$

The free energy is then given by:

$$\mathcal{F} = -k_b T \ln(Z).$$

The correlation function, $G(S_1, S_2)$ can be written in the following manner:

$$G(S_1, S_2) = \frac{1}{Z} \sum_{S_1} \sum_{S_2} S_1 S_2 e^{-\beta \mathcal{H}} - \langle S_1 \rangle \langle S_2 \rangle. \tag{1}$$

We compute the two partial derivatives of $\mathcal{F}$ with respect to H_1 and H_2:

$$\begin{aligned}
\frac{\partial^2 \mathcal{F}}{\partial H_1 \partial H_2} &= \frac{k_b T}{Z} \frac{\partial^2 Z}{\partial H_1 \partial H_2} \\
&= \frac{k_b T}{Z} \left(\beta^2 \sum_{S_1} \sum_{S_2} S_1 S_2 e^{\beta(H_1 S_1 + H_2 S_2 + J S_1 S_2)}\right) \\
&= \frac{\beta}{Z} \left(\sum_{S_1} \sum S_2 e^{\beta \mathcal{H}_i}\right)
\end{aligned} \tag{2}$$

Comparing (1) and (2) we see that:

$$G(S_1, S_2) = \frac{1}{\beta} \frac{\partial^2 \mathcal{F}}{\partial H_1 \partial H_2} - \langle S_1 \rangle \langle S_2 \rangle.$$

And thus one has proved that the connected correlation function can be written as the second derivative of the free energy.