FK7058: Handin2

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Date: February 2, 2024

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 $S_2 = 1$, $-\mathcal{H} = 2H + J$.
2. $S_1 = 1$ and $S_2 = -1$, $-\mathcal{H} = -J$.
3. $S_1 = -1$ and $S_2 = 1$, $-\mathcal{H} = -J$.
4. $S_1 = -1$ and $S_2 = -1$, $-\mathcal{H} = -2H + J$.

The probability of the states is given by the following:

$$\begin{aligned}
P(S_1, S_2) &= \frac{e^{-\beta E_i}}{Z}, \\
P(1,1) &= \frac{e^{\beta(2H+J)}}{Z}, \\
P(1,-1) &= \frac{e^{\beta(-J)}}{Z}, \\
P(-1,1) &= \frac{e^{\beta(-J)}}{Z}, \\
P(-1,-1) &= \frac{e^{\beta(-2H+J)}}{Z}.
\end{aligned}$$

2)

Calculate the partition function.

Answer: The partition function is given as:

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

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:

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

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:

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

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: The magnetization per unit spin M is defined as:

$$
M = \frac{1}{N}\sum_{i=1}^{N}\langle S_i\rangle = \frac{\langle S_1\rangle + \langle S_2\rangle}{2}
$$

We can now write, that in general, the magnetization per unit spin is given by:

$$
\begin{aligned}
M &= -\frac{1}{N}\frac{\partial \mathcal{F}}{\partial H} \\
&= -\frac{1}{2}\frac{\partial \mathcal{F}}{\partial H}.
\end{aligned}
$$

Thus, one has that the magnetization per unit spin is related to the free energy of the system, and to the average sin of the system. One computes the derivative of the free energy with respect to H:

$$\begin{aligned}
M &= -\frac{1}{2}\frac{\partial F}{\partial H} = -\frac{1}{2}\frac{\partial}{\partial H}\left(-k_b T \ln(Z)\right) \\
&= \frac{k_b T}{2}\frac{\partial}{\partial H}\left[\ln\left(e^{\beta J}\left[2e^{-2\beta J} + 2\cosh(2\beta H)\right]\right)\right] \\
&= \frac{k_b T}{2}\frac{\partial}{\partial H}\left(\ln\left[2e^{-2\beta J} + 2\cosh(2\beta H)\right]\right) \\
&= \frac{1}{2}\frac{2\sinh(2\beta H)}{e^{-J\beta} + 2\cosh(2\beta H)}.
\end{aligned}$$

When $H = 0$ one has that the magnetization per unit spin is given by:

$$M(H=0) = \frac{1}{2}\frac{2\cdot 0}{e^{-J\beta} + 2} = 0.$$

6)

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

Answer: We can rewrite the limit as $\beta \to \infty$, which gives the following:

$$\begin{aligned}
\lim_{\beta\to\infty} M &= \lim_{\beta\to\infty}\left(\frac{1}{2}\frac{2\sinh(2\beta H)}{e^{-J\beta} + 2\cosh(2\beta H)}\right) \\
&= \lim_{\beta\to\infty}\left(\frac{\sinh(2\beta H)}{\cosh(2\beta H)}\right) = \lim_{\beta\to\infty}\left(\tanh(2\beta H)\right) = \mp 1,
\end{aligned}$$

The magnetization per unit spin M is then given by ∓ 1 in the limit $T \to 0$, depending on the sign of H.

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:

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

Thus $\langle S_1 \rangle = \langle S_2 \rangle$. We now compute $\langle S_1 \cdot S_2 \rangle$:

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

Thus, the connected correlation function is given by:

$$
\begin{aligned}
G(S_1, S_2) &= \langle S_1 \cdot S_2 \rangle - \langle S_1 \rangle \langle S_2 \rangle \\
&= \frac{2\cosh(2\beta H) - 2e^{-2\beta J}}{2e^{-2\beta J} + 2\cosh(2\beta H)} - \left(\frac{\sinh(2H\beta)}{\left[2e^{-2\beta J} + 2\cosh(2\beta H)\right]}\right)^2 \\
&= \frac{\left(2\cosh(2\beta H) - 2e^{-2\beta J}\right) \cdot (2e^{-2\beta J} + 2\cosh(2\beta H))}{(2e^{-2\beta J} + 2\cosh(2\beta H))^2} - \left(\frac{\sinh(2H\beta)}{\left[2e^{-2\beta J} + 2\cosh(2\beta H)\right]}\right)^2 \\
&= \frac{4\cosh^2(2H\beta) - 4e^{-4\beta J} - \sinh^2(2H\beta)}{(2e^{-2\beta J} + 2\cosh(2\beta H))^2} \\
&= \frac{4 - 4e^{-4\beta J}}{(2e^{-2\beta J} + 2\cosh(2\beta H))^2} \\
&= \frac{1 - e^{-4\beta J}}{\left(e^{-2\beta J} + 2\cosh(2\beta H)\right)^2}.
\end{aligned}
$$

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:

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

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.