

PROBLEM SET 3

1. a. From $P \propto e^{-\beta E}$, we get that

$$\frac{P_1}{P_0} = e^{-\beta \hbar \omega}$$

- b. First we calculate the partition function only counting the first two states

$$Z = e^{-\beta \frac{1}{2} \hbar \omega} + e^{-\beta \frac{3}{2} \hbar \omega} = e^{-\beta \hbar \omega} 2 \cosh\left(\frac{1}{2} \beta \hbar \omega\right)$$

$$\log Z = -\beta \hbar \omega + \log 2 + \log \cosh\left(\frac{1}{2} \beta \hbar \omega\right)$$

$$\begin{aligned} \langle E \rangle &= -\frac{\partial}{\partial \beta} \log Z \\ &= \hbar \omega + \frac{1}{\cosh(\beta \hbar \omega / 2)} \frac{\partial}{\partial \beta} \cosh\left(\frac{1}{2} \beta \hbar \omega\right) \\ &= \hbar \omega - \frac{1}{2} \hbar \omega \tanh\left(\frac{1}{2} \beta \hbar \omega\right) \\ &= \hbar \omega \left(1 - \frac{1}{2} \tanh\left(\frac{\hbar \omega}{2 k_B T}\right)\right) \end{aligned}$$

2. a. Because the spinners are independent the partition function factors into a product partition functions of single spinners.

$$Z = Z_1^N = (e^{-\beta\mu B} + e^{\beta\mu B})^N$$

$$\log Z = N \log(2 \cosh(\beta\mu B))$$

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log Z = -N\mu B \tanh(\beta\mu B)$$

Because $\langle E \rangle = -MB$ where M is the expectation value of the magnetization

$$M = N\mu \tanh(\beta\mu B) = N\mu \tanh\left(\frac{\mu B}{\tau}\right)$$

$$\chi \equiv \frac{dM}{dB} = \frac{N\mu^2\beta}{\cosh^2\left(\frac{\mu B}{\tau}\right)} = 4N\mu^2\beta (e^{-\mu\beta B} + e^{\mu\beta B})^{-2}$$

$$\chi = \frac{4N\mu^2/\tau}{(e^{-\mu B/\tau} + e^{\mu B/\tau})^2}$$

- b. When $\tau \ll \mu B$ the second term in parentheses dominates,

$$\lim_{\mu B/\tau \rightarrow \infty} \chi = 4N\mu^2\beta (e^{-2\mu\beta B})$$

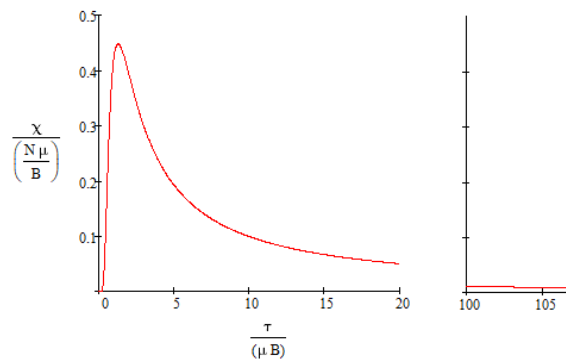
which goes to zero because the exponential term outruns the linear term.

When $\tau \gg \mu B$ we can Taylor expand the exponentials,

$$\chi = \frac{4N\mu^2/\tau}{(1 - \mu B/\tau + \dots + 1 + \mu B/\tau + \dots)^2}$$

$$\lim_{\mu B/\tau \rightarrow 0} \chi = 4N\mu^2\beta (2)^{-2} = N\mu^2\beta$$

- c. For the plot I will nondimensionalize τ by μB and χ by $N\mu/B$



3. (K&K 3.4) It is usually easier to work with β rather than τ .

$$\left(\frac{\partial U}{\partial \tau}\right)_V = \frac{\partial \beta}{\partial \tau} \frac{\partial U}{\partial \beta} = -\beta^2 \frac{\partial}{\partial \beta} \left(-\frac{\partial}{\partial \beta} \log Z\right) = \beta^2 \frac{\partial^2}{\partial \beta^2} \log Z$$

On the other hand,

$$\langle (E - \langle E \rangle)^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2 = \frac{1}{Z} \frac{\partial^2}{\partial \beta^2} Z - \left(\frac{1}{Z} \frac{\partial Z}{\partial \beta}\right)^2 = \frac{\partial}{\partial \beta} \left(\frac{1}{Z} \frac{\partial Z}{\partial \beta}\right) = \frac{\partial^2}{\partial \beta^2} \log Z$$

So we see that

$$\langle (E - \langle E \rangle)^2 \rangle = \tau^2 \left(\frac{\partial U}{\partial \tau}\right)_V$$

4. (K&K 3.5) The Boltzmann factor is ratio of probabilities of two microstates of the system. Let's denote these states as S with energy ϵ and S' with energy ϵ' .

$$\frac{P(S')}{P(S)} = \frac{g_R(S')}{g_R(S)} = e^{\sigma_R(S') - \sigma_R(S)}$$

First we write the entropy of the reservoir in terms of the energy of the reservoir, ϵ_R .

$$\begin{aligned} \sigma_R(S') - \sigma_R(S) &= \sigma_R(\epsilon'_R) - \sigma_R(\epsilon_R) \\ &\approx \sigma_R(\epsilon_R) + \frac{d\sigma_R}{d\epsilon} (\epsilon'_R - \epsilon_R) - \sigma_R(\epsilon_R) \\ &= \beta (\epsilon'_R - \epsilon_R) \end{aligned}$$

Whenever energy flows into the system a net amount $1 - \alpha$ flows out of the reservoir, that is,

$$\Delta \epsilon_R = (\alpha - 1) \Delta \epsilon$$

therefore

$$\sigma_R(S') - \sigma_R(S) = -\beta (1 - \alpha) \Delta \epsilon$$

$$\frac{P(S')}{P(S)} = e^{-(1-\alpha)\Delta\epsilon\beta}$$

Therefore $P(S')$ is proportional to $e^{-(1-\alpha)\epsilon\beta}$, where the proportionality constant depends on the baseline state we are comparing it to, in this case $P(S)$. Regardless, this constant is taken care of by the partition function.

5. (K&K 3.7)

- a. The energy of state s , where links 1 through s are open, is $s\varepsilon$. Therefore the partition function is

$$Z = \sum_{s=0}^N e^{-\beta s\varepsilon}$$

which is just a geometric sum where $r = e^{-\beta\varepsilon}$, so

$$Z = \frac{1 - r^{N+1}}{1 - r} = \frac{1 - e^{-\beta(N+1)\varepsilon}}{1 - e^{-\beta\varepsilon}}$$

b.

$$\begin{aligned} \langle s \rangle &= \frac{1}{Z} \sum_{s=0}^N s e^{-\beta s\varepsilon} = \frac{1}{Z} \left(-\frac{1}{\varepsilon} \right) \frac{\partial Z}{\partial \beta} \\ &= \frac{-1}{Z\varepsilon} \left(\frac{e^{-\beta\varepsilon(N+1)}\varepsilon(N+1)}{1 - e^{-\beta\varepsilon}} + \frac{(1 - e^{-\beta\varepsilon(N+1)})(-\varepsilon)(e^{-\varepsilon\beta})}{(1 - e^{-\beta\varepsilon})^2} \right) \\ &= \left(\frac{1}{1 - e^{-\beta(N+1)\varepsilon}} \right) \left(-e^{-\beta\varepsilon(N+1)}(N+1) + \frac{(1 - e^{-\beta\varepsilon(N+1)})(e^{-\varepsilon\beta})}{(1 - e^{-\beta\varepsilon})} \right) \end{aligned}$$

When $\beta\varepsilon \gg 1$,

$$\langle s \rangle \approx \frac{e^{-\varepsilon\beta}}{1 - e^{-\beta\varepsilon}} = \frac{1}{e^{\beta\varepsilon} - 1} \approx e^{-\beta\varepsilon}$$

6. (K&K 3.9) Let's say we have a combined state s , where the first system is in state a and the second system is in state b . Since they are independent, $P(s) = P(a)P(b)$, and therefore $Z(1+2) = \sum_s P(a)P(b)$. In addition, every possible combination of a and b is possible (once again because they are independent). Therefore summing over s is equivalent to summing over a and over b separately, so $Z(1+2) = \sum_a P(a) \sum_b P(b) = Z(1)Z(2)$.

7. (K&K 3.3)

- a. First we need to calculate the partition function, and then we can calculate the free energy.

$$Z = \sum_{s=0}^{s=\infty} e^{-s\hbar\omega\beta} = \frac{1}{1 - e^{-\hbar\omega\beta}}$$

$$F = -\tau \ln Z = -\tau \ln \left[\frac{1}{1 - e^{-\hbar\omega\beta}} \right] = \tau \ln [1 - e^{-\hbar\omega\beta}]$$

- b.

$$\begin{aligned} \sigma &= -\frac{\partial F}{\partial \tau} = -\ln(1 - e^{-\hbar\omega\beta}) - \frac{\tau}{1 - e^{-\hbar\omega\beta}} (-e^{-\hbar\omega\beta})(-\hbar\omega)(-\tau^{-2}) \\ &= \frac{(e^{-\hbar\omega\beta})(\hbar\omega\beta)}{1 - e^{-\hbar\omega\beta}} - \ln(1 - e^{-\hbar\omega\beta}) \\ &= \frac{\hbar\omega\beta}{e^{\hbar\omega\beta} - 1} - \ln(1 - e^{-\hbar\omega\beta}) \end{aligned}$$