PHY 410 - Homework 3 solutions

1. K+K Ch. 3, #9 Show $Z(1+2) = Z(1)\,Z(2)$ for independent systems 1 + 2.

$$\left.\begin{aligned} Z(1) &= \sum_{s_1} e^{-\varepsilon_{s1}/\tau} \\ Z(2) &= \sum_{s_2} e^{-\varepsilon_{s2}/\tau} \end{aligned}\right\} \quad Z(1+2) = \sum_{s} e^{-\varepsilon_s/\tau}$$

Since the 2 systems are independent, the sum over s is a double sum over s_1 and s_2, and

$$\varepsilon_s = \varepsilon_{s1} + \varepsilon_{s2}$$

So $$Z(1+2) = \sum_{s_1}\sum_{s_2} e^{-(\varepsilon_{s1}+\varepsilon_{s2})/\tau}$$

$$= \left(\sum_{s_1} e^{-\varepsilon_{s1}/\tau}\right)\left(\sum_{s_2} e^{-\varepsilon_{s2}/\tau}\right)$$

$$Z(1+2) = Z(1)\,Z(2) \quad \checkmark$$

2. K+K. Ch 3, #1 2-state system: $\overline{}\ \varepsilon$ / $\overline{}\ 0$

a) $$Z = \sum_s e^{-\varepsilon_s/\tau} = 1 + e^{-\varepsilon/\tau}$$

$$F = -\tau \ln Z = \underline{\underline{-\tau \ln\left(1 + e^{-\varepsilon/\tau}\right)}}$$

b) $$\sigma = -\left(\frac{\partial F}{\partial \tau}\right)_{V,N} = \frac{\tau}{1+e^{-\varepsilon/\tau}} e^{-\varepsilon/\tau} \frac{\varepsilon}{\tau^2} + \ln\left(1+e^{-\varepsilon/\tau}\right)$$

$$\underline{\underline{\sigma = \frac{\varepsilon/\tau}{1+e^{\varepsilon/\tau}} + \ln\left(1+e^{-\varepsilon/\tau}\right)}}$$

$$F = U - \tau\sigma \Rightarrow U = F + \tau\sigma$$

$$U = \cancel{-\tau \ln\left(1+e^{-\varepsilon/\tau}\right)} + \frac{\varepsilon}{1+e^{\varepsilon/\tau}} + \cancel{\tau \ln\left(1+e^{-\varepsilon/\tau}\right)}$$

$$\underline{\underline{U = \frac{\varepsilon}{1+e^{\varepsilon/\tau}}}}$$

You could also calculate U directly from $U = \tau^2 \frac{\partial \ln Z}{\partial \tau}$ without using F. Or here is an even easier method:

$$U = \langle \varepsilon \rangle = \sum_s \varepsilon_s P_s = \frac{0 + \varepsilon e^{-\varepsilon/\tau}}{1+e^{-\varepsilon/\tau}} = \frac{\varepsilon}{1+e^{\varepsilon/\tau}} \quad \checkmark$$

3. K + K. Ch 3, # 3 Free energy of a harmonic oscillator

a)
$$Z = \sum_s e^{-\varepsilon_s/\tau} = \sum_{s=0}^{\infty} e^{-s\hbar\omega/\tau}$$

neglect zero-point energy, so $\varepsilon_s = s\hbar\omega$

$$Z = \sum_{s=0}^{\infty}\left(e^{-\hbar\omega/\tau}\right)^s = \frac{1}{1-e^{-\hbar\omega/\tau}}$$

geometric series

b)
$$F = -\tau \ln Z = \tau \ln\left(1-e^{-\hbar\omega/\tau}\right)$$

$$U = \tau^2 \frac{\partial \ln Z}{\partial \tau} = -\tau^2 \frac{\partial}{\partial \tau} \ln\left(1-e^{-\hbar\omega/\tau}\right)$$

$$= -\tau^2 \frac{-e^{-\hbar\omega/\tau}}{1-e^{-\hbar\omega/\tau}} \cdot \frac{\hbar\omega}{\tau^2} = \frac{\hbar\omega}{e^{\hbar\omega/\tau}-1}$$

c) $\sigma = \dfrac{-\partial F}{\partial \tau}$ or $F = U - \tau\sigma \Rightarrow \sigma = \dfrac{U-F}{\tau}$

$$\sigma = \frac{1}{\tau}\left[\frac{\hbar\omega}{e^{\hbar\omega/\tau}-1} - \tau \ln\left(1-e^{-\hbar\omega/\tau}\right)\right]$$

$$\sigma = \frac{\hbar\omega}{\tau}\frac{1}{e^{\hbar\omega/\tau}-1} - \ln\left(1-e^{-\hbar\omega/\tau}\right)$$

d) In problem 3 of the previous homework set, we found

$$U_N = \frac{N\hbar\omega}{e^{\hbar\omega/\tau} - 1} \qquad \text{for } N \text{ harmonic oscillators}$$

U_N is indeed N times the result we found here.

On the previous homework we also found:

$$\sigma_N(U) = N \ln\left(1 + \frac{U_N}{N\hbar\omega}\right) + \frac{U_N}{\hbar\omega} \ln\left(1 + \frac{N\hbar\omega}{U_N}\right)$$

Substitute $U_N = \frac{N\hbar\omega}{e^{\hbar\omega/\tau} - 1}$ so $\frac{U_N}{N\hbar\omega} = \frac{1}{e^{\hbar\omega/\tau} - 1}$

$$\sigma_N(N,\tau) = N \ln\left(1 + \frac{1}{e^{\hbar\omega/\tau} - 1}\right) + \frac{N}{e^{\hbar\omega/\tau} - 1} \ln\left(1 + e^{\hbar\omega/\tau} - 1\right)$$

$$= N \ln\left(\frac{e^{\hbar\omega/\tau}}{e^{\hbar\omega/\tau} - 1}\right) + \frac{N}{e^{\hbar\omega/\tau} - 1} \ln\left(e^{\hbar\omega/\tau}\right)$$

$$= -N \ln\left(1 - e^{-\hbar\omega/\tau}\right) + \frac{N\hbar\omega}{\tau} \frac{1}{e^{\hbar\omega/\tau} - 1}$$

This is indeed N times the result we found in part (c) on the previous page.

$\Rightarrow$ Conclusion: Calculations in the Microcanonical Ensemble and the Canonical Ensemble give the <u>same answers</u> for $U(\tau)$, $\sigma(\tau)$.

4. K + K Ch 3, #2 Magnetic Susceptibility of N spins

a) For a single spin: $\varepsilon_s = -2mBs$ with $s = \pm\frac{1}{2}$

$$Z_1 = \sum_s e^{-\varepsilon_s/\tau} = e^{mB/\tau} + e^{-mB/\tau} = \underline{\underline{2\cosh\frac{mB}{\tau}}}$$

For N spins, $Z_N = (Z_1)^N = \underline{\underline{2^N\left(\cosh\frac{mB}{\tau}\right)^N}}$

$$\ln Z_N = N\ln 2 + N\ln\left(\cosh\frac{mB}{\tau}\right)$$

b) The magnetization per unit volume is defined in Eqn. (46) in Ch. 3: $M = \frac{\langle 2s\rangle m}{V}$

Method A:

use trick from class: $$\langle 2s\rangle = \frac{\sum_s (2s)\, e^{2mBs/\tau}}{Z} = \frac{-\frac{\tau^2}{mB}\frac{\partial}{\partial\tau}\sum_s e^{2mBs/\tau}}{Z}$$

$$= -\frac{\tau^2}{mB}\frac{1}{Z}\frac{\partial Z}{\partial\tau} = -\frac{\tau^2}{mB}\cdot\frac{\partial\ln Z}{\partial\tau}$$

$$= -\frac{\tau^2}{mB}N\frac{\sinh\frac{mB}{\tau}}{\cosh\frac{mB}{\tau}}\cdot\left(\frac{-mB}{\tau^2}\right) = N\tanh\frac{mB}{\tau}$$

$$M = \frac{\langle 2s\rangle m}{V} = \frac{Nm}{V}\tanh\frac{mB}{\tau} = \underline{\underline{nm\tanh\frac{mB}{\tau}}}$$

Method B: Since $\varepsilon_s = -2s\,m B$, $U = \langle \varepsilon \rangle = -\langle 2s \rangle m B$ we can re-write M as $M = \frac{\langle 2s \rangle m}{V} = \frac{-U}{BV}$

Then use the result we derived in class:

$$U = \tau^2 \frac{\partial \ln Z_N}{\partial \tau} = \tau^2 N \tanh \frac{mB}{\tau}\left(\frac{-mB}{\tau^2}\right)$$

$$= -m B N \tanh \frac{mB}{\tau}$$

$$M = \frac{-U}{BV} = \frac{mN}{V} \tanh \frac{mB}{\tau} = \underbrace{n m \tanh \frac{mB}{\tau}}_{} \qquad n \equiv N/V$$

c) $$\chi = \frac{dM}{dB} = n m \operatorname{sech}^2\left(\frac{mB}{\tau}\right) \cdot \frac{m}{\tau} = \frac{n m^2}{\tau} \frac{1}{\cosh^2 \frac{mB}{\tau}}$$

At high temperature, $\cosh \frac{mB}{\tau} \to 1$

so $\chi(\tau \to \infty) = \frac{n m^2}{\tau}$

d) On problem 2 of the previous homework set, we found $M = \frac{N m^2 B}{\tau}$, so $\chi = \frac{dM}{dB} = \frac{N m^2}{\tau}$

That agrees with our result in part (c) if we divide by volume.

5. K + K Ch 3, # 4 Energy fluctuations

Show that $\langle (\Delta\varepsilon)^2 \rangle = \tau^2 \left(\frac{\partial U}{\partial \tau}\right)_V$

L.H.S. $\langle (\Delta\varepsilon)^2 \rangle = \langle (\varepsilon - \langle\varepsilon\rangle)^2 \rangle = \langle \varepsilon^2 \rangle - 2\langle\varepsilon\rangle^2 + \langle\varepsilon\rangle^2$

$= \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2$ we showed this in class

R.H.S. $U = \dfrac{\sum_s \varepsilon_s e^{-\varepsilon_s/\tau}}{Z} \equiv \langle \varepsilon \rangle$

quotient rule:

$$\frac{\partial U}{\partial \tau} = \frac{1}{Z} \cdot \sum_s \varepsilon_s e^{-\varepsilon_s/\tau}\left(\frac{\varepsilon_s}{\tau^2}\right) - \left(\sum_s \varepsilon_s e^{-\varepsilon_s/\tau}\right)\frac{1}{Z^2}\frac{\partial Z}{\partial \tau}$$

$$= \frac{1}{Z}\frac{1}{\tau^2}\sum_s \varepsilon_s^2 e^{-\varepsilon_s/\tau} - \langle \varepsilon \rangle \frac{1}{Z}\frac{\partial Z}{\partial \tau}$$

$$= \frac{1}{\tau^2}\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle \frac{1}{Z}\frac{\partial Z}{\partial \tau}$$

But we also know that $U = \tau^2 \dfrac{1}{Z}\dfrac{\partial Z}{\partial \tau} \equiv \langle \varepsilon \rangle$

so $\dfrac{\partial U}{\partial \tau} = \dfrac{1}{\tau^2}\left[\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2\right]$

$$\tau^2 \frac{\partial U}{\partial \tau} = \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2$$

So the L.H.S. and R.H.S. match. ✓