PS 48: Problem 4.28

(a) The energy levels of a single 1D harmonic oscillator is given by

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{1}$$

and the corresponding partition function is

$$\begin{aligned} Z_1 &= \sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)} \\ &= e^{-\frac{1}{2}\beta\hbar\omega} \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega} \\ &= e^{-\frac{1}{2}\beta\hbar\omega} \sum_{n=0}^{\infty} \left(e^{-\beta\hbar\omega}\right)^n \end{aligned}$$

For $x < 1$, we can use the identity

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \tag{2}$$

so that

$$Z_1 = \frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \tag{3}$$

The free energy per particle is given by

$$\begin{aligned} f &= -kT \ln Z_1 && (4) \\ &= -kT \ln\left(\frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right) \\ &= -kT\left[\ln\left(e^{-\frac{1}{2}\beta\hbar\omega}\right) - \ln\left(1 - e^{-\beta\hbar\omega}\right)\right] \\ &= \frac{1}{2}kT\beta\hbar\omega + kT\ln\left(1 - e^{-\beta\hbar\omega}\right) && (5) \end{aligned}$$

We use the fact that $\beta = \frac{1}{kT}$ so that

$$\boxed{f = \frac{1}{2}\hbar\omega + kT\ln\left(1 - e^{-\beta\hbar\omega}\right)} \quad \square \tag{6}$$

The mean energy per particle is given by

$$\begin{aligned} \bar{e} &= -\frac{\partial}{\partial\beta}\ln Z_1 && (7) \\ &= -\frac{\partial}{\partial\beta}\ln\left(\frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\right) \\ &= -\frac{\partial}{\partial\beta}\left[\ln\left(e^{-\frac{1}{2}\beta\hbar\omega}\right) - \ln\left(1 - e^{-\beta\hbar\omega}\right)\right] \\ &= \frac{1}{2}\hbar\omega + \frac{e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}\hbar\omega \\ &= \frac{1}{2}\hbar\omega + \frac{e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} \cdot \frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}}\hbar\omega \end{aligned}$$

$$\boxed{\bar{e} = \hbar\omega\left[\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega} - 1}\right]} \quad \square \tag{8}$$

The entropy per particle is given by

$$\begin{aligned} s &= -\left(\frac{\partial f}{\partial T}\right)_V && (9) \\ &= -\frac{\partial}{\partial T}\left[\frac{1}{2}\hbar\omega + kT\ln\left(1 - e^{-\beta\hbar\omega}\right)\right]_V \\ &= -\frac{\partial}{\partial T}\left[\frac{1}{2}\hbar\omega + kT\ln\left(1 - e^{-\hbar\omega/kT}\right)\right]_V \\ &= \frac{1}{T}\frac{\hbar\omega e^{-\hbar\omega/kT}}{1 - e^{-\hbar\omega/kT}} - k\ln\left(1 - e^{-\hbar\omega/kT}\right) \\ &= k\frac{\beta\hbar\omega e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} - k\ln\left(1 - e^{-\beta\hbar\omega}\right) \\ &= k\frac{\beta\hbar\omega e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} \cdot \frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}} - k\ln\left(1 - e^{-\beta\hbar\omega}\right) \\ &= k\frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} - k\ln\left(1 - e^{-\beta\hbar\omega}\right) \end{aligned}$$

$$\boxed{s = k\left[\frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} - \ln\left(1 - e^{-\beta\hbar\omega}\right)\right]} \quad \square \tag{10}$$

(b) From (8), the mean energy of a system of N harmonic oscillator in equilibrium with a heat bath at temperature T is

$$\boxed{\bar{e} = N\hbar\omega\left[\frac{1}{2} + \frac{1}{e^{\hbar\omega/kT} - 1}\right]} \tag{11}$$

(c) The result for the energy of N harmonic oscillators calculated in the microcanonical ensemble in Problem 4.22 is

$$E(T) = \frac{N\hbar\omega}{2}\left(\frac{e^{\hbar\omega/kT}+1}{e^{\hbar\omega/kT}-1}\right) \tag{12}$$

Massaging the terms,

$$\begin{aligned}
E(T) &= \frac{N\hbar\omega}{2}\left(\frac{e^{\hbar\omega/kT}+1+1-1}{e^{\hbar\omega/kT}}\right) \\
&= \frac{N\hbar\omega}{2}\left(\frac{e^{\hbar\omega/kT}-1}{e^{\hbar\omega/kT}-1} + \frac{2}{e^{\hbar\omega/kT}-1}\right) \\
&= \frac{N\hbar\omega}{2}\left(1 + \frac{2}{e^{\hbar\omega/kT}-1}\right) \\
&= N\hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega/kT}-1}\right)
\end{aligned}$$

$$\boxed{E(T) = N\hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega}-1}\right)} \tag{13}$$

The two results are the same.