

PS 48: Problem 4.28

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

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

and the corresponding partition function is

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

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

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad (2)$$

so that

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

The free energy per particle is given by

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

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

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

The mean energy per particle is given by

$$\bar{e} = -\frac{\partial}{\partial\beta} \ln Z_1 \quad (7)$$

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

$$= \frac{1}{2}\hbar\omega + \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}\hbar\omega$$

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

The entropy per particle is given by

$$s = -\left(\frac{\partial f}{\partial T} \right)_V \quad (9)$$

$$= -\frac{\partial}{\partial T} \left[\frac{1}{2}\hbar\omega + kT \ln \left(1 - e^{-\beta\hbar\omega} \right) \right]_V$$

$$= -\frac{\partial}{\partial T} \left[\frac{1}{2}\hbar\omega + kT \ln \left(1 - e^{-\hbar\omega/kT} \right) \right]_V$$

$$= \frac{1}{T} \frac{\hbar\omega e^{-\hbar\omega/kT}}{1 - e^{-\hbar\omega/kT}} - k \ln \left(1 - e^{-\hbar\omega/kT} \right)$$

$$= k \frac{\beta\hbar\omega e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} - k \ln \left(1 - e^{-\beta\hbar\omega} \right)$$

$$= k \frac{\beta\hbar\omega e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \cdot \frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}} - k \ln \left(1 - e^{-\beta\hbar\omega} \right)$$

$$= k \frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} - k \ln \left(1 - e^{-\beta\hbar\omega} \right)$$

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

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

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

- (c) The answer differs from the result for the energy of N harmonic oscillators calculated in the microcanonical ensemble in Problem 4.22:

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