PHYS 301: Thermodynamics and Statistical Mechanics
Solutions to Problem Set #4

February 11, 2026

Question 1: The Quantum Harmonic Oscillator

(a) Compute the partition function Z

The energy levels of a quantum harmonic oscillator are given by:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \ldots \tag{1}$$

The partition function is defined as:

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta E_n} \tag{2}$$

Substitute the energy levels into the sum:

$$Z = \sum_{n=0}^{\infty} e^{-\beta(n+1/2)\hbar\omega} \tag{3}$$

We can factor out the term corresponding to the zero-point energy, which does not depend on n:

$$Z = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\beta n\hbar\omega} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} (e^{-\beta\hbar\omega})^n \tag{4}$$

Let $x = e^{-\beta\hbar\omega}$. Since $x < 1$ for any positive temperature, we can use the geometric series formula $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$:

$$\boxed{Z = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}} \tag{5}$$

Note: This can be further simplified using the identity $2\sinh(y) = e^y - e^{-y}$. Multiplying the numerator and denominator by $e^{\beta\hbar\omega/2}$ yields $Z = \frac{1}{2\sinh(\beta\hbar\omega/2)}$.

(b) Compute the average energy $\langle E \rangle$

The average energy is defined as:

$$\langle E \rangle = \sum_{n=0}^{\infty} E_n p(n) = \sum_{n=0}^{\infty} E_n \frac{e^{-\beta E_n}}{Z} \tag{6}$$

Substituting our expressions for E_n and Z:

$$\langle E \rangle = \frac{1}{Z} \sum_{n=0}^{\infty} \left(n + \frac{1}{2} \right) \hbar\omega \, e^{-\beta(n+1/2)\hbar\omega} \tag{7}$$

Factor out the constants and the zero-point energy term from the sum:

$$\langle E \rangle = \frac{\hbar\omega \, e^{-\beta\hbar\omega/2}}{Z} \left[\sum_{n=0}^{\infty} n(e^{-\beta\hbar\omega})^n + \frac{1}{2} \sum_{n=0}^{\infty} (e^{-\beta\hbar\omega})^n \right] \tag{8}$$

Recall the standard series results for $x = e^{-\beta\hbar\omega}$:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$$
$$\sum_{n=0}^{\infty} n x^n = x \frac{d}{dx} \left(\sum_{n=0}^{\infty} x^n \right) = \frac{x}{(1-x)^2}$$

Substitute these into our equation, along with $Z = \frac{e^{-\beta\hbar\omega/2}}{1-x}$:

$$\begin{aligned} \langle E \rangle &= \hbar\omega(1-x) \left[\frac{x}{(1-x)^2} + \frac{1}{2(1-x)} \right] \\ &= \hbar\omega \left[\frac{x}{1-x} + \frac{1}{2} \right] \end{aligned}$$

Substitute $x = e^{-\beta\hbar\omega}$ back into the equation:

$$\langle E \rangle = \hbar\omega \left[\frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} + \frac{1}{2} \right] \tag{9}$$

Multiplying the first fraction by $e^{\beta\hbar\omega}/e^{\beta\hbar\omega}$ gives the final expression:

$$\boxed{\langle E \rangle = \hbar\omega \left[\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right]} \tag{10}$$

(c) Compute $-\frac{\partial}{\partial\beta} \ln Z$ and compare

First, take the natural logarithm of the partition function from part (a):

$$\ln Z = \ln \left(\frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \right) = -\frac{\beta\hbar\omega}{2} - \ln(1 - e^{-\beta\hbar\omega}) \tag{11}$$

Now, differentiate with respect to β:

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

Multiply the second term by $e^{\beta\hbar\omega}/e^{\beta\hbar\omega}$ to simplify:

$$\boxed{-\frac{\partial}{\partial\beta}\ln Z = \hbar\omega\left[\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right]} \tag{12}$$

Comparison and Generality: Comparing the result from part (c) with part (b), we see they are exactly identical. This is not a coincidence; it is a completely **general result** for any system in the canonical ensemble.

Relationship between $\langle E\rangle$ and Z: The average energy of a system in thermal equilibrium with a reservoir is always given by the negative derivative of the natural logarithm of the partition function with respect to β:

$$\langle E\rangle = -\frac{\partial \ln Z}{\partial\beta} \tag{13}$$

Proof of generality:

$$-\frac{\partial \ln Z}{\partial\beta} = -\frac{1}{Z}\frac{\partial Z}{\partial\beta} = -\frac{1}{Z}\frac{\partial}{\partial\beta}\sum_n e^{-\beta E_n} = \frac{1}{Z}\sum_n E_n e^{-\beta E_n} = \sum_n E_n p(n) = \langle E\rangle$$