

Consider a system of N classical and distinguishable, harmonic oscillators. Their energy is,

$$E = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i=1}^N \frac{K}{2} |\vec{r}_i - \vec{r}_i^{(0)}|^2$$

where $\vec{r}_i^{(0)}$ is the equilibrium position of the i -th oscillator particle.

1. Calculate the canonical partition function of this system of classical oscillators.
2. Show that this result agrees with the quantum mechanical calculation in the limit of high temperatures. Recall that $\omega = \sqrt{K/m}$

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a) Quantum Mechanical oscillator:

$$Z = \prod_{i=1}^{3N} Z_i \quad \text{as Hamiltonian is separable in } 3N \text{ degrees of freedom.}$$

For each:

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

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

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

b) Classical calculation (distinguishable):

$$Z = \int \frac{d^3 \vec{r} d^3 \vec{p}}{h^{3N}} e^{-\beta E} = \frac{1}{h^{3N}} \left[\int_{-\infty}^{\infty} dp_x e^{-\beta p_x^2 / 2m} \right]^{3N}$$

$$\cdot \left[\int_{-\infty}^{\infty} dx e^{-\beta \frac{k}{2} (x-x_0)^2} \right]^{3N}$$

$$= \frac{1}{h^{3N}} \left(\sqrt{\frac{2m\hbar}{\beta}} \right)^{3N} \left(\sqrt{\frac{2\pi}{\beta k}} \right)^{3N} = \left(\beta \hbar \omega \right)^{-3N} = Z$$

c) In the limit of

$$T \rightarrow \infty, \beta \rightarrow 0$$

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

Rewrite:
$$Z = \left(\frac{1}{e^{\beta \hbar \omega / 2} - e^{-\beta \hbar \omega / 2}} \right)^{3N} = \left(e^{\beta \hbar \omega / 2} - e^{-\beta \hbar \omega / 2} \right)^{-3N}$$

Expand the exponential: $T \rightarrow \infty, \beta \rightarrow 0$

$$Z \approx \left(1 - \cancel{\beta \hbar \omega / 2} - \cancel{\beta \hbar \omega / 2} \right)^{-3N} = (\beta \hbar \omega)^{-3N} \checkmark$$