Consider a set of independent ~~and~~ classical harmonic oscillators, so that the energy levels of each oscillator are discrete and given by:

$$\epsilon_k = \left(k + \frac{1}{2}\right) h\nu \,, \quad k = 0, 1, 2, \dots$$

$h$ is Planck's constant and $\nu$ the frequency of the oscillator.

(a) Show that the ~~partition function~~ single particle partition function $Z_1 = \sum_k e^{-\beta\epsilon_k}$ is given by

$$Z_1 = \frac{e^{-h\nu/2k_BT}}{1 - e^{-h\nu/k_BT}}$$

(b) Define a characteristic temperature $\theta$ through $k_B\theta = h\nu$, and calculate the value of $\theta$ for a ~~r~~frequency in the infrared region of the energy spectrum (say $\nu = 10^{13}$ Hz).

(c) Calculate the ~~fract~~ ~~occ~~ fractional occupation number of the energy levels $\langle n_k\rangle / \langle N\rangle$. Obtain specific values of this ratio for $T = \theta$, and for the four lowest energy levels $k = 0, 1, 2$, and $3$.

(d) Obtain the ~~A~~ internal energy $\langle E\rangle$, and the heat capacity at constant volume. Study the limits of both quantities as $T \ll \theta$ and $T \gg \theta$.

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$$Z_1 = \sum_k e^{-\beta\epsilon_k} = \sum_k e^{-\frac{h\nu}{k_BT}\left(k+\frac{1}{2}\right)} = e^{-\frac{h\nu}{2k_BT}} \underbrace{\sum_k \left(e^{-\frac{h\nu}{k_BT}}\right)^k}_{\text{geometric series}}$$

$$Z_1 = \frac{e^{-h\nu/2k_BT}}{1 - e^{-h\nu/k_BT}}$$

(b) $\theta = \frac{h\nu}{k_B} = \frac{6.62 \cdot 10^{-34} J \cdot s \times 10^{13} s^{-1}}{1.38 \cdot 10^{-23} J/k} \simeq 500\,k$

(c). $\frac{\langle n_k \rangle}{\langle N \rangle} = \frac{e^{-\beta \epsilon_k}}{Z_1} = \frac{1}{Z_1} e^{-\beta (k + \frac{1}{2}) h\nu}$

$\Rightarrow \frac{\langle n_k \rangle}{\langle N \rangle} = \frac{(1 - e^{-h\nu/k_B T})\, e^{-\beta(k + \cancel{\frac{1}{2}}) h\nu}}{\cancel{e^{-h\nu/2k_B T}}} = (1 - e^{-h\nu/k_B T}) e^{-\frac{h\nu}{k_B T} \cdot k}$

For $\theta = T$, $\frac{\langle n_k \rangle}{\langle N \rangle} = 0.632\, e^{-k}$

$\frac{\langle n_0 \rangle}{\langle N \rangle} = 0.632$, $\frac{\langle n_1 \rangle}{\langle N \rangle} = 0.232$, $\frac{\langle n_2 \rangle}{\langle N \rangle} = 0.085$, $\frac{\langle n_3 \rangle}{\langle N \rangle} = 0.032$

(d) . . .

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Classical limit:

$$Z_1 = \frac{e^{-h\nu/2k_B T}}{1 - e^{-h\nu/k_B T}} = \frac{1}{e^{h\nu/2k_B T} - e^{-h\nu/2k_B T}}$$

$T \to \infty$, $\beta \to 0$

$$Z_1 \simeq \frac{1}{1 + \frac{h\nu}{2k_B T} - 1 + \frac{h\nu}{2k_B T}} = \frac{k_B T}{h\nu}$$

(Callen 16.5-5)

Consider a harmonic oscillator such that its energy levels are discrete and given by:

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_0$$

where $\hbar$ is Planck's constant, and $\omega_0$ the angular frequency of the oscillator.

(a) Calculate the probability that the oscillator is in a state of odd quantum number $n = 1, 3, 5 \ldots$ at a temperature $T$. (b) Find the dominant behavior of the probability near $T = 0$ and the high temperature region. Interpret the results.

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Odd states: $m = 1, 3, 5, \ldots$ or $m = 2n+1$, $n = 0, 1, 2, \ldots$

The probability is:

$$P_{odd} = \frac{\sum_{n=0}^{\infty} e^{-\beta\hbar\omega_0\left[\cancel{\frac{1}{2}} + (2n+1)\right]}}{\sum_{n=0}^{\infty} e^{-\beta\hbar\omega_0\left(\cancel{\frac{1}{2}} + n\right)}} = \frac{e^{-\beta\hbar\omega_0}\sum_{n=0}^{\infty}\left(e^{-2\beta\hbar\omega_0}\right)^n}{\sum_{n=0}^{\infty}\left(e^{-\beta\hbar\omega_0}\right)^n}$$

Geometric series sum $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$

$$\boxed{P_{odd} = \frac{e^{-\beta\hbar\omega_0}\left(1 - e^{-\beta\hbar\omega_0}\right)}{1 - e^{-2\beta\hbar\omega_0}}}$$

(b) High $T$: $\frac{\hbar\omega_0}{k_B T} \to 0$

$$P_{odd} \cong \frac{(1 - \beta\hbar\omega_0)(+\beta\hbar\omega_0)}{(+2\beta\hbar\omega_0)} \simeq \frac{1}{2}$$ equally populated

Low $T$: $\frac{\hbar\omega_0}{k_B T} \to \infty$

$$P_{odd} = \frac{e^{-\beta\hbar\omega_0}}{1} \to 0$$ all in ground state. The first odd level is an excited state.