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Phys 242

Assignment #3 / Midterm
(Handwritten part)

① 2D Harmonic oscillator $\rightarrow$ $E = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m\omega^2 (x^2 + y^2)$

(a) Thermal average energy $\mathcal{E}(T)$

$$Z = \int e^{-E(\vec{p},\vec{r})/k_BT} \, d^2p \, d^2r$$
$$= \int e^{\frac{-p_x^2}{2mk_BT}} dP_x \int e^{-p_y^2/2mk_BT} dP_y \int e^{-\frac{m\omega^2 x^2}{2k_BT}} dx \int e^{-\frac{m\omega^2 y^2}{2k_BT}} dy$$
$$= 2\pi m k_BT \cdot \frac{2\pi k_BT}{m\omega^2}$$
$$= \frac{4\pi^2 k_B^2 T^2}{\omega^2} \leftarrow \text{Partition function!}$$

$$* \ \mathcal{E}(T) = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial\beta} \ln\left(\frac{4\pi^2}{\omega^2} \cdot \frac{1}{\beta^2}\right) = \frac{\partial}{\partial\beta} \ln\left(\frac{\omega^2 \beta^2}{4\pi^2}\right) = 2/\beta = 2k_BT$$

$\beta = 1/k_BT$

$\boxed{\mathcal{E}(T) = 2k_BT}$ ← Makes sense... in 1D, $\mathcal{E}(T) = k_BT$, and for 2D we are just doubling the number of degrees of freedom...

② (a) Same, but for quantum electron, so that energies are now discrete $\Rightarrow \int \rightarrow \Sigma$
in 1D

$* E_n = \frac{\hbar\omega}{2}(2n+1)$

$$Z = \sum_{n=0}^{\infty} e^{-E_n/k_BT} = \sum_{n=0}^{\infty} e^{-\frac{\hbar\omega}{2k_BT}(2n+1)}$$
$$= \sum_{n=0}^{\infty} e^{-\frac{\hbar\omega}{2k_BT}} \cdot e^{-\frac{\hbar\omega n}{k_BT}}$$

$* \text{Geometric sum } \sum_{k=0}^{\infty} a \cdot r^k = \frac{a}{1-r}$

$$= \frac{e^{-\hbar\omega/2k_BT}}{1 - e^{-\hbar\omega/k_BT}} \leftarrow \text{Partition function}$$

$$\mathcal{E}(T) = -\frac{\partial}{\partial\beta} \ln\left(\frac{e^{-\frac{\hbar\omega}{2}\beta}}{1 - e^{-\hbar\omega\beta}}\right) = -\left[\frac{\frac{(1-e^{-\hbar\omega\beta})\cdot(-\frac{\hbar\omega}{2} e^{-\frac{\hbar\omega}{2}\beta}) - e^{-\frac{\hbar\omega}{2}\beta}(\hbar\omega e^{-\hbar\omega\beta})}{(1-e^{-\hbar\omega\beta})^2}}{\frac{e^{-\frac{\hbar\omega}{2}\beta}}{1-e^{-\hbar\omega\beta}}}\right] = \frac{\frac{\hbar\omega}{2}(1-e^{-\hbar\omega\beta}) + \hbar\omega e^{-\hbar\omega\beta}}{1-e^{-\hbar\omega\beta}}$$
$$= \hbar\omega\left[\frac{1}{2} + \frac{e^{-\hbar\omega/k_BT}}{1-e^{-\hbar\omega/k_BT}}\right]$$

$$\Rightarrow \boxed{\mathcal{E}(T) = \hbar\omega\left(\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1} + \frac{1}{2}\right)}$$

← Makes sense because $\langle n \rangle = \sum n e^{-E_n/k_BT} = \frac{1}{e^{\hbar\omega/k_BT}-1}$ (Bose-Einstein distribution)
so we can rewrite this as...
$\mathcal{E}(T) = \frac{\hbar\omega}{2}(2\langle n\rangle + 1)$

(d) Specific heat and classical + quantum limits

$$C_v = \frac{\partial \varepsilon(T)}{\partial T} = \frac{-\hbar\omega \cdot \frac{-\hbar\omega}{k_B T^2}}{\left(e^{\frac{\hbar\omega}{k_B T}}-1\right)^2} = \boxed{k_B\left[\frac{\hbar\omega}{k_B T}\cdot\frac{1}{e^{\hbar\omega/k_B T}-1}\right]^2}$$

Classical limit, $T \to \infty$

$$e^{\hbar\omega/k_B T} \approx 1 + \frac{\hbar\omega}{k_B T} \Rightarrow C_v \approx k_B\left[\frac{\hbar\omega}{k_B T}\cdot\frac{1}{1+\frac{\hbar\omega}{k_B T}-1}\right] \approx \boxed{k_B}$$

checks out with equipartition theorem.

$V = \text{const.}$, so

$E_{int} = Q = N \cdot \frac{f}{2} k_B T = N c_v k_B T$

$\Rightarrow C_v = \frac{f}{2} k_B$, where $f = 2$ in this case...

Quantum limit, $T \to 0$

$$e^{\hbar\omega/k_B T} \gg 1 \rightarrow \boxed{C_v \approx k_B \cdot \left(\frac{\hbar\omega}{k_B T}\right)^2 \cdot e^{-2\hbar\omega/k_B T}}$$