PHYS 630 S'24 Problem Set 8 Solutions

Kardar 6.9

a) $$Z_p = \sum_{\ell \in 2\mathbb{Z}^+} (2\ell+1) e^{-\beta\hbar^2 \ell(\ell+1)/2I}$$

$$= \sum_{n=0}^{\infty} \left(2(2n)+1\right) e^{-\beta\hbar^2 2n(2n+1)/2I}$$

Low-T: $$Z_p = 1 + (2\cdot 2+1) e^{-\beta\hbar^2(2(2+1))/2I} + \cdots$$

$$\boxed{Z_p \approx 1 + 5e^{-3\beta\hbar^2/I}}$$

High-T: $$Z_p = \sum_{n=0}^{\infty} (4n+1) e^{-\beta\hbar^2 n(2n+1)/I}$$

Let $x = \sqrt{\frac{\beta\hbar^2}{I}}\, n$

$$Z_p = \sqrt{\frac{I}{\beta\hbar^2}} \sum_n \left(4x + \sqrt{\frac{\beta\hbar^2}{I}}\right) e^{-x\left(2x + \sqrt{\frac{\beta\hbar^2}{I}}\right)/I}$$

$\frac{\beta\hbar^2}{I} \ll 1$, $\sum_n \to \sqrt{\frac{I}{\beta\hbar^2}}\, dx$

$$\to Z_p \approx \frac{I}{\beta\hbar^2} \int_0^{\infty} 4x\, e^{-2x^2}\, dx$$

Let $u = 2x^2$, $$Z_p \approx \frac{I}{\beta\hbar^2} \int_0^{\infty} e^{-u}\, du$$

$$\boxed{Z_p \approx \frac{I}{\beta\hbar^2}}$$

6.9 b)

$$Z_o = 3 \sum_{\ell \in 2\mathbb{Z}^+ - 1} (2\ell+1)\, e^{-\beta\hbar^2 \ell(\ell+1)/2I}$$

triply degenerate spin state

$$= 3 \sum_{n=0}^{\infty} \left(2(2n+1)+1\right) e^{-\beta\hbar^2 (2n+1)(2n+2)/2I}$$

$$= 3 \sum_{n=0}^{\infty} (4n+3)\, e^{-\beta\hbar^2 (2n+1)(n+1)/I}$$

Low-T: $\boxed{Z_0 \approx 9 e^{-\beta\hbar^2/I}}$

n=0 contribution

High-T: $Z_0 = \sum_{n=0}^{\infty} (4n+3)\, e^{-\beta\hbar^2 (2n+1)(n+1)/I}$

let $x = \sqrt{\frac{\beta\hbar^2}{I}}\, n$, $\quad \sum_{n=0}^{\infty} \rightarrow \sqrt{\frac{I}{\beta\hbar^2}} \int_0^{\infty} dx$, $\quad \frac{\beta\hbar^2}{I} \ll 1$

$$\boxed{Z_0 \approx \frac{3I}{\beta\hbar^2} \int_0^{\infty} 4x\, e^{-2x^2} = \frac{3I}{\beta\hbar^2}}$$

c) N_p para., $N_0 = N - N_p$ ortho.

$$Z = \sum_{N_p=0}^{N} \frac{1}{(N-N_p)_0!\, N_p!}\, Z_p^{N_p} Z_0^{N-N_p}$$

$$= \frac{1}{N_0!} (Z_0 + Z_p)^N \quad \text{(binomial expansion)}$$

6.9 d) $\langle E_{rot} \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial}{\partial \beta}\left(N \ln (Z_0 + Z_p)\right)$

low-T: $Z_0 + Z_p \approx 1 + 9e^{-\beta \hbar^2/I}$

$\boxed{\langle E_{rot} \rangle} \approx -\frac{\partial}{\partial \beta}\left(N \cdot 9e^{-\beta\hbar^2/I}\right)$ (using $\ln(1+\epsilon) \approx \epsilon$ for $\epsilon \ll 1$)

$\boxed{= \frac{9N\hbar^2}{I} e^{-\beta\hbar^2/I}}$

High-T: $Z_0 + Z_p \approx \frac{4I}{\beta\hbar^2}$

$\boxed{\langle E_{rot} \rangle} \approx -\frac{\partial}{\partial \beta}\left(N \ln\left(\frac{4I}{\beta\hbar^2}\right)\right)$

$= \frac{N}{\beta}$ $\boxed{= N k_B T}$ — $\frac{1}{2} k_B T$ per rotational degree of freedom

H — H

10. $\mathcal{H} = \sum_{i=1}^{N} \frac{1}{2m} (\vec{p}_i - e\vec{A})^2 + U(\vec{q}_1, \dots, \vec{q}_N)$

where $\vec{B} = \nabla \times \vec{A}$

$$Z(\vec{B}) = \sum_{\mu_s} e^{-\beta \mathcal{H}(\mu_s)}$$

$$= \int \prod_{n=1}^{N} \frac{d^3p_n \, d^3q_n}{h^3} \, e^{-\beta \left[\sum_{i=1}^{N} \frac{1}{2m} (\vec{p}_i - e\vec{A})^2 + U(\vec{q}_1, \dots, \vec{q}_N) \right]}$$

Define $\left.\begin{array}{l} \vec{p}_i{}' = \vec{p}_i - e\vec{A} \\ \vec{q}_i{}' = \vec{q}_i \end{array}\right\}$ Jacobian $\det \left| \frac{\partial(p', q')}{\partial(p, q)} \right| = 1$

$$Z(\vec{B}) = \int \prod_{n=1}^{N} \frac{d^3p'_n \, d^3q'_n}{h^3} \, e^{-\beta \left[\sum_{i=1}^{N} \frac{1}{2m} \vec{p}_i{}'^2 + U(\vec{q}_1{}', \dots, \vec{q}_N{}') \right]}$$

$\Rightarrow \boxed{Z(\vec{B}) = Z(\vec{0})}$, independent of $\vec{B}$.