Physics 6311: Statistical Mechanics - Homework Solutions 7

Problem 1: Three-dimensional rotor

Problem 1:

a) $$\langle S_x \rangle = \int d\theta d\varphi \, P_{\theta\varphi}(\theta,\varphi) \cos\varphi \sin\theta = \frac{1}{4\pi}\int_0^{\pi} d\theta \sin^2\theta \underbrace{\int_0^{2\pi} d\varphi \cos\varphi}_{0} = 0$$

$$\langle S_y \rangle = \int d\theta d\varphi \, P_{\theta\varphi}(\theta,\varphi) \sin\varphi \sin\theta = \frac{1}{4\pi}\int_0^{\pi} d\theta \sin^2\theta \int_0^{2\pi} d\varphi \cos\varphi = 0$$

$$\langle S_z \rangle = \int d\theta d\varphi \, P_{\theta\varphi}(\theta,\varphi) \cos\theta = \frac{1}{2}\int_0^{\pi} d\theta \sin\theta \cos\theta = \frac{1}{2}\int_{-1}^{1} d\eta \, \eta = 0$$

b) $$\langle S_z^2 \rangle = \int d\theta d\varphi \, P_{\theta\varphi}(\theta,\varphi) \cos^2\theta = \frac{1}{2}\int_{-1}^{1} d\eta \, \eta^2 = \frac{1}{3}$$

$$\sigma_{S_z}^2 = \langle S_z^2 \rangle - \langle S_z \rangle^2 = \frac{1}{3}$$

c) $$P_{S_z}(S_z) = \int d\theta d\varphi \, P_{\theta\varphi}(\theta,\varphi) \, \delta(S_z - \cos\theta) = \frac{1}{2}\int_{-1}^{1} d\eta \, \delta(S_z - \eta)$$

$$= \frac{1}{2} \quad \text{for} \quad -1 \le S_z \le 1$$

Problem 2: Schottky peak in two-level system

Set $\epsilon_2 = \epsilon_1 + \epsilon$.

a)

$$\begin{aligned} Q &= e^{-\beta\epsilon_1} + e^{-\beta\epsilon_2} = e^{-\beta\epsilon_1}(1 + e^{-\beta\epsilon}) \\ \langle E \rangle &= -\frac{\partial}{\partial\beta}\ln Q = \epsilon_1 + \frac{\epsilon}{1 + e^{\beta\epsilon}} \end{aligned}$$

b)

$$\begin{aligned} C &= \frac{\partial\langle E\rangle}{\partial T} = \frac{\partial\beta}{\partial T}\frac{\partial\langle E\rangle}{\partial T} \\ &= k_B \frac{(\beta\epsilon)^2 e^{\beta\epsilon}}{(e^{\beta\epsilon}+1)^2} \end{aligned}$$

For $T \to 0$ or $\beta \to \infty$ heat capacity vanishes because denominator is quadratic in large term $e^{\beta\epsilon}$. For $T \to \infty$ or $\beta \to 0$ heat capacity vanishes because of power law prefactor $(\beta\epsilon)^2$.

c) Set $x = \beta\epsilon$.

$$\begin{aligned} \frac{dC}{dx} &= k_b \left[\frac{2xe^x + x^2e^x}{(e^x+1)^2} - \frac{2x^2e^{2x}}{(e^x+1)^3}\right] = 0 \\ 0 &= 2 + x - \frac{2xe^x}{e^x+1} \\ e^x &= \frac{x+2}{x-2} \qquad x_s \approx 2.4 \\ \epsilon/(k_BT_s) &= 2.4 \\ k_BT_s &= 0.417\epsilon \end{aligned}$$

Problem 3: Polymer on a lattice

Problem 2

a) N joints independent of each other

$$Q_N = Q_1^N$$

at each joint, 3 possibilities → ↱ ↳

$$Q_1 = 1 + 2e^{-\beta\varepsilon}$$

$$Q_N = 4\left(1+2e^{-\beta\varepsilon}\right)^N$$

↑ 4 orientations of first segment

$$A = -k_BT \ln Q_N = -k_BTN \ln\left(1+2e^{-\beta\varepsilon}\right) - k_BT\ln 4$$

b) $$E = -\frac{\partial}{\partial\beta}\ln Q_N = -N\frac{\partial}{\partial\beta}\ln\left(1+2e^{-\beta\varepsilon}\right) + O(N^0)$$

$$= \frac{2N\varepsilon e^{-\beta\varepsilon}}{1+2e^{-\beta\varepsilon}} = \frac{2N\varepsilon}{e^{\beta\varepsilon}+2}$$

$$C = \frac{\partial E}{\partial T} = \frac{\partial E}{\partial\beta}\frac{d\beta}{dT} = \frac{2N\varepsilon^2 e^{\beta\varepsilon}}{\left(e^{\beta\varepsilon}+2\right)^2}\;\frac{1}{k_BT^2}$$

$$= 2Nk_B\left(\frac{\varepsilon}{k_BT}\right)^2\frac{e^{\beta\varepsilon}}{\left(e^{\beta\varepsilon}+2\right)^2}$$

c) $$p_{st} = \frac{1}{1+2e^{-\beta\varepsilon}} \qquad N_{st} = Np_{st} = \frac{N}{1+2e^{-\beta\varepsilon}}$$

d) $T\to 0:\; N_{st}\to N \quad , \quad T\to\infty:\; N_{st}\to N/3$

Problem 4: Absorbed atoms

a) $$Q_N = \frac{1}{N!}\int \frac{d^{3N}p\, d^{3N}q}{h^{3N}} \quad e^{-\beta \sum_i \frac{p_i^2}{2m}}$$

$$= \frac{V^N}{N!\,h^{3N}} \left(2\pi m k_B T\right)^{3/2 N}$$

$$A = -k_B T \ln Q_N = -N k_B T\left[\ln \frac{V}{N} + 1 + \ln\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\right]$$

$$\mu_{gas} = \left(\frac{\partial A}{\partial N}\right)_{T,V} = -k_B T\left[\ln \frac{V}{N} + 1 + \ln\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\right] - N k_B T\left(-\frac{1}{N}\right)$$

$$\mu_{gas} = -k_B T\left[\ln \frac{V}{N} + \ln\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\right]$$

b) $$pV = N k_B T \quad \Rightarrow \quad V/N = k_B T/p$$

$$\mu_{gas} = -k_B T\left[\ln \frac{k_B T}{p} + \ln\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}\right]$$

c) $$Q_G = 1 + e^{-\beta(-\varepsilon - \mu_{sl})} = 1 + e^{\beta(\varepsilon + \mu_{sl})}$$

d) $$\langle n \rangle = \frac{e^{\beta(\varepsilon+\mu_{sl})}}{1+e^{\beta(\varepsilon+\mu_{sl})}} = \frac{1}{1+e^{-\beta(\varepsilon+\mu_{sl})}}$$

e) $$\mu_{sl} = \mu_{gas}$$

$$\langle n \rangle = \frac{1}{1 + e^{\ln(k_B T/p) + \ln(2\pi m k_B T/h^2)^{3/2}}\, e^{-\beta\varepsilon}}$$

$$\langle n \rangle = \frac{1}{1 + \frac{k_B T}{p} \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} e^{-\beta \varepsilon}}$$

$$p \to 0 \qquad \Rightarrow \qquad \langle n \rangle \to 0$$

$$p \to \infty \qquad \Rightarrow \qquad \langle n \rangle \to 1$$