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Problem 1

a) $$Z_g = \sum_{N=0}^{\infty} \frac{e^{\beta\mu N}}{N!\, h^{3N}} \cdot I_p \cdot Q_N$$

$$I_p = \int d^3p_1 \cdots d^3p_N \, e^{-\frac{\beta}{2m}\sum_{i=1}^{N} \vec{p}_i^{\,2}}$$

$$= (I)^N$$

$$I = \int d^3p \, e^{-\frac{\beta \vec{p}^{\,2}}{2m}} = I_0^{\,3}$$

$$I_0 = \int_{-\infty}^{\infty} dp_x \, e^{-\frac{\beta}{2m}p_x^2} = \sqrt{\frac{2\pi m}{\beta}}$$

$$Z_g = \sum_{N=0}^{\infty} \frac{e^{\beta\mu N}}{N!\, h^{3N}} \left(\frac{2\pi m}{\beta}\right)^{\frac{3N}{2}} Q_N$$

Introducing $\Lambda = \frac{h}{\sqrt{2\pi m k_B T}} \Rightarrow$

$$Z_g = \sum_{N=0}^{\infty} \frac{e^{\beta\mu N}}{\Lambda^{3N}} \frac{1}{N!} Q_N = \sum_{N=0}^{\infty} \frac{z^N}{N!} Q_N$$

$$\underline{\underline{z = \frac{e^{\beta\mu}}{\Lambda^3}}}$$

b) $Z_g = e^{\beta p V}$

$$\beta p V = \ln Z_g$$

$$\langle N \rangle = \frac{\partial \ln Z_g}{\partial \beta\mu} = z \frac{\partial \ln Z_g}{\partial z} = z \frac{\partial(\beta p V)}{\partial z}$$

$$Z_g = 1 + \underbrace{z Q_1 + \frac{z^2}{2} Q_2 + \cdots}_{\equiv x}$$

$$\beta p V = \ln(1+x) = x - \frac{x^2}{2} + \cdots$$

$$\beta p V = z Q_1 + \frac{z^2}{2} Q_2 - \frac{1}{2} z^2 Q_1^2 + \cdots$$

$$= z Q_1 + \frac{1}{2}(Q_2 - Q_1^2) z^2 + \cdots$$

$$\langle N \rangle = z Q_1 + (Q_2 - Q_1^2) z^2$$

Defining

$$A_1 \equiv Q_1 / V$$

$$A_2 \equiv \frac{1}{2V}(Q_2 - Q_1^2)$$

$$\beta p = A_1 z + A_2 z^2 + \cdots$$

$$\rho = A_1 z + 2 A_2 z^2 + \cdots$$

c) Virial expansion

$$\beta p = \rho + \sum_{l=2} B_l(T)\,\rho^l$$

First term : Ideal classical gas

Second term : Corrections to ideal classical gas equation of state, due to interactions between particles.

$$V_{ext}(\vec{r}_1, \dots \vec{r}_N) = \sum_{i=1}^{N} \phi(\vec{r}_i)$$

$$Q_N = \int d^3r_1 \cdots \int d^3r_N \, e^{-\beta(\varphi(\vec{r}_1) + \cdots \varphi(\vec{r}_N))}$$

$$= \int d^3r_1 \cdots \int d^3r_N \, e^{-\beta\varphi(\vec{r}_1)} \cdots\cdots e^{-\beta\varphi(\vec{r}_N)}$$

$$= \left(\int d^3r \, e^{-\beta\varphi(\vec{r})}\right)^N = Q_1^N$$

$$Z_g = \sum_{N=0}^{\infty} \frac{z^N}{N!} Q_N = \sum_{N=0}^{\infty} \frac{(zQ_1)^N}{N!}$$

$$= e^{zQ_1}$$

$$\underline{\beta p V = z Q_1}$$

$$\langle N \rangle = z \frac{\partial \ln Z_g}{\partial z} = z Q_1$$

$$\beta p V = \langle N \rangle \Rightarrow p V = \langle N \rangle k_B T$$

$$\Rightarrow \underline{\beta p = \rho} \Rightarrow \underline{\underline{B_l(T) = 0 \, ; \, l \geq 2}}$$

All virial coefficients $B_\ell(T)$, $\ell \geq 2$ vanish.

This is so, since $V_p = \sum_i \phi(\bar{r}_i)$ does not include forces between the particles in the gas. This particular V_p only describes external forces acting on the particles.

Problem 2

$$H = -\vec{B} \cdot \sum_i \vec{S_i}$$

$$= -B \sum_i \sigma_i \quad ; \quad \sigma_i \in (-m, \cdots +m)$$

a) $Z = (Z_1)^N$

since the spins are independent

$$Z_1 = \sum_{\sigma=-m}^{m} e^{\beta B \sigma}$$

Introduce $\omega = \beta B$

Using the given formula on the formula sheet, we have

$$Z_1 = \frac{e^{\omega(m+\frac{1}{2})} - e^{-\omega(m+\frac{1}{2})}}{e^{\frac{\omega}{2}} - e^{-\frac{\omega}{2}}}$$

$$= \frac{\sinh(\omega(m+\frac{1}{2}))}{\sinh \frac{\omega}{2}}$$

$$Z = (Z_1)^N$$

b) $\langle H \rangle = \frac{1}{Z} \sum_{\{\sigma_i\}} H e^{-\beta H}$

$$= -\frac{\partial \ln Z}{\partial \beta} = -B \frac{\partial \ln Z}{\partial \beta B}$$

$$M = \frac{1}{Z} \sum_{\{\sigma_i\}} \left(\sum_i \sigma_i\right) e^{\beta B \sum_i \sigma_i}$$

$$= \frac{\partial \ln Z}{\partial \beta B}$$

We see that $\langle H \rangle = -BM$

so it suffices to compute one of these quantities.

$$M = \frac{\partial \ln Z}{\partial \omega} = \frac{N}{Z_1} \frac{\partial Z_1}{\partial \omega}$$

$$= \frac{N}{Z_1} \left\{ \frac{(m+\frac{1}{2}) \cosh(\omega(m+\frac{1}{2}))}{\sinh(\frac{\omega}{2})} - \frac{1}{2} \frac{\cosh(\frac{\omega}{2}) \cdot \sinh(\omega(m+1/2))}{\sinh^2(\frac{\omega}{2})} \right\}$$

$$M = N\left\{\left(m+\tfrac{1}{2}\right)\coth\left(\omega\left(m+\tfrac{1}{2}\right)\right) - \tfrac{1}{2}\coth\left(\tfrac{\omega}{2}\right)\right\}$$

$$\langle H\rangle = -BM$$

$\omega \gg 1$: $\coth\left(\omega\left(m+\tfrac{1}{2}\right)\right) \to 1$

$\coth\left(\tfrac{\omega}{2}\right) \to 1$

$$M = N\left\{m+\tfrac{1}{2}-\tfrac{1}{2}\right\} = Nm$$

Fully spin-polarized system.

$\omega \ll 1$: $\coth x \simeq \frac{1}{x} + \frac{x}{3}$

$$M = N\left\{\left(m+\tfrac{1}{2}\right)\left\{\frac{1}{\omega\left(m+\tfrac{1}{2}\right)} + \frac{\omega\left(m+\tfrac{1}{2}\right)}{3} + \dots\right\} - \frac{1}{2}\left(\frac{1}{\frac{\omega}{2}} + \frac{1}{3}\frac{\omega}{2} + \dots\right)\right\}$$

$$= \frac{N}{3}\omega\left[\left(m+\tfrac{1}{2}\right)^2 - \left(\tfrac{1}{2}\right)^2\right]$$

$$= \frac{N\omega}{3} m(m+1) = \frac{N}{3} m(m+1) \frac{B}{k_B T}$$

Magnetization vanishes at very high T due to thermal fluctuations.

c) $$\chi = \left(\frac{\partial M}{\partial B}\right)_T = \beta \left(\frac{\partial M}{\partial \omega}\right)_T$$

$$= N\beta \left[\left(\frac{1/2}{\sinh(\frac{\omega}{2})} \right)^2 - \left(\frac{(m+1/2)}{\sinh(\omega(m+\frac{1}{2}))} \right)^2 \right]$$

d)

$\omega \gg 1$: First term dominates

$$\underline{\underline{\chi \simeq N\beta e^{-\beta B}}} \xrightarrow{T \to 0} 0$$

At very low T, the system tends to fully ordered state, and there is no further increase in M by increasing B.

$\omega \ll 1$: Do it in two ways

i) Use result for M from b), for $\omega \ll 1$

$$M = \frac{N}{3} m(m+1) \frac{B}{k_B T}$$

$$\chi = \left(\frac{\partial M}{\partial B}\right)_T = \frac{N}{3} m(m+1) \frac{1}{k_B T}$$

ii) Use directly the general expression for χ, which is of the form

$$\chi = N\beta\left[\left(\frac{\alpha}{\sinh\alpha\omega}\right)^2 - \left(\frac{\gamma}{\sinh\gamma\omega}\right)^2\right]$$

$$\alpha = \frac{1}{2}$$

$$\gamma = m + \frac{1}{2}$$

$\omega << 1$: Using $\sinh\alpha\omega \simeq \alpha\omega + \frac{(\alpha\omega)^3}{3!} + \cdots$

$$\left(\frac{\alpha}{\sinh\alpha\omega}\right)^2 \simeq \frac{1}{\omega^2}\left(1 - \frac{2}{3!}\alpha^2\omega^2 + \cdots\right)$$

$$\chi \simeq N\beta\,\frac{1}{\omega^2}\left[1 - \frac{2}{3!}\alpha^2\omega^2 - 1 + \frac{2}{3!}\gamma^2\omega^2\right]$$

$$= N\beta\,\frac{2}{3!}\left(\gamma^2 - \alpha^2\right) = \frac{N\beta}{3}\left[\left(m+\frac{1}{2}\right)^2 - \left(\frac{1}{2}\right)^2\right]$$

$$= \frac{N\beta}{3}\,m(m+1)$$

Spin disorder more and more with increasing temperature, and the increase in magnetization by increasing the B-field therefore is reduced when increasing the temperature.

High-T limit of $Z=(Z_1)^N$:

$$Z_1 = \frac{\sinh\left(\omega\left(m+\frac{1}{2}\right)\right)}{\sinh\left(\frac{\omega}{2}\right)}$$

$\omega \ll 1 \Rightarrow$

$$Z_1 \simeq \frac{\omega\left(m+\frac{1}{2}\right)}{\frac{\omega}{2}} = 2m+1$$

This is just the number of possible spin-states on each lattice site.

$$Z = (2m+1)^N$$

is therefore just the total possible # spin states in the system

(Z is a weighted sum over all states, and when $\beta \to 0$ $(T \to \infty)$ all states have the same weight $=1 \Rightarrow$ $Z = (2m+1)^N$)

Problem 3

a) $$\ln Z_g = -\sum_{\vec{k}} \ln\left(1 - z e^{-\beta \varepsilon_k}\right)$$

$$\langle N \rangle = z \frac{\partial \ln Z_g}{\partial z}$$

$$= \sum_{\vec{k}} \frac{z e^{-\beta \varepsilon_k}}{1 - z e^{-\beta \varepsilon_k}} = \sum_{\vec{k}} \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1}$$

$k = 0$: $\varepsilon_k = 0$

$$\langle N \rangle = \underbrace{\frac{1}{z^{-1} - 1}}_{\equiv N_0} + \sum_{\vec{k} \neq 0} \frac{z e^{-\beta \varepsilon_k}}{1 - z e^{-\beta \varepsilon_k}}$$

$$N_0 = \frac{1}{z^{-1} - 1} \quad ; \quad z = e^{\beta \mu}$$

b) $$N_0 = \frac{1}{\frac{1}{z} - 1} \Rightarrow z = \frac{1}{1 + \frac{1}{N_0}}$$

$N_0 \gg 1$, macroscopic occupation of ground state $\Leftrightarrow$ Bose-Einstein condensation

$$z = e^{\beta \mu} \Rightarrow \mu = k_B T \ln z = -k_B T \ln\left(1 + \frac{1}{N_0}\right)$$

$$\mu \simeq -\frac{k_B T}{N_0} \rightarrow 0^- \quad \Rightarrow: \quad z = 1$$

c) We proceed by computing $\langle N \rangle$ when $T \leq T_c$, i.e. the ground state is macroscopically occupied

$\mu \to 0^-$, $z = 1$ (but keep z for the moment)

$$\langle N \rangle = N_0 + \sum_{\vec{k} \neq 0} z \frac{e^{-\beta \epsilon_k}}{1 - z e^{-\beta \epsilon_k}}$$

$$= N_0 + \underbrace{\sum_{\vec{k} \neq 0} \sum_{l=1}^{\infty} z^l e^{-\beta \epsilon_k l}}_{\equiv N_{>0}}$$

$$N_{>0} = \sum_{l=1}^{\infty} z^l \sum_{\vec{k} \neq 0} e^{-\beta \epsilon_k l}$$

Consider the $\vec{k}$-summation:

$$\sum_{\vec{k} \neq 0} e^{-\beta \epsilon_k l} = \frac{V}{(2\pi)^3} \int d^3k \, e^{-\beta A l |\vec{k}|^{1/2}}$$

$$= \frac{V}{(2\pi)^3} 4\pi \int_0^{\infty} dk \, k^2 e^{-\beta A l k^{1/2}}$$

$$x \equiv \beta A l k^{1/2} \Rightarrow k = \frac{x^2}{(\beta A l)^2}$$

$$dk = \frac{2x\,dx}{(\beta A l)^2}$$

$$\sum_{\vec{k}\neq 0} e^{-\beta \varepsilon_k l}$$

$$= \frac{V}{(2\pi)^3}\, 8\pi\, \frac{1}{(\beta A l)^6} \underbrace{\int_0^\infty dx\, x^5 e^{-x}}_{\equiv \Gamma(6)}$$

$$= \frac{V}{\pi^2} \frac{\Gamma(6)}{(\beta A l)^6}$$

$$\langle N \rangle = N_0 + V \frac{1}{\pi^2} \frac{\Gamma(6)}{(\beta A)^6} \underbrace{\sum_{l=1}^{\infty} \frac{z^l}{l^6}}_{Li_6(z)}$$

$T > T_c$: N_0 not macroscopically large $\Rightarrow$ $z \neq 1$

$T < T_c$: N_0 macroscopically large, $z = 1$

$$Li_6(z=1) = \zeta(6)$$

$\zeta(6)$: Riemann-zeta function

$\underline{T < T_c}$:

$$n = n_0 + \frac{1}{\pi^2}\left(\frac{\Gamma(6)\zeta(6)}{(\beta A)^6}\right)$$

$$\frac{n_0}{n} = 1 - \frac{1}{\pi^2} \frac{1}{n} \frac{\Gamma(6)\zeta(6)}{(\beta A)^6}$$

$T \to T_c^-$: $n_0 \to 0$

$$(\beta A)^6 = \frac{\Gamma(6)\zeta(6)}{\pi^2 n}$$

$$\beta A = \left(\frac{\Gamma(6)\zeta(6)}{\pi^2 n}\right)^{1/6}$$

$$\underline{\underline{k_B T_c = A \left(\frac{\pi^2 n}{\Gamma(6)\zeta(6)}\right)^{1/6}}}$$

$\frac{n_0}{n}$ when $T = \frac{T_c}{2} \Leftrightarrow \beta = 2\beta_c$

$$\frac{n_0}{n} = 1 - \underbrace{\frac{1}{\pi^2}\frac{1}{n}\frac{\Gamma(6)\zeta(6)}{(\beta_c A)^6}}_{=1}\left(\frac{\beta_c}{\beta}\right)^6$$

$$= 1 - \left(\frac{T}{T_c}\right)^6 = 1 - \left(\frac{1}{2}\right)^6 = \underline{\underline{\frac{63}{64} \simeq 0.98}}$$

d)

$$n = n_0 + C\sum_{l=1}^{\infty} \frac{z^l}{l^6} = n_0 + C\, Li_6(z)$$

$$\beta p = C\sum_{l=1}^{\infty} \frac{z^l}{l^7} = C\, Li_7(z)$$

$$C = \frac{1}{\pi^2}\frac{\Gamma(6)}{(\beta A)^6}$$

$T > T_c$: $n_0 = 0$

$$\underline{\frac{\beta p}{n} = \frac{Li_7(z)}{Li_6(z)}}$$

Ideal gas, classical case:

$$\frac{\beta p}{n} = 1$$

From the definition of $Li_s(z)$, it is clear that $\underline{Li_{s'}(z) < Li_s(z); \; s' > s}$

Thus, $\frac{Li_7(z)}{Li_6(z)} < 1$ for all $z > 0$

and hence

$$\left(\frac{\beta p}{n}\right)_{\text{ideal Bose gas}} < \left(\frac{\beta p}{n}\right)_{\text{ideal gas}}$$

$\Rightarrow$ (for given n):

$$\underline{(\beta p)_{\text{ideal Bose gas}} < (\beta p)_{\text{ideal gas}}}$$

$T \to T_c^+$: $z \to 1$

$$Li_s(z=1) = \zeta(s)$$

$\zeta(s)$: Riemann ζ-function

$T = T_c$

$$\frac{(\beta p)_{Bose}}{(\beta p)_{classical}} = \frac{p_{Bose}}{p_{classical}} = \frac{\zeta(7)}{\zeta(6)}$$

$$\simeq \underline{\underline{0.991}}$$