HW #2 solutions

1) $S = -\left(\frac{\partial F}{\partial T}\right)_{NV}$ $\qquad Q = \sum_{E_s} e^{-E_s/kT}$

$$= k \frac{\partial}{\partial T}\left(T \ln Q\right)$$

$$= k \ln Q + \frac{kT}{Q}\frac{\partial Q}{\partial T}$$

$$= k \ln Q + \frac{kT}{Q}\frac{1}{kT^2}\sum E_s e^{-E_s/kT}$$

$$= \frac{k}{Q}\left[Q \ln Q + \frac{1}{kT}\sum E_s e^{-E_s/kT}\right]$$

$$= \frac{k}{Q}\sum_s e^{-E_s/kT}\left[\ln Q + E_s/kT\right]$$

$$= -\frac{k}{Q}\sum_s e^{-E_s/kT}\left[\ln \frac{1}{Q} - E_s/kT\right]$$

$$= -k\sum_s \frac{e^{-E_s/kT}}{Q} \ln \frac{e^{-E_s/kT}}{Q}$$

$$= -k \sum_s \rho_s \ln \rho_s$$

An ideal gas of N particles is confined to a two-dimensional disk of radius R. Each particle is attracted to the center by a force that increases proportional to its distance from the center, so the Hamiltonian is

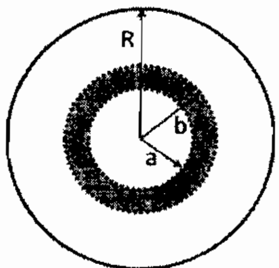
$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} k r_i^2 \right)$$

where k is the effective spring constant of the central force and m is the mass of the particles.

(a) (15 points) Write down the partition function for the full system.

(b) (15 points) Calculate the average energy of the system. pressure & C_v

(c) (15 points) Using the single particle partition function, compute the probability that a given particle is in the shaded region of the figure (greater than a distance a from the center but less than b).



a) $Q_N = \frac{Q_1^N}{N!}$

$$\boxed{= \frac{1}{h^{2N} N!} \left[\int e^{-\frac{p^2}{2m}\beta} e^{-\frac{kr^2}{2}\beta} d^2r\, d^2p \right]^N}$$

b) Evaluate $Q_1 = \frac{1}{h^2} \int e^{-\frac{\beta p^2}{2m}} d^2 p \int e^{-\frac{\beta k r^2}{2}} d^2 r$

$$= \frac{1}{h^2} \frac{2m\pi}{\beta} \underbrace{2\pi}_{\text{angular}} \int_0^R e^{-\beta k R^2/2} R\, dR \qquad x = \frac{\beta k R^2}{2}, \quad dx = \beta k R\, dR$$

$$= \frac{4m\pi^2}{\beta h^2} \int_0^{\beta k R^2/2} e^{-x} \frac{dx}{\beta k}$$

$$= \frac{4m\pi^2}{\beta^2 k h^2} \left[-e^{-\beta k R^2/2} + 1 \right]$$

$$\langle E \rangle = \frac{-\partial \ln Q_N}{\partial \beta} = \frac{-\partial}{\partial \beta} \left[N \ln Q_1 - \cancel{\ln N!} \right] \quad \text{Constant}$$

$$= +\frac{\partial}{\partial \beta} \left[N \ln \frac{\beta^2 k h^2}{4m\pi^2} - N \ln \left(1 - e^{-\beta k R^2/2} \right) \right]$$

$$= \boxed{\frac{2N}{\beta} - N \frac{\frac{kR^2}{2} e^{-\beta k R^2/2}}{1 - e^{-\beta k R^2/2}}}$$

$\xrightarrow{R \to \infty} \frac{2}{\beta} = 2kTN$ (equipartition)

$\xrightarrow{k \to 0} \frac{2N}{\beta} - \frac{\frac{kR^2}{2} N}{1 - (1 - \frac{\beta k R^2}{2})} = \frac{N}{\beta} = kTN$ (equipartition)

Pressure $\quad P = -\frac{\partial F}{\partial V}$ $\quad$ in this case we are in two dimensions so "Volume" is really the area $= \pi R^2$

$$P = -\frac{\partial F}{\partial A} = \frac{\partial R}{\partial A}\frac{\partial F}{\partial R} \qquad A = \pi R^2$$

$$= \frac{-1}{2\pi R}\frac{\partial F}{\partial R} \qquad \frac{\partial A}{\partial R} = 2\pi R$$

$$F = -kT \ln Q_N = -kT \ln \frac{Q_1^N}{N!} = -Nk_BT \ln Q_1 + k_BT N \ln N - k_BT N$$

$$= -Nk_BT \ln \frac{Q_1}{N} - NkT$$

$$= -Nk_BT \ln\left[\frac{4m\pi^2}{N\beta^2 k h^2}\left[1 - e^{-\beta k R^2/2}\right]\right] - NkT$$

$$= -Nk_BT \ln\left[\frac{\pi}{\beta k N \lambda^2}\left(1 - e^{-\beta k R^2/2}\right)\right] - NkT \qquad \lambda = \frac{h}{\sqrt{2m\pi k_BT}}$$

$$\frac{\partial F}{\partial R} = \frac{\beta k R \; e^{-\beta k R^2/2}}{1 - e^{-\beta k R^2/2}}(-Nk_BT)$$

$$P = \frac{-1}{2\pi \cancel{R}}(-N\cancel{k_BT})\frac{\cancel{\beta}k\cancel{R} \quad 1}{e^{\beta k R^2/2} - 1} = \boxed{\frac{Nk}{2\pi\left(e^{\beta k R^2/2} - 1\right)}}$$

limit $k \to 0$ $\qquad P \to \frac{Nk}{2\pi\left(\cancel{1} + \beta k R^2/2 - \cancel{1}\right)}$

so $\quad P(\pi R^2) = Nk_BT$ ✓

$$C_V = \frac{\partial E}{\partial T} = \frac{\partial \beta}{\partial T}\frac{\partial E}{\partial \beta} \qquad \frac{\partial \beta}{\partial T} = \frac{-1}{kT^2}$$

$$= \frac{-1}{kT^2}\left[-\frac{2N}{\beta^2} - \frac{NkR^2}{2}\frac{\partial}{\partial \beta}\left(\frac{1}{e^{\beta k R^2/2} - 1}\right)\right]$$

$$= -\frac{\beta}{T}\left[\frac{-2N}{\beta^2} - \frac{NkR^2}{2}\frac{-(kR^2/2)\,e^{\beta k R^2/2}}{\left(e^{\beta k R^2/2} - 1\right)^2}\right]$$

$$= \frac{\beta}{T}\left[\frac{2N}{\beta^2} - N\left(\frac{kR^2}{2}\right)^2\frac{e^{\beta k R^2/2}}{\left(e^{\beta k R^2/2} - 1\right)^2}\right] \longleftarrow$$

c) $$Q_{ab} = \frac{1}{h^2} \underbrace{\frac{2m\pi}{\beta}}_{\text{momentum integral}} 2\pi \int_a^b e^{-\beta k R^2/2} R\,dR$$

$$\text{Probability} = \frac{Q_{ab}}{Q_1} = \frac{\int_a^b e^{-\beta k R^2/2} R\,dR}{\int_0^R e^{-\beta k R^2/2} R\,dR}$$

$$= \boxed{\frac{e^{-\beta k a^2/2} - e^{-\beta k b^2/2}}{1 - e^{-\beta k R^2/2}}}$$

P 3.15

$$Q_N = \frac{1}{N!} Q_1^N \qquad Q_1 = \frac{1}{h^3}\int e^{-\beta pc}\, d^3p\, d^3q$$

$$= \frac{4\pi V}{h^3}\int e^{-\beta pc}\, p^2 dp$$

$x = \beta pc$

$dx = \beta c\, dp$

$$= \frac{4\pi V}{(\beta hc)^3}\underbrace{\int e^{-x} x^2 dx}$$

$$= \cancel{-x^2 e^{-x}\Big|_0^{\infty}} + 2\underbrace{\int x e^{-x} dx}$$

$u = x^2 \quad v = -e^{-x}$

$du = 2x\,dx \quad dv = e^{-x} dx$

$$\cancel{-xe^{-x}} + \int e^{-x} dx$$

$$= \frac{8\pi V}{(\beta hc)^3}$$

$$\boxed{Q_N = \frac{1}{N!}\left(8\pi V\left(\frac{kT}{hc}\right)^3\right)^N}$$

$$F = -kTN\left[\ln\left(\frac{8\pi V}{N}\left(\frac{kT}{hc}\right)^3\right) + 1\right]$$

$$\boxed{P = -\left(\frac{\partial F}{\partial V}\right) = \frac{NkT}{V}}$$

$$E = -\frac{\partial}{\partial \beta}\ln Q = \frac{\partial}{\partial \beta}\left[3N\ln\beta + \text{constants}\right]$$

$$\boxed{E = 3NkT}$$

$$\boxed{PV = NkT = \frac{E}{3}}$$

$$C_V = \frac{\partial E}{\partial T} = 3Nk \qquad C_p = \frac{\partial(E+PV)}{\partial T} = \frac{\partial}{\partial T}(3NkT + NkT)$$

$$= 4Nk$$

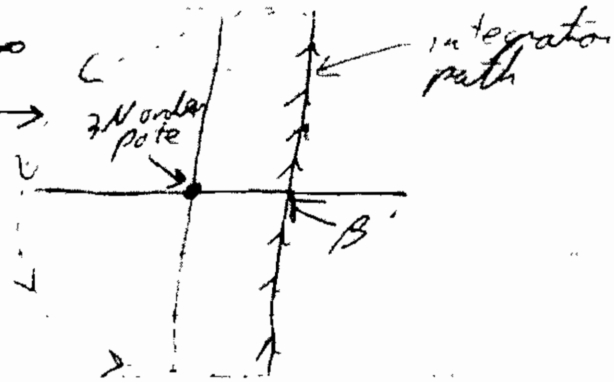
$$\boxed{\gamma = \frac{C_p}{C_V} = \frac{4Nk}{3Nk} = \frac{4}{3}}$$

Pathria 3.15 (cont.)

$$g(E) = \frac{1}{2\pi i}\int_{\beta'-i\infty}^{\beta'+i\infty} e^{\beta E} Q_N(\beta)\,d\beta$$

$$= \frac{1}{2\pi i}\,\frac{1}{N!}\left(\frac{8\pi V}{(hc)^3}\right)^N \int \frac{e^{\beta E}}{\beta^{3N}}\,d\beta$$

Close contour with $R=\infty$ loop in ~~right~~ left half plane →



Loop does not contribute due to factor β^{-3N}
(note: exponential factor is bounded $< e^{\beta' E}$ due to closure on left)

$$\oint e^{\beta E}\beta^{-3N}\,d\beta = 2\pi i \underbrace{\text{Res}(\beta=0)}_{\lim_{\beta\to 0}\frac{1}{(3N-1)!}E^{(3N-1)}e^{\beta E}}$$

$$\boxed{g(E) = \frac{E^{3N-1}}{N!\,(3N-1)!}\left(\frac{8\pi V}{(hc)^3}\right)^N}$$

4) (a) N dipoles $\quad N_+$ with energy ε

N_- with energy $-\varepsilon \qquad N_+ + N_- = N$

$$E = N_+\varepsilon - N_-\varepsilon = (N_+ - N_-)\varepsilon = (2N_+ - N)\varepsilon$$

$$N_+ = \frac{E/\varepsilon + N}{2} \qquad N_- = N - N_+ = \frac{N - E/\varepsilon}{2}$$

# of state

$$\Omega = \binom{N}{N_+} = \frac{N!}{N_+!\,N_-!}$$

$$S/k_B = \ln\Omega$$

$$\cong \underbrace{N\ln N}_{(N_+ + N_-)\ln N} - \cancel{N} - N_+\ln N_+ + \cancel{N_+} - N_-\ln N_- + \cancel{N_-}$$

$$= -N_+\ln\frac{N_+}{N} - N_-\ln\frac{N_-}{N}$$

$$\frac{S}{Nk_B} = -\frac{N_+}{N}\ln\frac{N_+}{N} - \frac{N_-}{N}\ln\frac{N_-}{N}$$

$$\frac{N_+}{N} = \frac{N\varepsilon + E}{2N\varepsilon} \qquad \frac{N_-}{N} = \frac{N\varepsilon - E}{2N\varepsilon}$$

$$\frac{S}{Nk_B} = -\frac{N\varepsilon + E}{2N\varepsilon}\ln\frac{N\varepsilon + E}{2N\varepsilon} - \frac{N\varepsilon - E}{2N\varepsilon}\ln\frac{N\varepsilon - E}{2N\varepsilon}$$

✓

b) Canonical version

$$Q = \sum_E g(E)\, e^{-\beta E}$$

E goes from $-N\varepsilon$ to $N\varepsilon$ in steps of 2ε

or

$$= \sum_{N_+=0}^{N} g(N_+)\, e^{-\beta(N_+\varepsilon - N_-\varepsilon)}$$

$$= \sum_{N_+} g(N_+)\, e^{-\beta(2N_+ - N)\varepsilon}$$

$$g(N_+) = \binom{N}{N_+} = \frac{N!}{N_+!(N-N_+)!}$$

$$= e^{N\beta\varepsilon} \sum_{N_+=0}^{N} \binom{N}{N_+} e^{-\beta 2N_+\varepsilon}$$

← Binomial Series!

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

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

$$= Q_1^{\,N}$$

Homework 3 Solutions

1) a)

$$Q_1 = \sum_{m=-J}^{J} e^{-\beta\mu g H m} = \sum_{-J}^{J} e^{-mx} \qquad x = \beta\mu g H$$

$$= e^{xJ}\sum_{n=0}^{2J} e^{-nx}$$

$$= e^{xJ}\left[\sum_{n=0}^{\infty} e^{-nx} - \sum_{n=2J+1}^{\infty} e^{-nx}\right]$$

$$= e^{xJ}\left[\frac{1}{1-e^{-x}} - e^{-x(2J+1)}\frac{1}{1-e^{-x}}\right]$$

$$= \frac{e^{xJ}}{1-e^{-x}}\left[1-e^{-x(2J+1)}\right] = \frac{e^{xJ}-e^{-xJ-x}}{e^{-x/2}\left(e^{x/2}-e^{-x/2}\right)} = \boxed{\frac{\sinh\left(x(J+\frac{1}{2})\right)}{\sinh\left(\frac{x}{2}\right)}}$$

b)

$$M_z = \frac{\partial \ln Q}{\partial(\beta H)} = \frac{\partial x}{\partial(\beta H)}\frac{\partial}{\partial x}\left[\ln\left\{\sinh\left(x(J+\tfrac{1}{2})\right)\right\} - \ln\left(\sinh\left(\tfrac{x}{2}\right)\right)\right]$$

$$= \mu g\left[(J+\tfrac{1}{2})\coth\left\{x(J+\tfrac{1}{2})\right\} - \tfrac{1}{2}\coth\left(\tfrac{x}{2}\right)\right]$$

c) $J \to \frac{1}{2}$ $\qquad M_z = \mu g\left[\coth(x) - \frac{1}{2}\coth\left(\frac{x}{2}\right)\right]$

$$= \mu g\left[\frac{2\cosh x \sinh\frac{x}{2} - \cosh\frac{x}{2}\sinh x}{2\sinh x\,\sinh\frac{x}{2}}\right]$$

$$= \mu g\left[\frac{2\left(\sinh\frac{x}{2}\cosh^2\left(\frac{x}{2}\right) + \sinh^3\frac{x}{2}\right) - 2\cosh^2\frac{x}{2}\sinh\frac{x}{2}}{2\sinh^2\frac{x}{2}\cosh\frac{x}{2}}\right]$$

$$= \mu g\,\frac{\sinh\frac{x}{2}}{\cosh\frac{x}{2}} = \mu g\tanh(\beta\mu g H)$$

equivalent to lecture if $g=2$

c (cont.)

$J \to \infty \quad (g \to 0)$

$$M_z = \mu g\left[J\coth\left\{x\left(J+\tfrac{1}{2}\right)\right\} + \tfrac{1}{2}\cancel{\mu g}\coth\left\{x\left(J+\tfrac{1}{2}\right)\right\}\right] - \frac{\mu g}{2}\underbrace{\coth\left(\frac{x}{2}\right)}$$

$\coth x \to \frac{1}{x}$ as $x \to 0$

$$= \mu_0 \coth\left\{\beta\mu g H J + \cancel{\tfrac{1}{2}\beta\mu g H}\right\} - \frac{\mu g}{x}$$

$$= \mu_0 \coth(\beta H \mu_0) - \frac{1}{\beta H} \leftarrow \text{classical result}$$

d) $$\lim_{x\to 0} M_z = \mu g\left[\cancel{\left(J+\tfrac{1}{2}\right)}\frac{1}{x\cancel{\left(J+\tfrac{1}{2}\right)}}\left(1+\tfrac{1}{3}x^2\left(J+\tfrac{1}{2}\right)^2\right) - \frac{1}{2}\,\frac{2}{x}\left(1+\tfrac{1}{3}\left(\frac{x}{2}\right)^2\right)\right]$$

$$= \mu g\left[\frac{1}{x}\left(\cancel{1}+\tfrac{1}{3}x^2\left(J+\tfrac{1}{2}\right)^2\right) - \frac{1}{x}\left(\cancel{1}+\left(\frac{x}{2}\right)^2\frac{1}{3}\right)\right]$$

$$= \mu g\,\frac{x}{3}\left(J^2+J\right)$$

Curie constant is : $\frac{(\mu g)^2}{k_B\, 3} J(J+1)$