Homework Ch. 2-4

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2.1

3D gas, N non-interacting atoms, volume V

$$H = \frac{(p_x^2 + p_y^2 + p_z^2)}{2m}$$

partition function $Z = \int dp\,dq\, e^{-\beta H(p,q)}$

$$\bar{E} = -\frac{\partial}{\partial \beta} \ln Z = \frac{\int dp\,dq\, H(p,q)\, e^{-\beta H(p,q)}}{\int dp\,dq\, e^{-\beta H(p,q)}}$$

a.) $Z = \int e^{-\frac{\beta}{2m}(p_x^2 + p_y^2 + p_z^2)}\, dp\,dq$

$$= V^N \int e^{-\frac{\beta}{2m} p^2}\, dp = V^N \left(\frac{2\pi m}{\beta}\right)^{3N/2}$$

$\bar{E} = -\frac{\partial}{\partial \beta}\left[\ln\left[V^N\left(\frac{2\pi m}{\beta}\right)^{3N/2}\right]\right]$

$$E = -\frac{\partial}{\partial\beta}\left\{ \ln\left[V^{N} \left(\frac{2\pi m}{\beta}\right)^{3N/2} \right] \right.$$

$$= -\left\{ -\frac{3N}{2} V^{N} \frac{2\pi m}{\beta} \right\} = \frac{3N\pi m V^{N}}{\beta}$$

b.) $dE = -P\,dV$

$$P = -\frac{dE}{dV} = -\frac{3N\pi m}{\beta}\frac{d}{dV}\left(V^{N}\right)$$

$$= -\frac{3N^{2}\pi m}{\beta} V^{N-1}$$

c.) $PV = nRT$

$$-\frac{3N^{2}\pi m}{\beta} V^{N-1} V = nRT$$

$$-3N^{2}\pi m V^{N} = nRT$$

$$\overline{\qquad\qquad}$$
$$\beta$$

$$R = -\frac{3N^2 \pi m V^N}{\beta n T}$$

d.) $C_V = \left(\frac{\partial E}{\partial T}\right)_V = 3N\pi m V^N k_B T$

$$= 3N\pi m V^N k_B$$

2.2) $H = \frac{p_x^2}{2m} + \frac{1}{2} m \omega_0^2 x^2$

$$Z = \int dp\,dq\, e^{-\beta H(p,q)}$$

$$= \int e^{-\beta\left[\frac{p_x^2}{2m} + \frac{1}{2} m \omega_0^2 x^2\right]} dp_x\, dx$$

p_x x

$$= \int_0 \int_0 \left(1 - \frac{\beta p_x'^2}{2m} - \frac{\beta}{2} m\omega_0^2 x'^2\right) dp_x'\, dx'$$

$$= \int_0^{p_x} \left(x - \frac{\beta p_x'^2}{2m} x - \frac{\beta}{2} m\omega_0^2 \frac{x^3}{3}\right) dp_x'$$

$$= px - \frac{\beta p_x'^3 x}{6m} - \frac{\beta m\omega_0^3 x^4}{24}$$

$$\bar{E} = -\frac{\partial}{\partial\beta}\ln Z = -\frac{\partial}{\partial\beta}\ln\left(px - \frac{\beta p^3 x}{6m} - \frac{\beta m\omega_0^3 x^4}{24}\right)$$

$$= \frac{6m}{\beta p^3 x} + \frac{24}{\beta m\omega_0^3 x^4}$$

b.) $C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{6mk_B}{p^3 x} + \frac{24 k_B}{m\omega_0^3 x^4}$

c.) $P = -\frac{dE}{dV} = \frac{-d}{dV}\left(\frac{6m}{\beta p^3 x} + \frac{24}{\beta m \omega_0^3 x^4}\right)$

$\boxed{\text{assume } x \longrightarrow V}$

$= \frac{-6m}{\beta p^3 V^2} - \frac{6}{\beta m \omega_0^3 V^5}$

$PV = nRT$

$R = \frac{PV}{nT} = \left(\frac{-6mk_BT}{p^3V^2} - \frac{6k_BT}{m\omega_0^3 V^5}\right)\frac{V}{nT}$

$= \frac{-6mk_B}{p^3 V n} - \frac{6k_B}{m\omega_0^3 V^4 n}$

3.1 eqn 2.31

$-\frac{\partial}{\partial\beta}\ln Z = \frac{\int dp\,dq\, H(p,q)\, e^{-\beta H(p,q)}}{\int dp\,dq\, e^{-\beta H(p,q)}} = \bar{E}$

a.)

$$Z = \sum_n e^{-\beta E_n} \qquad E_n = n\hbar\omega$$

$$Z = \sum_n e^{-\beta n \hbar\omega}$$

$$= \sum_n \left(e^{-\beta\hbar\omega}\right)^n = \frac{1}{1-e^{-\beta\hbar\omega}}$$

$$\bar{E} = -\frac{\partial}{\partial\beta}\ln Z = \frac{-\partial}{\partial\beta}\ln\left(\frac{1}{1-e^{-\beta\hbar\omega}}\right)$$

$$= \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}$$

b.) $$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{\partial}{\partial T}\left(\frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}}-1}\right)$$

$$= \hbar\omega\left(\frac{\hbar\omega}{k_B}\right)e^{\frac{\hbar\omega}{k_B T}} \qquad = \frac{(\hbar\omega)^2 e^{\beta\hbar\omega}}{}$$

$$\overline{T^2\left(e^{\frac{\hbar\omega}{k_BT}}-1\right)^2} \qquad \overline{k_BT^2\left(e^{\beta\hbar\omega}-1\right)^2}$$

3.2) $$E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n^2$$

a.) $$Z = \sum_n e^{-\beta E_n} = \sum_n e^{-\beta\frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n^2}$$

$$= \sum_n \underbrace{e^{\left[-\frac{\beta\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2\right]}}_{a}{}^{n^2} = \sum_n a^n \sum_n a^n$$

$$= \left(\frac{1}{1-a}\right)\left(\frac{1}{1-a}\right) = \frac{1}{1+a^2-2a}$$

$$= \frac{1}{1+e^{-\frac{\beta\hbar^2}{m}\left(\frac{\pi}{L}\right)^2} - 2e^{-\frac{\beta\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2}}$$

$$\bar{E} = -\partial \ln Z = -\partial \ln\left[\frac{1}{1 - \beta a \quad - \beta a}\right]$$

$$E = -\frac{\partial}{\partial\beta}\ln Z = -\frac{\partial}{\partial\beta}\ln\left[1+e^{-\beta a} - 2e^{-\frac{\beta a}{2}}\right]$$

$$\boxed{a = \frac{\hbar^2}{m}\left(\frac{\pi}{L}\right)^2}$$

$$= \frac{-a\left(e^{-\beta a/2} - e^{-\beta a}\right)}{\left(1+e^{-\beta a} - 2e^{-\frac{\beta a}{2}}\right)^2}$$

b.) $$C_L = \left(\frac{\partial E}{\partial T}\right)_L = \frac{-a\left(e^{\frac{-a}{2k_BT}} - e^{\frac{-a}{k_BT}}\right)}{\left(1+e^{-a/k_BT} - 2e^{-a/2k_BT}\right)^2}$$

$$= \frac{a^2\left(e^{\frac{3a}{2Tk_B}} - 3e^{\frac{a}{2Tk_B}} + 2\right)e^{\frac{5a}{2Tk_B}}}{2T^2\left[\left(e^{\frac{a}{2Tk_B}} - 2\right)e^{\frac{a}{Tk_B}} + e^{\frac{a}{2Tk_B}}\right]^3}$$