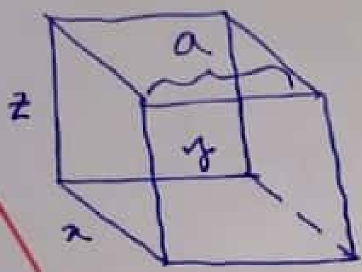
TOPIC : TRANSLATIONAL PARTITION F^{n} (MONOATOMIC GAS)

Page (3-4)

Dr. R.K. Hazra

Energy of a particle in 3-D box



$$\varepsilon_{n_x,n_y,n_z} = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

where $n_x, n_y, n_z = 1, 2, 3, \ldots$

$$\Rightarrow \quad q_t = q_{trans} = \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty} e^{-\beta\varepsilon_{n_x,n_y,n_z}}$$

$$= \left(\sum_{n_x=1}^{\infty} e^{-\frac{\beta h^2 n_x^2}{8ma^2}}\right) \times \left(\sum_{n_y=1}^{\infty} e^{-\frac{\beta h^2 n_y^2}{8ma^2}}\right) \times \left(\sum_{n_z=1}^{\infty} e^{-\frac{\beta h^2 n_z^2}{8ma^2}}\right)$$

$$= \left(\sum_{n=1}^{\infty} e^{-\frac{\beta h^2 n^2}{8ma^2}}\right)^3 = q_1^3$$

q_1 cannot be evaluated in closed form. Thus discretized Summation can be expressed in integral form.

Scanned with CamScanner

$$q_1 = \int_0^{\infty} e^{-(\beta h^2 n^2/8ma^2)}\, dn$$

Using standard integral

$$\int_0^{\infty} e^{-\alpha x^2}\, dx = \frac{1}{2}\left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$$

$$q_1 = \frac{1}{2}\left(\pi / (\beta h^2/8ma^2)\right)^{\frac{1}{2}}$$

$$\boxed{q_1 = \left(\frac{2\pi m k_B T}{h^2}\right) a}$$

$$\Rightarrow q_{trans} = q_1^3 = \left(\frac{2\pi m k_B T}{h^2}\right)^3 a^3$$

$$= \left(\frac{2\pi m k_B T}{h^2}\right)^3 V \quad \text{where } V = a^3 = \text{volume}$$

If we consider rectangular parallelopiped

$$q_{trans} = \left(\frac{2\pi m k_B T}{h^2}\right) a \left(\frac{2\pi m k_B T}{h^2}\right) b \times \left(\frac{2\pi m k_B T}{h^2}\right) c$$

$$\boxed{q_{trans} = \left(\frac{2\pi m k_B T}{h^2}\right)^3 V} \quad \text{where, } V = abc = \text{volume}$$

The same result.