* Rotational Partition function :-

From Quantum mechanics, the rotational energy (E_r) is given as -

$$E_J = \frac{h^2 J(J+1)}{8\pi^2 I}$$

where, J = Rotational quantum no.

$J = 0, 1, 2, 3 \ldots\ldots$

I = Moment of Inertia

$I = \mu r^2$

μ = reduced mass.

The rotational partition in terms of rotational energy is given as -

$$q_r = \sum_{J=0}^{\infty} g_j \exp\left(-\varepsilon_j / kT\right)$$

for rotational motion, degree of degeneracy

$$g_j = (2J+1)$$

$$\therefore q_r = \sum_{J=0}^{\infty} \exp\left(\frac{-h^2 J(J+1)}{8\pi^2 I\, kT}\right)(2J+1)$$

Rotational energy levels are so closely spaced that summation may be replaced by integration -

$$q_r = \int_{J=0}^{\infty} (2J+1) \exp \frac{-h^2 J(J+1)}{8\pi^2 I kT} \cdot dJ$$

on solving this equation, we get -

$$q_r = \frac{8\pi^2 I kT}{h^2}$$

where, σ = symmetry no.

$$\text{or} \quad \boxed{q_r = \frac{8\pi^2 I kT}{\sigma h^2}}$$

* Sackur - Tetrode equation

Entropy of mono-atomic Gas.

The entropy and partition function are related as -

$$S = KT\left(\frac{\partial \ln Q}{\partial T}\right)_V + K \ln Q.$$

and Energy -

$$E = KT^2\left(\frac{\partial \ln Q}{\partial T}\right)_V$$

$$\therefore S = \frac{E}{T} + K \ln Q.$$

and also molar partition function -

$$Q = \frac{q^N}{N!}$$

on using stirling approximation -

$$\ln Q = N \ln q - N \ln N + N$$
$$= N \ln q - (N \ln N - N)$$

The no. of molecules of sample (N), moles (n) and Avogadros no are related as -

$$N = n N_A$$

$$\therefore S = \frac{E}{T} + nK N_A \ln q - (nK N_A \ln N - nK N_A)$$

since, Rot. Energy $E = \frac{3nRT}{2}$ & $KN_A = R$

$$\therefore S = \left(\frac{3nR}{2}\right) + nR\left(\ln q - \ln n N_A + 1\right)$$

Now, Substituting

$$q = \left(\frac{2\pi m KT}{h^2}\right)^{3/2} V \quad \text{we get}-$$

$$S = \left(\frac{3nR}{2}\right) + nR\left[\ln\left(\frac{2\pi m KT}{h^2}\right)\right]^{3/2} V - \ln(nN_0 + 1)$$

This eqn is called Sackur Tetrode eqn for the entropy of mono atomic gas.

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