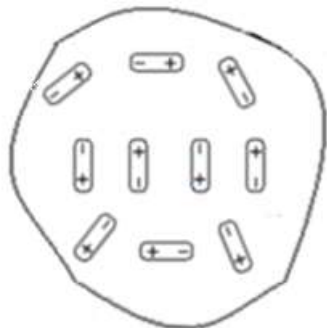


Quadrant II – Transcript and Related Materials

Programme	: Bachelor of Science (Third Year)
Subject	: Physics
Paper Code	: PYC 107
Paper Title	: Mathematical Physics & Electromagnetic Theory - I
Unit 4	: Microscopic Theory of Dielectrics
Module Name	: Polar molecules, Langevin- Debye formula
Module No	: 17
Name of the Presenter	: Mr. Yatin P. Desai

Notes

Polar Molecules in a Dielectric: [The Langevin – Debye Formula]



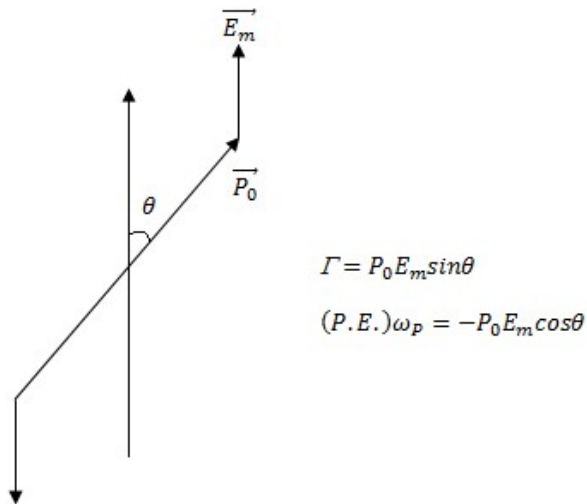
In absence of external
electric field

$$\vec{P} = \frac{\sum \vec{P}_m}{\Delta V}$$

In the absence of external electric field, all dipoles are randomly oriented so that,

$$\sum \vec{P}_m = 0$$

$$i.e. \vec{P} = 0 \text{ when } \vec{E}_{ext} = 0$$

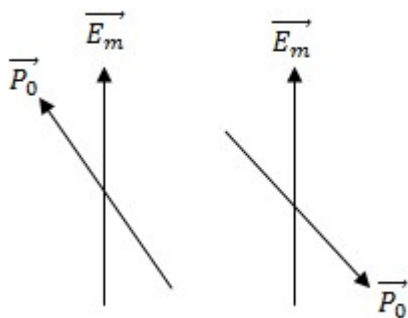


When external electric field is applied all the molecular dipoles experience torque which try to rotate dipoles and make them parallel to the applied field. At sufficiently strong electric field we expect all the dipoles to be perfectly aligned and polarization \vec{P} to attain saturation value. But this is not observed in practice with sufficiently strong electric field. Polarization is far from saturation point. This lack of complete alignment is due to thermal energy of molecules which tend to produce randomness in their orientation.

The average effective dipole moment per molecule is calculated using a principle of statistical mechanics which states that at temperature T, the probability of finding a molecule with energy ω is proportional to $e^{-\frac{\omega}{kT}}$, where, $\omega = \omega_K + \omega_P$ [ω_K : K.E. and ω_P : P.E.], K is the Boltzmann constant and T is absolute temperature.

The potential energy of permanent dipole \vec{P}_0 in an electric field \vec{E}_m is;

$$\omega_P = -\vec{P}_0 \cdot \vec{E}_m = -P_0 E_m \cos \theta; [\theta \text{ is an angle between } \vec{P}_0 \text{ and electric field}]$$

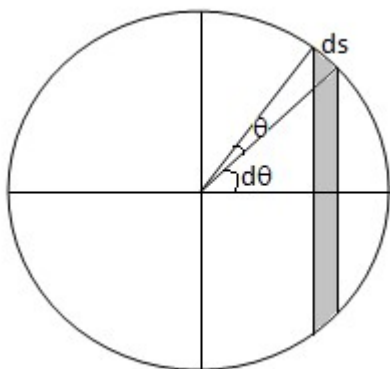


Effective dipole moment of a molecule is its component in the direction of \vec{E}_m i.e. $P_0 \cos \theta$.

It is different for different molecules.

Average value of effective dipole moment;

$$\langle P_0 \cos \theta \rangle = \frac{\int P_0 \cos \theta e^{-\frac{\omega}{KT}} d\omega}{\int e^{-\frac{\omega}{KT}} d\omega}$$



$$d\omega = \text{elementary solid angle} = \frac{ds}{r^2} = \frac{2\pi(r \sin \theta) r d\theta}{r^2} = 2\pi \sin \theta d\theta$$

$$\langle P_0 \cos \theta \rangle = \frac{\int P_0 \cos \theta e^{-\frac{\omega}{KT}} \sin \theta d\theta}{\int e^{-\frac{\omega}{KT}} \sin \theta d\theta} \text{-----(1)}$$

In equation (1), $e^{-\frac{\omega}{KT}} = e^{-\frac{\omega_K + \omega_P}{KT}}$; $e^{-\frac{\omega_K}{KT}}$ is not a function of θ and therefore it can be taken out of the integral of both numerator and denominator and can be cancelled.

$$\therefore \langle P_0 \cos \theta \rangle = \frac{\int P_0 \cos \theta e^{-\frac{\omega_P}{KT}} 2\pi \sin \theta d\theta}{\int e^{-\frac{\omega_P}{KT}} 2\pi \sin \theta d\theta}$$

$$\because \omega_P = -P_0 E_m \cos \theta$$

$$\langle P_0 \cos \theta \rangle = \frac{P_0 \int e^{\frac{P_0 E_m \cos \theta}{KT}} \cos \theta \sin \theta d\theta}{\int e^{\frac{P_0 E_m \cos \theta}{KT}} \sin \theta d\theta} \text{-----(2)}$$

$$\text{Put, } \frac{P_0 E_m}{KT} = y$$

$$\langle P_0 \cos \theta \rangle = \frac{P_0 \int e^{y \cos \theta} \cos \theta \sin \theta d\theta}{\int e^{y \cos \theta} \sin \theta d\theta} \text{-----(3)}$$

$$\text{Let } \cos \theta = x$$

$$\therefore -\sin\theta d\theta = dx$$

When, $\theta = 0$, $x=1$ and when $\theta = \pi$, $x = -1$

Therefore equation (3) can be rewritten as;

$$\langle P_0 \cos\theta \rangle = \frac{P_0 \int_{-1}^1 e^{y^x} x(-dx)}{\int_{-1}^1 e^{y^x} (-dx)}$$

$$\therefore \langle P_0 \cos\theta \rangle = \frac{P_0 \int_{-1}^1 e^{y^x} x dx}{\int_{-1}^1 e^{y^x} dx} \text{----- (4)}$$

Integrating by parts:

$$\langle P_0 \cos\theta \rangle = P_0 \left[\frac{\left\{ \frac{e^{y^x}}{y} x \right\}_{-1}^1 - \int_{-1}^1 \frac{e^{y^x}}{y} 1 dx}{\int_{-1}^1 e^{y^x} dx} \right]$$

$$\therefore \langle P_0 \cos\theta \rangle = P_0 \left[\frac{\left\{ \frac{e^{y^x}}{y} x \right\}_{-1}^1 - \frac{\int_{-1}^1 e^{y^x} 1 dx}{\int_{-1}^1 e^{y^x} dx}}{\int_{-1}^1 e^{y^x} dx} \right] = P_0 \left[\frac{\left\{ \frac{e^{y^x}}{y} x \right\}_{-1}^1 - \frac{\int_{-1}^1 e^{y^x} 1 dx}{\int_{-1}^1 e^{y^x} dx}}{\left\{ \frac{e^{y^x}}{y} \right\}_{-1}^1 - \frac{1}{y}} \right]$$

$$\therefore \langle P_0 \cos\theta \rangle = P_0 \left[\frac{\left\{ \frac{e^y}{y} + \frac{e^{-y}}{y} \right\}}{\left\{ \frac{e^y}{y} - \frac{e^{-y}}{y} \right\}} - \frac{1}{y} \right]$$

$$\therefore \langle P_0 \cos\theta \rangle = P_0 \left[\frac{\{e^y + e^{-y}\}}{\{e^y - e^{-y}\}} - \frac{1}{y} \right] \text{----- (5)}$$

We have, $e^{i\theta} = \cos\theta + i\sin\theta$ and $e^{-i\theta} = \cos\theta - i\sin\theta$

$$\therefore \cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2} \text{ and } \sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$

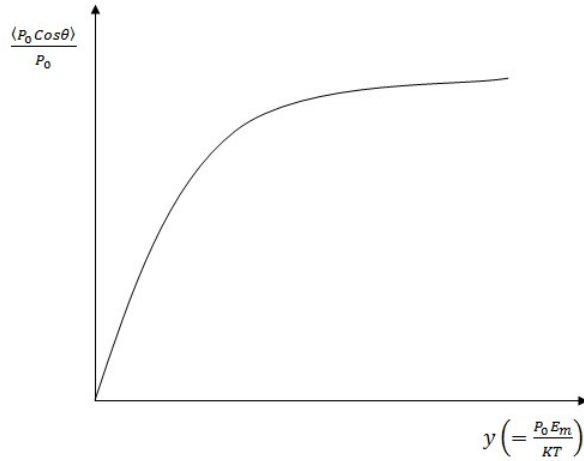
$$\cosh\theta = \frac{e^{\theta} + e^{-\theta}}{2} \text{ and } \sinh\theta = \frac{e^{\theta} - e^{-\theta}}{2}$$

$$\coth\theta = \frac{e^{\theta} + e^{-\theta}}{e^{\theta} - e^{-\theta}}$$

Therefore equation (5) is;

$$\langle P_0 \cos\theta \rangle = P_0 \left[\coth y - \frac{1}{y} \right] \text{----- (6)}$$

Equation (6) is known as **Lagrangian Formula**.



For most dielectric, P_0 is such that, y is much smaller than 1 [$y \ll 1$].

$$\coth y = \frac{e^y + e^{-y}}{e^y - e^{-y}} = \frac{\left(1 + y + \frac{y^2}{2!} + \frac{y^3}{3!}\right) + \left(1 - y + \frac{y^2}{2!} - \frac{y^3}{3!}\right)}{\left(1 + y + \frac{y^2}{2!} + \frac{y^3}{3!}\right) - \left(1 - y + \frac{y^2}{2!} - \frac{y^3}{3!}\right)}$$

$$\therefore \coth y = \frac{2 + y^2}{\left(2y + \frac{y^3}{3}\right)} = \frac{2\left(1 + \frac{y^2}{2}\right)}{2y\left(1 + \frac{y^2}{6}\right)} = \frac{1}{y} \left(1 + \frac{y^2}{2}\right) \left(1 + \frac{y^2}{6}\right)^{-1}$$

$$\therefore \coth y \cong \frac{1}{y} \left(1 + \frac{y^2}{2}\right) \left(1 - \frac{y^2}{6}\right) \quad [\text{using binomial theorem}]$$

$$\therefore \coth y = \frac{1}{y} \left(1 - \frac{y^2}{6} + \frac{y^2}{2} - \frac{y^4}{12}\right) = \frac{1}{y} \left(1 + \frac{y^2}{3}\right) \cong \frac{1}{y} + \frac{y}{3} - - - - - (7)$$

Substituting equation (7) in equation (6);

$$\langle P_0 \cos \theta \rangle = P_0 \left[\frac{1}{y} + \frac{y}{3} - \frac{1}{y} \right] = P_0 \frac{y}{3}$$

$$\therefore \langle P_0 \cos \theta \rangle = P_0^2 \frac{E_m}{3KT} - - - - - (8) \quad \left[\because y = \frac{P_0 E_m}{KT} \right]$$

Let N be number of molecules per unit volume.

$$\therefore P = N \langle P_0 \cos \theta \rangle$$

$$\therefore \frac{P}{N} = \langle P_0 \cos \theta \rangle = \frac{P_0^2 E_m}{3KT}$$

$$\frac{P}{N} = P_m = \propto E_m$$

$$\therefore \propto E_m = \frac{P_0^2 E_m}{3KT}$$

$$\therefore \propto \frac{P_0^2}{3KT} \text{ --- (9) --- } \textit{Orientational polarisability}$$

Considering non-polar molecules only;

$$\alpha_0 = 4\pi\epsilon_0 R_0^3 \text{ --- (10) --- } \textit{Deformation polarisability}$$

\therefore total molecular polarisability of a dielectric is;

$$\therefore \propto \alpha_0 + \frac{P_0^2}{3KT} \text{ --- } \textit{Langevin - Debye Equation}$$