Dispersion of Light - $n(\omega)$

- A field $\vec{\mathbf{E}}$ applied to a (isotropic) dielectric, i.e., an insulator that can be polarized by an applied electric field, separates positive and negative charges within the material. Hence, electric dipole moments are created.
- The resultant dipole moment per unit volume = **electric polarization** $\vec{\mathbf{P}}$.
- In many materials, $\vec{\mathbf{P}}$ and $\vec{\mathbf{E}}$ are proportional, and is related by:

$$\vec{\mathbf{P}} = (\epsilon - \epsilon_0)\vec{\mathbf{E}} \qquad (1a) \qquad \text{(SI units C/m}^2\text{)}$$

or, since $\epsilon = K_E \epsilon_o$, (1b)

$$\vec{\mathbf{P}} = \epsilon_0 (K_E - 1)\vec{\mathbf{E}} \qquad (1c)$$

- Another common way of writing eqn (1c) is

$$\vec{\mathbf{P}} = \epsilon_0 \chi \vec{\mathbf{E}} \qquad (1d)$$

χ: ***susceptibility***

- By comparing (1c) and (1d),

$$K_E = 1 + \chi \qquad (1e)$$

- For non-magnetic materials, via Maxwell's relation (see previous handout),

$$\boxed{n = \sqrt{K_E} = \sqrt{1 + \chi}} \qquad (2a)$$

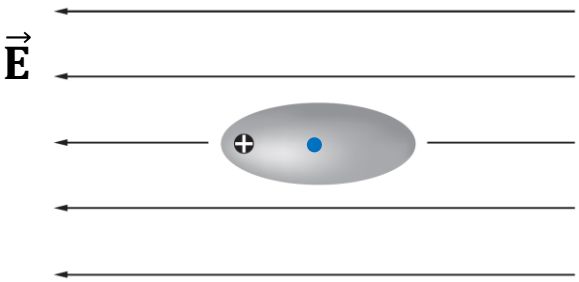
or

$$\boxed{n^2 = K_E = 1 + \chi} \qquad (2b)$$

$\Rightarrow$ Eqns (1d) and (2) will be useful for calculating $n(\omega)$.

Some Mechanisms for Polarization:

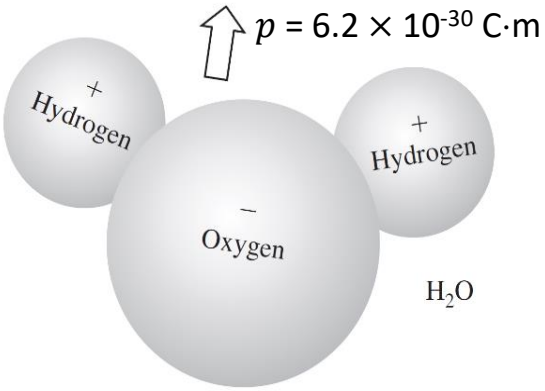
• In *nonpolar molecules* and *atoms*, e.g. H atom, the applied $\vec{\mathbf{E}}$ distorts the electron cloud, shifting it relative to the nucleus, hence inducing a dipole moment. This is *electronic polarization.* (We will focus on modelling this situation.)



Center of electron cloud does not coincide with the nucleus. This can be modelled as a dipole.

• In crystals, the applied $\vec{\mathbf{E}}$ can also distort the position of the ions (e.g. the Na^+ and Cl^- ions in NaCl). The resultant induced dipole moment is due to *ionic* or *atomic polarization.*

• Some molecues have permanent dipole moments (e.g. H_2O). The applied $\vec{\mathbf{E}}$ can align these dipoles, and the material takes on an *orientational polarization*.



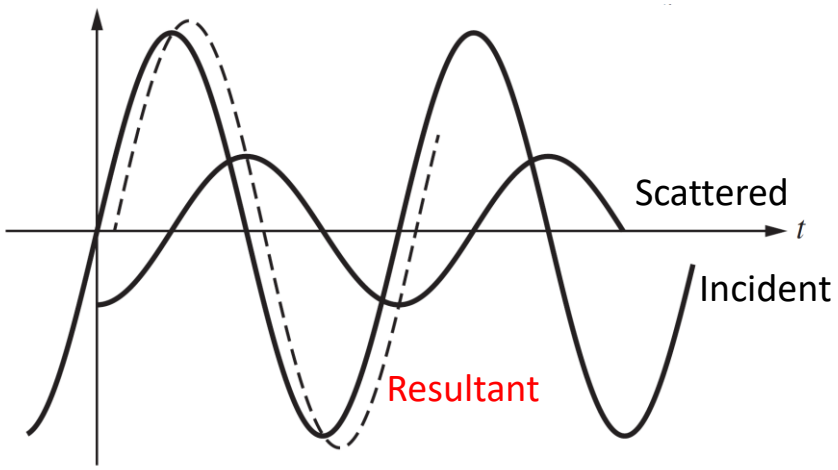
Frequency dependence of n: (Qualitative description)

• If a harmonic EM wave is incident on a dielectric, the internal charges will experience *time-varying* forces. The ability of the charges to "follow" $\vec{\mathbf{E}}(t)$ plays an important role in producing a frequency dependence of the index of refraction n.

$\Rightarrow$ Oscillating $\vec{\mathbf{E}}(t)$ creates oscillating electric dipoles.

$\Rightarrow$ These oscillating dipoles radiate at the same frequency as the incident wave, but usually with a phase delay, e.g. because of inertia of the charges involved.

$\Rightarrow$ The light wave travelling in the medium is the superposition of the original wave plus the phase delayed waves radiated by all the oscillating dipoles.



$\Rightarrow$ An observer in the forward direction will see the resultant wave which is phase-shifted (e.g. recall discussion of superposition of harmonic plane waves in Sec 1). This wave will appear to have a speed different than c.

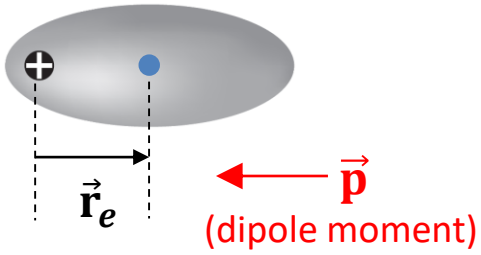
e.g. In the above figure, the peak of the resultant wave occurs at a later time compared to the peak of the incident wave; the resultant wave appears to have a speed less than c.

$\Rightarrow$ The cumulative phase shift builds as the light penetrates further into the medium.

Dispersion: Lorentz Model (classical theory)

- The Lorentz Model is a microscopic atomic model used to derive the frequency dependence of $\vec{\mathbf{P}}$, and hence χ (or K_E), and therefore n.

- The Lorentz model of the atom uses Newton's equation of motion to describe the displacement of the center of the electron cloud (indicated by the blue dot in the figure below) from equilibrium when an electric field $\vec{\mathbf{E}}$ is applied.



(Nucleus is assumed to be immobile because it is much more massive than electron.)

- The system is modelled as a dipole consisting of a point nucleus (positive) and a point electron (negative) separated by $\vec{\mathbf{r}}_e$. The attractive force between the nucleus and electron is modelled as a spring.

k_s = elastic (spring) constant

m_e = electron mass

q_e = magnitude of electron charge (> 0)

ω = EM wave's angular frequency

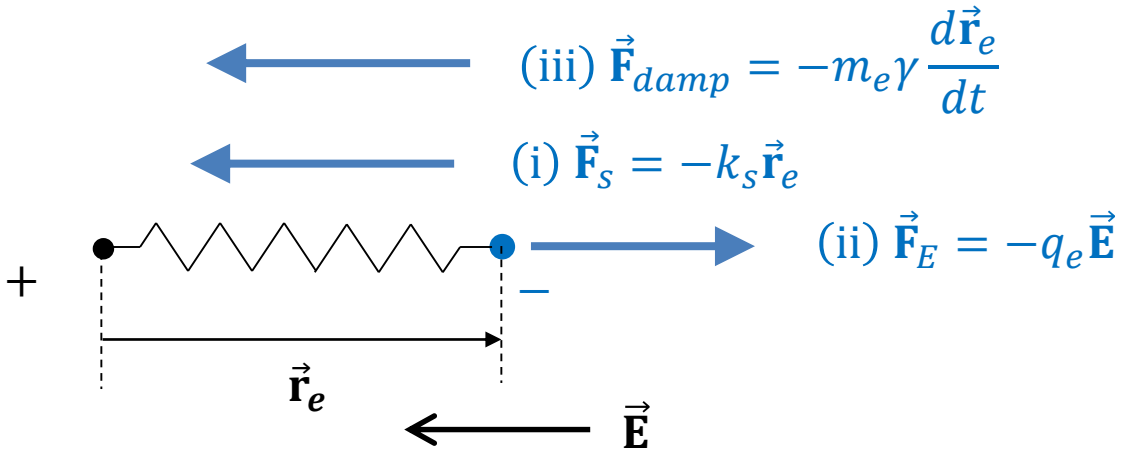
γ = damping constant

$\vec{\mathbf{E}} = \vec{\mathbf{E}}_0 e^{-i\omega t}$ = harmonic incident wave

- Suppose N is the number of contributing electrons per unit volume. Each electron contributes a dipole moment $\vec{\mathbf{p}} = -q_e\vec{\mathbf{r}}_e$ (recall that direction of the dipole moment is from the negative towards the positive charge). Hence, the **electric polarization**, i.e., density of dipole moments, is given by

$$\vec{\mathbf{P}} = -Nq_e\vec{\mathbf{r}}_e \qquad (3)$$

• The model assumes three forces acting on the electron:



(i) Assume electron is bound to the nucleus by a spring-like force:

$$\vec{\mathbf{F}}_s = -k_s\vec{\mathbf{r}}_e \qquad \text{(Hooke's Law)}$$

natural or *resonance* frequency $\omega_0 = \sqrt{k_s/m_e}$ (e.g. from 1st year Physics)

so $\vec{\mathbf{F}}_s = -m_e\omega_0^2\vec{\mathbf{r}}_e$

(ii) Harmonic EM wave exerts a (Lorentz) force: $\vec{\mathbf{F}}_E = -q_e\vec{\mathbf{E}}(t)$

(iii) A damping force ("drag force" or "friction force"):

$$\vec{\mathbf{F}}_{damp} = -m_e\gamma\frac{d\vec{\mathbf{r}}_e}{dt}$$

• Newton's 2nd Law hence gives the following "Equation of Motion" for the electron:

$$\vec{\mathbf{F}}_{net} = \vec{\mathbf{F}}_s + \vec{\mathbf{F}}_E + \vec{\mathbf{F}}_{damp}$$

$$m_e\frac{d^2\vec{\mathbf{r}}_e}{dt^2} = -m_e\omega_0^2\vec{\mathbf{r}}_e - q_e\vec{\mathbf{E}} - m_e\gamma\frac{d\vec{\mathbf{r}}_e}{dt} \qquad (4)$$

• Suppose $\vec{\mathbf{E}}$ is a harmonic field described by by $\vec{\mathbf{E}} = \vec{\mathbf{E}}_0 e^{-i\omega t}$ and that the oscillations respond with a similar dependence, $\vec{\mathbf{r}}_e = \vec{\mathbf{r}}_0 e^{-i\omega t}$. Hence, $d\vec{\mathbf{r}}_e/dt = -i\omega\vec{\mathbf{r}}_e$ and $d^2\vec{\mathbf{r}}_e/dt^2 = -\omega^2\vec{\mathbf{r}}_e$, and eqn (4) yields:

$$-m_e\omega^2\vec{\mathbf{r}}_e = -m_e\omega_0^2\vec{\mathbf{r}}_e - q_e\vec{\mathbf{E}} + im_e\gamma\omega\vec{\mathbf{r}}_e \qquad (5a)$$

or

$$\vec{\mathbf{r}}_e = -\left(\frac{q_e}{m_e}\right)\frac{\vec{\mathbf{E}}}{\omega_0^2 - \omega^2 - i\omega\gamma} \qquad (5b)$$

• Substitute eqn (5b) into eqn (3) [$\vec{\mathbf{P}} = -Nq_e\vec{\mathbf{r}}_\mathbf{e}$]:

$$\vec{\mathbf{P}} = \left(\frac{Nq_e^2}{m_e}\right)\frac{\vec{\mathbf{E}}}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

$$\vec{\mathbf{P}} = \epsilon_0\left(\frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}\right)\vec{\mathbf{E}} \qquad (6)$$

where the ***plasma frequency*** ω_p is

$$\boxed{\omega_p = \sqrt{\frac{Nq_e^2}{\epsilon_0 m_e}}} \qquad (7)$$

• Substitute eqn (6) into eqn (1d) [$\vec{\mathbf{P}} = \epsilon_0\chi\vec{\mathbf{E}}$] to get

$$\chi(\omega) = \left(\frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}\right) \qquad (8)$$

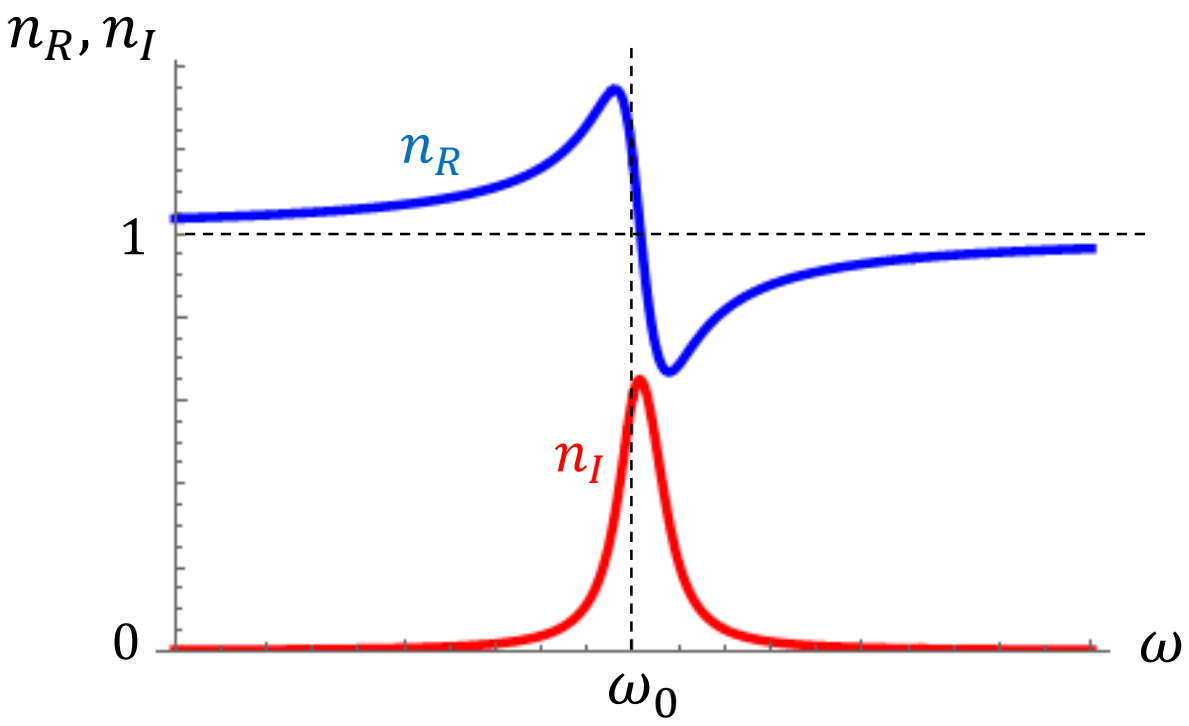
• To obtain the refractive index, we now substitute eqn (8) into eqn (2b) [$n^2 = 1 + \chi$] :

$$n^2 = 1 + \chi(\omega) = 1 + \left(\frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma} \right) \quad (9)$$

Dispersion Equation

- Note from (9) that n is complex, with real part n_R and an imaginary part n_I . In the context of the complex n, the n_R is commonly called the "refractive index" while the n_I is called the "extinction coefficient".

- Schematically, $n_R(\omega)$ and $n_I(\omega)$ look like the following:



- The n_I corresponds to the attenuation of the EM wave (e.g. such as through absorption) by the medium [see following discussion]. The attenuation is only strong **near the resonant frequencies**. These regions of significant attenuation are called *absorption bands*.

- The n_R affects the EM wave's phase speed, etc., as "usual" [see following discussion]. (Note that $n_R = 1$ at very high frequencies.)

Complex refractive index $\tilde{n}$ and its affect on the plane wave

- The complex index of refraction can be written as

$$\tilde{n} = n_R + in_I \qquad \text{(A-1)}$$

where the real and imaginary parts of $\tilde{n}$ are the n_R and n_I, respectively.

- Suppose an EM plane wave traveling within the dielectric is described by

$$\vec{\mathbf{E}} = \vec{\mathbf{E}}_0 e^{i(\tilde{k}z - \omega t)} \qquad \text{(A-2)}$$

- Assume that the propagation number, denoted by $\tilde{k}$, is complex:

$$\tilde{k} = \frac{\omega}{c}\tilde{n} = \frac{\omega}{c}(n_R + in_I) = \frac{\omega n_R}{c} + i\frac{\omega n_I}{c} = k + i\frac{\alpha}{2} \qquad \text{(A-3)}$$

where k represents the real part of the complex $\tilde{k}$ and is given by

$$k = \frac{\omega n_R}{c} = \frac{\omega}{v} \quad \text{with} \quad v = \frac{c}{n_R} \qquad \text{(A-4)}$$

where α is the absorption coefficient (units: m^{-1})

$$\boxed{\alpha = \frac{2\omega n_I}{c}} \qquad \text{(A-5)}$$

- The traveling EM wave is now given by

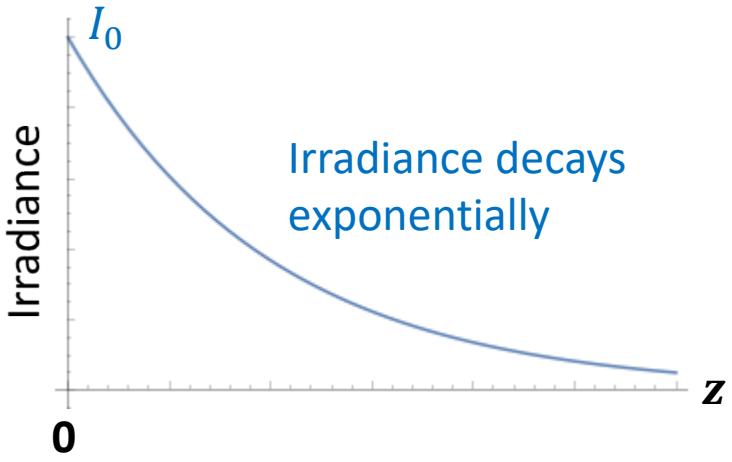
$$\vec{\mathbf{E}} = \vec{\mathbf{E}}_0 e^{-\frac{\alpha}{2}z} e^{i(kz - \omega t)} \qquad \text{(A-6)}$$

- Hence, the imaginary part of the refractive index corresponds to an attenuation of the wave. The real part of the refractive index affects the phase speed, as “usual”.

Complex $\tilde{n}$ and its affect on the plane wave (con't)

- Note that the irradiance is proportional to the square of the amplitude in (A-6) and hence

$$\boxed{I = I_0 e^{-\alpha z}} \qquad \text{(Beer-Lambert Law)}$$



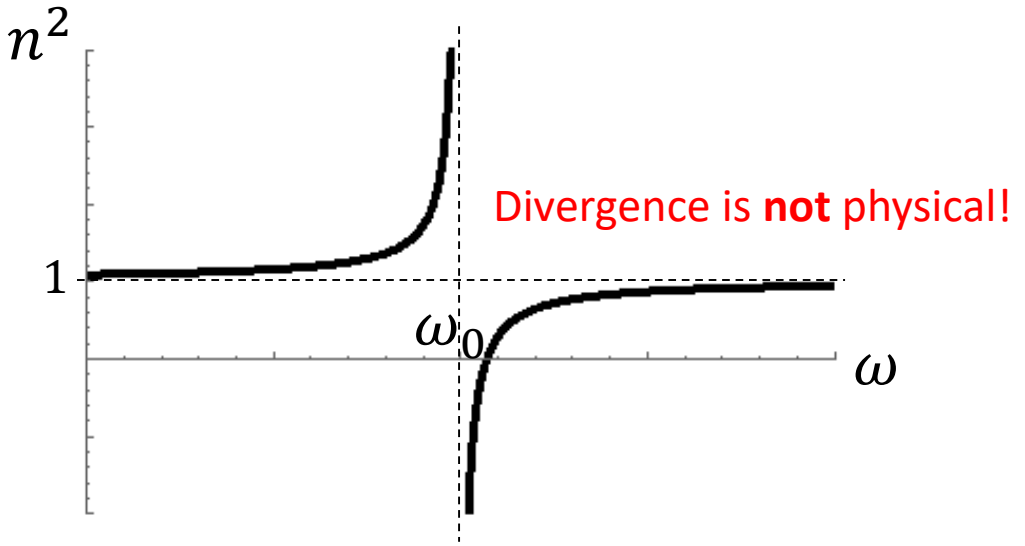
Extensions & Simplifications of Eqn (9):

(1) Suppose we are interested in frequencies that are far from the resonant frequency ω_0. It is also reasonable to assume that there is no absorption (n_I is small). Eqn (9) is then real, and can be approximated as :

$$n^2(\omega) = 1 + \left(\frac{\omega_p^2}{\omega_0^2 - \omega^2}\right) = 1 + \frac{Nq_e^2}{\epsilon_0 m_e}\left(\frac{1}{\omega_0^2 - \omega^2}\right) \qquad (10)$$

Sellmeier Equation

- Regarding the Sellmeier equation, note that n^2 diverges at $\omega = \omega_0$:



- Hence, the equation is only applicable for frequencies far away from ω_0.

---

(2) Most materials have more than one species of "active" electrons, and each is characterized by a different spring constant, damping constant γ_j, and resonant frequency ω_{0j} (where $j = 1,2,3, \ldots.$). If N is the number of contributing electrons per unit volume, and s_j is the fraction of electrons per unit volume with resonant frequency ω_{0j}, then (9) can be generalized to:

$$n^2(\omega) = 1 + \chi(\omega) = 1 + \sum_j \left(\frac{s_j \omega_p^2}{\omega_{0j}^2 - \omega^2 - i\omega\gamma_j} \right) \qquad \text{(11a)}$$

$$\text{where } \sum_j s_j = 1 \qquad \text{(11b)}$$

Note:

In the context of quantum mechanics, the interpretation is

ω_{0j} = frequencies at which an atom may absorb or emit radiant energy

s_j = *oscillator strength* or *transition probability*

(s_j measures the likelihood that a given atomic transition will occur)

[e.g. 1s, 2s, etc. electrons have different binding to the nucleus]

(3) We can also apply a variation of eqn (9) or (11) to ions bound to fixed atomic sites if we replace the electron mass with the (much larger) ion mass, and q_e with the ionic charge.

(4) Extra Information: Clausius-Mossotti relation

Eqn (9) applies well for rarefied media such as gases. But in dense dielectric media, atoms can experience an additional induced field set up by the other atoms which can be shown (e.g. Kittel, *Intro. to Solid State Physics*) to be $P(t)/3\epsilon_0$. It can be further shown that this leads to:

$$\frac{n^2-1}{n^2+2} = \frac{Nq_e^2}{3\epsilon_0 m_e}\sum_j \left(\frac{s_j}{\omega_{0j}^2 - \omega^2 + i\gamma_j\omega}\right) \qquad (11)$$

(one formulation of the Clausius–Mossotti relation)

- Qualitatively, $n_R(\omega)$ and $n_I(\omega)$ for eqn (11) look like those for eqn (9):