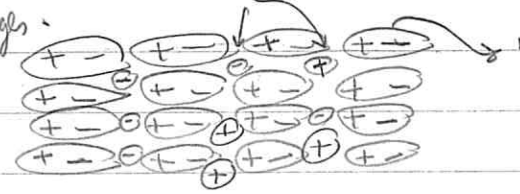
Lecture #13 : Electromagnetic waves in crystals

Same classical wave eqn method can be applied to propagation of light in crystals.
→ Important effects such as birefringence ⇒ double refraction, light ray splits up into two rays (ordinary and extraordinary). Show Calcite crystal.

Charge density ρ and current density $\vec{J}$ in a material

Materials can be thought as formed by free and bound charges.

"free" (mobile) charges, electrons ⊖ or holes ⊕.



"Bound" molecular charges

The electrostatic potential inside a material can be approximated by

$$\Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int d^3r' \left\{ \frac{\rho_{Free}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} + \vec{P}(\vec{r}\,')\cdot \underbrace{\frac{(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^3}}_{=\vec{\nabla}'\left(\frac{1}{|\vec{r}-\vec{r}\,'|}\right)} + \underbrace{\frac{1}{2}\frac{(\vec{r}-\vec{r}\,')\cdot \overleftrightarrow{Q}(\vec{r}\,')\cdot(\vec{r}-\vec{r}\,')}{|\vec{r}-\vec{r}\,'|^5} + \ldots}_{\text{Quadrupole and higher orders, neglect!}} \right\}$$

where $\rho_{Free}(\vec{r}\,') = \sum_{\text{Free charges } i} q_i\, \delta(\vec{r}-\vec{R}_i)$

$$\vec{P}(\vec{r}\,') = \sum_{\text{molecules } m} \vec{p}_m\, \delta(\vec{r}-\vec{R}_m) \,,$$

$$\boxed{\begin{array}{l}\text{molecular dipole moment} \\ \vec{p}_m = \int \rho_{molecule}(\vec{r}\,')\,\vec{r}\,' d^3r' \\ \text{integral with origin at center of mass of molecule.}\end{array}}$$

Write $\vec{P}(\vec{r}\,')\cdot\vec{\nabla}'\left(\frac{1}{|\vec{r}-\vec{r}\,'|}\right) = \vec{\nabla}'\cdot\left[\frac{\vec{P}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\right] - \frac{\vec{\nabla}'\cdot\vec{P}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}$ and integrate out the full divergence

to get

$$\boxed{\Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int d^3r' \frac{\left[\rho_{Free}(\vec{r}\,') - \vec{\nabla}'\cdot\vec{P}(\vec{r}\,')\right]}{|\vec{r}-\vec{r}\,'|}}$$

So that we can interpret $-\vec{\nabla}\cdot\vec{P} \equiv \rho_{Bound}(\vec{r}\,')$ "Bound charge density".

From $\vec{E} = -\vec{\nabla}\Phi \Rightarrow \vec{\nabla}\cdot\vec{E} = -\nabla^2\Phi$ so that

$$\vec{\nabla}\cdot\vec{E} = \frac{1}{4\pi\varepsilon_0}\int d^3r' \underbrace{\left[-\nabla^2\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\right]}_{=4\pi\delta(\vec{r}-\vec{r}')}\left[\rho_{Free}(\vec{r}') - \vec{\nabla}'\cdot\vec{P}(\vec{r}')\right]$$

$$\Rightarrow \boxed{\vec{\nabla}\cdot\vec{E} = \frac{1}{\varepsilon_0}\left[\rho_{Free}(\vec{r}) - \vec{\nabla}\cdot\vec{P}(\vec{r})\right]}$$ (First Maxwell eqn in a material)

Note: 1) A more careful derivation (see Jackson 6.6) shows that this eqn holds for $\vec{E} = \langle\vec{E}_{microscopic}\rangle$, where $\langle\cdot\rangle$ is a "coarse grained average" over a volume element with many molecules.

2) It is customary to define the displacement vector $\vec{D} = \varepsilon_0\vec{E} + \vec{P}$ so that $\vec{\nabla}\cdot\vec{D} = \rho_{Free}(\vec{r})$. We will not work with $\vec{D}$ here.

The same consideration applies for the current density $\vec{J}$ inside a material.

To find $\vec{J}$, consider the conservation law for charge:

$$\frac{\partial\rho}{\partial t} = -\vec{\nabla}\cdot\vec{J}$$

$$\Rightarrow \frac{\partial}{\partial t}\left[\rho_{Free} - \vec{\nabla}\cdot\vec{P}\right] = -\vec{\nabla}\cdot\vec{J}$$

$$\Rightarrow \vec{\nabla}\cdot\vec{J} = \underbrace{-\frac{\partial\rho_{Free}}{\partial t}}_{\equiv\vec{\nabla}\cdot\vec{J}_{Free}} + \vec{\nabla}\cdot\underbrace{\left(\frac{\partial\vec{P}}{\partial t}\right)}_{\text{current due to change of polarization of bound charges!}}$$

$$\Rightarrow \vec{J} = \vec{J}_{Free} + \left(\frac{\partial\vec{P}}{\partial t}\right) + \vec{J}_M \quad \text{where } \vec{\nabla}\cdot\vec{J}_M = 0. \Rightarrow \vec{J}_M = \vec{\nabla}\times\vec{M},$$

where $\vec{M}$ is magnetization:

$$\vec{M}(\vec{r}) = \sum_{\text{molecules } n} \vec{\mu}_n \, \delta(\vec{r} - \vec{R}_n)$$

and $\vec{\mu}_n = \frac{e}{2m_e} \sum_{i \in \text{electrons in molecule}} (2\vec{S}_i + \vec{L}_i)$ is magnetic moment.

$\vec{S}_i$: spin; $\vec{L}_i$: orbital angular momentum.

Using this expression for $\vec{J}$ the other Maxwell eqn becomes

$$\vec{\nabla} \times \vec{B} = \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t} + \mu_0 \vec{J}$$

$$\Rightarrow \vec{\nabla} \times \vec{B} = \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t} + \mu_0 \left(\vec{J}_{Free} + \frac{\partial \vec{P}}{\partial t} + \vec{\nabla} \times \vec{M} \right)$$

Again, this eqn can be formally justified with $\vec{B} \to \langle \vec{B}_{\text{microscopic}} \rangle$.

$$\nabla \times \underbrace{\left[\frac{1}{\mu_0} \vec{B} - \vec{M} \right]}_{\text{customary to call this } \vec{H}} = \frac{\partial}{\partial t} \underbrace{\left(\varepsilon_0 \vec{E} + \vec{P} \right)}_{= \vec{D}} + \vec{J}_{Free} \Rightarrow \vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}_{Free}.$$

For a non-magnetic material $(\vec{M} = \vec{0})$ Maxwell's eqns become:

$$\begin{cases} \vec{\nabla} \cdot \vec{E} = \frac{1}{\varepsilon_0} \left(\rho_{Free}(\vec{r}) - \vec{\nabla} \cdot \vec{P} \right) \\ \vec{\nabla} \cdot \vec{B} = 0 \\ \vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{B} = \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t} + \mu_0 \left(\vec{J}_{Free} + \frac{\partial \vec{P}}{\partial t} \right) \end{cases}$$

Let's derive the wave eqn for propagation of light in an insulator with:

$$\rho_{Free} = 0 \;, \quad \vec{J}_{Free} = \vec{0} .$$

Take $\frac{\partial}{\partial t}$ of 4th eqn:

$$\vec{\nabla} \times \frac{\partial \vec{B}}{\partial t} = \mu_0 \varepsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} + \mu_0 \frac{\partial^2 \vec{P}}{\partial t^2}$$

Take curl of 3rd eqn:

$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = -\vec{\nabla} \times \left(\frac{\partial \vec{B}}{\partial t} \right)$, and plug in to get

$$\Rightarrow \boxed{-\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = \mu_0 \varepsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} + \mu_0 \frac{\partial^2 \vec{P}}{\partial t^2}}$$

Wave eqn for $\vec{E}$ in a non-magnetic insulator

Note: In vacuum $\vec{P} = 0$ and $-\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = \nabla^2 \vec{E} - \vec{\nabla}(\underbrace{\vec{\nabla} \cdot \vec{E}}_{= -\frac{\vec{\nabla} \cdot \vec{P}}{\varepsilon_0} = 0 \text{ in vacuum}})$

$$\Rightarrow \nabla^2 \vec{E} = \underbrace{\mu_0 \varepsilon_0}_{\equiv \frac{1}{c^2}} \frac{\partial^2 \vec{E}}{\partial t^2}$$

, c speed of light.

Crystals are usually anisotropic. Assuming $\vec{E}$ is "weak" we assume linear response

$$\vec{P} = \varepsilon_0 \overleftrightarrow{\chi} \cdot \vec{E} \quad \text{or} \quad P_i = \varepsilon_0 \chi_{ij} E_j$$

where $\overleftrightarrow{\chi}$ is the electric susceptibility tensor. Define the dielectric tensor $\overleftrightarrow{\varepsilon}$ as

$\varepsilon_{ij} = \varepsilon_0 (\delta_{ij} + \chi_{ij})$ so that our wave eqn becomes

$$\boxed{-\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = \mu_0 \overleftrightarrow{\varepsilon} \cdot \frac{\partial^2 \vec{E}}{\partial t^2}} .$$

5)

Let's solve this by plugging the plane wave ansatz:

$$\vec{E} = \vec{E}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)} : \begin{cases} \vec{\nabla}\cdot\vec{E} = i\vec{k}\cdot\vec{E} \\ \vec{\nabla}\times\vec{E} = i\vec{k}\times\vec{E} \end{cases}$$

$$-(i)^2\, \vec{k}\times(\vec{k}\times\vec{E}_0)\cancel{e^{i(\vec{k}\cdot\vec{r}-\omega t)}} = -\omega^2\mu_0 \overleftrightarrow{\varepsilon}\cdot\vec{E}_0\, \cancel{e^{i(\vec{k}\cdot\vec{r}-\omega t)}}$$

$$\vec{k}\times(\vec{k}\times\vec{E}_0) + \omega^2\mu_0\overleftrightarrow{\varepsilon}\cdot\vec{E}_0 = \vec{0}$$

$$(\vec{k}\cdot\vec{E}_0)\vec{k} - k^2\vec{E}_0 + \omega^2\mu_0\overleftrightarrow{\varepsilon}\cdot\vec{E}_0 = \vec{0}$$

$$k_j E_j^{(0)} k_i \hat{e}_i - k^2 E_i^{(0)}\hat{e}_i + \omega^2 \hat{e}_i \varepsilon_{ij} E_j^{(0)} = 0$$

$$\boxed{\sum_j \left[\left(k_i k_j - k^2\delta_{ij}\right) + \omega^2\mu_0\varepsilon_{ij}\right] E_j^{(0)} = 0} \qquad i = x, y, z$$

Three eqns, each for $i = x, y, z$.

Electromagnetic equivalent of the Christoffel eqn.

By proper choice of axis, $\overleftrightarrow{\varepsilon}$ can be diagonalized: $\overleftrightarrow{\varepsilon} = \begin{pmatrix} \varepsilon_1 & & 0 \\ & \varepsilon_2 & \\ 0 & & \varepsilon_3 \end{pmatrix}$, assume $\hat{z}$ // axis 3 and

Assume $\vec{k} = k\hat{z}$:

$$\begin{pmatrix} n_1^2\frac{\omega^2}{c^2} - k^2 & & \\ & n_2^2\frac{\omega^2}{c^2} - k^2 & \\ & & n_3^2\frac{\omega^2}{c^2} \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Solutions:

$$\left(n_1^2 \frac{\omega^2}{c^2} - k^2\right) E_1 = 0 \quad \Rightarrow \quad \omega = \left(\frac{c}{n_1}\right) k \,, \quad \vec{E} \parallel \hat{x}$$

$$\left(n_2^2 \frac{\omega^2}{c^2} - k^2\right) E_2 = 0 \quad \Rightarrow \quad \omega = \left(\frac{c}{n_2}\right) k \,, \quad \vec{E} \parallel \hat{y}$$

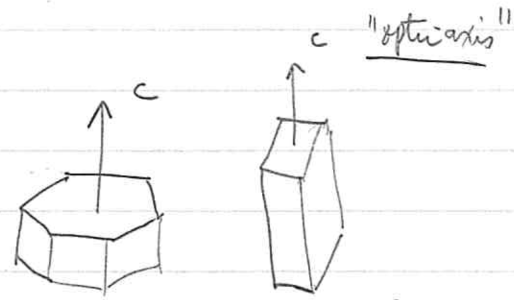
$$E_3 = 0 \qquad \text{for } \omega \neq 0 .$$

Only two polarizations $\parallel \hat{x}$ and $\parallel \hat{y}$. Since $\vec{\nabla}\cdot\vec{E} = 0$, EM wave has no Longitudinal polarization. These two polarizations can propagate with different speeds.

Uniaxial Crystals

$n_1 = n_2 = n_o$ ("ordinary axis")

$n_3 = n_e$ ("extraordinary axis" or "optic axis" or "c-axis")



Examples of uniaxial crystals.

wave eqn using these axis:

$$\begin{pmatrix} n_o^2 \frac{\omega^2}{c^2} - k_2^2 - k_3^2 & k_1 k_2 & k_1 k_3 \\ k_1 k_2 & n_o^2 \frac{\omega^2}{c^2} - k_1^2 - k_3^2 & k_2 k_3 \\ k_1 k_3 & k_2 k_3 & n_e^2 \frac{\omega^2}{c^2} - k_1^2 - k_2^2 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix} = \vec{0}$$

$$\det() = 0 \Rightarrow \left(k^2 - n_o^2 \frac{\omega^2}{c^2}\right)\left[(k_1^2 + k_2^2) n_o^2 \frac{\omega^2}{c^2} + k_3^2 n_e^2 \frac{\omega^2}{c^2} - n_o^2 n_e^2 \frac{\omega^4}{c^4}\right] = 0$$

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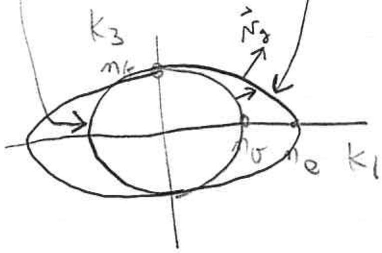
Two sols: $K^2 = n_o^2 \frac{\omega^2}{c^2}$ (sphere in k space)

$$\frac{k_1^2}{n_e^2} + \frac{k_2^2}{n_e^2} + \frac{k_3^2}{n_o^2} = \frac{\omega^2}{c^2} \quad \text{(ellipsoid)} \qquad (\star)$$



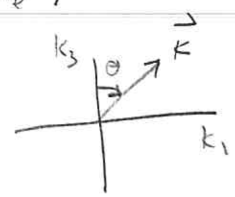
<u>Rays of light</u> point along $\vec{N}_g = \vec{\nabla}_{\vec{k}}\, \omega(\vec{k})$.

For the ordinary ray: $\omega = \frac{c}{n_o}|\vec{k}| \Rightarrow \vec{N}_g = \frac{c}{n_o}\hat{k}$

For the extraordinary ray: $\vec{N}_g = \left(\frac{\partial \omega}{\partial k_1}, \frac{\partial \omega}{\partial k_2}, \frac{\partial \omega}{\partial k_3}\right) = \frac{c^2}{\omega}\left(\frac{k_1}{n_e^2}, \frac{k_2}{n_e^2}, \frac{k_3}{n_o^2}\right)$

$$\frac{2k_1}{n_e^2} = \frac{2\omega}{c^2}\frac{\partial \omega}{\partial k_1} \Rightarrow \frac{\partial \omega}{\partial k_1} = \frac{c^2}{n_e^2}\frac{k_1}{\omega} = \frac{c^2}{\omega}\left(\frac{k_1}{n_e^2}\right)$$

Focus on 1-3 plane: $k_1 = k\sin(\theta)$
$k_3 = k\cos(\theta)$



$$\vec{N}_g = \frac{c^2}{\omega}k\left(\frac{\sin(\theta)}{n_e^2}, \frac{\cos(\theta)}{n_o^2}\right) = |\vec{N}_g|\,(\sin\theta', \cos\theta') \Rightarrow \boxed{\tan(\theta') = \frac{n_o^2}{n_e^2}\tan(\theta)}$$

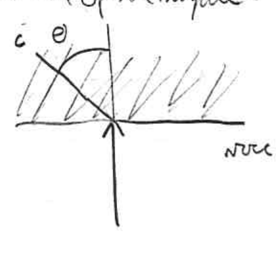
$\vec{N}_g$ <u>does not</u> point along $\hat{k}$!

<u>Example</u>: Suppose a crystal is cut with c-axis at $\theta = 30°$ from the normal of the surface. What happens to light incident normal to the surface?

$n_o = 1.5$, $n_e = 1.6$.

$\tan(\theta) = \tan(30°) = \frac{1}{\sqrt{3}}$

$\tan(\theta') = \left(\frac{1.5}{1.6}\right)^2 \frac{1}{\sqrt{3}} = 0.507 \Rightarrow \theta' = 26.9°$

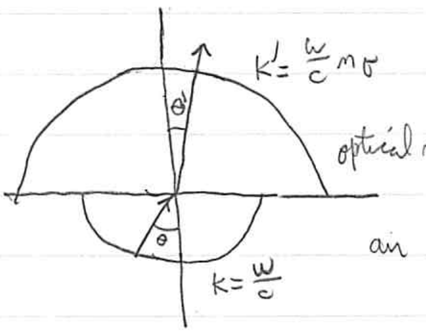


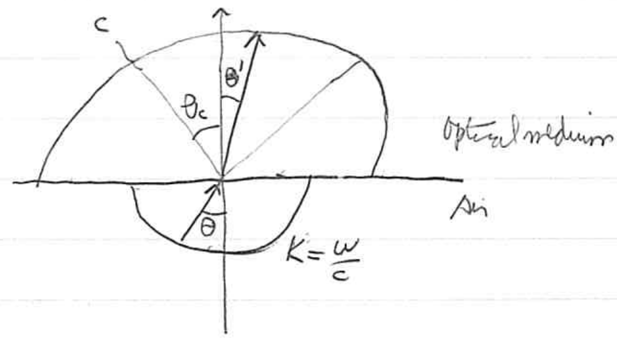
Double refraction!

Generalized Snell's law

General rule for refraction at an interface: $\begin{cases} \omega \text{ is the same in both sides;} \\ \text{In plane component of } \vec{k} \; (k_{\parallel}) \text{ must be conserved;} \\ \text{Normal component of } \vec{k} \, (k_{\perp}) \text{ need not be conserved;} \end{cases}$

⇒ Photon momentum perpendicular to surface is not conserved because the surface "recoils" when light hits it.





Ordinary ray

$$K' \sin(\theta') = K \sin\theta$$

$$\frac{\omega}{c} n_o \sin(\theta') = \frac{\omega}{c} \sin\theta$$

$$\boxed{n_o \sin(\theta') = \sin\theta}$$

Usual Snell's law.

Angle between ray and c-axis: $\tilde{\theta} \equiv \theta_c + \theta'$

Eqn of the Ellipse: From (☆) ⇒ $\frac{[K'\cos(\tilde{\theta})]^2}{n_o^2} + \frac{[K'\sin(\tilde{\theta})]^2}{n_e^2} = \frac{\omega^2}{c^2}$

Matching in plane components:

$$K \sin(\theta) = K' \sin(\theta') \Rightarrow K' = \frac{K \sin(\theta)}{\sin(\theta')}$$

Subst. this into ellipse:

$$\frac{1}{n_o^2}\left[K \frac{\sin(\theta)}{\sin(\theta')} \cos(\tilde{\theta})\right]^2 + \frac{1}{n_e^2}\left[K \frac{\sin(\theta)}{\sin(\theta')} \sin(\tilde{\theta})\right]^2 = \frac{\omega^2}{c^2} = K^2$$

$$\Rightarrow \frac{\sin^2(\theta)}{\sin^2(\theta')}\left[\frac{\sin^2(\tilde{\theta})}{n_e^2} + \frac{\cos^2(\tilde{\theta})}{n_o^2}\right] = 1$$

$$\boxed{\sin(\theta) = \frac{1}{\underbrace{\sqrt{\frac{\sin^2(\tilde{\theta})}{n_e^2} + \frac{\cos^2(\tilde{\theta})}{n_o^2}}}_{n(\tilde{\theta})}} \sin(\theta')}$$

generalized Snell's law.

$\tilde{\theta} = \theta_c + \theta'$

Note: when $n_e = n_o$ ⇒ get usual Snell's law.