PHY 712 Electrodynamics
9-9:50 AM MWF Olin 105

Plan for Lecture 33:

Special Topics in Electrodynamics:

Some optical properties of materials

23	Fri: 03/22/2019	Chap. 9 and 10	Radiation from oscillating sources	#17	3/27/2019
24	Mon: 03/25/2019	Chap. 11	Special Theory of Relativity	Pick topic	3/29/2019
25	Wed: 03/27/2019	Chap. 11	Special Theory of Relativity	#18	4/01/2019
26	Fri: 03/29/2019	Chap. 11	Special Theory of Relativity	#19	4/03/2019
27	Mon: 04/01/2019	Chap. 14	Radiation from accelerating charged particles	#20	4/05/2019
28	Wed: 04/03/2019	Chap. 14	Synchrotron radiation		
29	Fri: 04/05/2019	Chap. 14	Synchrotron radiation	#21	4/10/2019
30	Mon: 04/08/2019	Chap. 15	Radiation from collisions of charged particles	#22	4/12/2019
31	Wed: 04/10/2019	Chap. 13	Cherenkov radiation		
32	Fri: 04/12/2019		Special topic: E & M aspects of superconductivity		
33	Mon: 04/15/2019		Special topic: Aspects of optical properties of materials		
34	Wed: 04/17/2019	Chap. 1-15	Review		
	Fri: 04/19/2019	No class	*Good Friday*		
35	Mon: 04/22/2019	Chap. 1-15	Review		
36	Wed: 04/24/2019	Chap. 1-15	Review		
	Fri: 04/26/2019		Presentations I		
	Mon: 04/29/2019		Presentations II		
	Wed: 05/01/2019		Presentations III		

Schedule for PHY 712 presentations
Friday, April 26, 2019

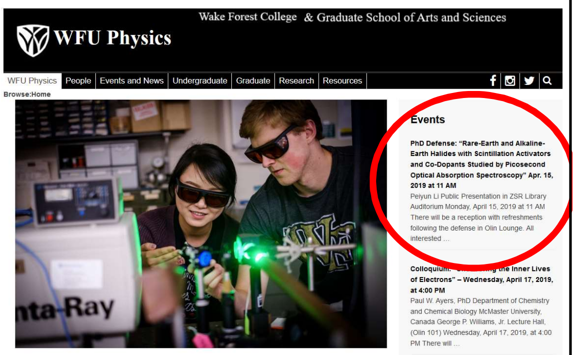
	Name	Topic
9:00-9:16	Ian Newsome	Current density from particle production in classical background E-field coupled to quantum scalar field. :)
9:17-9:31	Dizhou Wu	Ewald
9:32-9:48	Leda Gao	Hyperfine Hamiltonian

Monday, April 29, 2019

	Name	Topic
9:00-9:16	Shohreh Gholizadeh	3D FEM
9:17-9:31	Lindsey Gray	
9:32-9:48		

Wednesday, May 1, 2019

	Name	Topic
9:00-9:16	Eric	TBD
9:17-9:31	Ryan	Planetary Magnetism?
9:32-9:48		



04/15/2019 PHY 712 Spring 2019 -- Lecture 33 4

Aspects of optical properties of solids

1. **Quantum effects cause discrete energy levels for electrons; EM radiation can couple the ground state of a material to its excited states**
2. **In solid materials with ~10^{23} atoms, discrete states become bands of states**
   a. **Metals**
   b. **Insulators**
3. **Anisotropic effects**
4. **Non-linear effects**

Note: We can analyze effectively single particle systems with high accuracy. Analysis of several/many particle systems can be accomplished with a series of approximations. We will use a linear combination of atomic orbital approach to get the qualitative picture.

04/15/2019 PHY 712 Spring 2019 -- Lecture 33 5

Electronic structure of an atom

For simplicity we will first consider a single electron system; a H-like ion with atomic charge *Ze and one electron of charge –e:*

According to Quantum Mechanics:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$H\Psi_{nlm}(r,\theta,\phi) = E_{nlm}\Psi_{nlm}(r,\theta,\phi)$$

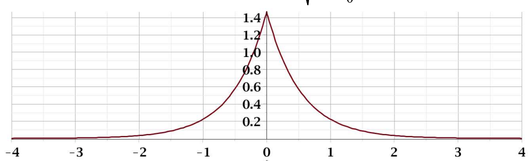
$$E_{nlm} = -\frac{Z^2e^2}{4\pi\epsilon_0 a_0}\frac{1}{2n^2} \equiv \frac{E_{100}}{n^2} \qquad a_0 \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2}$$

E_{100}=-13. 60569253 Z^2 eV
a_0 = 0. 52917721092 Å

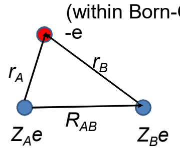
04/15/2019 PHY 712 Spring 2019 -- Lecture 33 6

Probability amplitude for electron in the ground state:

$$\Psi_{100}(r,\theta,\phi) = \sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0}$$



Now consider one electron in the presence of two H-like ions:
Electronic structure of H-like molecular ion
(within Born-Oppenheimer approximation)



$r_A = |\mathbf{r} - \mathbf{R}_A|$ $r_B = |\mathbf{r} - \mathbf{R}_B|$
$R_{AB} = |\mathbf{R}_B - \mathbf{R}_A|$

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Z_A e^2}{4\pi\epsilon_0 r_A} - \frac{Z_B e^2}{4\pi\epsilon_0 r_B} + \frac{Z_A Z_B e^2}{4\pi\epsilon_0 R_{AB}}$$

Approximate wavefunction:

$$\Psi(\mathbf{r},\mathbf{R}_A,\mathbf{R}_B) = X_A \Psi_{100}(\mathbf{r}-\mathbf{R}_A) + X_B \Psi_{100}(\mathbf{r}-\mathbf{R}_B)$$

X_A and X_B can be determined variationally by optimizing

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Electronic structure of H-like molecular ion – continued
Ref. Pauling and Wilson, *Introduction to Quantum Mechanics* (1935) (now published by Dover)

Necessary integrals:

$$\Delta \equiv \int d^3r \Psi^*_{100}(\mathbf{r}-\mathbf{R}_A)\Psi_{100}(\mathbf{r}-\mathbf{R}_B)$$

$$H_{AA} \equiv \int d^3r \Psi^*_{100}(\mathbf{r}-\mathbf{R}_A) H \Psi_{100}(\mathbf{r}-\mathbf{R}_A) = H_{BB}$$

$$H_{AB} \equiv \int d^3r \Psi^*_{100}(\mathbf{r}-\mathbf{R}_A) H \Psi_{100}(\mathbf{r}-\mathbf{R}_B)$$

Generalized eigenvalue problem for energy E in the variational approximation:

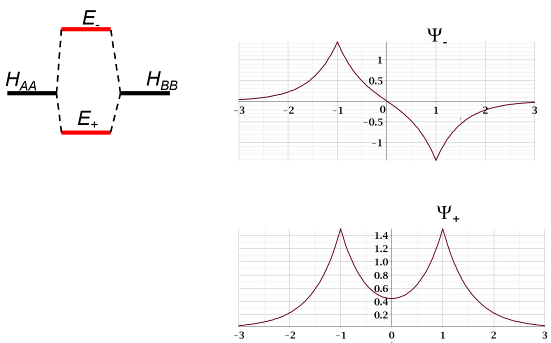
$$\begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix}\begin{pmatrix} X_A \\ X_B \end{pmatrix} = E\begin{pmatrix} 1 & \Delta \\ \Delta & 1 \end{pmatrix}\begin{pmatrix} X_A \\ X_B \end{pmatrix}$$

Eigenstates:

$$\begin{pmatrix} X_A \\ X_B \end{pmatrix}_+ = \frac{1}{\sqrt{2(1+\Delta)}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \mathrm{E}_+ = \frac{H_{AA}+H_{AB}}{1+\Delta}$$

$$\begin{pmatrix} X_A \\ X_B \end{pmatrix}_- = \frac{1}{\sqrt{2(1-\Delta)}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \mathrm{E}_+ = \frac{H_{AA}-H_{AB}}{1-\Delta}$$

Electronic structure of H-like molecular ion – continued

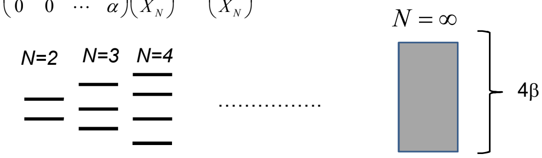


Formation of "energy bands" with a large number of atoms --

Extension of approximate "linear combination of atomic orbital" idea to larger systems

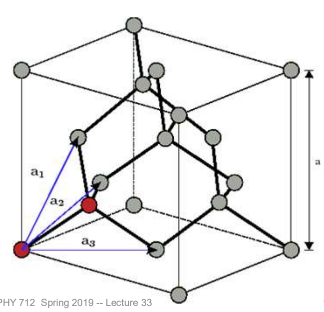
Idealized model Hamiltonian with only nearest neighbor interactions:

$$\begin{pmatrix} \alpha & \beta & \cdots & 0 \\ \beta & \alpha & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \alpha \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{pmatrix} = E \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{pmatrix}$$



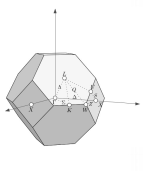
In practice, the "energy band" structure of materials is affected by competing effects of structure and composition

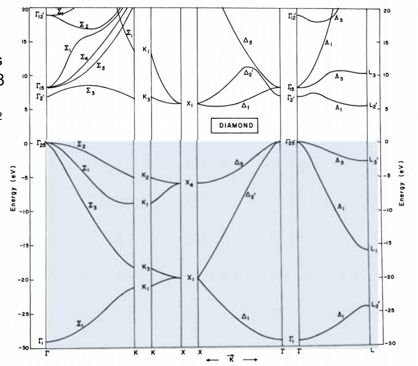
Example: Diamond lattice (2 C atoms per unit cell)



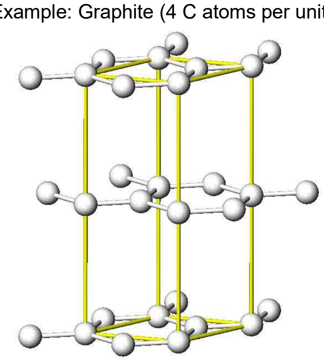
Ref. PRB **2**, 2054 (1970) $E_n(k)$

Note: Valence bands must accommodate 8 valence electrons from two C $1s^2 2s^2 2p^2$ atoms per unit cell



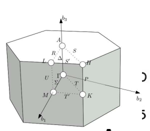


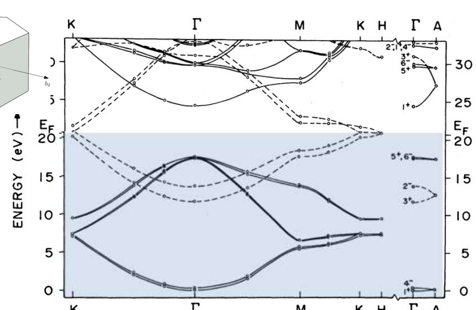
Example: Graphite (4 C atoms per unit cell)



Ref. *PRB* **26**, 5382 (1982)

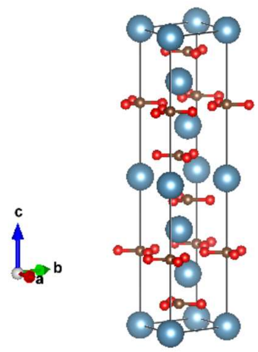
Note: Valence bands must accommodate 16 valence electrons from four C $1s^2 2s^2 2p^2$ atoms per unit cell



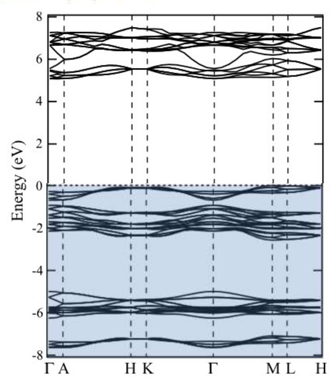


Band diagram for graphite

Example: Calcite $CaCO_3$

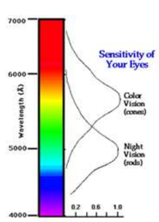


F.M. Hossain et al. / Solid State Communications 149 (2009) 1201–1203

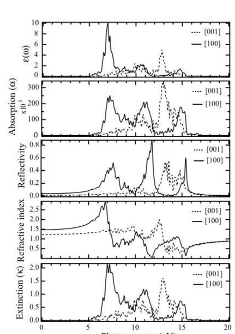


$CaCO_3$
Calculated optical properties

2 eV



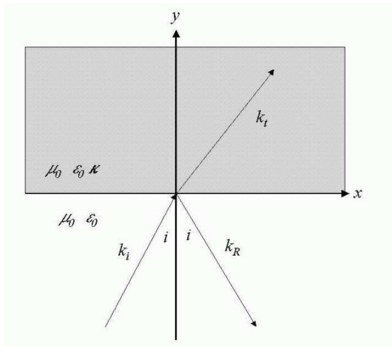
3 eV



n_o=1.7
n_e=1.5

Fig. 3. The frequency dependent optical properties evaluated for the two directions (dashed and solid lines are along [001] and [100] directions respectively) of incoming light w.r.t. the crystal axis.

Reflectance and transmittance in an anisotropic crystal --



Consider the problem of determining the reflectance from an anisotropic medium with isotropic permeability μ_0 and anisotropic permittivity $\varepsilon_0\,\boldsymbol{\kappa}$ where:

$$\boldsymbol{\kappa} \equiv \begin{pmatrix} \kappa_{xx} & 0 & 0 \\ 0 & \kappa_{yy} & 0 \\ 0 & 0 & \kappa_{zz} \end{pmatrix}$$

By assumption, the wave vector in the medium is confined to the *x-y* plane and will be denoted by

$$\mathbf{k}_t \equiv \frac{\omega}{c}(n_x\hat{\mathbf{x}} + n_y\hat{\mathbf{y}}), \text{where } n_x \text{ and } n_y \text{ are to be determined.}$$

The electric field inside the medium is given by:

$$\mathbf{E} = (E_x\hat{\mathbf{x}} + E_y\hat{\mathbf{y}} + E_z\hat{\mathbf{z}})e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}.$$

Inside the anisotropic medium, Maxwell's equations are:

$$\nabla \cdot \mathbf{H} = 0 \qquad \nabla \cdot \boldsymbol{\kappa} \cdot \mathbf{E} = 0$$

$$\nabla \times \mathbf{E} - i\omega\mu_0\mathbf{H} = 0 \qquad \nabla \times \mathbf{H} + i\omega\epsilon_0\boldsymbol{\kappa} \cdot \mathbf{E} = 0$$

After some algebra, the equation for **E** is:

$$\begin{pmatrix} \kappa_{xx} - n_y^2 & n_x n_y & 0 \\ n_x n_y & \kappa_{yy} - n_x^2 & 0 \\ 0 & 0 & \kappa_{zz} - (n_x^2 + n_y^2) \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} = 0.$$

From **E, H** can be determined from

$$\mathbf{H} = \frac{1}{\mu_0 c}\left\{E_z(n_y\hat{\mathbf{x}} - n_x\hat{\mathbf{y}}) + (E_y n_x - E_x n_y)\hat{\mathbf{z}}\right\} e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}.$$

The fields for the incident and reflected waves are the same as for the isotropic case.

$$\mathbf{k}_i = \frac{\omega}{c}(\sin i\hat{\mathbf{x}} + \cos i\hat{\mathbf{y}}),$$

$$\mathbf{k}_R = \frac{\omega}{c}(\sin i\hat{\mathbf{x}} - \cos i\hat{\mathbf{y}}).$$

Note that, consistent with Snell's law: $n_x = \sin i$
Continuity conditions at the *y=0* plane must be applied for the following fields:

$$\mathbf{H}(x,0,z,t),\ E_x(x,0,z,t),\ E_z(x,0,z,t),\ \text{and}\ D_y(x,0,z,t).$$

There will be two different solutions, depending of the polarization of the incident field.

Solution for s-polarization

$$E_x = E_y = 0 \qquad \Rightarrow n_y^2 = \kappa_{zz} - n_x^2$$

$$\mathbf{E} = E_z\hat{\mathbf{z}}e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t} \qquad \mathbf{H} = \frac{1}{\mu_0 c}\left\{E_z(n_y\hat{\mathbf{x}} - n_x\hat{\mathbf{y}})\right\}e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}$$

E_z must be determined from the continuity conditions:

$$E_0 + E_0'' = E_z \qquad (E_0 - E_0'')\cos i = E_z n_y \qquad (E_0 + E_0'')\sin i = E_z n_x$$

$$\frac{E_0''}{E_0} = \frac{\cos i - n_y}{\cos i + n_y}.$$

$$\frac{E_z}{E_0} = \frac{2\cos i}{\cos i + n_y}.$$

Some details for s-polarization

$$\mathbf{E}_0 = E_0\hat{\mathbf{z}}\ e^{i\frac{\omega}{c}(\sin i\ x + \cos i\ y) - i\omega t} \qquad \mathbf{E}_0^{"} = E_0^{"}\hat{\mathbf{z}}\ e^{i\frac{\omega}{c}(\sin i\ x - \cos i\ y) - i\omega t}$$

$$\mathbf{H}_0 = \frac{E_0}{\mu_0 c}\left(\hat{\mathbf{x}}\cos i - \hat{\mathbf{y}}\sin i\right)e^{i\frac{\omega}{c}(\sin i\ x + \cos i\ y) - i\omega t}$$

$$\mathbf{H}_0^{"} = \frac{E_0^{"}}{\mu_0 c}\left(-\hat{\mathbf{x}}\cos i - \hat{\mathbf{y}}\sin i\right)e^{i\frac{\omega}{c}(\sin i\ x - \cos i\ y) - i\omega t}$$

$$\mathbf{E} = E_z\hat{\mathbf{z}}e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t} \qquad \mathbf{H} = \frac{1}{\mu_0 c}\left\{E_z(n_y\hat{\mathbf{x}} - n_x\hat{\mathbf{y}})\right\}e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}$$

Continuity conditions:

$$E_0 + E_0'' = E_z \qquad (E_0 - E_0'')\cos i = E_z n_y \qquad (E_0 + E_0'')\sin i = E_z n_x$$

Solution for p-polarization

$$E_z = 0 \quad \Rightarrow n_y^2 = \frac{\kappa_{xx}}{\kappa_{yy}}(\kappa_{yy} - n_x^2).$$

Note that for $\kappa_{xx} = \kappa_{yy}$

$$n_y = \sqrt{\kappa_{xx} - sin^2 i}$$

$$\mathbf{E} = E_x \left(\hat{\mathbf{x}} - \frac{\kappa_{xx} n_x}{\kappa_{yy} n_y} \hat{\mathbf{y}} \right) e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}.$$

$$\mathbf{H} = -\frac{E_x}{\mu_0 c} \frac{\kappa_{xx}}{n_y} \hat{\mathbf{z}} e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}.$$

E_x must be determined from the continuity conditions:

$$(E_0 - E_0'')\cos i = E_x \quad (E_0 + E_0'') = \frac{\kappa_{xx}}{n_y} E_x \quad (E_0 + E_0'')\sin i = \frac{\kappa_{xx} n_x}{n_y} E_x.$$

$$\frac{E_0''}{E_0} = \frac{\kappa_{xx}\cos i - n_y}{\kappa_{xx}\cos i + n_y}. \qquad \frac{E_x}{E_0} = \frac{2\kappa_{xx}\cos i}{\kappa_{xx}\cos i + n_y}.$$

Some details for p-polarization

$$\mathbf{E}_0 = E_0 \left(\hat{\mathbf{x}}\cos i - \hat{\mathbf{y}}\sin i \right) e^{i\frac{\omega}{c}(\sin i\, x + \cos i\, y) - i\omega t}$$

$$\mathbf{E}_0'' = E_0'' \left(-\hat{\mathbf{x}}\cos i - \hat{\mathbf{y}}\sin i \right) e^{i\frac{\omega}{c}(\sin i\, x - \cos i\, y) - i\omega t}$$

$$\mathbf{H}_0 = -\frac{E_0}{\mu_0 c} \hat{\mathbf{z}}\, e^{i\frac{\omega}{c}(\sin i\, x + \cos i\, y) - i\omega t} \qquad \mathbf{H}_0'' = -\frac{E_0''}{\mu_0 c} \hat{\mathbf{z}}\, e^{i\frac{\omega}{c}(\sin i\, x - \cos i\, y) - i\omega t}$$

$$\mathbf{E} = E_x \left(\hat{\mathbf{x}} - \frac{\kappa_{xx} n_x}{\kappa_{yy} n_y} \hat{\mathbf{y}} \right) e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t} \qquad \mathbf{H} = -\frac{E_x}{\mu_0 c} \frac{\kappa_{xx}}{n_y} \hat{\mathbf{z}} e^{i\frac{\omega}{c}(n_x x + n_y y) - i\omega t}.$$

Continuity conditions:

$$(E_0 - E_0'')\cos i = E_x \quad (E_0 + E_0'') = \frac{\kappa_{xx}}{n_y} E_x \quad (E_0 + E_0'')\sin i = \frac{\kappa_{xx} n_x}{n_y} E_x.$$