3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

3.23 Fall 2007 – Lecture 23

FERMI'S GOLDEN RULE

Study

- Fox, Optical Properties of Solids: 3.1 to 3.6 (skip 3.3.5 and 3.3.6), 4.1, 4.2, and Appendix B.2

Boundary conditions

$$\hat{n}\cdot\left(\vec{B}_2 - \vec{}_1\right) = 0$$

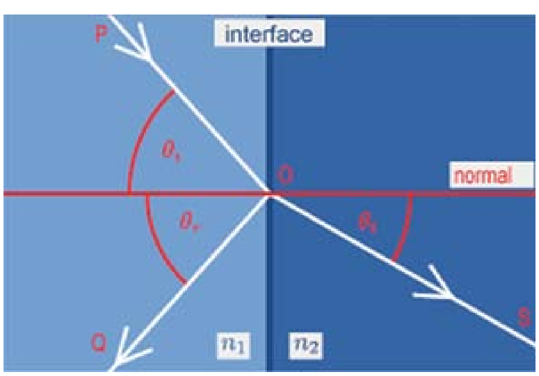
$$\hat{n}\cdot\left(\vec{D}_2 - \vec{D}_1\right) = \sigma \ \ (\sigma = \text{surface charge density})$$

$$\hat{n}\times\left(\vec{E}_2 - \vec{E}_1\right) = 0$$

$$\hat{n}\times\left(\vec{H}_2 - \vec{H}_1\right) = \vec{K}$$

$$\left(\vec{K} = \text{surface current density}\right)$$

Snell's law



$$\left(\vec{k}_{1t}\cdot\vec{r}_t\right) = \left(\vec{k}'_{1t}\cdot\vec{r}_t\right) = \left(\vec{k}_{2t}\cdot\vec{r}_t\right)$$

$$\left.\begin{aligned} k_{1z} &= \left|\vec{k}_1\right|\sin\theta_1 = n_1\frac{\omega}{c}\sin\theta_1 \\ k_{2z} &= \left|\vec{k}_2\right|\sin\theta_2 = n_2\frac{\omega}{c}\sin\theta_2 \end{aligned}\right\} n_1\sin\theta_1 = n_2\sin\theta_2$$

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Energy conservation

$$\int \vec{J} \cdot \vec{E} dv + \frac{\partial}{\partial t} \int \underbrace{\left(\vec{E} \cdot \vec{D} + \vec{H} \cdot \vec{B} \right)}_{\substack{\text{total energy stored in electrical} \\ \text{and magnetic field} \\ \text{per volume}}} dv + \int \underbrace{\left(\vec{E} \times \vec{H} \right)}_{\substack{\text{energy surface} \\ \text{flux per unit area}}} \cdot \hat{n} dS = 0$$

$$\vec{S} = \frac{c}{4\pi} \vec{E} \times \vec{H}$$

Optical processes

- Reflection and refraction
- Absorption
- Luminescence
- Scattering

Optical coefficients

POWER PER UNIT AREA

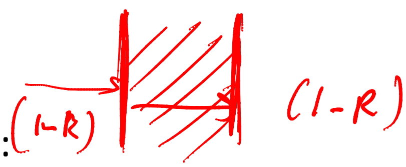
T: ratio of transmitted vs incident power

R+T=1 (no absorption, scattering)

$dI = -\alpha\, dz\, I(z) \Rightarrow I(z) = I_0 e^{-\alpha z}$

Absorption:

Transmission:



αl

$e^{-\alpha l}$

Modeling Optical Constants with a Damped Harmonic Oscillator

$$\varepsilon = (n + ik)^2 = \underbrace{n^2 - k^2}_{\varepsilon_1} + i\,\underbrace{2nk}_{\varepsilon_2}$$

$$\varepsilon = \underbrace{1 + 4\pi\chi + 4\pi \frac{Ne^2\left(\omega_0^2 - \omega^2\right)}{m_0\left(\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2\right)}}_{\varepsilon_1} - i\,\underbrace{4\pi \frac{Ne^2\gamma\omega}{m_0\left(\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2\right)}}_{\varepsilon_2}$$

Amorphous silica

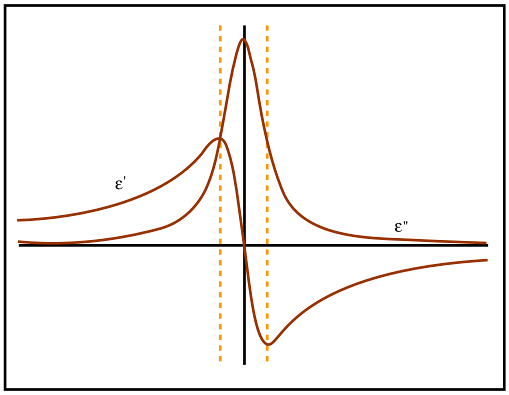
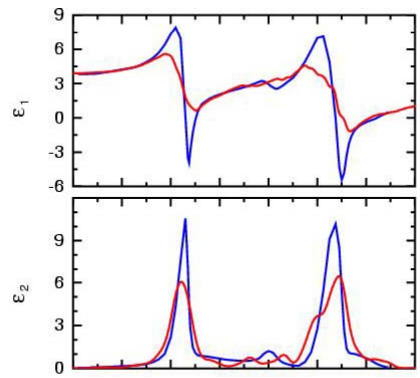


Figure by MIT OpenCourseWare.



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Kramers-Kronig relations

$$n(\omega) = 1 + \frac{1}{\pi} \, \mathsf{P} \int_{-\infty}^{\infty} \frac{\kappa(\omega')}{\omega' - \omega} \, d\omega'$$

$$\kappa(\omega) = -\frac{1}{\pi} \, \mathsf{P} \int_{-\infty}^{\infty} \frac{n(\omega') - 1}{\omega' - \omega} \, d\omega'$$

Optical materials

Infrared active modes

Excitations across this gap

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Please see: Fig. 1.4 in Fox, Mark. *Optical Properties of Solids.* Oxford, England: Oxford University Press, 2001.

Infrared active modes

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Please see Fig. 1a and 2a in Giannozzi, Paolo, et al. "*Ab initio* Calculation of Phonon Dispersions in Semiconductors." *Physical Review B* 43 (March 15, 1991): 7231-7242.

Optical materials

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Please see: Fig. 1.7 in Fox, Mark. *Optical Properties of Solids*. Oxford, England: Oxford University Press, 2001.

Optical materials

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Please see: Fig. 1.5 in Fox, Mark. *Optical Properties of Solids*. Oxford, England: Oxford University Press, 2001.

Interband absorption

$E_f - E_i = \hbar\omega$

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Please see: Fig. 3.1 in Fox, Mark. *Optical Properties of Solids.* Oxford, England: Oxford University Press, 2001.

Direct and indirect transitions

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Please see: Fig. 3.2 in Fox, Mark. *Optical Properties of Solids.* Oxford, England: Oxford University Press, 2001.

Transition rate for direct absorption

$$W_{i\to f} = \frac{2\pi}{\hbar} |M_{if}|^2 g(\hbar\omega)$$

$$\delta(E_f - E_i - \hbar\omega)$$

$$M = \langle f | H' | i \rangle$$

$$H' \Rightarrow -\vec{d}\cdot\vec{\mathcal{E}} = e\vec{r}\cdot\vec{\mathcal{E}}$$

Transition rates: perturbing Hamiltonian

$$\vec{p} \mapsto \vec{p} - q\vec{A}$$

$$\frac{p^2}{2m} \to \frac{1}{2m}(\vec{p} + e\vec{A})^2 \Rightarrow \hat{H}' = \frac{e}{2m}(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p})$$

$$\frac{e^2}{2m}A^2$$

$$[\vec{p}\cdot\vec{A} - \vec{A}\cdot\vec{p}]\psi =$$

$$= -i\hbar[\vec{\nabla}\cdot(\vec{A}\psi) - \vec{A}\cdot\vec{\nabla}\psi]$$

$$= -i\hbar[\psi\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}\psi - \vec{A}\vec{\nabla}\psi]$$

$$\vec{\nabla}\cdot\vec{A} = 0$$

$$\frac{e}{m}(\vec{p}\cdot\vec{A})$$

Transition rates: perturbing Hamiltonian

$$\frac{e}{m}\langle f^{(r,t)}|\vec{p}\cdot\vec{A}|i^{(r,t)}\rangle \quad \delta(E_f - E_i - \hbar\omega)$$

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t}$$

$$\vec{A}(\vec{r},t) = \vec{A}_0 e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

$$\frac{e}{m}\langle f|\vec{p}\cdot\vec{A}_0 e^{i\vec{k}\cdot\vec{r}}|i\rangle$$

$$e^{i\vec{k}\cdot\vec{r}} \cong 1 \Rightarrow e\langle f|\frac{d\vec{r}}{dt}|i\rangle\cdot\vec{A}_0$$

$$\vec{p} = m\frac{d\vec{r}}{dt}$$

$$\frac{dr}{dt} = \frac{i}{\hbar}[H_0, \vec{r}]$$

$$\frac{ie}{\hbar}\langle f|[H_0, r]|i\rangle\cdot\vec{A} = \frac{ie}{\hbar}(E_f - E_i)\langle f|\vec{r}|i\rangle\cdot\vec{A}$$

Transition rate for direct absorption

$$M_{12} = ie\frac{(E_f - E_i)}{\hbar}\langle f|\vec{r}|i\rangle\cdot\vec{A}_0$$

$$E = -\frac{\partial A}{\partial t} \qquad \vec{E}_0 = i\omega\vec{A}_0$$

$$= +e\frac{(E_f - E_i)}{\omega\hbar}\vec{E}_0\langle f|\vec{r}|i\rangle$$

$$= +e\,\vec{E}_0\,\langle f|\vec{r}|i\rangle$$