

MIT OpenCourseWare
<http://ocw.mit.edu>

3.23 Electrical, Optical, and Magnetic Properties of Materials

Fall 2007

For information about citing these materials or our Terms of Use, visit: <http://ocw.mit.edu/terms>.

3.23 Fall 2007 – Lecture 23

FERMI'S GOLDEN RULE

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Boundary conditions

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

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

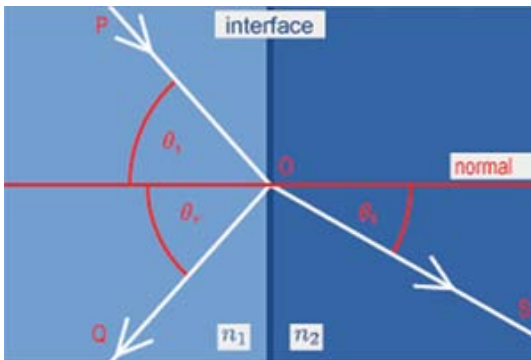
$$\hat{n} \times (\vec{E}_2 - \vec{E}_1) = 0$$

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

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Snell's law



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

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

Image from Wikimedia Commons, <http://commons.wikimedia.org>

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Energy conservation

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

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Optical processes

- Reflection and refraction
- Absorption
- Luminescence
- Scattering

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Optical coefficients

T: ratio of transmitted vs incident power

R+T=1 (no absorption, scattering)

Absorption:

Transmission:

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Modeling Optical Constants with a Damped Harmonic Oscillator

$$\epsilon = (n + ik)^2 = \underbrace{n^2 - k^2}_{\epsilon_1} + i \underbrace{2nk}_{\epsilon_2}$$

$$\epsilon = 1 + 4\pi\chi + 4\pi \underbrace{\frac{Ne^2(\omega_0^2 - \omega^2)}{m_0((\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2)}}_{\epsilon_1} - i4\pi \underbrace{\frac{Ne^2\gamma\omega}{m_0((\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2)}}_{\epsilon_2}$$

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Amorphous silica

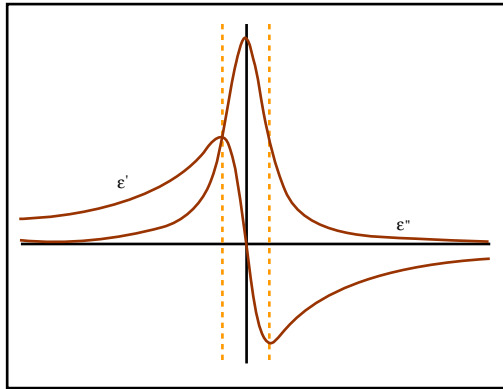
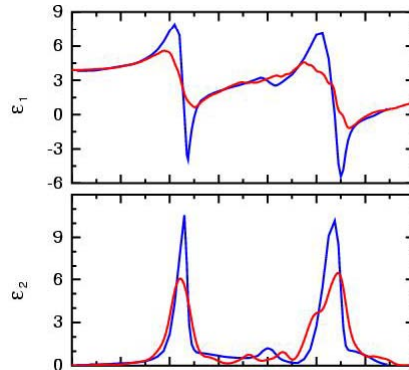


Figure by MIT OpenCourseWare.



Courtesy of Elsevier, Inc., <http://www.sciencedirect.com>.
Used with permission.

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Kramers-Kronig relations

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

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Optical materials

Image removed due to copyright restrictions.

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Infrared active modes

Image removed due to copyright restrictions.

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.

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Optical materials

Image removed due to copyright restrictions.

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Optical materials

Image removed due to copyright restrictions.

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Interband absorption

Image removed due to copyright restrictions.

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Direct and indirect transitions

Image removed due to copyright restrictions.

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

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Transition rate for direct absorption

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Transition rates: perturbing Hamiltonian

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Transition rates: perturbing Hamiltonian

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)

Transition rate for direct absorption

3.23 Electronic, Optical and Magnetic Properties of Materials - Nicola Marzari (MIT, Fall 2007)