3.024 Electrical, Optical, and Magnetic Properties of Materials Spring 2012
Recitation 15
Outline:

Final Exam Toolbox Review
1. Quantum Mechanics
    a) Fundamental Postulates & Schrödinger's Equation
    b) Fundamental Systems by Hamiltonian
    c) Periodic Potentials: Bloch Waveforms & Electronic Band Diagrams
2. Solid State Physics
    a) Density of States & Fermi-Dirac Distribution
    b) Charge Carrier Density in Semi-Conductors (Intrinsic & Extrinsic)
    c) ***p-n*** Junction Devices: Solar Cells & LEDs
3. Electrodynamics, Optics, & Magnetism
    a) Maxwell's Equations, Constitutive Relations, & The Damped Harmonic Oscillator
    b) Optical Constants, Boundary Conditions, Snell's Law, & Light Interaction with Matter
    c) Origins of Magnetism, Magnetic Hysteresis, & Magnetic Exchange Energy

1. Quantum Mechanics

a) Fundamental Postulates & Schrödinger's Equation

I $\quad (x,t)$ $\int_{-\infty}^{\infty}\psi_n^*(x)\psi_m(x)dx = \begin{cases}1 & n=m\\ 0 & n\neq m\end{cases}$ $(x,t)\ \neq \infty$ If $\psi(x) = \begin{cases}\psi_I(x) & x\epsilon(-\infty,a]\\ \psi_{II}(x) & x\epsilon[a,\infty)\end{cases}$ $\psi_I(a)=\psi_{II}(a)$ $\frac{\partial\psi_I}{\partial x}(a)=\frac{\partial\psi_{II}}{\partial x}(a)$	IV Total State $\quad (x) = \sum_n c_n\psi_n(x)$ $P(a_n) = \lvert\langle\ \ (x)\lvert\psi_n(x)\rangle\rvert^2$ $\lvert\langle\ \ (x)\lvert\psi_n(x)\rangle\rvert^2 = \left\lvert\int_{-\infty}^{\infty}\ \ ^*(x)\psi_n(x)\,dx\right\rvert^2$ $\left\lvert\int_{-\infty}^{\infty}\ \ ^*(x)\psi_n(x)\,dx\right\rvert^2 = \lvert c_n\rvert^2$
II Probability Density $\rho(x) = \psi^*(x)\psi(x)$ $P(a\leq x\leq b) = \int_a^b \psi^*(x)\psi(x)dx$ $1 = \int_{-\infty}^{\infty}\psi^*(x)\psi(x)dx$	V If $\hat{A}\ \ (x) = a_n\psi_n(x) \rightarrow \quad (x) = \psi_n(x)$
III $\langle\psi\lvert\hat{A}\rvert\psi\rangle = \int_{-\infty}^{\infty}\psi^*(x)\hat{A}\psi(x)dx$ $\hat{A}\psi_n(x) = a_n\psi_n(x)$	VI $\quad \hat{H}\ \ (x,t) = i\hbar\frac{\partial\ \ (x,t)}{\partial t}$ $(x,t) = \psi(x)\phi(t)$ $\phi(t) = e^{-i\frac{E}{\hbar}t}$ $\hat{H}\psi(x) = E\psi(x)$

1D Position $\hat{x} \rightarrow x$

1D Momentum $\hat{p}_x \rightarrow -i\hbar\frac{\partial}{\partial x}$

1D Hamiltonian $\hat{H} \rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

<u>Fundamental Constants</u>

$$h = 6.626\times10^{-34}\ \mathrm{J\cdot s} = 4.136\times\ 10^{-15}\mathrm{eV\cdot s} \quad \hbar = \frac{h}{2\pi}$$

$$c_0 = 3.00\times10^8\,\frac{\mathrm{m}}{\mathrm{s}}$$

$$m = 9.11\times10^{-31}\mathrm{kg} = 5.11\times10^5\,\frac{\mathrm{eV}}{\mathrm{c_0^2}}$$

$$k_B = 1.381\times10^{-23}\,\frac{\mathrm{J}}{\mathrm{K}} = 8.617\times10^{-5}\,\frac{\mathrm{eV}}{\mathrm{K}}.$$

b) Fundamental Systems by Hamiltonian

System / Hamiltonian	Eigenenergies	Eigenfunctions
Free Electron $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ $V(x) = 0$	$E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$ $p = \hbar k = \sqrt{2mE}$	$u(x) = Ce^{\pm ikx}$
Particle-In-A-Box $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ $V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x > L \cup x < 0 \end{cases}$	$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} = \frac{h^2 n^2}{8mL^2}$ $n = 1,2,3,\ldots$	$u_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}$ $n = 1,2,3,\ldots$
Simple Harmonic Oscillator $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m\omega^2 x^2}{2}$	$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ $\omega = \sqrt{\frac{K}{m}}$ $n = 0,1,2,\ldots$	$u_n(x) = \sqrt{\frac{1}{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)$ $H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)$ are the Hermite polynomials.
Hydrogen Atom $\hat{H} = -\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{4\pi\epsilon_0 r}$	$E_n = -\frac{E_I}{n^2} \cong -\frac{13.6\text{ eV}}{n^2}$ $n = 1,2,3,\ldots$	$u_n(x) = R_{n,l}(r)Y_l^m(\theta,\phi)$ $l \leq n\,;\, 0 \leq l \leq n-1\,;\, -l+1 \leq m \leq l-1$
Periodic Potential $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_G V_G e^{iGx}$	$E_n(k)$ Energy Band Diagram	$u_{n,k}(x) = e^{ikx}\sum_G C_{k-G}e^{-iGx}$ $-\frac{g}{2} \leq k \leq \frac{g}{2}\,;\, g = \frac{2\pi}{a}$

c) Periodic Potentials: Bloch Waveforms & Electronic Band Diagrams

<u>Periodic Trends</u>

N = Atomic Number

$N \uparrow \rightarrow V \downarrow, a \uparrow, K \downarrow, m \uparrow$

Periodic Potentials

$$V(x) = \sum_G V_G e^{iGx}$$

Central Equation

$$\left(\frac{\hbar^2}{2m}k^2 - E\right)C_k + \sum_G V_G C_{k-G} = 0$$

$$u_{n,k}(x) = e^{ikx}\sum_G C_{k-G}e^{-iGx}$$

Near the band-edge:

$$E_c = E_g + \frac{\hbar^2}{2m_c^*}k^2$$

$$E_v = -\frac{\hbar^2}{2m_c^*}k^2$$

2. Solid State Physics

a) Density of States & Fermi-Dirac Distribution

Finding an ηD system density of states:

First calculate the total number of states *N*

$$N = \#\text{ of Fermions per State (Based off of spin)}\frac{\eta\text{D } k - \text{space volume of entire Brillouin Zone}}{\eta\text{D } k - \text{space volume between atoms}}$$

$$N = 2\frac{Ck^{\eta}}{\left(\frac{2\pi}{L}\right)^{\eta}} = \frac{2Ck^{\eta}L^{\eta}}{(2\pi)^{\eta}}$$

Next use free electron energy to express *N* as a function of *E*

$$k = \frac{\sqrt{2mE}}{\hbar} \rightarrow N = \frac{2C(2mE)^{\frac{\eta}{2}}L^{\eta}}{(2\pi\hbar)^{\eta}}$$

Divide *N* by the ηD real space volume to get the volume state density *n*

$$n = \frac{N}{V} = \frac{N}{L^{\eta}} = \frac{2C(2mE)^{\frac{\eta}{2}}}{(2\pi\hbar)^{\eta}}$$

Finally, find $g(E)$ by taking the derivative of *n* with respect to *E*

$$g(E) = \frac{dn}{dE} = \frac{\eta C(2m)^{\frac{\eta}{2}}}{(2\pi\hbar)^{\eta}}E^{\frac{\eta}{2}-1}$$

The Fermi-Dirac distribution gives the probability at a temperature *T* and energy *E* that a fermion will occupy that state. Electrons are fermions, so we apply this distribution when calculating total charge carrier densities.

$$f(E,T) = \frac{1}{e^{\frac{E-E_F}{k_BT}} + 1}$$

b) Charge Carrier Density in Semi-Conductors (Intrinsic & Extrinsic)

General formula to calculate the electron charge carrier density in material with lowest conduction energy E_0.

$$n(T) = \int_{E_0}^{\infty} f(E,T)g(E)dE$$

For semiconductors, using the degenerate semiconductor approximation, the carrier densities can be calculated as follows:

$$n_c(T) = \int_{E_c}^{\infty} f(E,T)g_c(E)dE$$

$$p_v(T) = \int_{-\infty}^{E_v} (1 - f(E,T))g_v(E)dE$$

$$n_c(T) \cong N_c(T)e^{\frac{-(E_C-\mu)}{k_BT}} \qquad N_c(T) \cong \frac{1}{4}\left(\frac{2m_c^*k_BT}{\pi\hbar^2}\right)^{\frac{3}{2}}$$

$$p_v(T) \cong P_v(T)e^{\frac{(E_v-\mu)}{k_BT}} \qquad P_v(T) \cong \frac{1}{4}\left(\frac{2m_v^*k_BT}{\pi\hbar^2}\right)^{\frac{3}{2}}$$

Law of Mass Action

$$n_c(T)p_v(T) = N_c(T)P_v(T)e^{\frac{-E_g}{k_BT}}$$

Intrinsic SC

$$n_c = p_v = n_i$$

$$n_cp_v = n_i^2 = N_c(T)P_v(T)e^{\frac{-E_g}{k_BT}}$$

$$\mu = \ _F = E_v + \frac{E_g}{2} + \frac{3}{4}k_BT\ln\left(\frac{m_v^*}{m_c^*}\right)$$

Extrinsic SC

p-type material (dopant is electron acceptor)

$$p_v \approx N_A$$

$$n_c \approx \frac{n_i^2}{N_A}$$

$$_F = +\frac{E_g}{2} + \frac{3}{4}k_B T \ln\left(\frac{m_v^*}{m_c^*}\right) - k_B T \ln\left(\frac{N_A}{n_i}\right)$$

n-type material (dopant is electron donor)

$$p_v \approx \frac{n_i^2}{N_D}$$

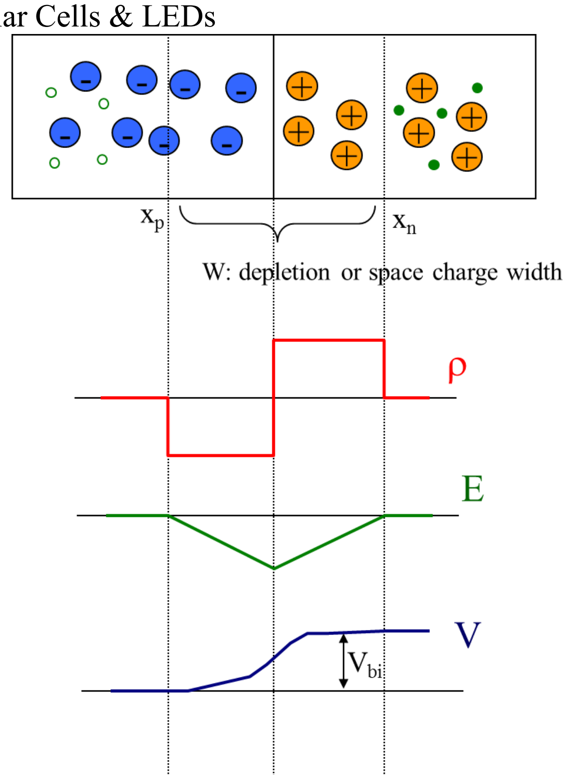
$$n_c \approx N_D$$

$$_F = +\frac{E_g}{2} + \frac{3}{4}k_B T \ln\left(\frac{m_v^*}{m_c^*}\right) + k_B T \ln\left(\frac{N_D}{n_i}\right)$$

Conductivity

$$\sigma = n_c e \mu_e + p_v e \mu_h$$

c) ***p-n*** Junction Devices: Solar Cells & LEDs



$$qV_{BI} = E_{Fn} - E_{Fp}$$

For LEDs

$$I = I_s\left(e^{\frac{qV}{k_B T}} - 1\right)$$

$$h\nu = E_g + \frac{k_B T}{2}$$

For Solar Cells

$$I = I_S\left(e^{\frac{qV}{k_B T}} - 1\right) - I_{PH}(\lambda)$$

3. Electrodynamics, Optics, & Magnetism
   a) Maxwell's Equations, Constitutive Relations, & The Damped Harmonic Oscillator

Maxwell's Equations

$$\vec{\nabla}\cdot\vec{D} = \rho$$
$$\vec{\nabla}\cdot\vec{B} = 0$$
$$\vec{\nabla}\times\vec{E} + \frac{\partial\vec{B}}{\partial t} = 0$$
$$\vec{\nabla}\times\vec{H} - \frac{\partial\vec{D}}{\partial t} = \vec{J}$$

Constitutive Relations

$$\vec{D} = \varepsilon\vec{E} = \varepsilon_0\vec{E} + \vec{P}$$
$$\vec{B} = \mu\vec{H} = \mu_0\vec{H} + \vec{M}$$

Damped Harmonic Oscillator

$$\vec{P} = \frac{\omega_0^2\varepsilon_0\chi_0}{\omega_0^2 - \omega^2 - i\sigma\omega}\vec{E} = \varepsilon_0\chi(\omega)\vec{E}$$
$$\chi = \chi' + i\chi''$$
$$\varepsilon = \varepsilon_0(1+\chi)$$

   b) Optical Constants, Boundary Conditions, Snell's Law, & Light Interaction with Matter

Optical Constants & Relations

$$\frac{1}{c^2} = \mu\varepsilon$$
$$c = \frac{c_0}{n}$$
$$\mu = \mu_r\mu_0$$
$$\varepsilon = \varepsilon_r\varepsilon_0$$
$$\omega = c|\vec{k}| = \frac{c_0}{n}\frac{2\pi}{\lambda}$$
$$n' \equiv n + i\alpha$$
$$\vec{E}\times\vec{H} = \vec{S}$$

Boundary Conditions

$$B_1 = B_2$$
$$\sigma = D_2 - D_1$$
$$\vec{E}_{1||} = \vec{E}_{2||}$$
$$\vec{K} = \vec{H}_{2||} - \vec{H}_{1||}$$

Reflection & Snell's Law

$$\theta_i = \theta_r$$
$$n_1\sin\theta_i = n_2\sin\theta_t$$

Wave Guides

$$\sin\theta_c = \frac{n_2}{n_1} \qquad n\sin\theta_{MAX} = \sqrt{n_1^2 - n_2^2}$$

Anti-Reflective Coatings & Quarter Wave Stacks

$$n_I = \sqrt{n_0 n_S} \qquad d = \frac{\lambda_0}{4n_I}$$

Photonic Dispersion Relationship

$$\cos K(\beta,\omega)a = \frac{1}{2}(M_{11} + M_{22})$$

c) Origins of Magnetism, Magnetic Hysteresis, & Magnetic Exchange Energy

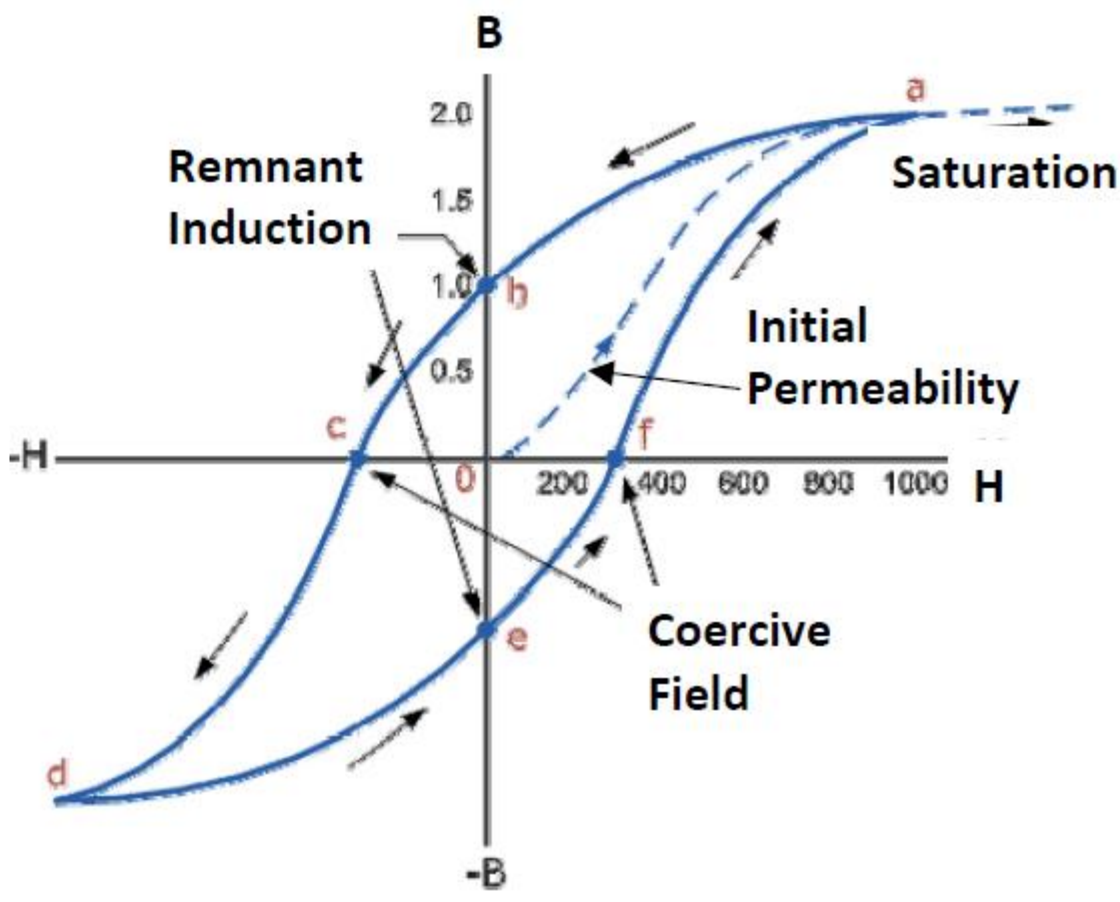
Origins of Magnetism

$$\vec{B} = \mu_0 \vec{H} + \vec{M}$$
$$\vec{M} = \mu_0 \chi_M \vec{H}$$
$$\vec{M} = N\vec{\mu} \neq N q_{mag} \vec{x}$$
$$\mu_B = \gamma \hbar$$
$$\gamma = \frac{q}{2m}$$

Total Angular Momentum

$$\vec{J} = \vec{S} + \vec{L}$$
$$\hat{J}^2 \Psi = \hbar^2 j(j+1) \Psi$$
$$\mu = \mu_B \sqrt{j(j+1)}$$

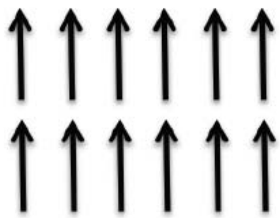
Magnetic Hysteresis



Hard Magnets = High Coercivity
Soft Magnets = Low Coercivity

Magnetic Exchange Energy

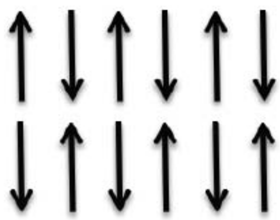
$$\hat{H}_{magnetic} = -\sum_{i,j} J_{ij}\hat{S}_i \cdot \hat{S}_j + \frac{\mu_B}{\hbar}\sum_i \vec{B} \cdot \hat{S}_i = \sum_i \left(-\sum_j J_{ij}\hat{S}_j + \frac{\mu_B}{\hbar}\vec{B} \right) \cdot \hat{S}_i = \sum_i \left(\frac{\mu_B}{\hbar}\left(\vec{B}_{ex} + \vec{B}\right) \right) \cdot \hat{S}_i$$



Ferromagnetic:

$J_{ex} > 0 \Rightarrow$ exchange energy is minimized when $\hat{S}_i \uparrow\uparrow \hat{S}_j$

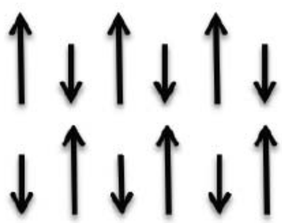
Large spontaneous magnetization at $T < T_C$



Anti-ferromagnetic:

$J_{ex} < 0 \Rightarrow$ exchange energy is minimized when $\hat{S}_i \uparrow\downarrow \hat{S}_j$

No net magnetization, but ordering at $T < T_N$



Ferrimagnetic:

$J_{ex} < 0 \Rightarrow$ exchange energy is minimized when $\hat{S}_i \uparrow\downarrow \hat{S}_j$

Reduced net magnetization (as compared to ferromagnetic materials), spontaneous ordering at $T < T_N$