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

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3.23 Fall 2007 – Lecture 1

WAVES MECHANICS

Courtesy of Jon Sullivan, http://pdphoto.org


The 3.23 Team

• Lectures
• Recitations

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Roadmap

• Sep 6. From particles to waves: the Schrödinger equation
• Sep 11. The mechanics of quantum mechanics: operators, expectation values
• Sep 13. Measurements and probabilities. The harmonic oscillator.
• Sep 18. The hydrogen atom and the periodic table
• Sep 20. Periodicity and phonons
• Sep 25. Electrons in a lattice: Bloch’s theorem
• Sep 27. The nearly-free electron model
• Oct 2. The tight-binding model. Band structures
• Oct 4. Semiconductors and insulators
• Oct 11. Band structure engineering
• Oct 16. Transport of heat and electricity
• Oct 18. Inhomogeneous and hot carriers in semiconductors
• Oct 23. Mid-term exam (during class, 1:30 hours)
• Oct 25. The p-n diode


Roadmap

• Oct 30. Optical materials and refractive index
• Nov 1. Electromagnetism in dielectric media
• Nov 6. Classic propagation of waves
• Nov 8. Interband absorption
• Nov 13. Fundamental of ferromagnetic materials
• Nov 15. Hysteresis loop and driving energies
• Nov 20. Hard materials and permanent magnets
• Nov 27. Soft materials: thin films and nanoparticles. Spintronics and GMR
• Nov 29. Spin valves, spin switches, and spin tunneling
• Dec 4. Excitons
• Dec 6. Luminescence
• Dec 11. Semiconductor quantum wells

• Dec 17 – Dec 21: Final exam (3 hours, date will be fixed by Schedules’ office)

DO NOT BOOK YOUR FLIGHTS YET!

Grading: Exams, Problem Sets

• 30% Problem Sets
• 30% Mid-term Exam (Oct 23)
• 40% Final Exam (Final’s week – Dec 17-21)
• Exams are not “open book”, but you can bring one 2-sided, Letter-sized sheet of mnemonic aids
• For the exams, you’ll probably need a very basic calculator

Academic Integrity

Collaboration Policy for 3.23 - Fall Term 2007

Before preparing your problem set, you are welcome to discuss it with your fellow students.

Data and figures may not be shared.

All writing in a problem set must be original: do not copy any portion from reference material or the problem sets of other students, previous or current.
Textbooks

The class is based on these two required textbooks:

John Singleton
*Band Theory and Electronic Properties of Solids*
Paperback, Oxford University Press (2001)

Mark Fox
*Optical Properties of Solids*
Paperback, Oxford University Press (2001)
(Errata can be found at [www.mark-fox.staff.shef.ac.uk/ops_errata.html](http://www.mark-fox.staff.shef.ac.uk/ops_errata.html))

These can be found at any academic bookstore. They are also available from Oxford University Press ([www.oup.com](http://www.oup.com)). Last, [www.addall.com](http://www.addall.com) is a very good site to compare prices across


Other Textbooks

**Hayden Reserves**

- Stephen Blundell *Magnetism in Condensed Matter*, Oxford University Press
- Ashcroft and Mermin *Solid-state physics*
- Charles Kittel *Introduction to solid-state physics* (Wiley)

**Other**

- Bransden & Joachain *Physics of Atoms and Molecules (2nd ed)*
Life at MIT (@ Prof Fink)

- Your experience should be wonderful and enjoyable (when averaged appropriately 😊)
- Finding an advisor (junior vs. senior, work style, group members, resources...)
- You can change the world! (It might require some work)
- Are you stuck? Unhappy? Making progress? Is it only you?
- What if things don’t work out initially? (what are your options)
- Have a life (friends, home, gym, travel, music, museums...)

Materials Breakthroughs (so 20th century...)

- Steel and cement - building and engines
- Aluminum alloys - air transportation
- Polymers - safe packaging, medical materials
- Silicon - computing
- Cobalt alloys - data storage
- Silica fibers - communications
- Transition-metal alloys – catalytic converters
Advanced Materials


Courtesy Nicola Marzari and Young-Su Lee. Used with permission.

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Physical Origin of Material Properties

Image removed due to copyright restrictions. Please see: Fig. 12 in Landman, Uzi, et al. "Factors in Gold Nanocatalysis: Oxidation of CO in the Non-scalable Size Regime." Topics in Catalysis 44 (June 2007): 145-158.

U. Landman @ Georgia Tech

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From Classical to Quantum

Round Up the Usual Suspects

- Particles and electromagnetic fields
- Forces
- Dynamics
Particles and Fields

- Electrons
- Nuclei (protons, neutrons)

Image courtesy NASA.

Forces

- Electromagnetic interactions
- (Gravity, electroweak, strong)
Dynamics of a Particle

\[ m \frac{d^2 \vec{r}}{dt^2} = F(\vec{r}) \quad \rightarrow \quad \vec{r}(t) \quad \vec{v}(t) \]

The sum of the kinetic and potential energy (E=T+V) is conserved

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Electromagnetic Waves / Photons

\[ E = h\nu = h\frac{c}{\lambda} = kT \]

\( h \) is Planck’s constant = \( 6.626 \times 10^{-34} \) J s

\( k \) is Boltzmann’s constant = \( 1.381 \times 10^{-23} \) J/K

THE ELECTROMAGNETIC SPECTRUM

Penetrates Earth Atmosphere?

Wavelength (meters)

About the size of...

Frequency (Hz)

Temperature of bodies emitting the wavelength (K)

Examples: http://imagers.gsfc.nasa.gov/ems/ems.html
Standard Model of Matter

- Atoms are made by massive, point-like nuclei (protons+neutrons)
- Surrounded by tightly bound, rigid shells of core electrons
- Bound together by a glue of valence electrons (gas vs. atomic orbitals)

Material Properties From First-Principles

- Energy at our living conditions (300 K): 0.04 eV (kinetic energy of an atom in an ideal gas).
- Differences in bonding energies are within one order of magnitude of 0.29 eV (hydrogen bond).
- Binding energy of an electron to a proton (hydrogen): 13.6058 eV = 0.5 atomic units (a.u)
- Everything, from the muscles in our hands to the minerals in our bones is made of atomic nuclei and core electrons bonded together by valence electrons (standard model of matter)
Why do we need quantum mechanics?
Structural properties (fracture in silicon)

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Electronic, optical, magnetic properties

Courtesy of Prof. M. Bawendi and Felice Frankel. Used with permission.
Wave-particle Duality

- Waves have particle-like properties:
  - Photoelectric effect: quanta (photons) are exchanged discretely
  - Energy spectrum of an incandescent body looks like a gas of very hot particles

- Particles have wave-like properties:
  - Quantum mechanics: Electrons in atoms are standing waves – just like the harmonics of an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926...)

Courtesy of flickr user holisticgeek.
Description of a Wave

The wave is an excitation (a vibration): We need to know the amplitude of the excitation at every point and at every instant

\[ \Psi = \Psi(\vec{r}, t) \]

Principle of linear superposition

Wave Interactions

Constructive Interference
- $A_1$
- $A_2$

Destructive Interference
- $A_1 - A_2$

Resultant $A_1 + A_2$

Resultant $A_1 - A_2$

Interference in Action

Figure by MIT OpenCourseWare.

Interference in Action

Figure by MIT OpenCourseWare.

Harmonic Oscillator (I)

A mass on a spring. This system can be represented by a harmonic oscillator.

\[ ma = F \]
\[ m \frac{d^2x(t)}{dt^2} = -\frac{d}{dz} V(z) \]
\[ V(z) = \frac{1}{2} k z^2 \]

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Figure by MIT OpenCourseWare.
Harmonic Oscillator (II)

\[ \frac{\ddot{x}}{m} + \frac{k}{m} x = 0 \]

\[ e^{i\alpha x}, e^{i\beta x} \]

Image from Wikimedia Commons, [http://commons.wikimedia.org](http://commons.wikimedia.org).

Harmonic Oscillator (III)

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Please see any graph of harmonic oscillator position and velocity, such as [http://commons.wikimedia.org/wiki/File:HarmOsc2.png](http://commons.wikimedia.org/wiki/File:HarmOsc2.png).

The total energy of the system

- Kinetic energy $K$

- Potential energy $V$

A Traveling “Plane” Wave

$$\Psi(\vec{r},t) = A \exp[i(\vec{k} \cdot \vec{r} - \omega t)]$$
When is a particle like a wave?

Wavelength • momentum = Planck

\[ \lambda \cdot p = h \]

( \( h = 6.626 \times 10^{-34} \text{ J s} = 2\pi \text{ a.u.} \) )

Time-dependent Schrödinger’s equation

(Newton’s 2nd law for quantum objects)

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + V(\vec{r}, t) \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} \]

1925-onwards: E. Schrödinger (wave equation), W. Heisenberg (matrix formulation), P.A.M. Dirac (relativistic)
Plane waves as free particles

Our free particle \( \Psi(\vec{r}, t) = A \exp[i(\vec{k} \cdot \vec{r} - \omega t)] \) satisfies the wave equation:

\[
\frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} \quad \text{(provided} \quad E = \hbar \omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \text{)}
\]