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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

Nicola Marzari (Instructor)
David Paul (I, Magnetic)
Nicolas Poilvert (TA, Electronic)
Nicephore Bonnet (TA, Optical/Magn)

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 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)
ISBN-10: 0198506449, ISBN-13: 978-0198506447

Mark Fox
Optical Properties of Solids
Paperback, Oxford University Press (2001)
ISBN-10: 0198506120, ISBN-13: 978-0198506126
(Errata can be found at 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). Last, 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 *Quantum Mechanics (2nd ed),* Prentice Hall (2000)**
- **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

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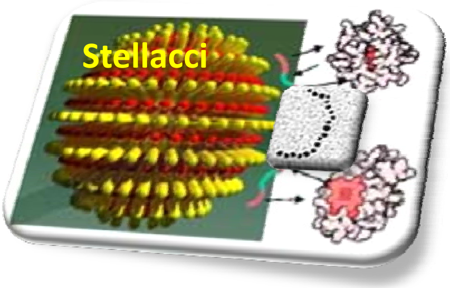
Please see http://mit-pbg.mit.edu/img/NatureFiberWeb.jpg.



Courtesy Francesco Stellacci.
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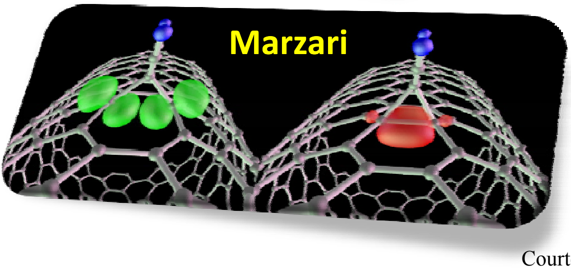
Image removed due to copyright restrictions. Please see any image of the microstructure of nacre, such as http://www.cas.org/ASSETS/E332CE654DC544398C837B46C102CA9D/abalone%20-%20200.jpg.



Courtesy Nicola Marzari and Young-Su Lee.
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Physical Origin of Material Properties

Courtesy flickr user dymero.

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U. Landman @ Georgia Tech

From Classical to Quantum

Round Up the Usual Suspects

- Particles and electromagnetic fields
- Forces
- Dynamics

Particles and Fields

- Electrons
- Nuclei (protons, neutrons)

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Please see http://www.cpepweb.org/images/chart_details/Structure.jpg.

Particles and Fields

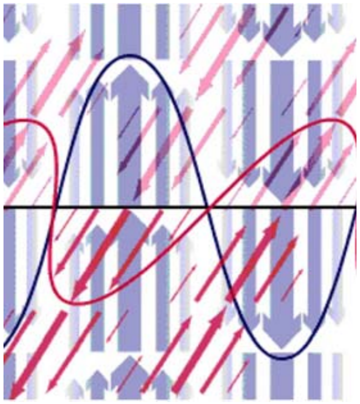


Image courtesy NASA.

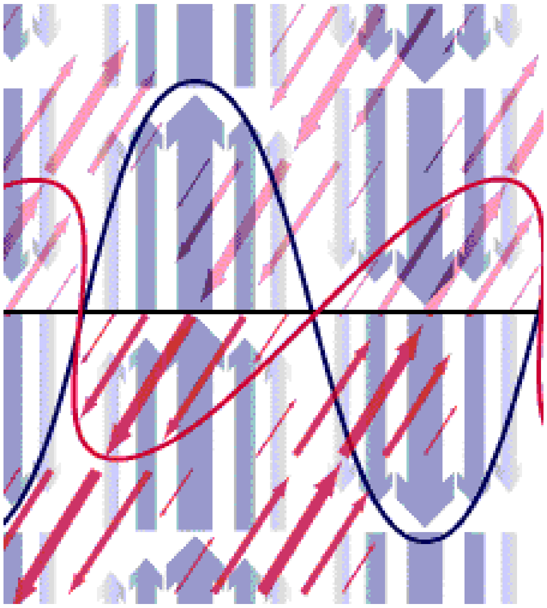


Image courtesy NASA.

Forces

- Electromagnetic interactions
- (Gravity, electroweak, strong)

Dynamics of a Particle

$$m\frac{d^2\vec{r}}{dt^2} = F(\vec{r}) \longrightarrow \begin{matrix}\vec{r}(t)\\ \vec{v}(t)\end{matrix}$$

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

Image from the Open Clip Art Library, http://openclipart.org

Dynamics of a Particle

$$m\frac{d^2\vec{r}}{dt^2} = F(\vec{r}) \longrightarrow \begin{matrix}\vec{r}(t)\\ \vec{v}(t)\end{matrix}$$

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

Electromagnetic Waves / Photons

$$E = h\nu = h\frac{c}{\lambda} = k\mathrm{T}$$

h is Planck's constant = 6.626 10^{-34} J s

k is Boltzmann's constant = 1.381 10^{-23} J/K

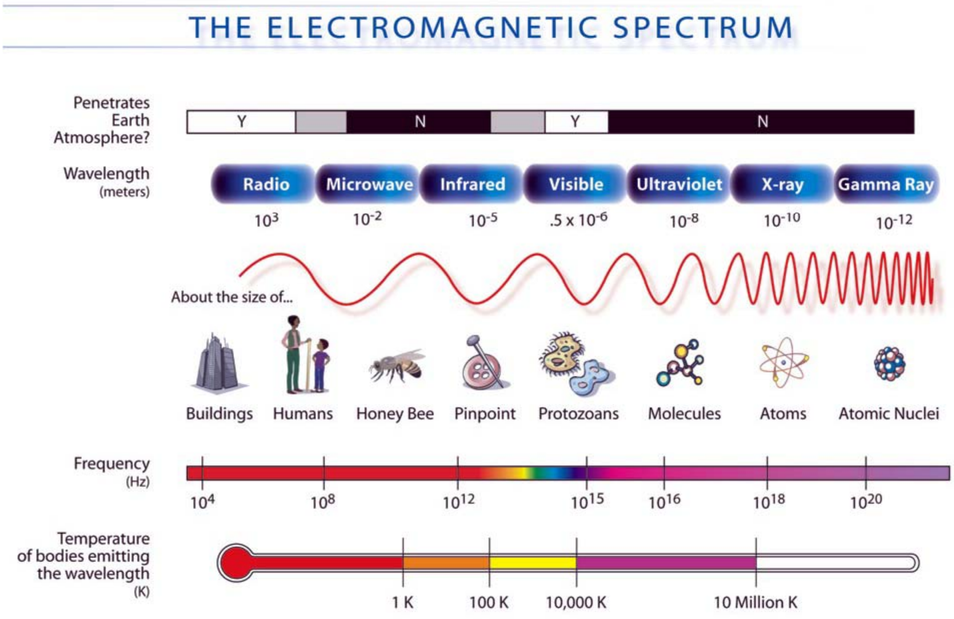


Image courtesy NASA.

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)**

Image removed due to copyright restrictions. Please see http://static.howstuffworks.com/gif/atom-quantum.jpg

Material Properties From First-Principles

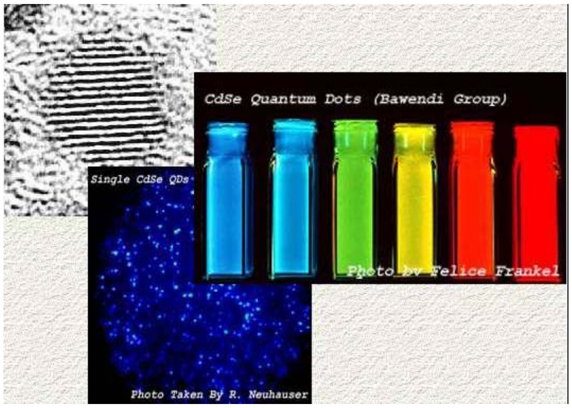
- Energy at our living conditions (300 K): 0.04 eV (kinetic energy of an atom in an ideal gas).
- Differences in bonding energies are within one order of magnitude of 0.29 eV (hydrogen bond).
- Binding energy of an electron to a proton (hydrogen): 13.6058 eV = 0.5 atomic units (a.u)
- Everything, from 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)

Images removed due to copyright restrictions. Please see Fig. 1 and 3 in Pérez, Rubén, and Peter Gumbsch. "Directional Anisotropy in the Cleavage Fracture of Silicon." *Physical Review Letters* 84 (June 5, 2000): 5347-5350.

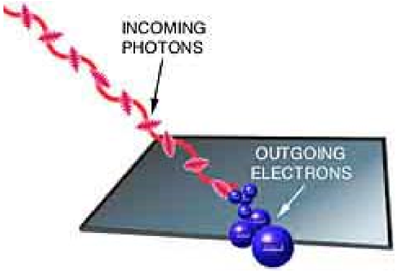
Electronic, optical, magnetic properties



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*



Courtesy Physics 2000, http://www.colorado.edu/physics/2000/cover.html. Used with permission.

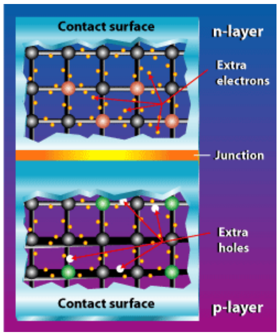
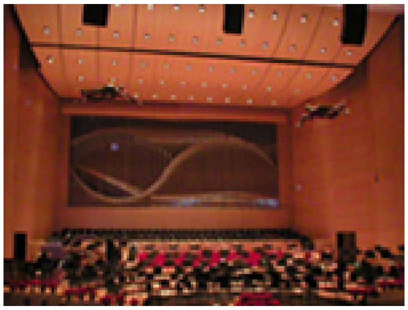


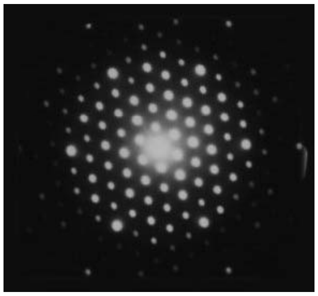
Image courtesy US Dept. of Energy.

Wave-particle Duality

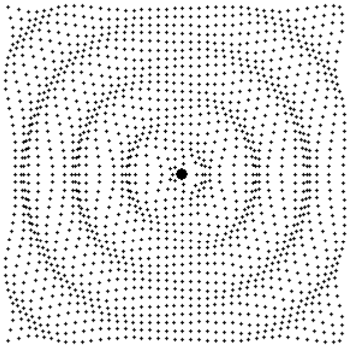
- Particles have wave-like properties:
  - Quantum mechanics: Electrons in atoms are standing waves – just like the harmonics of an organ pipe
  - Electrons beams can be diffracted, and we can see the fringes (Davisson and Germer, at Bell Labs in 1926…)



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

$$\Psi = \Psi(\vec{r}, t)$$

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

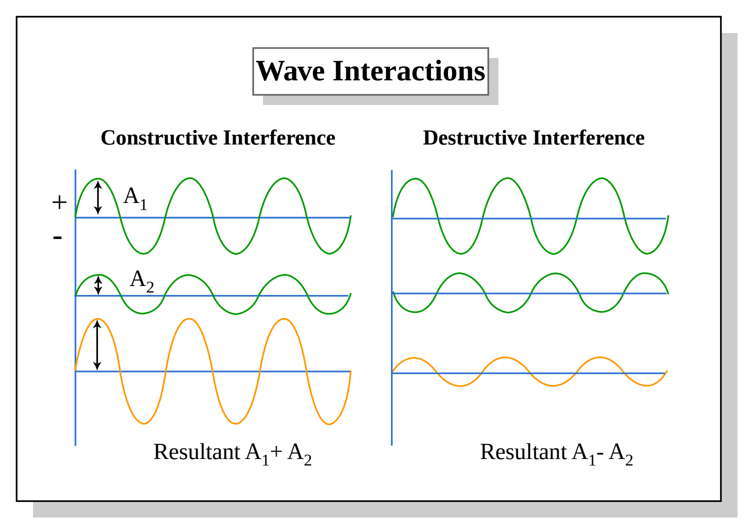
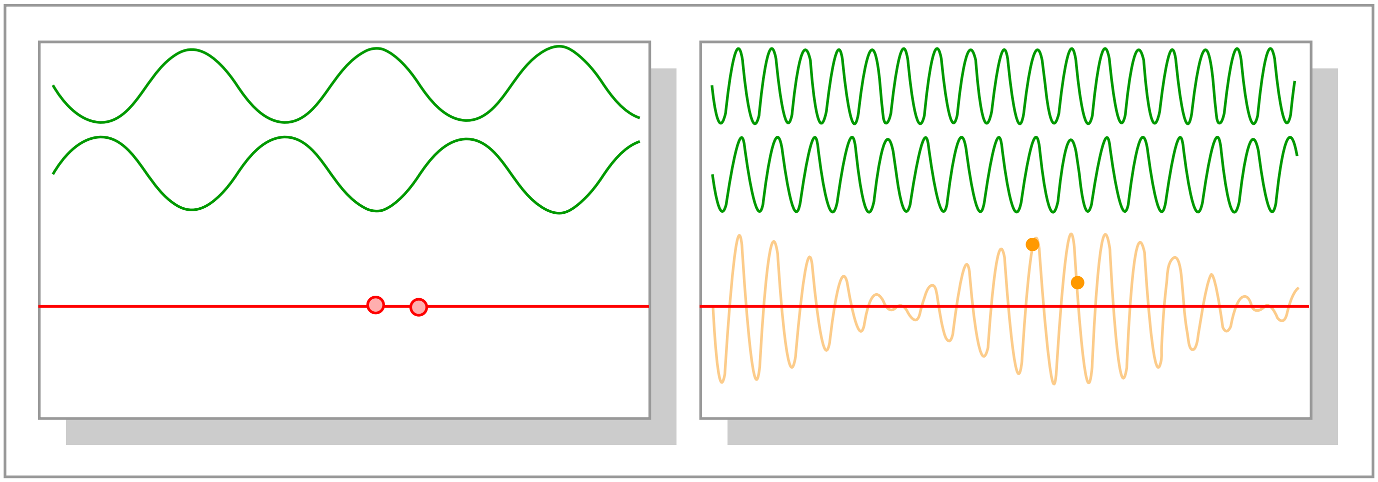


Figure by MIT OpenCourseWare.

Interference in Action



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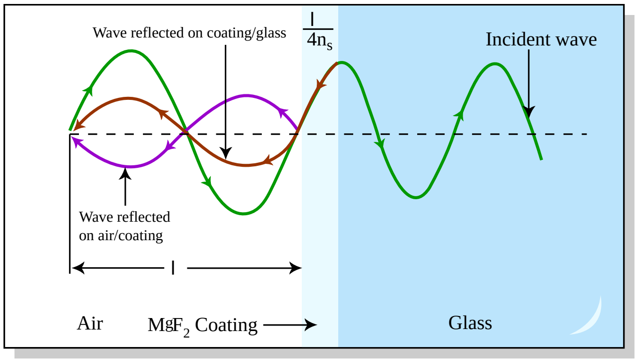
Interference in Action



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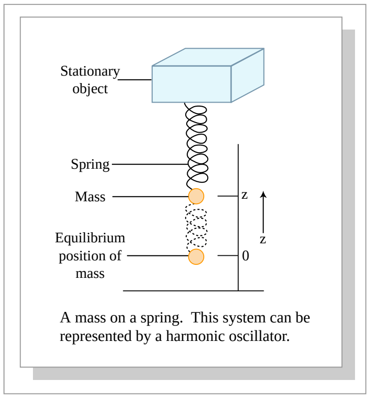
Harmonic Oscillator (I)



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

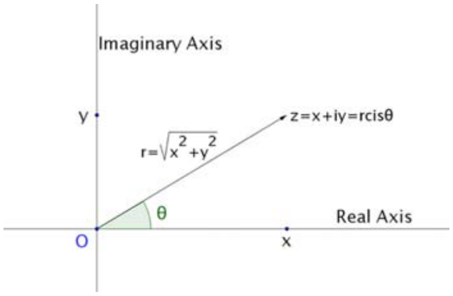
Figure by MIT OpenCourseWare.

$$ma = F$$

$$m \frac{d^2 z(t)}{dt^2} = -\frac{d}{dz} V(z)$$

$$V(z) = \frac{1}{2} k z^2$$

Harmonic Oscillator (II)



$$\frac{d^2z}{dt^2} = \boxed{-\frac{k}{m}}\,z$$

$$e^{i\alpha z} \quad , \quad e^{\alpha z}$$

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Harmonic Oscillator (III)

Image removed due to copyright restrictions.
Please see any graph of harmonic oscillator position and velocity, such as http://commons.wikimedia.org/wiki/File:HarmOsc2.png.

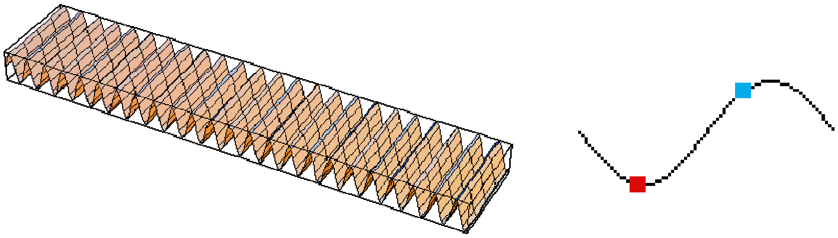
The total energy of the system

- 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

↕

Image of a double-slit experiment simulation removed due to copyright restrictions.
Please see "Double Slit Experiment." in *Visual Quantum Mechanics*.

λ • p = h

(h = 6.626 x 10^{-34} J s = 2π a.u.)

Time-dependent Schrödinger's equation

(Newton's 2^{nd} law for quantum objects)

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

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:

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