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

# 3.23 Fall 2007 – Lecture 1

# WAVES MECHANICS

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

# The 3.23 Team

- Lectures 4-231 Tue and Thu 10:00-11:30 am
- Recitations 13-5101 Wed 1-2 pm or 3-4pm

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 $20^{th}$ 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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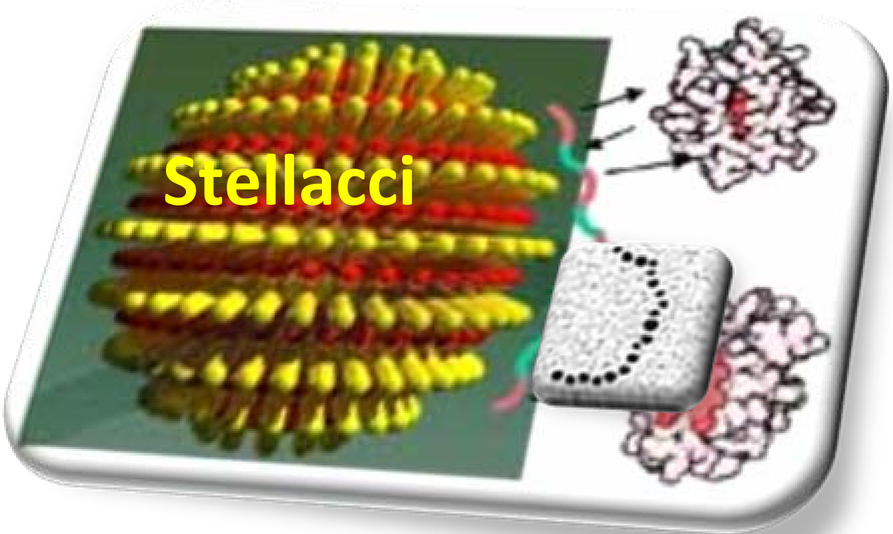
Please see http://mit-pbg.mit.edu/img/NatureFiberWeb.jpg.




Courtesy Francesco Stellacci. Used with permission.

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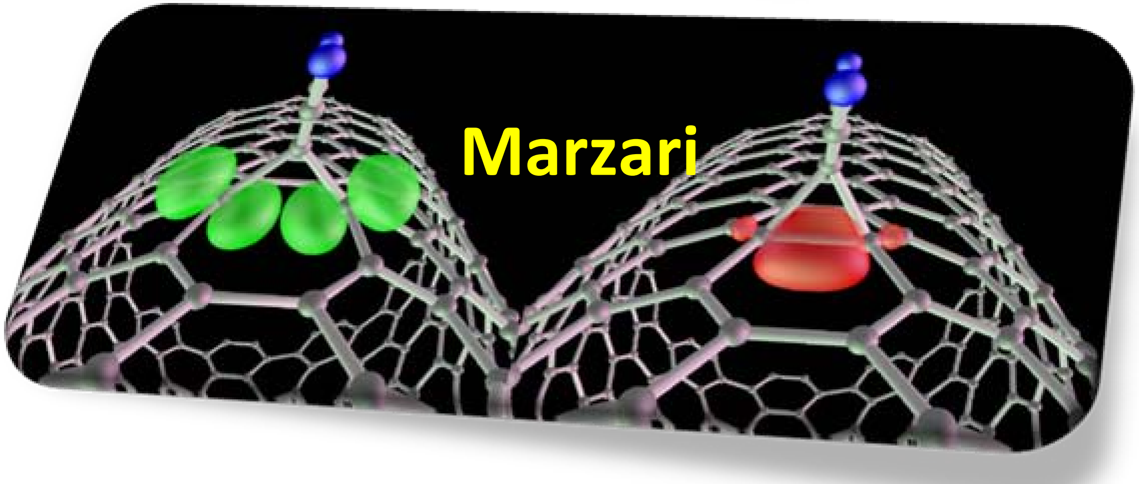
Please see any image of the microstructure of nacre, such as http://www.cas.org/ASSETS/E332CE654DC544398C837B46C102CA9D/abalone%20-%20200.jpg.




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

# Physical Origin of Material Properties

Courtesy flickr user dymero.

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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

# From Classical to Quantum

# Round Up the Usual Suspects

- Particles and electromagnetic fields
- Forces
- Dynamics

# Particles and Fields

- Electrons

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

- Nuclei (protons, neutrons)

# Particles and Fields

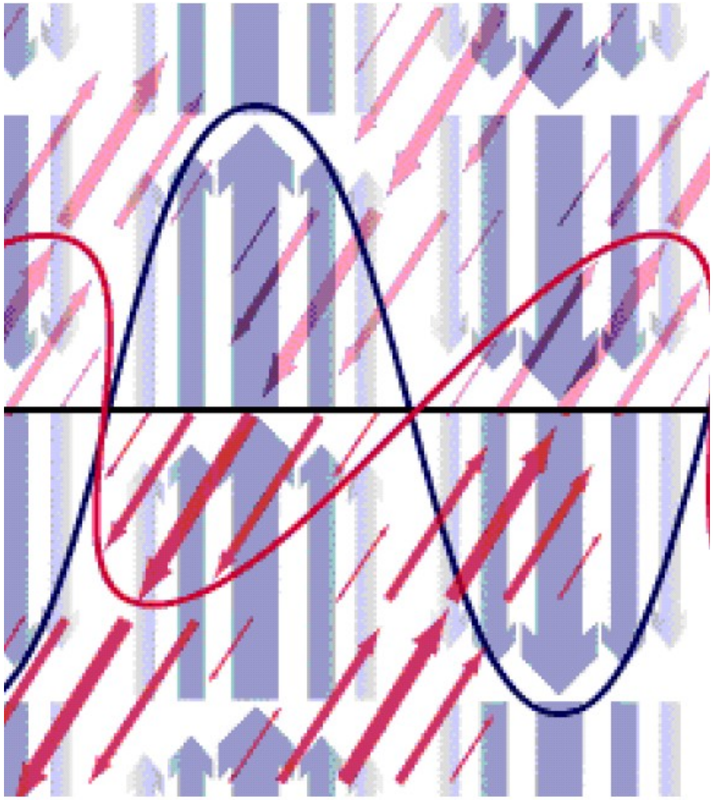


Image courtesy NASA.

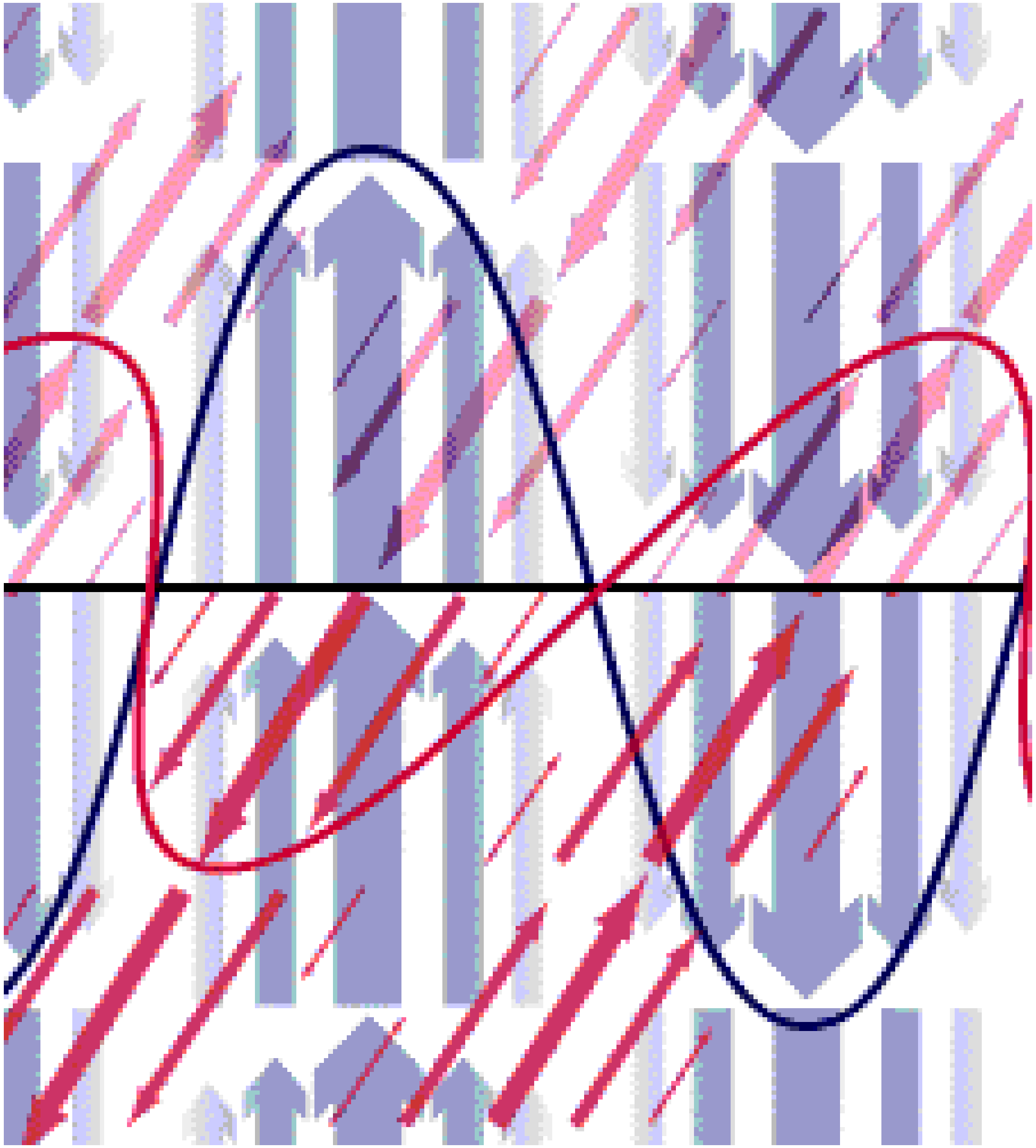


Image courtesy NASA.

# Forces

- Electromagnetic interactions
- (Gravity, electroweak, strong)

# Dynamics of a Particle

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

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

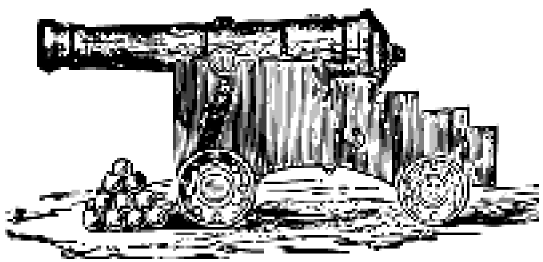


Image from the Open Clip Art Library, http://openclipart.org.

# 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

# THE ELECTROMAGNETIC SPECTRUM

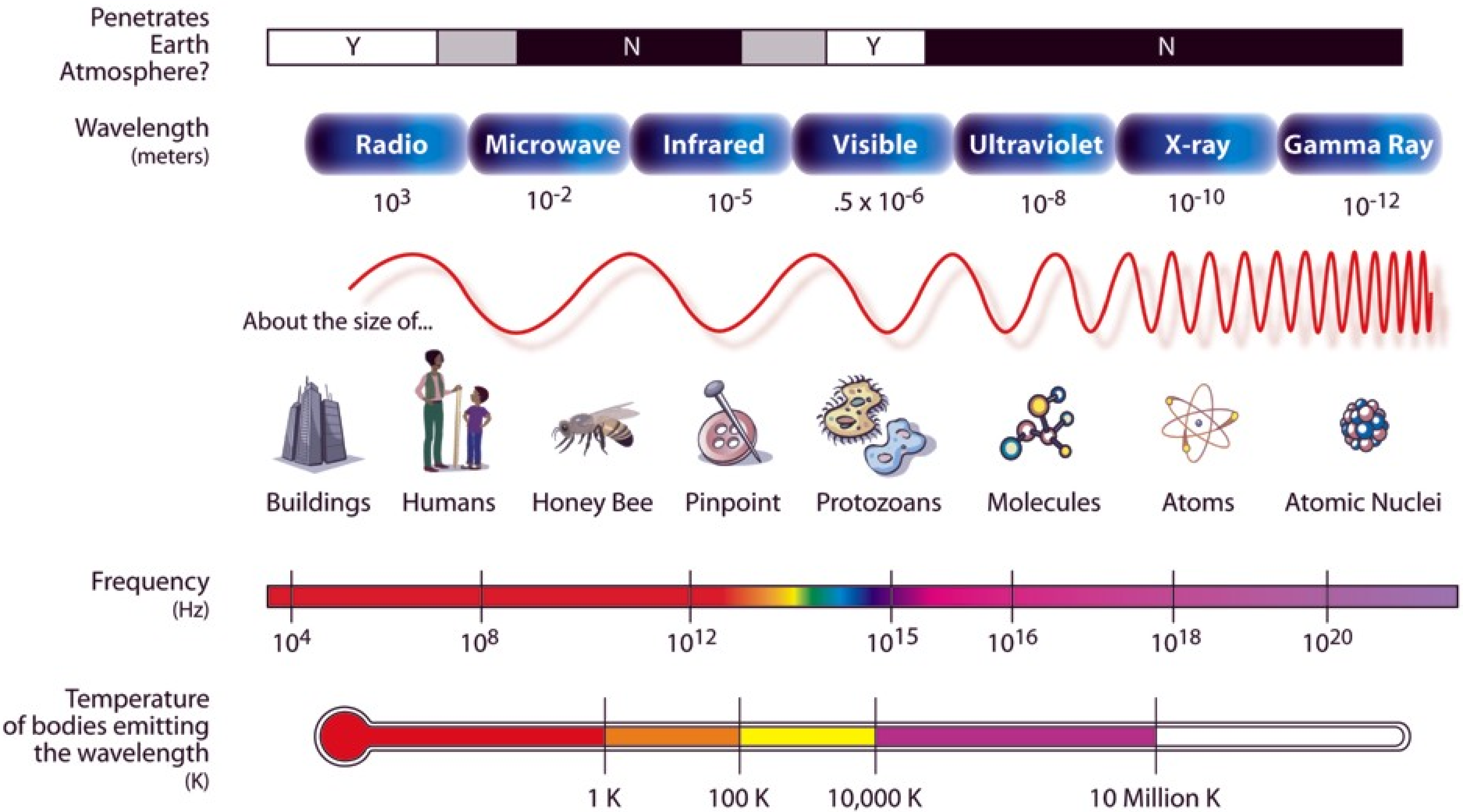



Image courtesy NASA.

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)**

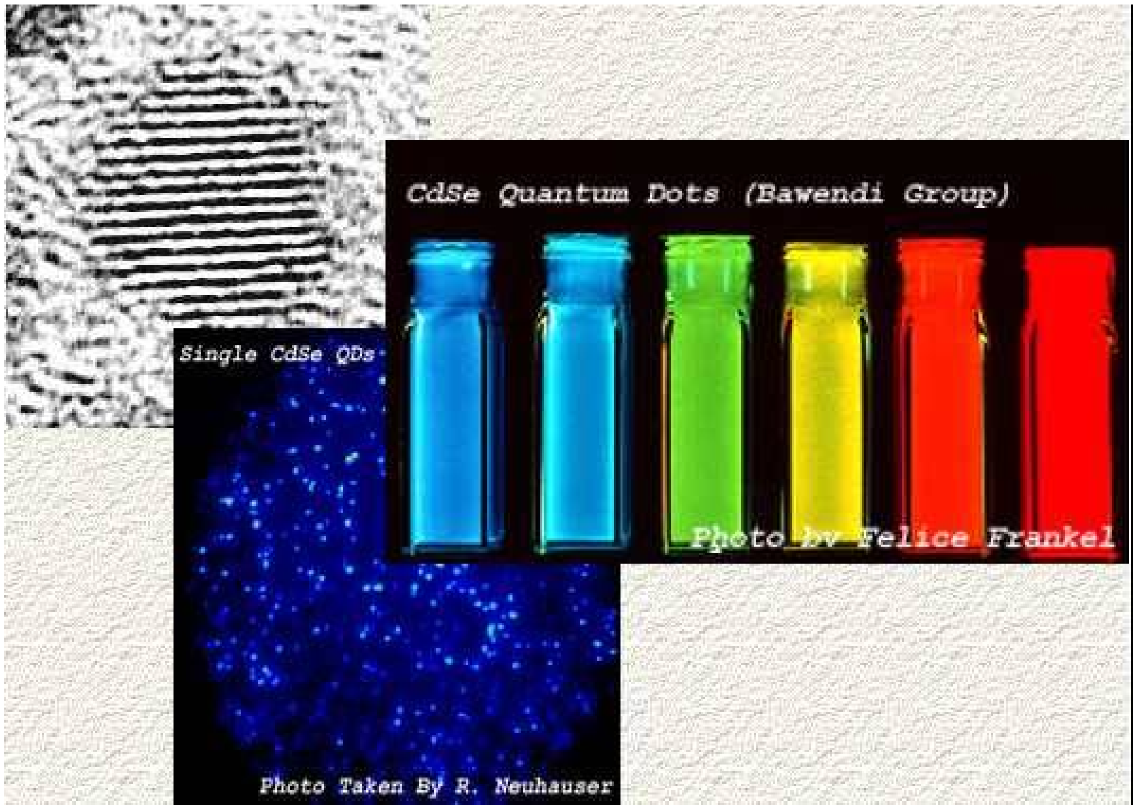
# Material Properties From First-Principles

- 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 ?

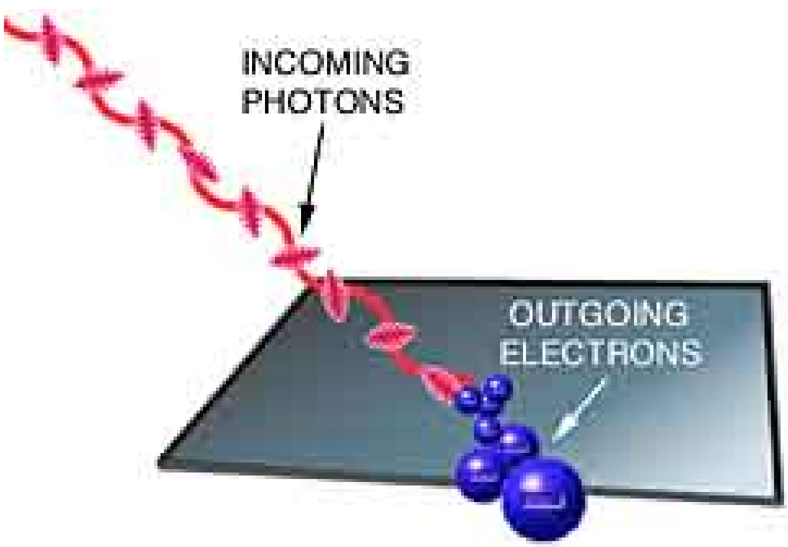
## Structural properties (fracture in silicon)

# Electronic, optical, magnetic properties



# *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.

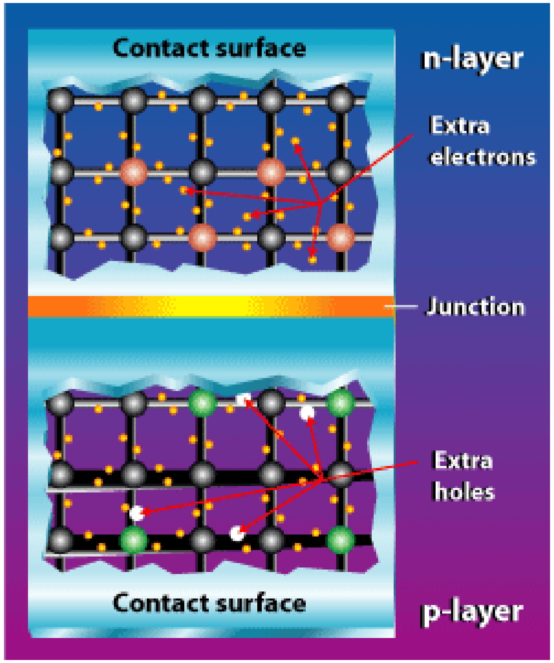
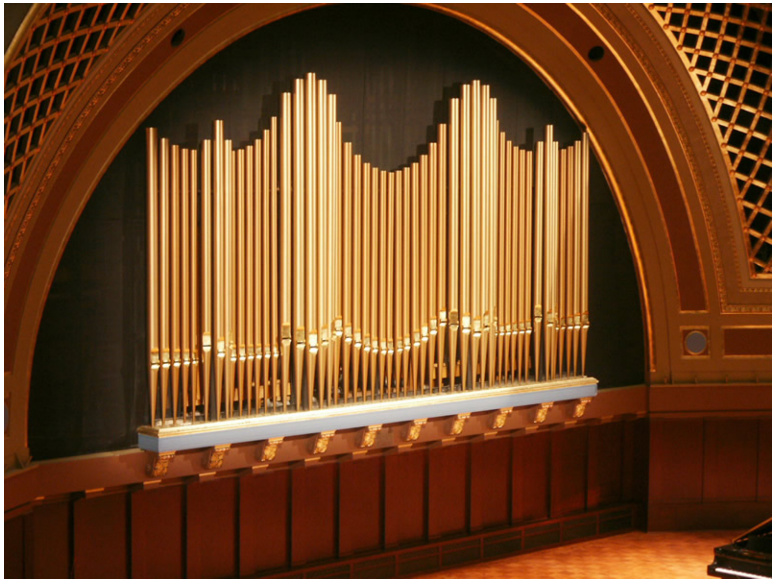
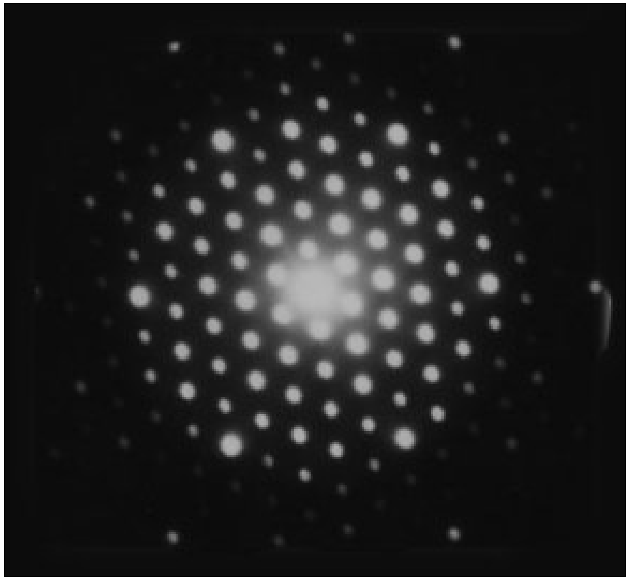



Image courtesy US Dept. of Energy.

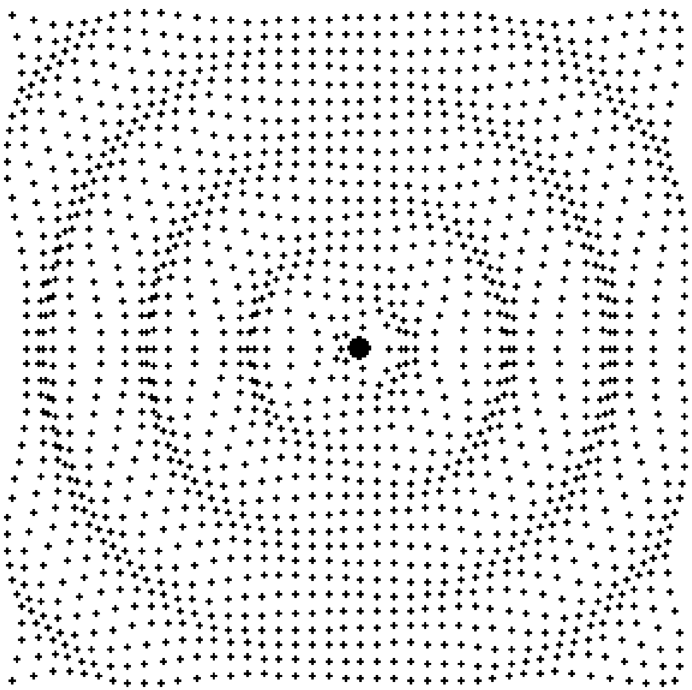
# *Wave*-particle Duality

- 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…)





# 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

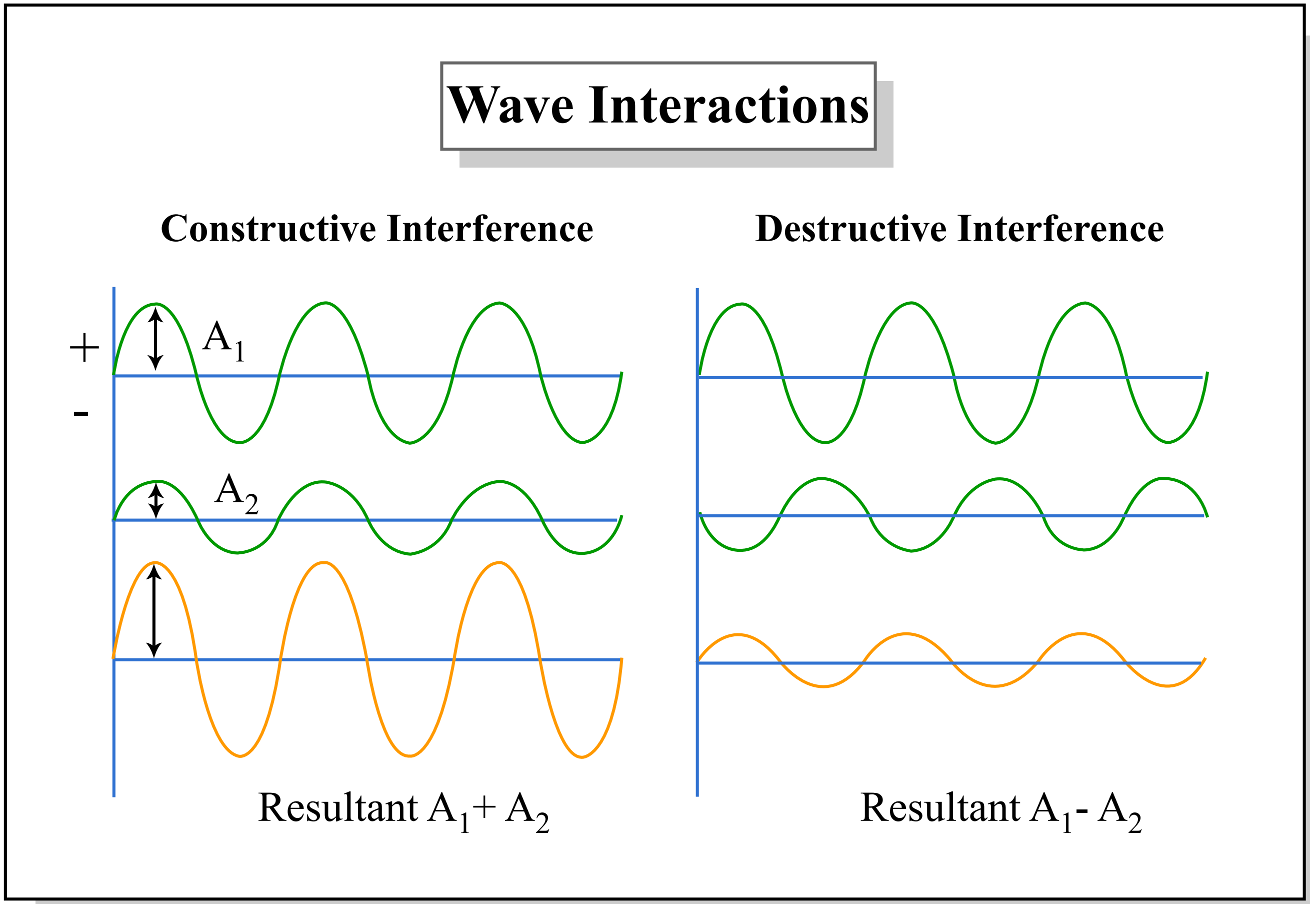



Figure by MIT OpenCourseWare.

# Interference in Action

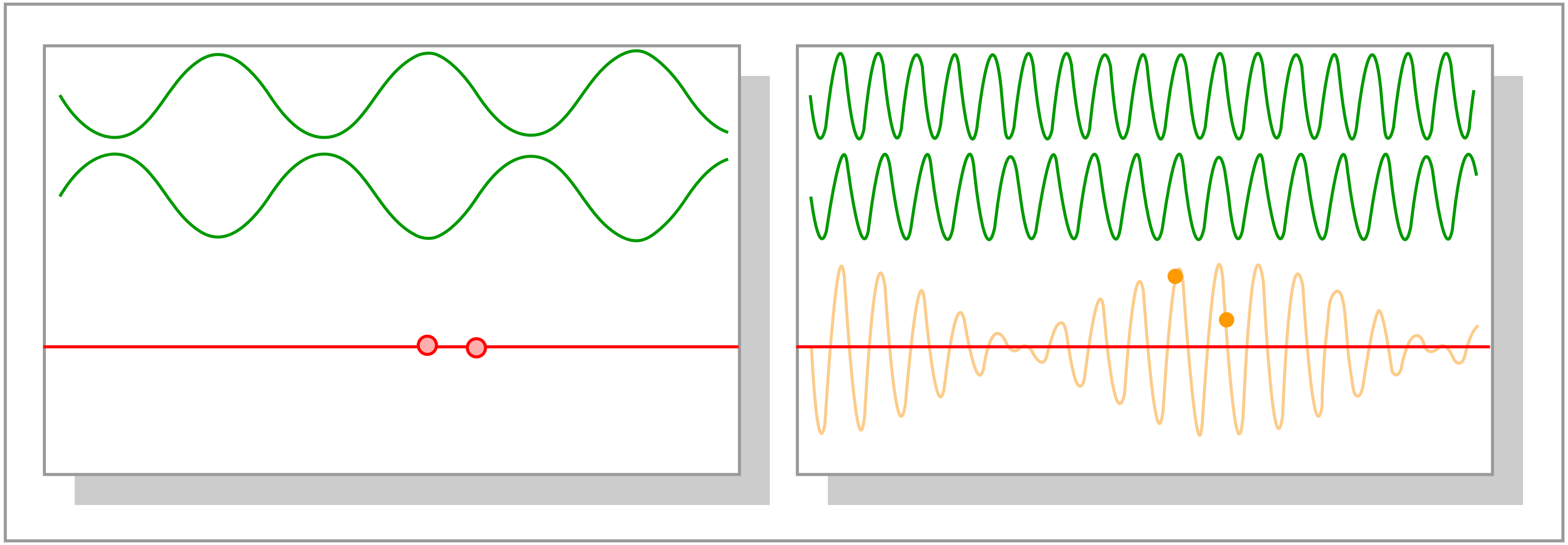


Figure by MIT OpenCourseWare.

# Interference in Action

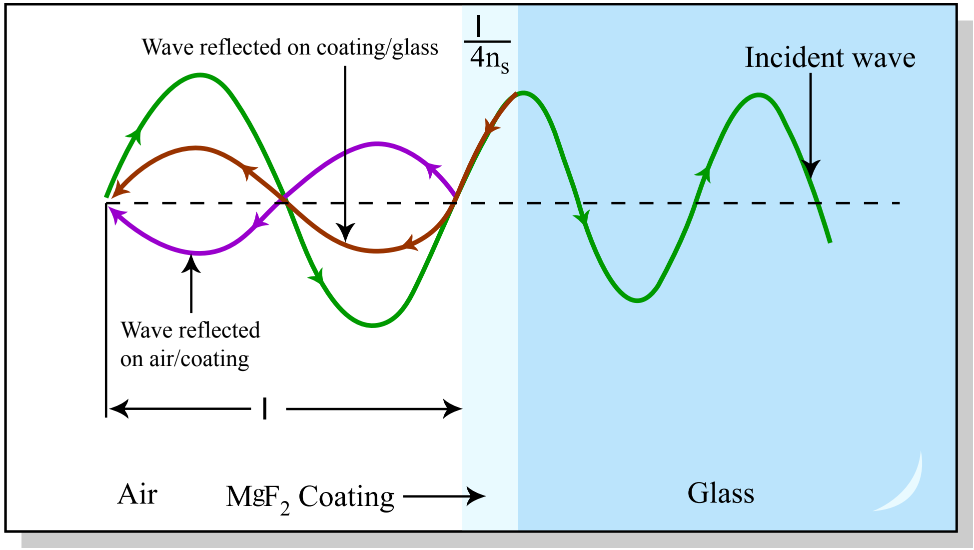



Figure by MIT OpenCourseWare.

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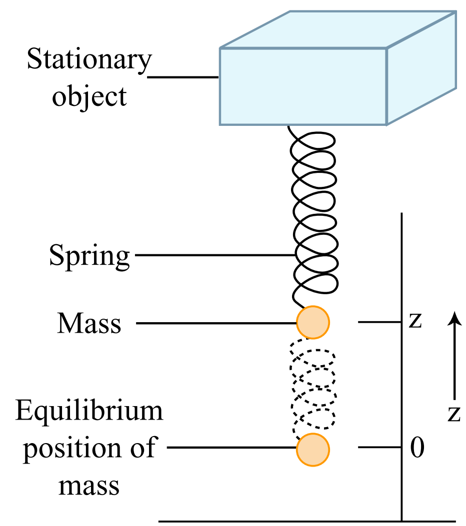
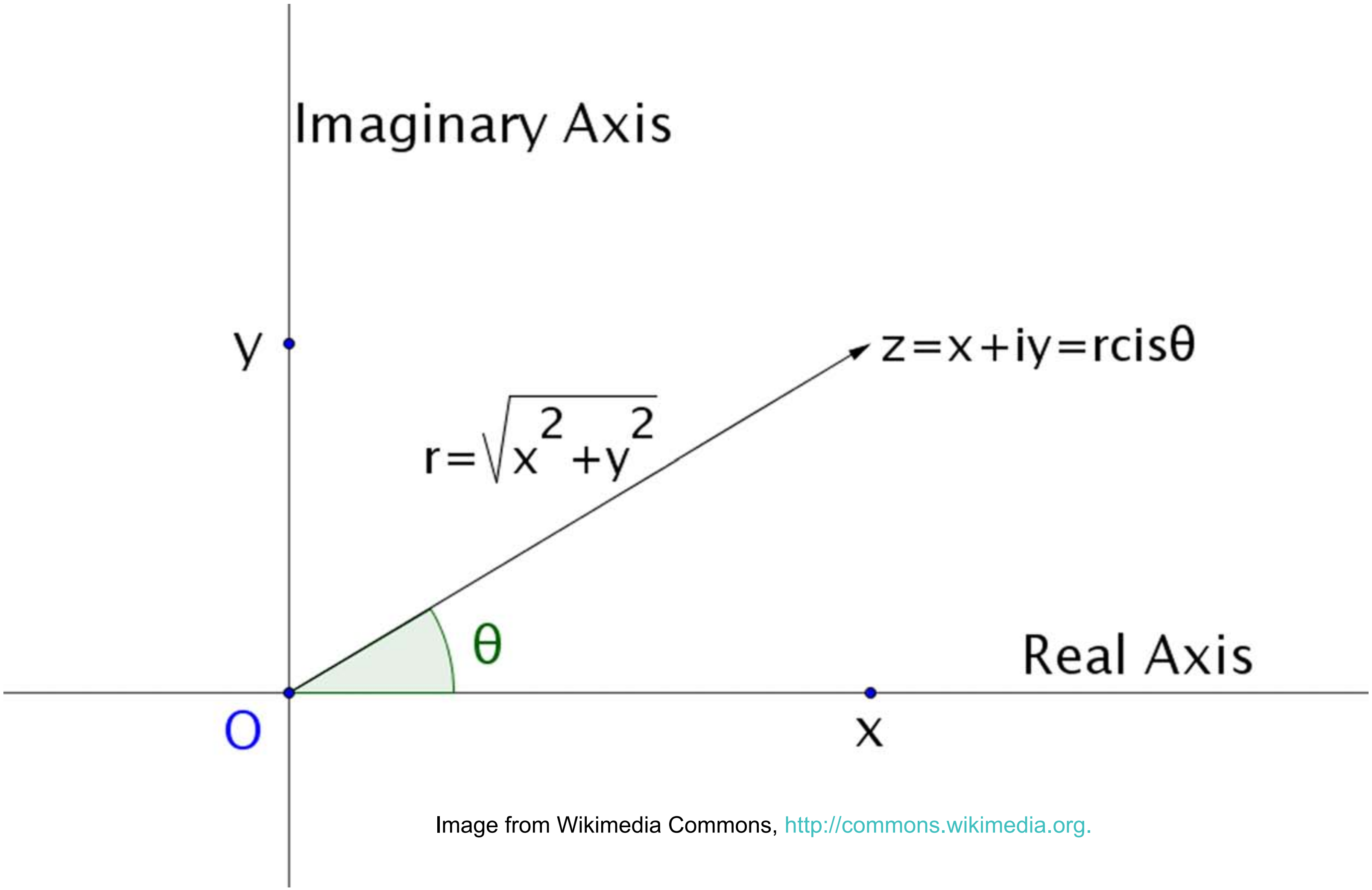
# Harmonic Oscillator (I)




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

Figure by MIT OpenCourseWare.

# Harmonic Oscillator (II)

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# Harmonic Oscillator (III)

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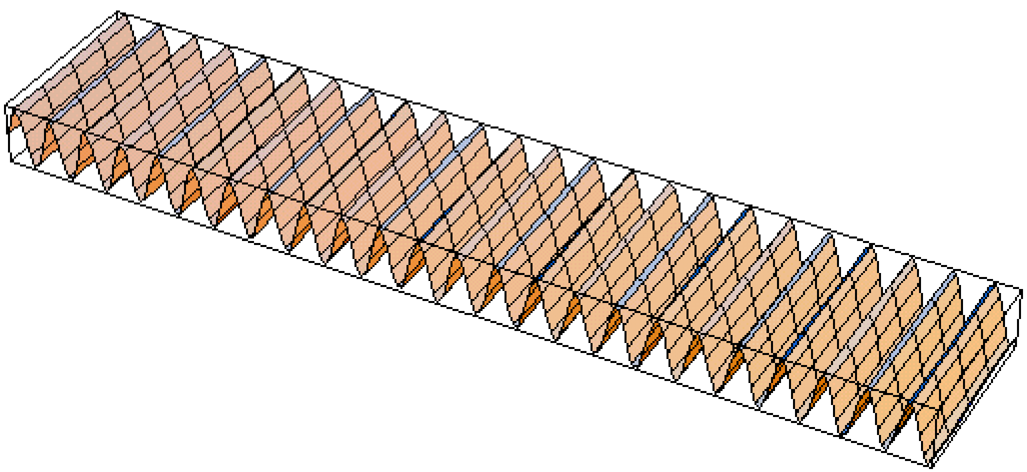
# The total energy of the system

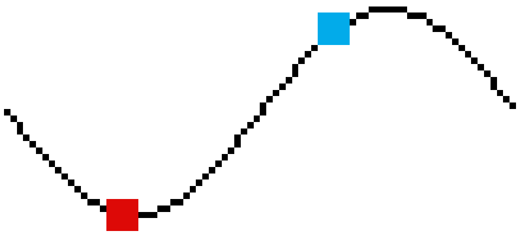
- Kinetic energy K

- 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

$\updownarrow$

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

$$\lambda \bullet p = h$$

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

# 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:

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

(provided $E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ )