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

3.23 Fall 2007 – Lecture 2

THINK OUTSIDE THE BOX

More practical info

- Problem sets – out on Wed (and posted on Stellar), due by 5pm of the following weekend (after that 75%, after Thu 5pm 50%, after Fri 5pm 25%)
- ~11 in total, 30% of the grade
- Sometimes I mention homework – it's not the "Problem Set" @ Poilvert, Bonnet

Homework

- Take notes
- Revise posted lecture
- Study posted or assigned material (TEXTBOOKS – do you have them ?)
- Meet with TAs or Instructor:

  Marzari Office Hours – Monday 4-5 pm
  Poilvert Office Hours – Tuesday 4-5pm

Last time: Wave mechanics

1. Particles, fields, and forces
2. Dynamics – from Newton to Schroedinger
3. De Broglie relation $\lambda \bullet p = h$
4. Waves and plane waves
5. Harmonic oscillator

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

Stationary Schrödinger's Equation (I)

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

ANSATZ

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

$$-\frac{\hbar^2}{2m}\nabla^2(\varphi f) + V(\vec{r})\varphi f = i\hbar\frac{\partial(\varphi f)}{\partial t}$$

$$-\frac{\hbar^2}{2m} f\nabla^2\varphi + V\varphi f = i\hbar\varphi\frac{\partial f}{\partial t} \Big/ \varphi f$$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\nabla^2\varphi}{\varphi} + V}_{\vec{r}} = \underbrace{i\hbar\frac{1}{f}\frac{\partial f}{\partial t}}_{t} =$$

$$= \text{CONSTANT} = E$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\nabla^2\varphi}{\varphi} + V = E} \qquad i\hbar\frac{1}{f}\frac{\partial f}{\partial t} = E$$

Stationary Schrödinger's Equation (II)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

Stationary Schrödinger's Equation (III)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

1. It's not proven – it's postulated, and it is confirmed experimentally
2. It's an "eigenvalue" equation: it has a solution only for certain values (discrete, or continuum intervals) of E
3. For those eigenvalues, the solution ("eigenstate", or "eigenfunction") is the complete descriptor of the electron in its equilibrium ground state, in a potenitial V(r).
4. As with all differential equations, boundary conditions must be specified
5. Square modulus of the wavefunction = probability of finding an electron

Free particle: Ψ(x,t)=ϕ(x)f(t)

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(x) = E\varphi(x)$$

$$\frac{d^2\varphi}{dx^2} = -\frac{2mE}{\hbar^2}\varphi \quad \Rightarrow \quad \varphi = e^{ikx}$$

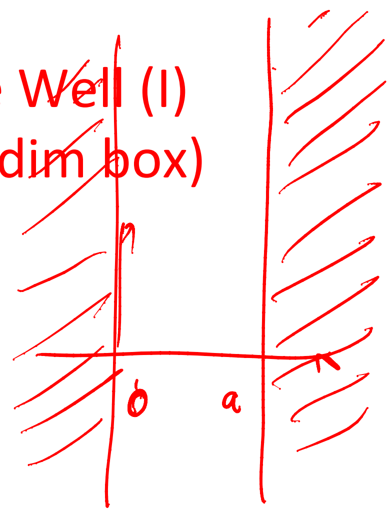
$$i\hbar\frac{d}{dt}f(t) = E\,f(t)$$

$$\frac{df}{dt} = -i\frac{E}{\hbar}f \quad \Rightarrow \quad f = e^{-i\frac{E}{\hbar}t}$$

HW

Infinite Square Well (I) (particle in a 1-dim box)

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x)$$



$$\varphi(x) = Ae^{ikx} + Be^{-ikx} = C\sin kx + D\cos kx \qquad D = 0$$

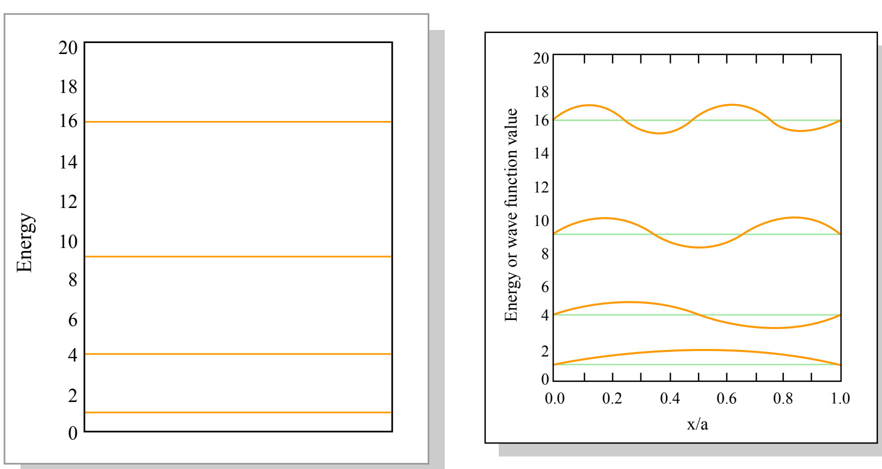
Infinite Square Well (II)

$$\left(C \sin kx \right)\Big|_{x=a} = 0$$

$$C \sin ka = 0$$

$$ka = n\pi \qquad n = 0, \pm 1, \pm 2, \ldots$$

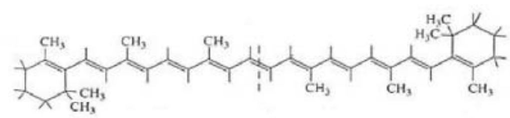
Infinite Square Well (III)



Figures by MIT OpenCourseWare.

The power of carrots

- β-carotene



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Physical Observables from Wavefunctions

- Eigenvalue equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\varphi(x)=E\varphi(x)$$

- Expectation values for the operator (energy)

H/W

$$E=\int\varphi^*(x)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\varphi(x)\,dx$$

$E = \frac{h^2}{8m}\left(\frac{n^2}{a^2}\right)$

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Particle in a 2-dim box

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi(x,y)=E\,\varphi(x,y)$$

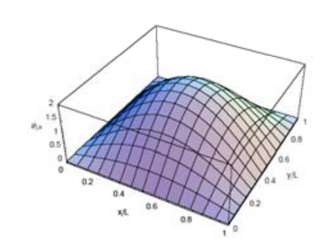
$$\varphi(x,y) = X(x)Y(y)$$

$$-\frac{\hbar^2}{2m} Y \frac{\partial^2 X}{\partial x} - \frac{\hbar^2}{2m} X \frac{\partial^2 Y}{\partial y^2} = E X Y$$

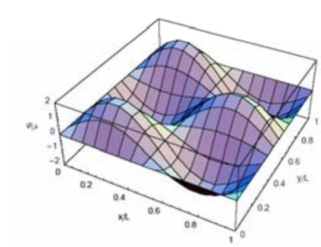
$$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = E \quad = -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}$$

Particle in a 2-dim box

$$\varphi(x,y)=C\sin\left(\frac{l\pi x}{a}\right)\sin\left(\frac{m\pi y}{b}\right)$$



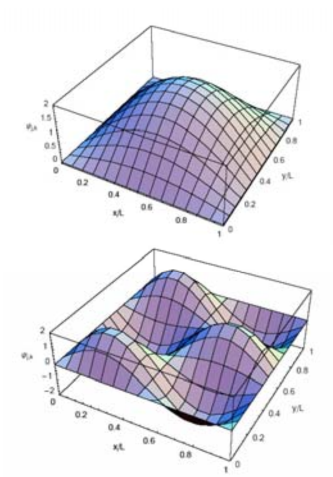
$$E=\frac{h^2}{8m}\left(\frac{l^2}{a^2}+\frac{m^2}{b^2}\right)$$



Particle in a 3-dim box

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z)=E\,\varphi(x,y,z)$$

Particle in a 3-dim box: *Farbe* defect in halides (e^- bound to a negative ion vacancy)



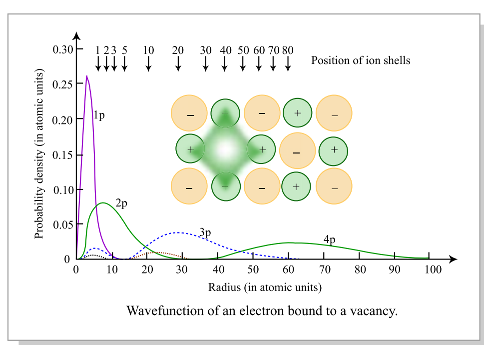


Figure by MIT OpenCourseWare.

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From Carl Zeiss to MIT…

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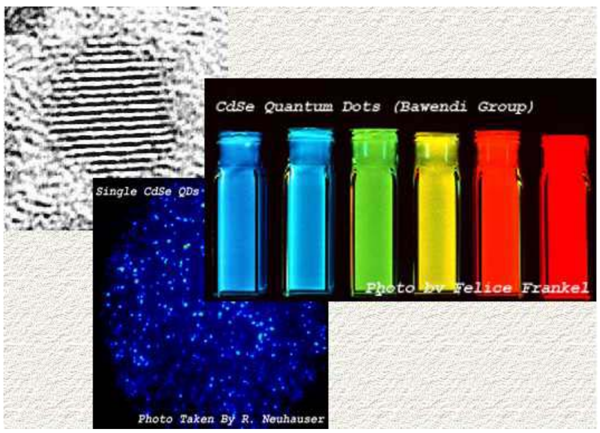
Avakian, P., and Smakula, A. "Color Centers in Cesium Halide Single Crystals."
Physical Review 120 (December 1960): 2007.

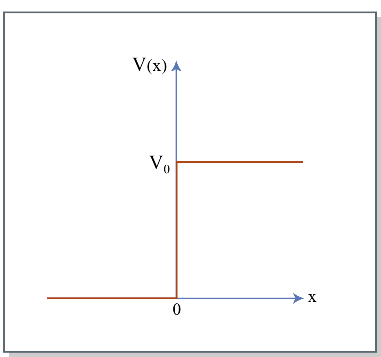
Light absorption/emission



MIT Research: Bawendi, Mayes, Stellacci

Metal Surfaces (I)

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\varphi(x)=E\varphi(x)$$



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$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}=E\varphi \quad \Big| \quad -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2}+V_0\varphi=E\varphi$$

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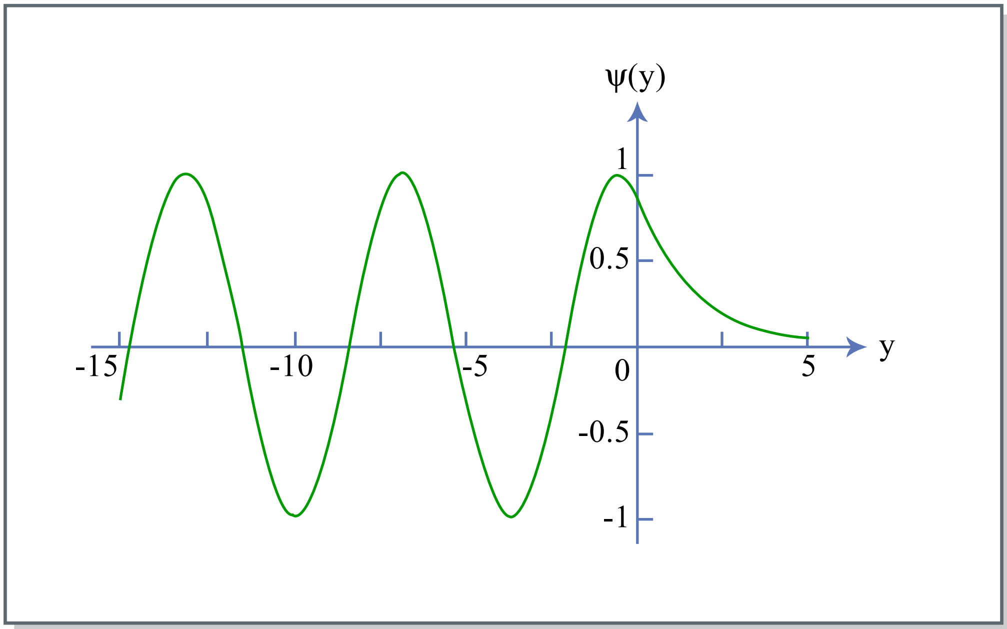
Metal Surfaces (II)



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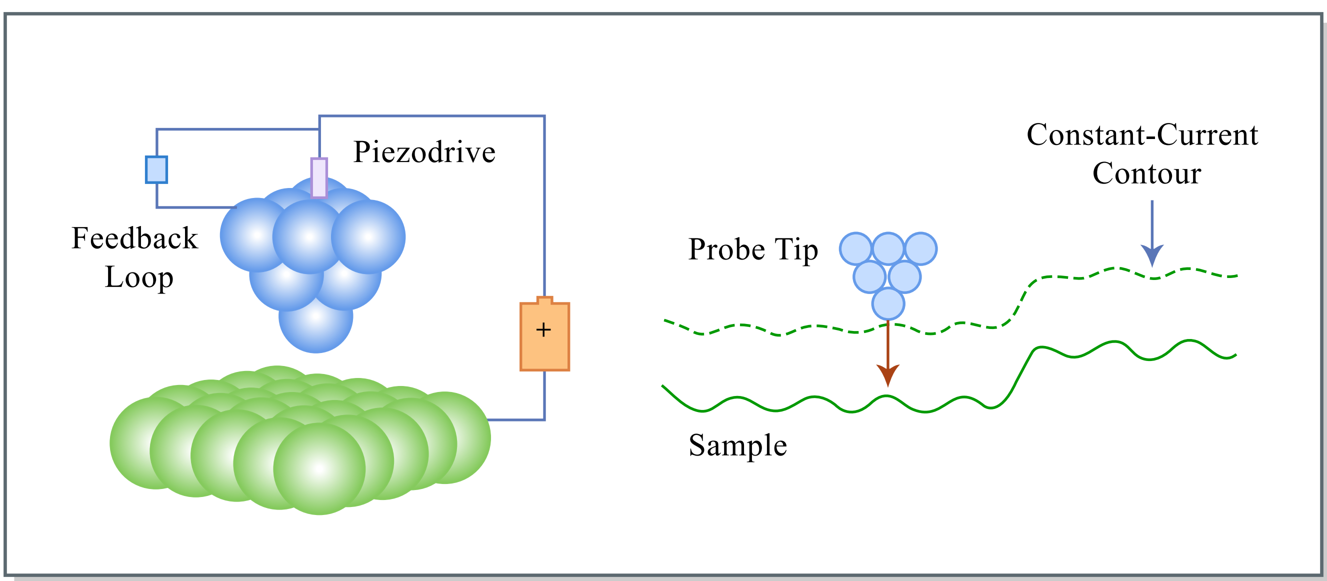
Scanning Tunnelling Microscopy



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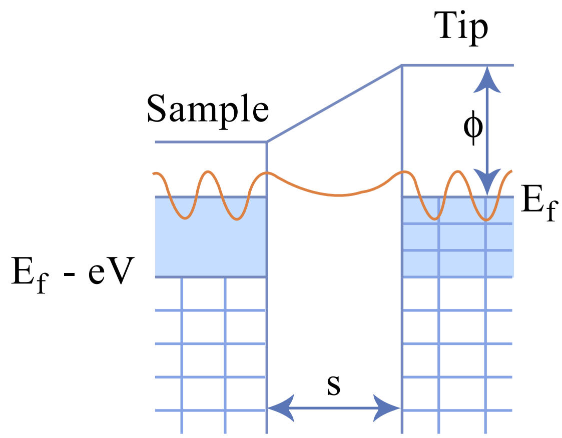
Scanning Tunnelling Microscopy, cont.



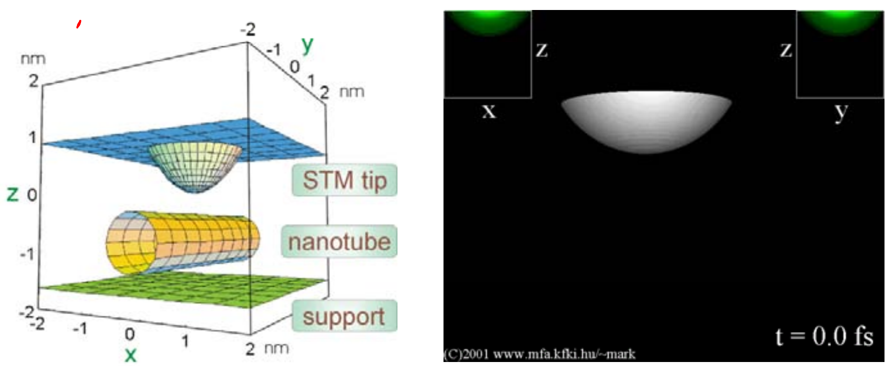
$$I/V \propto \rho e^{-2\kappa s}$$

$$\kappa = \left(\frac{2m\phi}{\hbar^2}\right)^{1/2} = 1.1\ \text{Å}^{-1}$$

ρ = density of states

Figure by MIT OpenCourseWare.

Wavepacket tunnelling through a nanotube



Images courtesy of Geza I. Mark. Used with permission.

http://newton.phy.bme.hu/education/schrd/index.html

http://www.quantum-physics.polytechnique.fr

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