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

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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:
Last time: Wave mechanics

1. Particles, fields, and forces
2. Dynamics – from Newton to Schroedinger
3. De Broglie relation $\lambda \cdot p = h$
4. Waves and plane waves
5. Harmonic oscillator
Time-dependent Schrödinger’s equation
(Newton’s 2\textsuperscript{nd} 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:

\[
- \frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} \quad \text{(provided} \quad E = \hbar \omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \text{)}
\]
Stationary Schrödinger’s Equation (I)

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

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

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 potential 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: \[ \Psi(x,t) = \varphi(x)f(t) \]

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

\[ i\hbar \frac{d}{dt} f(t) = E f(t) \]
Infinite Square Well (I)
(particle in a 1-dim box)

\[-\frac{\hbar^2}{2m} \frac{d^2 \varphi(x)}{dx^2} = E \varphi(x)\]
Infinite Square Well (II)
Infinite Square Well (III)

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The power of carrots

• β-carotene

Images removed due to copyright restrictions. Please see any spectrum of beta carotene, such as http://www.chm.bris.ac.uk/motm/carotene/beta-carotene_colourings.html.
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)

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

\[- \frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \varphi(x, y) = E \varphi(x, y)\]
Particle in a 2-dim box

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

\[ E = \frac{\hbar^2}{8m} \left(\frac{l^2}{a^2} + \frac{m^2}{b^2}\right) \]
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: \textit{Farbe} defect in halides (e\textsuperscript{-} bound to a negative ion vacancy)

Figure by MIT OpenCourseWare.
From Carl Zeiss to MIT…

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Light absorption/emission

Courtesy M. Bawendi and Felice Frankel.
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Metal Surfaces (I)

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

Figure by MIT OpenCourseWare.
Metal Surfaces (II)

Figure by MIT OpenCourseWare.

Scanning Tunnelling Microscopy

\[ I/V \propto e^{-2\kappa s} \]

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

\( \rho = \text{density of states} \)

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Wavepacket tunnelling through a nanotube

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