

Outline for Day 11 (and into Day 12)

Office hours: 2 - 4

In which we learn about the Schrödinger Equation and how to solve it for the particle in the box.

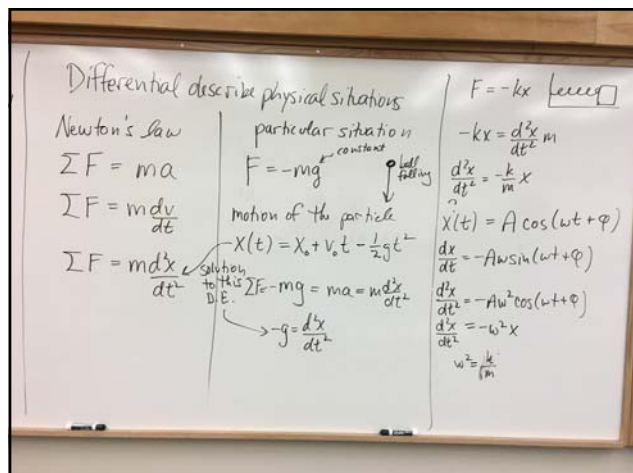
- Differential equations and their solutions describe physical situations in classical and quantum mechanics
 - Newton's law
 - The Schrödinger equation
- From time dependent to time independent Schrödinger equation: stationary states
- Real life examples of particle in a box
- Schrödinger equation solutions for particle in a box
- Using the particle in a box solutions to understand particle behavior (likely positions, expectation value, absorption spectra)

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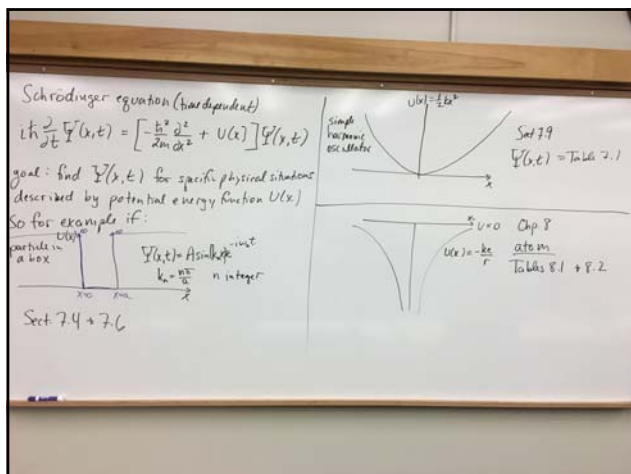


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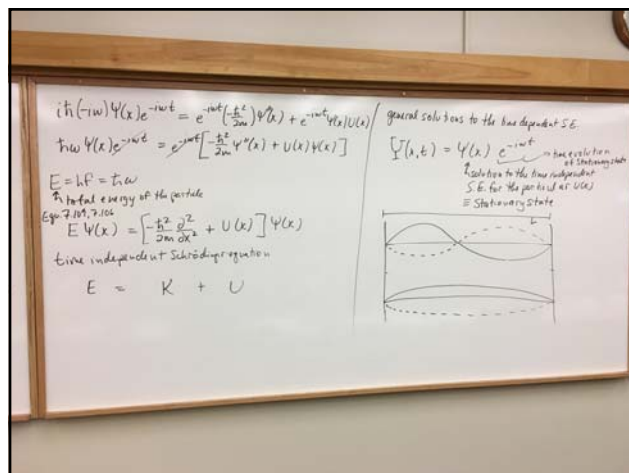
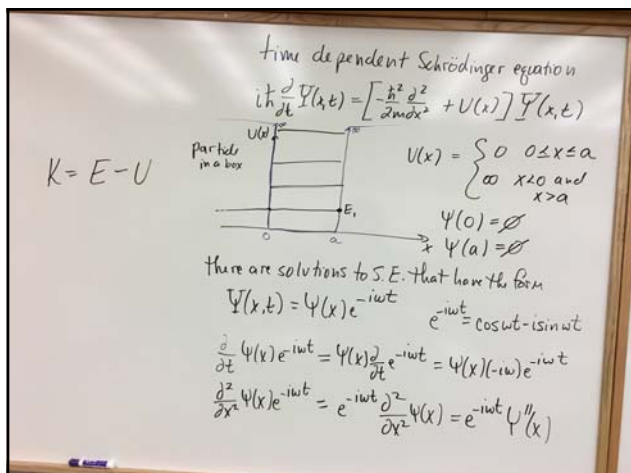


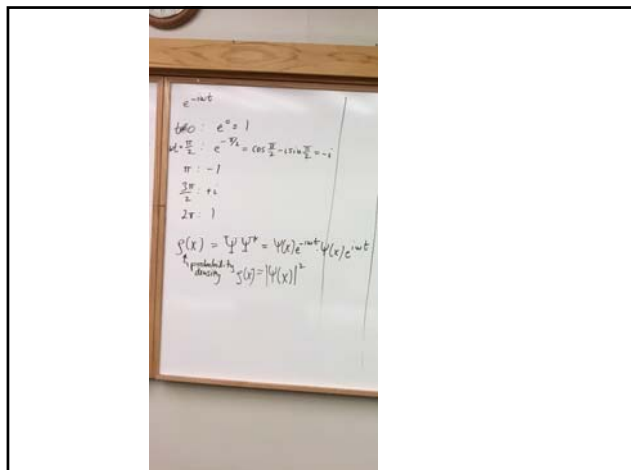
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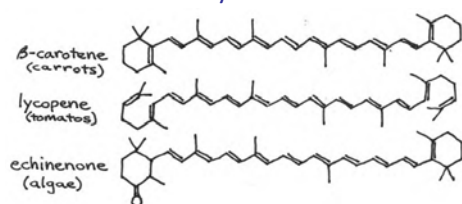
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Dye Molecules



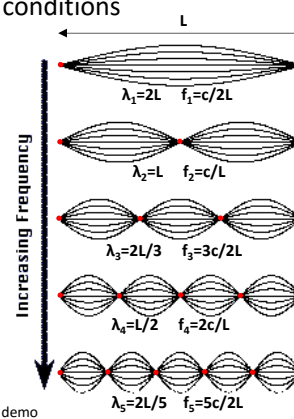
- Carbon atom at each vertex.
- Single vs double line tells what kind of bond.
- Typically one or two free electrons per carbon atom.
- Basic behavior predicted with ignoring internal structure.
- Free electrons = particles.
- Dye molecule = box.

Waves with boundary conditions

- Boundary conditions mean that waves only have discrete frequencies.
- e.g., guitar strings

$$\lambda_n = 2L/n$$
$$f_n = nc/2L$$

- = node = fixed point that doesn't move



PHET: normal modes + standing wave demo

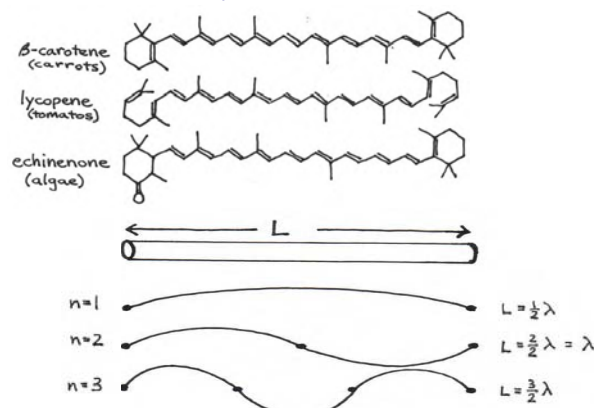
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Dye Molecules



Inside the box $U(x)=0$

$$\nabla^2 \psi = -\frac{2mE}{\hbar^2} \psi$$

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

$$\psi''(x) = -\frac{2mE}{\hbar^2} \psi(x)$$

$$\psi''(x) + k^2 \psi(x) = 0$$

$$\psi(x) = A \sin kx + B \cos kx$$

$$\psi'(x) = kA \cos kx - kB \sin kx$$

$$\psi''(x) = -k^2 A \sin kx - k^2 B \cos kx = -k^2 \psi(x)$$

to satisfy boundary conditions $\psi(0)=0$ and $\psi(L)=0$

$$kL = n\pi \quad n \text{ integer}$$

$$k^2 = \frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{a^2}$$

Diagram showing the wave functions for $n=1, 2, 3$ in a box of length a .

Energy levels $E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$ are the quantized energy levels for particle in a box. $\omega_n = \frac{E_n}{\hbar}$

Wave function $\psi(x) = A \sin\left(\frac{n\pi x}{a}\right)$ and time-dependent wave function $\Psi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i\omega_n t}$

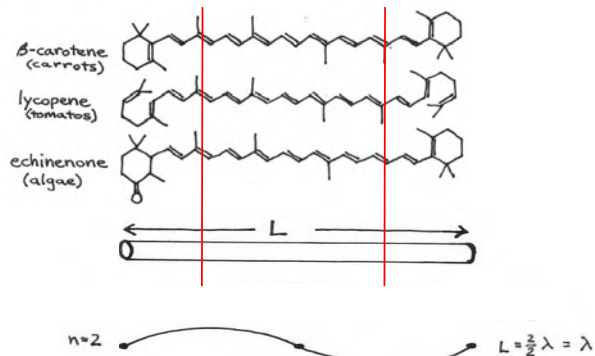
Normalization: $\int_0^a \psi^2(x) dx = 1$

$$\int_0^a \psi^2(x) dx = 1 = \int_0^a A^2 \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$A = \sqrt{\frac{2}{a}}$$

A - normalization constant

Most likely place to find the electron?



If we measure ^{position} x for a whole bunch of particles in the $n=2$ state, what is the average value of all measurements?
 What is expected average value of x ?
 "expectation value"

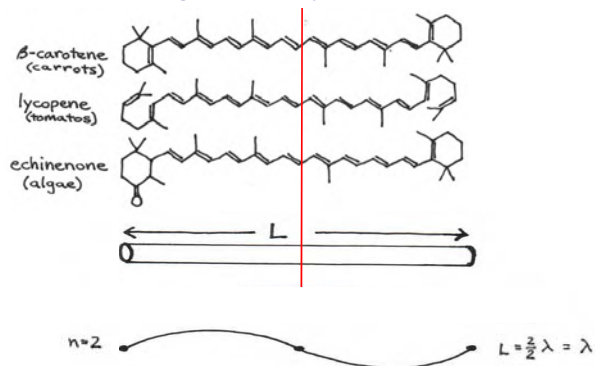
$$\langle x \rangle = \int_0^a \psi^* x \psi dx$$

$$= \int_0^a \frac{2}{a} \sin^2 \frac{2\pi x}{a} x dx$$

$$= \frac{2}{a} \cdot \frac{a^2}{4} = \frac{a}{2}$$

$\langle x \rangle = x_{avg} = \bar{x} = \int_{\text{box}} g(x) \cdot x dx$
 $g(x)$ how often we get a certain value of x

Average electron position?



Absorption of Photons

Energy spacing given by:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

$$E_{\text{photon}} = E_j - E_i$$

PHOTON

MOLECULE

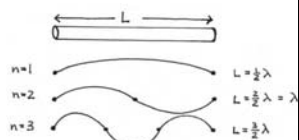
MOLECULE

BEFORE ABSORPTION

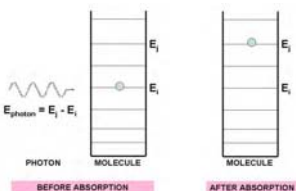
AFTER ABSORPTION

Two Wavelength Danger

length of box determines
allowed **electron** wavelengths
and hence energy levels



electron energy levels
determine allowed
light absorption wavelengths



Derive equation 10

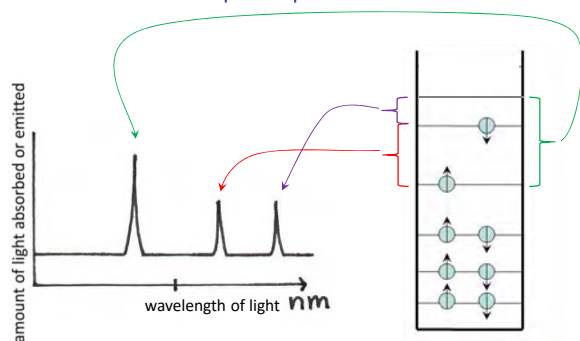
What is the wavelength of a photon
that can excite a particle from the
 m to n state? $n > m$

$$\Delta E_{nm} = E_n - E_m = (n^2 - m^2) \left(\frac{\pi^2 \hbar^2}{2ma^2} \right)$$

$$\Delta E_{nm} = hf_{nm} = \frac{hc}{\lambda_{nm}}$$

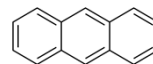
$$\lambda_{nm} = \frac{8cma^2}{h(n^2 - m^2)}$$

Absorption Spectrum

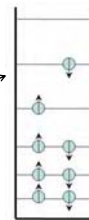


Absorption Spectra of Real Molecules

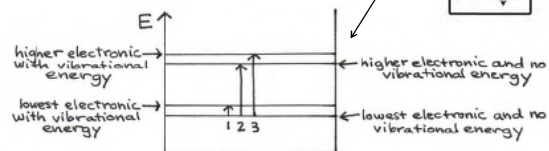
anthracene

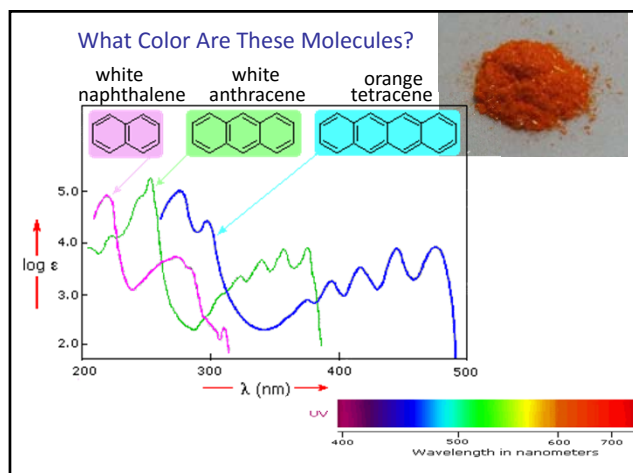
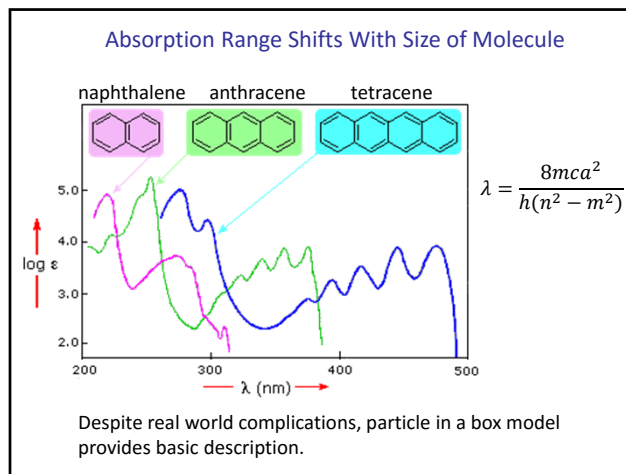
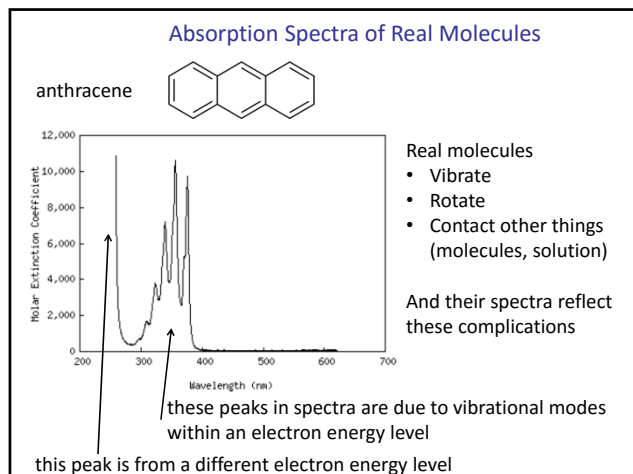


electron
energy
levels only



electron energy levels plus vibrational levels





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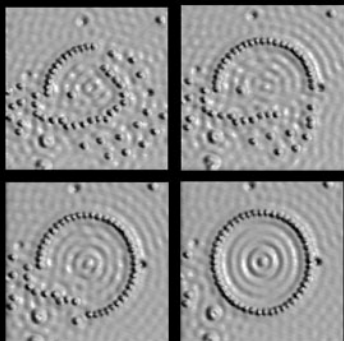
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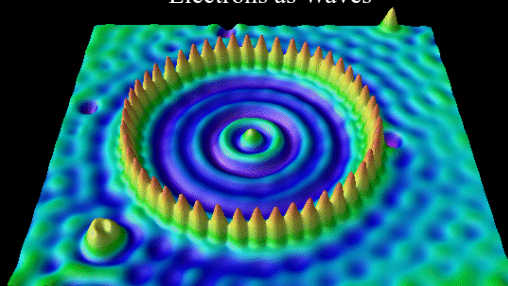
Moving Atoms with an STM

Fe atoms on Cu



M.F. Crommie, C.P. Lutz, D.M. Eigler.
Confinement of electrons to quantum corrals on a metal surface.
Science 262, 218-220 (1993).

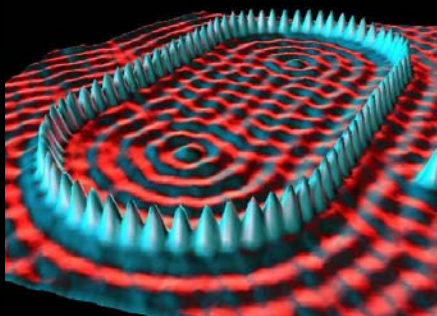
Electrons as Waves



48 Fe atoms and resulting electron standing wave pattern on a Cu(111) surface

M.F. Crommie, C.P. Lutz, D.M. Eigler.
Confinement of electrons to quantum corrals on a metal surface.
Science 262, 218-220 (1993).

Electron Wave Echo Chamber



M.F. Crommie, C.P. Lutz, D.M. Eigler, E.J. Heller.
Waves on a metal surface and quantum corrals.
Surface Review and Letters 2 (1), 127-137 (1995).