3.012 Fund of Mat Sci: Bonding – Lecture 3

GHOST IN THE MACHINE

Image of a quantum mirage produced by a Co atom placed in the focus of a Co elliptical corral, removed for copyright reasons. Don Eigler, IBM Almaden, *Nature (*2000). See http://domino.watson.ibm.com/comm/pr.nsf/pages/rscd.quantummirage-picb.html/$FILE/mirage2.jpg

Last time: Schrödinger equation

1. Time-dependent Schrödinger equation for one electron in a potential $V(r,t)$ (a plane wave satisfies this eqn.)
2. For a stationary potential $V(r)$, we introduced the method of separation of variables, and obtained a) the stationary Schrödinger equation for the spatial part $\varphi(x)$, and b) the equation for the time-dependent function $f(t)$
3. Homework: for a free particle it is easy to obtain $\varphi(x)$ and $f(t)$, and one obtains back the equation of a plane wave
4. Studied a free particle in an infinite well (particle in a box)

Homework for Fri 16

- Study: 15.3 (2-,3-dim box), 16.3 (π-electrons in conjugated molecules), 16.5-6 (scanning tunnelling microscope)
- Optional read: 1986 Nobel lecture by Binnig and Rohrer (on MIT Server)

Physical Observables from Wavefunctions

- Eigenvalue equation: (the operator is obtained via the "correspondence" principle)

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

- Expectation values for the operator (energy)

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

Normalization

$$\varphi(x) \longmapsto A\,\varphi(x)$$

$$\int_V \varphi^*(\vec{r})\,\varphi(\vec{r}) = 1$$

Infinite Square Well

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

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

$$= A' e^{ikx} + A'' e^{-ikx}$$

$$\varphi(x) = A \sin\frac{n\pi}{a}x$$

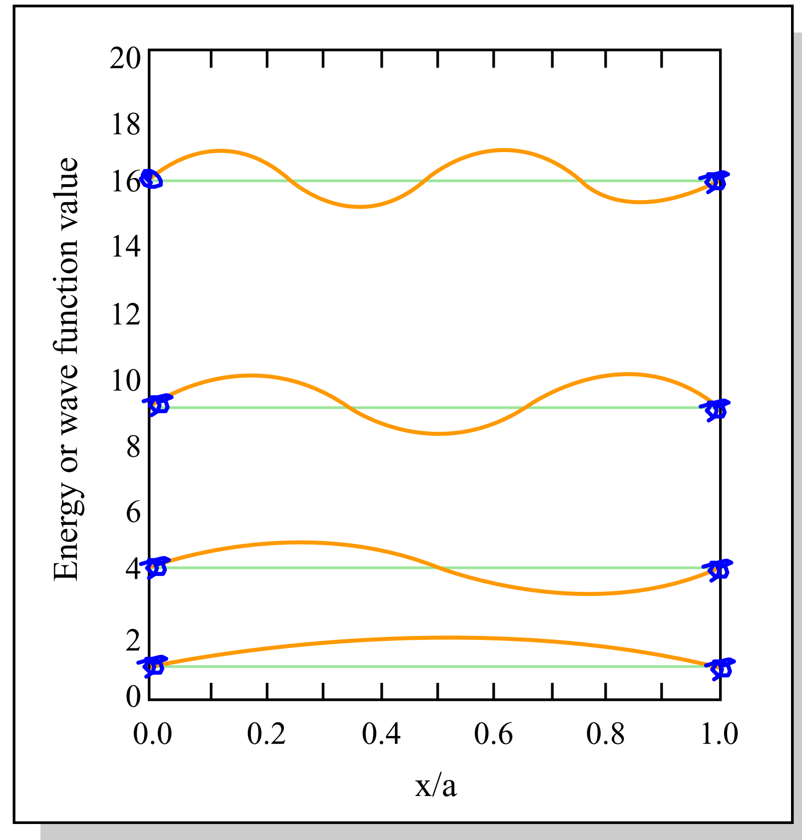


Figure by MIT OCW.

Infinite Square Well

$$\varphi(x) = A \sin\left(\frac{n\pi}{a}x\right)$$

$$\int_0^a \varphi^* \varphi \, dx = 1$$

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

$$\underbrace{\int_0^a \sin^2\left(\frac{n\pi}{a}x\right)}_{a/2}$$

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

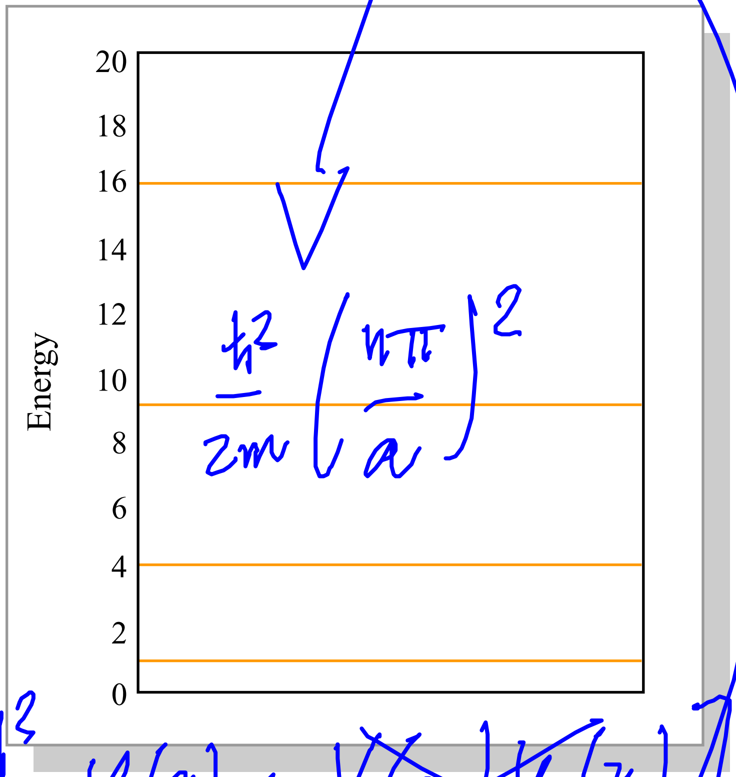


Figure by MIT OCW.

$$\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

$$E = \int \left(\sqrt{\frac{2}{a}} \sin \frac{n\pi}{a}x\right)^* \cdot \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) + V(x)\varphi(x)\right] dx$$

$$= +\frac{\hbar^2}{2m}\int \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a}x \cdot \sqrt{\frac{2}{a}}\left(\frac{n\pi}{a}\right)^2 \sin \frac{n\pi}{a}x \, dx$$

Absorption Lines (atomic units)

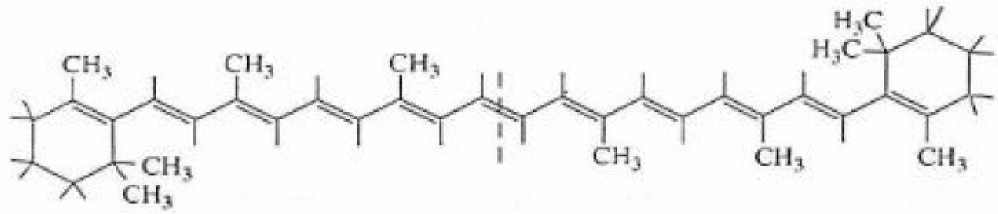
$E = h\nu$

$n = 2$ $\qquad E_2 = 4 E_1$

$n = 1$ $\qquad E_1 = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} 1$

The power of carrots

- β-carotene



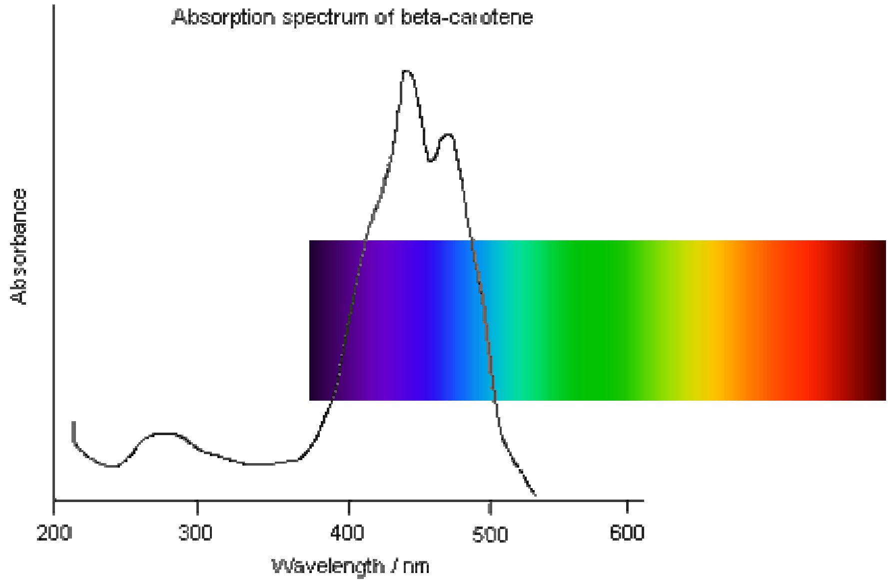


Photo courtesy of Andrew Dunn.

Particle in a 2-dim box

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

$$\Downarrow$$

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

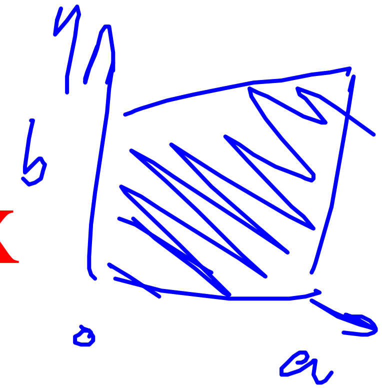
$$-\frac{\hbar^2}{2m}Y(y)\frac{\partial^2 X}{\partial x^2}-\frac{\hbar^2}{2m}X(x)\frac{\partial^2 Y}{\partial y^2}=E\,X(x)\,Y(y)$$

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

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2}=E_x$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}=E_y$$

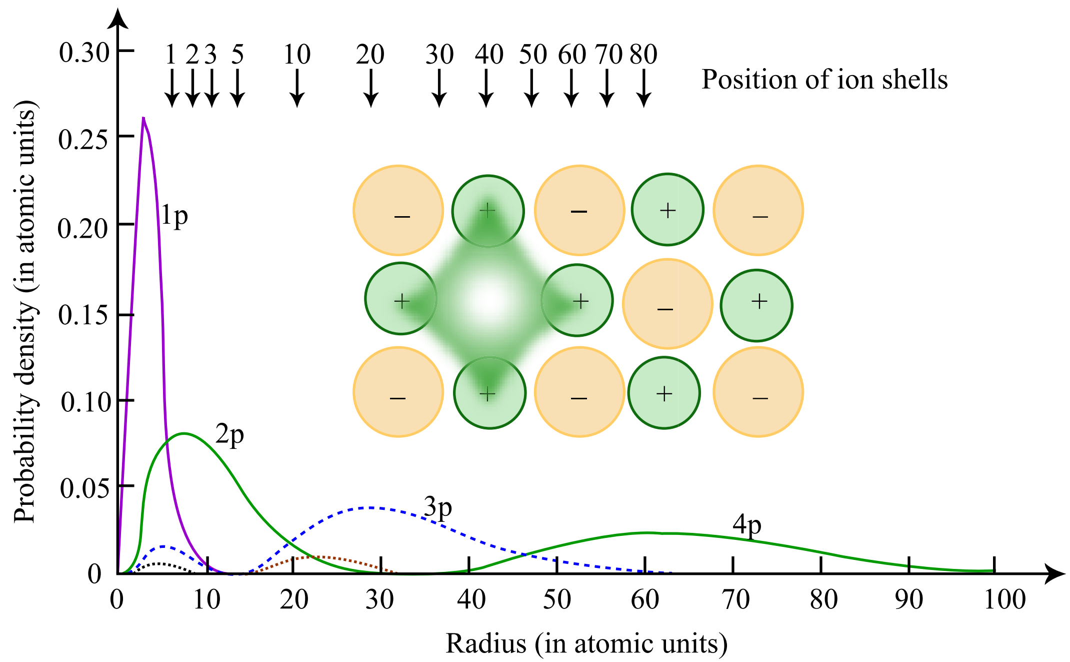
Particle in a 2-dim box



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

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

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



Wavefunction of an electron bound to a vacancy.

Figure by MIT OCW.

From Carl Zeiss to MIT…

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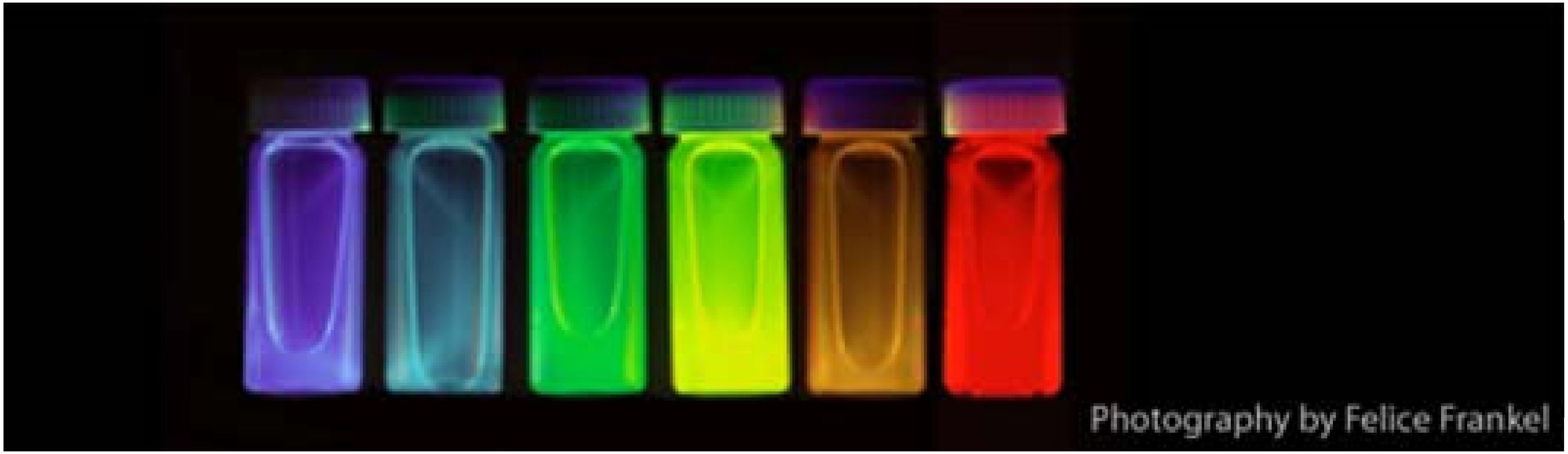
Light absorption/emission



MIT Research: Bawendi, Mayes, Stellacci

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See the chart of various diamondoids at http://www.physik.tu-berlin.de/cluster/diamondoids.html.

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