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

3.23 Fall 2007 – Lecture 4

CLOSE TO COLLAPSE

The collapse of the wavefunction

Travel

- Office hour (this time only)

Last time: Wave mechanics

1. The ket $|\Psi\rangle$ describe the system
2. The evolution is deterministic, but it applies to stochastic events
3. Classical quantities are replaced by operators
4. The results of measurements are eigenvalues, and the ket collapses in an eigenvector

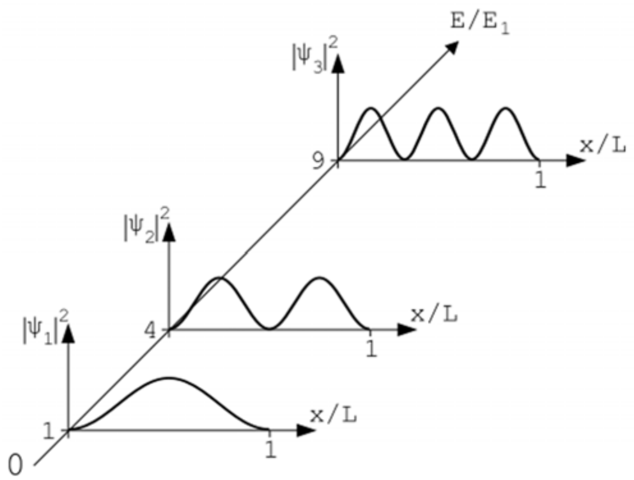
Commuting Hermitian operators have a set of common eigenfunctions

Fifth postulate

- If the measurement of the physical quantity A gives the result a_n , the wavefunction of the system immediately after the measurement is the eigenvector

$$\left|\varphi_n\right\rangle$$

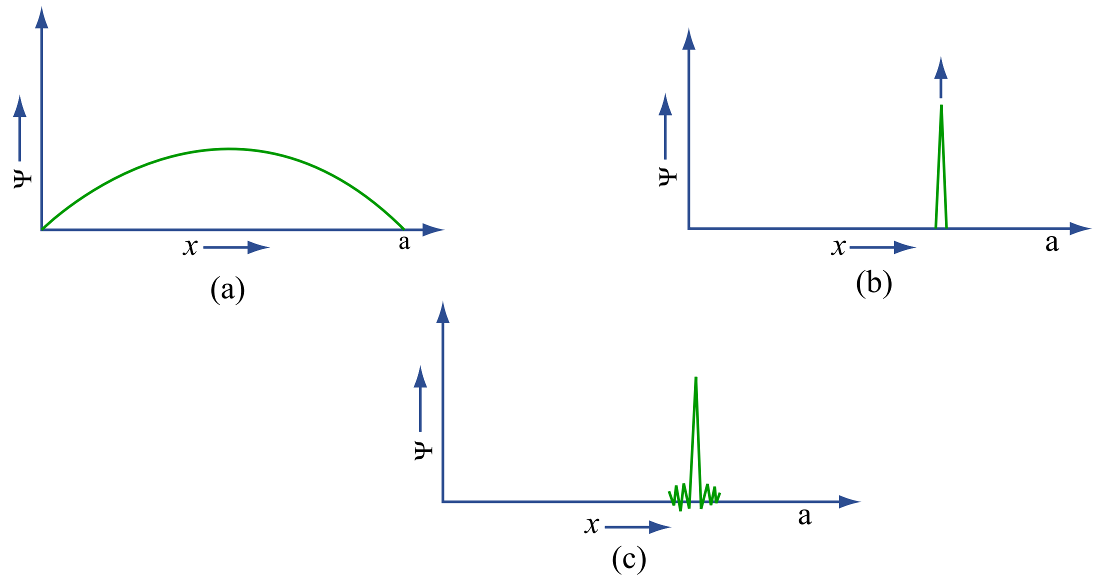
Position and probability



Graphs of the probability density for positions of a particle in a one-dimensional hard box according to classical mechanics removed for copyright reasons. See Mortimer, R. G. Physical Chemistry. 2nd ed. San Diego, CA: Elsevier, 2000, page 555, Figure 15.3.

Diagram showing the probability densities of the first 3 energy states in a 1D quantum well of width L.

"Collapse" of the wavefunction



The wave function of a particle in a box. (a) Before a position measurement (schematic). The probability density is nonzero over the entire box (except for the endpoints). (b) Immediately after the position measurement (schematic). In a very short time, the particle cannot have moved far from the position given by the measurement, and the probability density must be a sharply peaked function. (c) Shortly after a position measurement (schematic). After a short time, the probability density can be nonzero over a larger region.

Figure by MIT OpenCourseWare.

Quantum double-slit

Image removed due to copyright restrictions.

Please see any experimental verification of the double-slit experiment, such as
http://commons.wikimedia.org/wiki/Image:Doubleslitexperiment_results_Tanamura_1.gif

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

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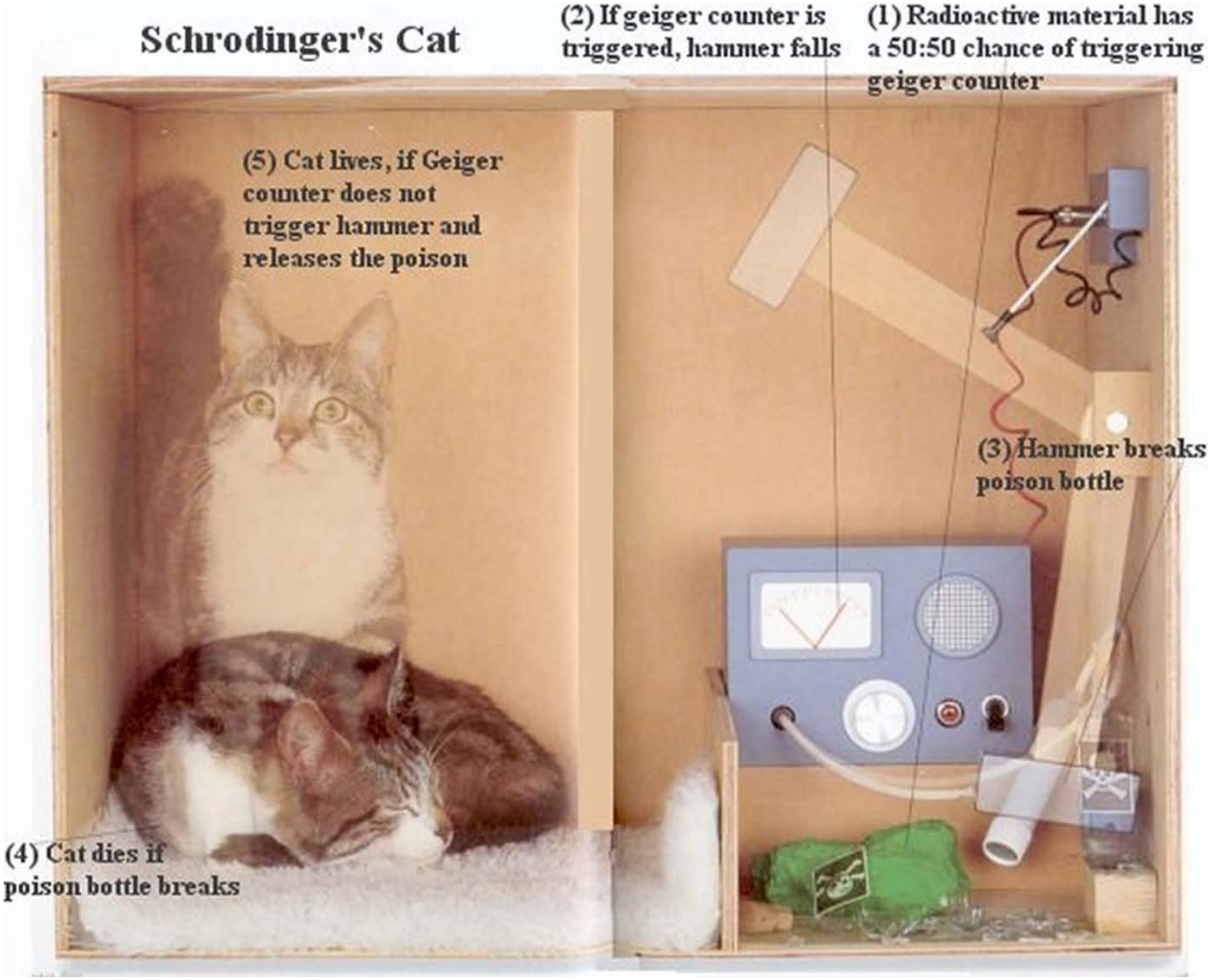
Deterministic vs. stochastic

- Classical, macroscopic objects: we have well-defined values for all dynamical variables at every instant (position, momentum, kinetic energy…)

- Quantum objects: we have well-defined probabilities of measuring a certain value for a dynamical variable, when a large number of identical, independent, identically prepared physical systems are subject to a measurement.

When scientists turn bad…



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Cat wavefunction

$$\left|\Psi_{cat}(t)\right\rangle = \left|\Psi_{alive}\right\rangle \left(\exp\left(-\frac{t}{\tau}\right)\right)^{\frac{1}{2}} + \left|\Psi_{dead}\right\rangle \left(1-\exp\left(-\frac{t}{\tau}\right)\right)^{\frac{1}{2}}$$

- There is not a value of the observable until it's measured (a conceptually different "statistics" from thermodynamics)

Uncertainties, and Heisenberg's Indetermination Principle

$$(\Delta A)^2 = \left\langle \left(A - \langle A \rangle\right)^2 \right\rangle = \left\langle A^2 \right\rangle - \langle A \rangle^2$$

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|$$

$$\left[x, -i\hbar \frac{d}{dx} \right] = i\hbar$$

Linewidth Broadening

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Top Three List

- ***Albert Einstein:* "***Gott wurfelt nicht!" [God does not play dice!]*
- ***Werner Heisenberg*** *"I myself . . . only came to believe in the uncertainty relations after many pangs of conscience. . ."*
- **Erwin Schrödinger:** *"Had I known that we were not going to get rid of this damned quantum jumping, I never would have involved myself in this business!"*

Spherical Coordinates

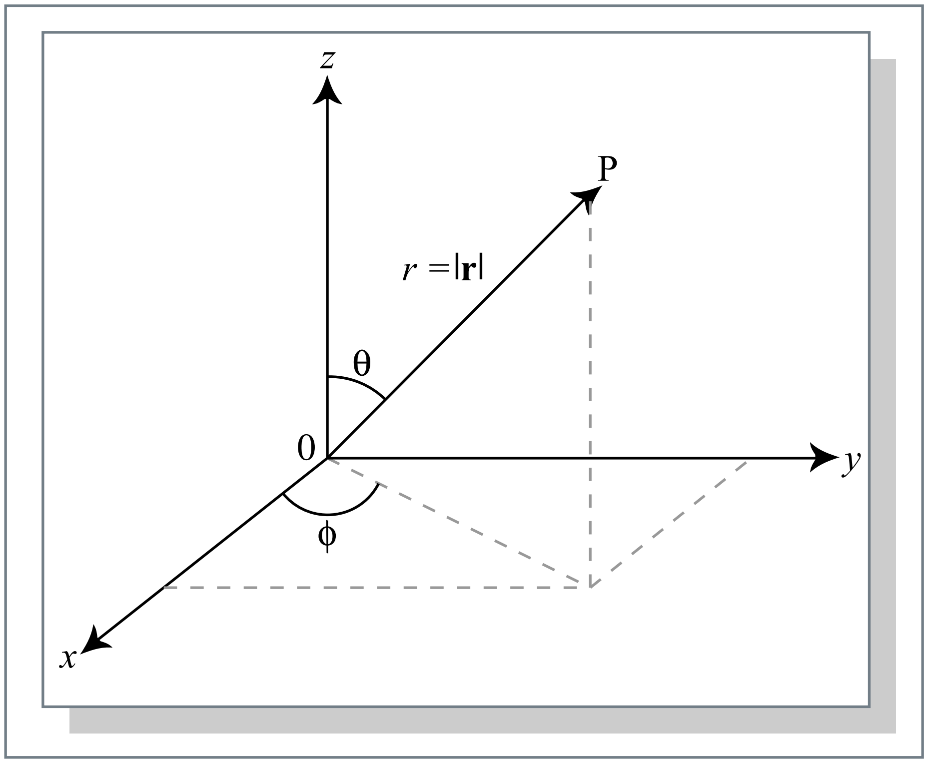


Figure by MIT OpenCourseWare.

$$x = r\sin\theta\cos\varphi$$

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta$$

Angular Momentum

Classical

$$\vec{L} = \vec{r} \times \vec{p}$$

Quantum

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right)$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right)$$

Commutation Relation

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$\left[\hat{L}^2, \hat{L}_x\right] = \left[\hat{L}^2, \hat{L}_y\right] = \left[\hat{L}^2, \hat{L}_z\right] = 0$$

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar \hat{L}_z \neq 0$$

Angular Momentum in Spherical Coordinates

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$$

$$\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right)$$

Eigenfunctions of L_z , L^2

$$\hat{L}_z Y_l^m(\theta,\varphi) = -i\hbar \frac{\partial}{\partial \varphi} Y_l^m(\theta,\varphi) = m\hbar Y_l^m(\theta,\varphi)$$

$$-\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right) Y_l^m(\theta,\varphi) = \hbar^2 l(l+1) Y_l^m(\theta,\varphi)$$

Simultaneous eigenfunctions of L^2, L_z

$$\hat{L}_z Y_l^m(\theta,\varphi) = m\hbar Y_l^m(\theta,\varphi)$$

$$\hat{L}^2 Y_l^m(\theta,\varphi) = \hbar^2 l(l+1) Y_l^m(\theta,\varphi)$$

$$Y_l^m(\theta,\varphi) = \Theta_l^m(\theta)\Phi_m(\varphi)$$

$$Y_0^0(\theta,\phi) = \frac{1}{(4\pi)^{1/2}}$$

$$Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$$

$$Y_1^{\pm1}(\theta,\phi) = \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta\, e^{\pm i\phi}$$

$$Y_2^0(\theta,\phi) = \left(\frac{5}{16\pi}\right)^{1/2} \left(3\cos^2\theta - 1\right)$$

$$Y_2^{\pm1}(\theta,\phi) = \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_2^{\pm2}(\theta,\phi) = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta\, e^{\pm 2i\phi}$$

Spherical Harmonics in Real Form

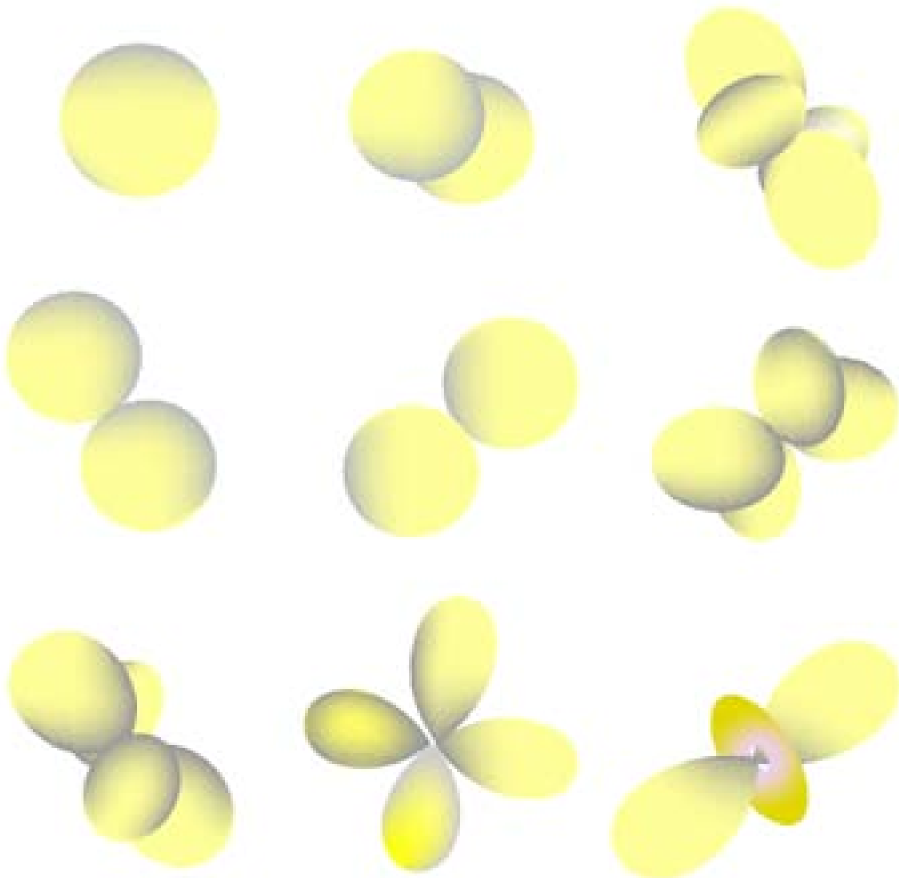


Figure by MIT OpenCourseWare.

$$p_x = \frac{1}{\sqrt{2}}\left(Y_1^1 + Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \cos\phi$$

$$p_y = \frac{1}{\sqrt{2}\, i}\left(Y_1^1 - Y_1^{-1}\right) = \sqrt{\frac{3}{4\pi}} \sin\theta \sin\phi$$

$$p_z = Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$d_{z^2} = Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$

$$d_{xz} = \frac{1}{\sqrt{2}}\left(Y_2^1 + Y_2^{-1}\right) = \sqrt{\frac{15}{4\pi}} \sin\theta \cos\theta \cos\phi$$

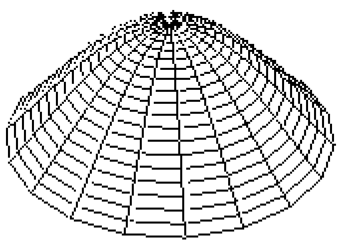
$$d_{yz} = \frac{1}{\sqrt{2}\, i}\left(Y_2^1 - Y_2^{-1}\right) = \sqrt{\frac{15}{4\pi}} \sin\theta \cos\theta \sin\phi$$

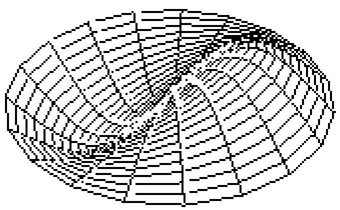
$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}\left(Y_2^2 + Y_2^{-2}\right) = \sqrt{\frac{15}{16\pi}} \sin^2\theta \cos 2\phi$$

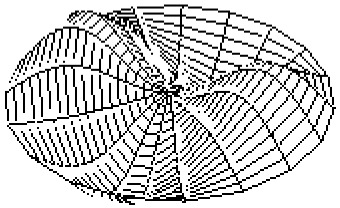
$$d_{xy} = \frac{1}{\sqrt{2}\, i}\left(Y_2^2 - Y_2^{-2}\right) = \sqrt{\frac{15}{16\pi}} \sin^2\theta \sin 2\phi$$

Same as a beating drum…

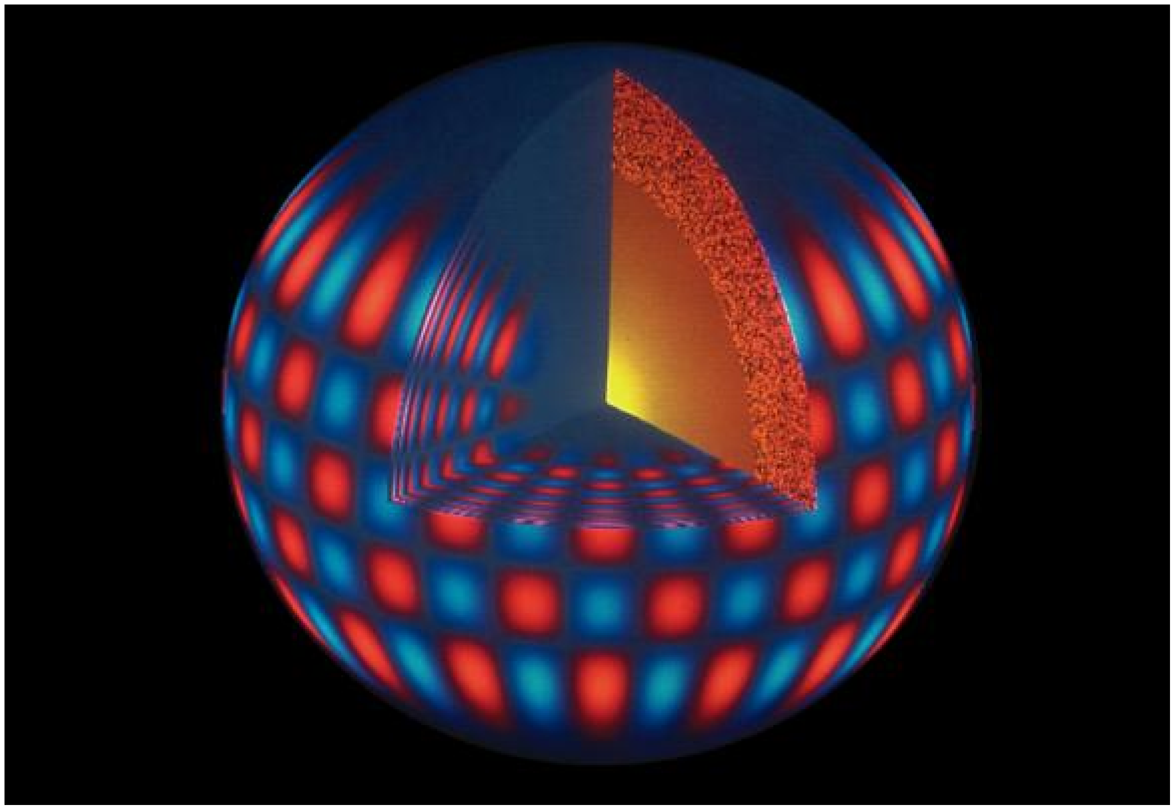
01 11 21





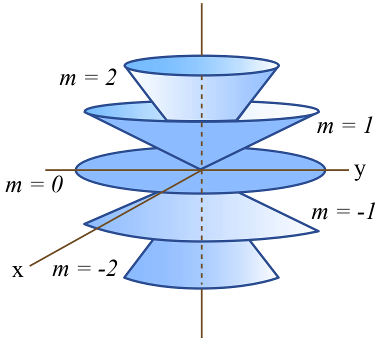


…for the career helioseismologist



Normal modes (i.e. sound, or seismic waves) for the Sun (basically jello in a 3d spherical box)

Angular Momentum, then…



Cones of possible angular momentum directions for $l = 2$. These cones are similar to the cones of precession of a gyroscope, and represent possible directions for the angular momentum vector. The z component is arbitrarily chosen as the one component that can have a definite value.

Figure by MIT OpenCourseWare.

$$L^2 = l(l+1)\hbar^2 = 0, \quad 2\hbar^2, \quad 6\hbar^2 \ldots$$

$$L_z = 0, \quad \pm\hbar, \quad \pm 2\hbar, \quad \pm 3\hbar \ldots$$

An electron in a central potential (I)

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})$$

∇^2 needs to be in spherical coordinates

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right] + V(r)$$

$$\hat{H} = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}\right] + V(r)$$

An electron in a central potential (II)

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{L^2}{2\mu r^2} + V(r)$$

$$\psi_{nlm}(\vec{r}) = R_{nlm}(r)Y_{lm}(\vartheta,\varphi)$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} + V(r)\right]R_{nl}(r) = E_{nl}\,R_{nl}(r)$$

An electron in a central potential (III)

$$u_{nl}(r) = r\,R_{nl}(r) \qquad V_{eff}(r) = \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2} - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{eff}(r)\right]u_{nl}(r) = E_{nl}\,u_{nl}(r)$$

What is the $V_{eff}(r)$ potential ?

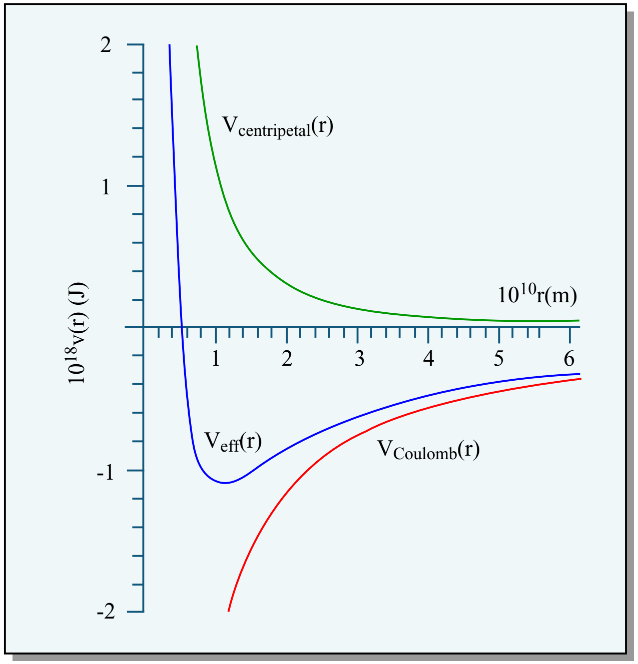
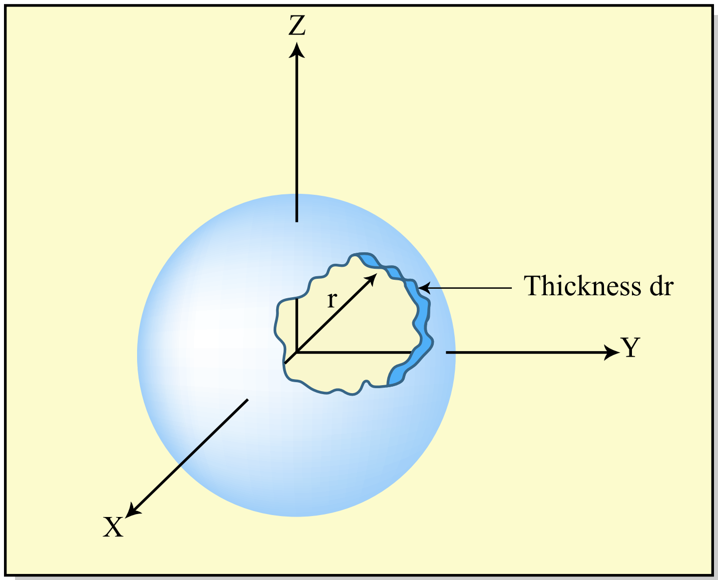
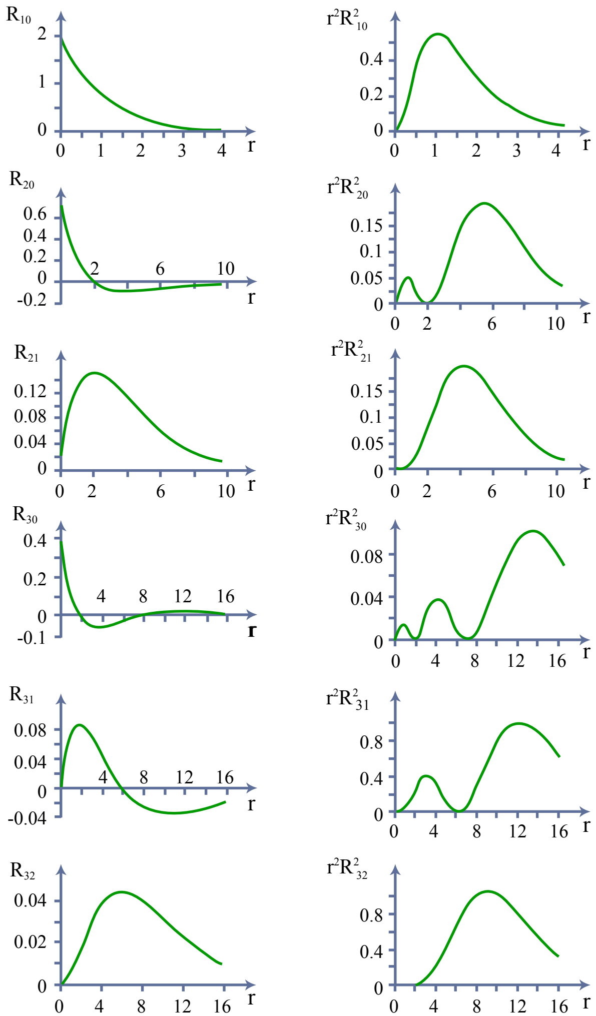


Figure by MIT OpenCourseWare.

The Radial Wavefunctions for Coulomb V(r)





Figures by MIT OpenCourseWare.

Radial functions $R_{nl}(r)$ and radial distribution functions $r^2R^2_{nl}(r)$ for atomic hydrogen. The unit of length is $a_\mu = (m/\mu)\, a_0$, where a_0 is the first Bohr radius.

The Grand Table

Shell	Quantum numbers n	l	m	Spectroscopic notation	Wave function $\Psi_{nlm}(r, \theta, \phi)$
K	1	0	0	1s	$\frac{1}{\sqrt{\pi}}(Z/a_0)^{3/2} \exp(-Zr/a_0)$
L	2	0	0	2s	$\frac{1}{2\sqrt{2\pi}}(Z/a_0)^{3/2}(1-Zr/2a_0)\exp(-Zr/a_0)$
	2	1	0	$2p_0$	$\frac{1}{4\sqrt{2\pi}}(Z/a_0)^{3/2}(Zr/a_0)\exp(-Zr/2a_0)\cos\theta$
	2	1	± 0	$2p_{\pm1}$	$\mp\frac{1}{8\sqrt{\pi}}(Z/a_0)^{3/2}(Zr/a_0)\exp(-Zr/2a_0)\sin\theta\exp(\pm i\phi)$
M	3	0	0	3s	$\frac{1}{3\sqrt{3\pi}}(Z/a_0)^{3/2}(1-2Zr/3a_0+2Z^2r^2/27a\ )\exp(-Zr/3a_0)$
	3	1	0	$3p_0$	$\frac{2\sqrt{2}}{27\sqrt{\pi}}(Z/a_0)^{3/2}(1-Zr/6a_0)(Zr/a_0)\exp(-Zr/3a_0)\cos\theta$
	3	1	± 1	$3p_{\pm1}$	$\mp\frac{2}{27\sqrt{\pi}}(Z/a_0)^{3/2}(1-Zr/6a_0)(Zr/a_0)\exp(-Zr/3a_0)\sin\theta\exp(\pm i\phi)$
	3	2	0	$3d_0$	$\frac{1}{81\sqrt{6\pi}}(Z/a_0)^{3/2}(Z^2r^2/a\ )\exp(-Zr/3a_0)(3\cos^2\theta-1)$
	3	2	± 1	$3d_{\pm1}$	$\mp\frac{1}{81\sqrt{\pi}}(Z/a_0)^{3/2}(Z^2r^2/a\ )\exp(-Zr/3a_0)\sin\theta\cos\theta\exp(\pm i\phi)$
	3	2	± 2	$3d_{\pm2}$	$\frac{1}{162\sqrt{\pi}}(Z/a_0)^{3/2}(Z^2r^2/a\ )\exp(-Zr/3a_0)\sin^2\theta\exp(\pm 2i\phi)$

The complete normalised hydrogenic wave functions corresponding to the first three shells, for an 'infinitely heavy' nucleus. The quantity $a_0 = 4\pi\varepsilon_0 h^2/me^2$ is the first Bohr radius. In order to take into account the reduced mass effect one should replace a_0 by $a_\mu = a_0(m/\mu)$

Figure by MIT OpenCourseWare.

Solutions in the central Coulomb Potential: the Alphabet Soup

http://www.orbitals.com/orb/orbtable.htm