PHY 741 Quantum Mechanics
12-12:50 PM MWF Olin 103

Plan for Lecture 15:
Review Chapters 1,3-7,9-12

1. Some relevant mathematical formalism
2. Quantum mechanical concepts
3. One-dimensional quantum systems
4. Commutators and uncertainty principle
5. Multiparticle systems
6. Eigenvalues and eigenvectors of angular momentum

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/28/2017	Chap. 1	Review of basic principles	#1	9/6/2017
2	Wed, 8/30/2017	Chap. 1	Linear vector spaces	#2	9/6/2017
3	Fri, 9/01/2017	Chap. 1	Linear vector spaces	#3	9/6/2017
4	Mon, 9/04/2017	Chap. 4	Principles of Quantum Mechanics	#4	9/8/2017
5	Wed, 9/06/2017	Chap. 5	Examples in 1 dimension		
6	Fri, 9/08/2017	Chap. 5	Schrödinger equation in one-dimension	#5	9/13/2017
7	Mon, 9/11/2017	Chap. 5	Schrödinger equation in one-dimension		
8	Wed, 9/13/2017	Chap. 7	Schrödinger equation in one-dimension	#6	9/15/2017
9	Fri, 9/15/2017	Chap. 7	Schrödinger equation in one-dimension	#7	9/20/2017
10	Mon, 9/18/2017	Chap. 5 and 7	Schrödinger equation in one-dimension		
11	Wed, 9/20/2017	Chap. 9	Commutator formalism	#8	9/22/2017
12	Fri, 9/22/2017	Chap. 10	Quantum mechanics of multiparticle systems	#9	9/25/2017
13	Mon, 9/25/2017	Chap. 10-12	Multiparticle systems and angular momentum		
14	Wed, 9/27/2017	Chap. 12	Eigenstates of angular momentum		
15	Fri, 9/29/2017	Chap. 1,4,5,7,9,10,12	Review		
	Mon, 10/02/2017		*Take-home exam -- No class*		
	Wed, 10/04/2017		*Take-home exam -- No class*		
16	Fri, 10/06/2017				

Next class on Oct. 6th

Operators and matrices, especially Hermitian and Unitary

An operator **O** can generally be evaluated using an orthgonal basis:

$$\mathbf{O} = \sum_{i,j=1}^{n} |i\rangle O_{ij} \langle j| \quad \text{where} \quad O_{ij} \equiv \langle i|\mathbf{O}|j\rangle$$

Properties of special operators: $\mathbf{O}|\Psi_\alpha\rangle = \lambda_\alpha |\Psi_\alpha\rangle$

Hermitian operators: $\mathbf{O} = \mathbf{O}^\dagger$ $\quad O_{ij} = O^*_{ji}$

$\Rightarrow$ Eigenvalues are real; eigenvectors are orthonormal

Unitary operators: $\mathbf{O}^{-1} = \mathbf{O}^\dagger$ $\quad O^{-1}_{ij} = O^*_{ji}$

$\Rightarrow |\lambda_\alpha| = 1$; eigenvectors are orthonormal

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Functions of Operators

An operator **O** can generally be evaluated within a spanning orthonormal basis:

$$\mathbf{O} = \sum_{i,j=1}^{n} |i\rangle O_{ij} \langle j| \quad \text{where} \quad O_{ij} \equiv \langle i|\mathbf{O}|j\rangle$$

It is often convenient to choose the spanning orthnormal basis from the eigenvectors:

$$\mathbf{O}|\Psi_\alpha\rangle = \lambda_\alpha |\Psi_\alpha\rangle$$

$$\Rightarrow \mathbf{O} = \sum_{\alpha=1}^{n} \lambda_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

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How can we evaluate functions of operators?

Assume that $f(\mathbf{O}) = f(0) + \mathbf{O}f'(0) + \frac{1}{2}\mathbf{O}^2 f''(0) + \frac{1}{3!}\mathbf{O}^3 f'''(0) + \cdots$

Properties of eigenvectors:

$$\mathbf{O}|\Psi_\alpha\rangle = \lambda_\alpha |\Psi_\alpha\rangle$$

$$\mathbf{O}^2|\Psi_\alpha\rangle = \lambda_\alpha^2 |\Psi_\alpha\rangle$$

$$\mathbf{O}^3|\Psi_\alpha\rangle = \lambda_\alpha^3 |\Psi_\alpha\rangle \quad \cdots$$

Example:

$$e^{\mathbf{O}} = 1 + \mathbf{O} + \frac{1}{2}\mathbf{O}^2 + \frac{1}{3!}\mathbf{O}^3 + \cdots$$

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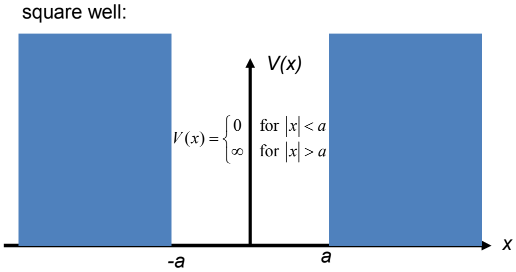
Quantum mechanical particles in one dimension

Energy eigenstates of the Schrödingder equation

$$H|E\rangle = E|E\rangle$$

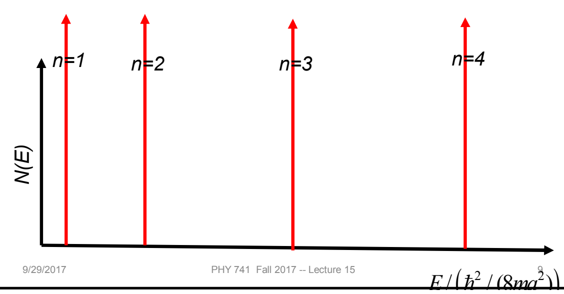
Example: Particle of mass *m* confined within an infinite square well:



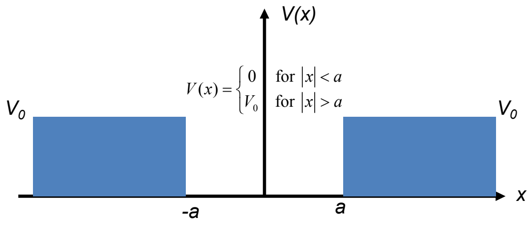
Summary of results: $E = \frac{\hbar^2 \pi^2 n^2}{8ma^2}$

For n odd: $\psi(x) = \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right)$ For n even: $\psi(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right)$

Summary: Energy eigenvalue spectrum for a particle of mass *m* confined within an infinite square well of width *2a*:



Example: Particle of mass *m* confined within an finite square well:



$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ V_0 & \text{for } |x| > a \end{cases}$$

Solution of transcendental equations:

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}a\right) = \sqrt{\frac{V_0 - E}{E}} \quad \Rightarrow \tan\left(\frac{\sqrt{2mV_0}a}{\hbar}\sqrt{\frac{E}{V_0}}\right) = \sqrt{\frac{1 - E/V_0}{E/V_0}}$$

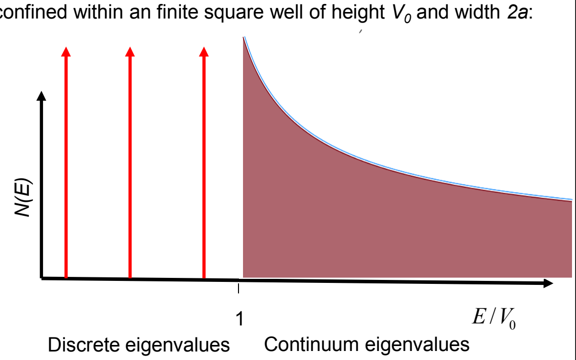
$$\cot\left(\frac{\sqrt{2mE}}{\hbar}a\right) = -\sqrt{\frac{V_0 - E}{E}} \quad \Rightarrow \cot\left(\frac{\sqrt{2mV_0}a}{\hbar}\sqrt{\frac{E}{V_0}}\right) = -\sqrt{\frac{1 - E/V_0}{E/V_0}}$$

$$\text{Let} \quad u \equiv \frac{\sqrt{2mV_0}a}{\hbar} \qquad \epsilon \equiv \sqrt{\frac{E}{V_0}}$$

$$\tan(u\epsilon) = \sqrt{\frac{1-\epsilon^2}{\epsilon^2}}$$

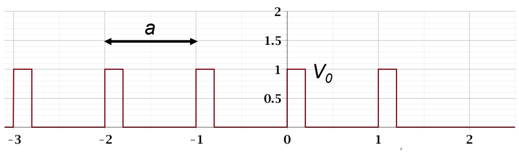
$$\text{or} \qquad \cot(u\epsilon) = -\sqrt{\frac{1-\epsilon^2}{\epsilon^2}}$$

Summary: Energy eigenvalue spectrum for a particle of mass *m* confined within an finite square well of height V_0 and width $2a$:



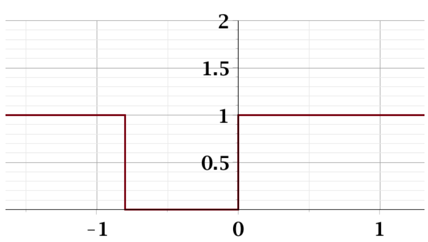
Another example of a one-dimensional system

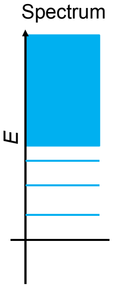
Consider an electron moving in a one-dimensional model potential (Kronig and Penney, *Proc. Roy. Soc. (London)* **130,** 499 (1931)



Consider a single potential well

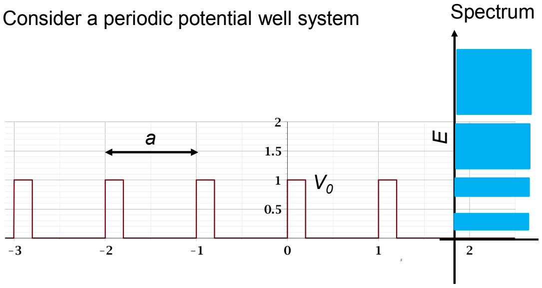
Spectrum





Consider a periodic potential well system

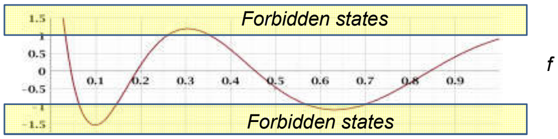
Spectrum



Some details of solution --

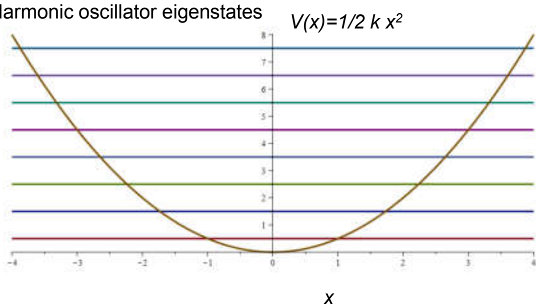
$$\cos(ka) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2} \cos\left(11.7\sqrt{f} - \Delta(f)\right)$$

$$\tan\Delta(f) = \frac{1-2f}{2\sqrt{f(1-f)}} \tanh\left(0.687\sqrt{1-f}\right)$$



$$X(f) = \left(1 + \frac{\sinh^2\left(0.687\sqrt{1-f}\right)}{4f(1-f)}\right)^{1/2} \cos\left(11.7\sqrt{f} - \Delta(f)\right)$$

Harmonic oscillator eigenstates $V(x)=1/2\ k\ x^2$



Comes from analysis of systems near equilibrium:

$$V(x) = V(x_0) + \left.\frac{dV}{dx}\right|_{x_0}(x - x_0) + \frac{1}{2!}\left.\frac{d^2V}{dx^2}\right|_{x_0}(x - x_0)^2 + \cdots$$

Complete solution including normalization

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right]$$

$$E_n = \hbar\omega\left(\frac{1}{2} + n\right) \qquad n = 0,1,2,.....$$

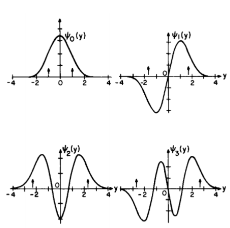


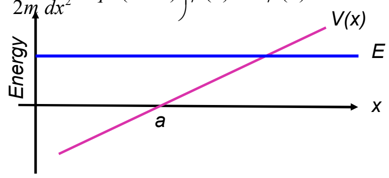
Figure 7.1. Normalized eigenfunctions for $n = 0, 1, 2,$ and 3. The small arrows at $|y| = (2n+1)^{1/2}$ stand for the classical turning points. Recall that $y = (m\omega/\hbar)^{1/2}x$.

Energy eigenstates of the Schrödinger equation for one-dimensional systems

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

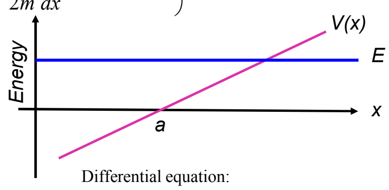
Suppose that the potential is due to an electrostatic field F and the particle has charge q such that $V(x)=qF(x-a)$:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+qF(x-a)\right)\psi(x)=E\psi(x)$$



One dimensional Schrödinger equation for charged particle in an electrostatic field – continued:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+qF(x-a)\right)\psi(x)=E\psi(x)$$



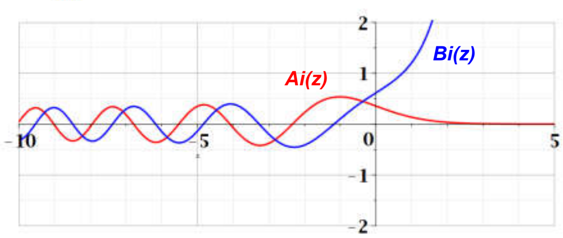
Differential equation:

$$\left(\frac{d^2}{dx^2}-\frac{2mqF}{\hbar^2}(x-b)\right)\psi(x)=0 \quad \text{where } b\equiv a+\frac{E}{qF}$$

$$\left(\frac{d^2}{du^2}-\alpha u\right)\psi(u)=0 \quad \text{where } u\equiv x-b \quad \alpha\equiv\frac{2mqF}{\hbar^2}$$

Airy functions

$$\frac{d^2w}{dz^2}=zw$$



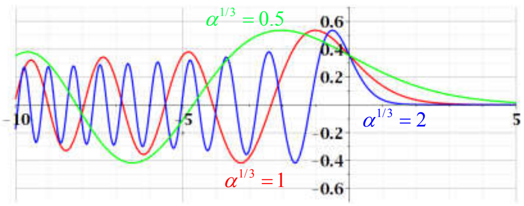
Summary of results

Differential equation:

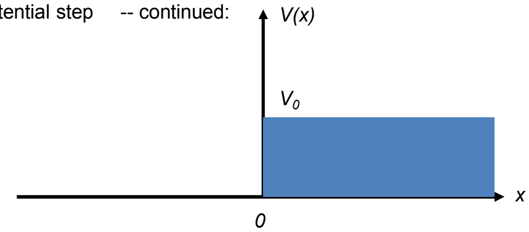
$$\left(\frac{d^2}{dx^2}-\frac{2mqF}{\hbar^2}(x-b)\right)\psi(x)=0 \qquad \text{where } b\equiv a+\frac{E}{qF}$$

$$\left(\frac{d^2}{du^2}-\alpha u\right)\psi(u)=0 \qquad \text{where } u\equiv x-b \qquad \alpha\equiv\frac{2mqF}{\hbar^2}$$

$$\psi(u)=\mathcal{N}Ai(\alpha^{1/3}u)$$



Consider a particle of mass *m* in the presence of an infinite potential step -- continued:



Eigenfunctions of the Schroedinger equation:

$x<0$

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

$x>0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)=\left(E-V_0\right)\psi(x)$$

Notion of current density for continuum wavefunctions

$$i\hbar\frac{\partial\psi}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right)\psi \qquad -i\hbar\frac{\partial\psi^*}{\partial t}=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right)\psi^*$$

$$i\hbar\psi^*\frac{\partial\psi}{\partial t}=\psi^*\left(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})\right)\psi$$

Define probability density: $\rho(\mathbf{r},t)\equiv P(\mathbf{r},t)=\psi^*(\mathbf{r},t)\psi(\mathbf{r},t)$

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0$$

where $\mathbf{j}\equiv\frac{\hbar}{2mi}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)$

Example: $\psi(\mathbf{r},t)=\psi(x,t)=\frac{1}{\sqrt{2\pi}}e^{ikx} \quad\Rightarrow\quad \mathbf{j}=\frac{\hbar k}{m}\hat{\mathbf{x}}$

Commutation relations

Commutator formalism in quantum mechanics

Definition:
Given two Hermitian operators A and B, their commutator is
$[A,B] \equiv AB - BA$

Theorem:
Given Hermitian operators A, B, C such that
$[A,B] = iC$,
it follows that $\Delta A \Delta B \geq \frac{1}{2}\left|\langle C \rangle\right|$

Example: $[X, P_x] = i\hbar$

Multi particle systems

Quantum mechanical treatment of multiparticle systems

For a non-interacting system:

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = H(\mathbf{r}_1) + H(\mathbf{r}_2) + ...H(\mathbf{r}_N)$$

Energy eigenstates:

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N)\psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = E\psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N)$$

Simplification for separable Hamiltonian

For: $H(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a\varphi_a(\mathbf{r}_1)$

$H(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b\varphi_b(\mathbf{r}_2)$

Solution to the many particle problem

$$\psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)...\varphi_z(\mathbf{r}_N)$$

$$E = \varepsilon_a + \varepsilon_b + ...\varepsilon_z$$

Quantum mechanical treatment of multiparticle systems – non-interacting particles

The treatment given on previous slides, assumes that the particles are distinguishable.
A more sophisticated treatment is needed for indistinguishable particles.

Two types of indistinguishable particles:

Fermi particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = -\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

Bose particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = +\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

Quantum mechanical treatment of multiparticle systems – non-interacting **Fermi** particles

Fermi particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = -\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

Example for N particles using Slater determinant:

$$\psi(\mathbf{r}_1,\mathbf{r}_2....\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_a(\mathbf{r}_1) & \varphi_a(\mathbf{r}_2) & \varphi_a(\mathbf{r}_3) & \cdots & \varphi_a(\mathbf{r}_N) \\ \varphi_b(\mathbf{r}_1) & \varphi_b(\mathbf{r}_2) & \varphi_b(\mathbf{r}_3) & \cdots & \varphi_b(\mathbf{r}_N) \\ \varphi_c(\mathbf{r}_1) & \varphi_c(\mathbf{r}_2) & \varphi_c(\mathbf{r}_3) & \cdots & \varphi_c(\mathbf{r}_N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \varphi_z(\mathbf{r}_1) & \varphi_z(\mathbf{r}_2) & \varphi_z(\mathbf{r}_3) & \cdots & \varphi_z(\mathbf{r}_N) \end{vmatrix}$$

$$E = \varepsilon_a + \varepsilon_b + ...\varepsilon_z$$

Eigenvalues and eigenvectors of angular momentum

Review of commutation relations for angular momentum

Angular momentum in three dimensions

$$L_x = YP_z - ZP_y$$
$$L_y = ZP_x - XP_z$$
$$L_z = XP_y - YP_x$$
$$[L_x, L_y] = i\hbar L_z \qquad [L_y, L_z] = i\hbar L_x \qquad [L_z, L_x] = i\hbar L_y$$
$$\left[\mathbf{L}^2, L_z\right] = \left[L_x^2 + L_y^2, L_z\right] = 0$$

Eigenvalues and eigenvectors of **J**^{2} and J_z -- continued

Spectrum generalizes to integer and half-integer j

$$\mathbf{J}^2 \left| jm \right\rangle = \hbar^2 j(j+1) \left| jm \right\rangle$$
$$J_z \left| jm \right\rangle = \hbar m \left| jm \right\rangle$$
$$J_+ \left| jm \right\rangle = \hbar \sqrt{j(j+1) - m^2 - m} \left| j(m+1) \right\rangle$$
$$J_- \left| jm \right\rangle = \hbar \sqrt{j(j+1) - m^2 + m} \left| j(m-1) \right\rangle$$

Example -- for $j = \frac{1}{2}$

$$\mathbf{J} = \frac{\hbar}{2}\left(\sigma_x \hat{\mathbf{x}} + \sigma_y \hat{\mathbf{y}} + \sigma_z \hat{\mathbf{z}}\right)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathbf{J}^2 = \frac{\hbar^2}{4}\left(\sigma_x^2 + \sigma_y^2 + \sigma_z^2\right) = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

For integer values of *j,* it is also possible to find spacial representations of the operators L^2 and L_z

$$L^2 \rightarrow (-\hbar^2)\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$L_z \rightarrow -i\hbar\frac{\partial}{\partial\phi}$$

$$\left|lm\right\rangle = Y_{lm}(\theta,\phi)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \; Y_{lm}^*(\theta,\phi) Y_{l'm'}(\theta,\phi) = \delta_{ll'}\delta_{mm'}$$

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}^*(\theta,\phi) Y_{lm}(\theta',\phi') = \delta(\phi-\phi')\delta(\cos\theta - \cos\theta')$$

Some spherical harmonic functions:

$$Y_{00}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1(\pm1)}(\hat{\mathbf{r}}) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta \, e^{\pm i\phi}$$

$$Y_{10}(\hat{\mathbf{r}}) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{2(\pm2)}(\hat{\mathbf{r}}) = \sqrt{\frac{15}{32\pi}}\sin^2\theta \, e^{\pm 2i\phi}$$

$$Y_{2(\pm1)}(\hat{\mathbf{r}}) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta \, e^{\pm i\phi}$$

$$Y_{20}(\hat{\mathbf{r}}) = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$

Note that:

$$Y_{lm}^*(\hat{\mathbf{r}}) = (-1)^m Y_{l-m}(\hat{\mathbf{r}})$$

(Condon & Shortley convention)

$$Y_{lm}(-\hat{\mathbf{r}}) = (-1)^l Y_{lm}(\hat{\mathbf{r}})$$