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

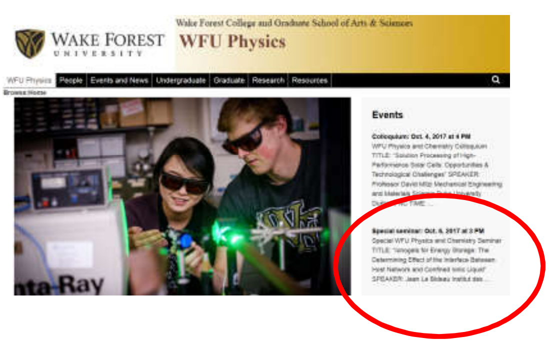
Plan for Lecture 16: Chapters 12-13

1. Eigenvalues and eigenvectors of angular momentum
2. Analysis of spherically symmetric system

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	Chap. 12-13	Spherically symmetric systems		



Review of commutation relations for angular momentum

Angular momentum in three dimensions

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

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Eigenvalues and eigenvectors of $\mathbf{J}^2$ and J_z -- continued

Spectrum generalizes to integer and half-integer j

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

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

$$L^2 \rightarrow (-\hbar^2)\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$
$$L_z \rightarrow -i\hbar\frac{\partial}{\partial\phi}$$
$$\left| lm \right\rangle = Y_{lm}(\theta,\phi)$$
$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta\; Y_{lm}^*(\theta,\phi) Y_{l'm'}(\theta,\phi) = \delta_{ll'}\delta_{mm'}$$
$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}^*(\theta,\phi) Y_{lm}(\theta',\phi') = \delta(\phi-\phi')\delta(\cos\theta - \cos\theta')$$

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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)

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

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Using eigenfunctions of orbital angular momentum to analyze spherically symmetric systems

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Using spherical polar coordinates

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

Note that: $\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y_{lm}(\theta,\phi) = -l(l+1)Y_{lm}(\theta,\phi)$

Try: $\Psi(\mathbf{r}) = R_{El}(r)Y_{lm}(\theta,\phi)$

$$\left(-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right\} + V(r)\right)R_{El}(r)Y_{lm}(\theta,\phi)$$
$$= ER_{El}(r)Y_{lm}(\theta,\phi)$$

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Using eigenfunctions of orbital angular momentum to analyze spherically symmetric systems -- continued

Try: $\Psi(\mathbf{r}) = R_{El}(r)Y_{lm}(\theta,\phi)$

$$\left(-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right\} + V(r)\right)R_{El}(r)Y_{lm}(\theta,\phi)$$
$$= ER_{El}(r)Y_{lm}(\theta,\phi)$$

Equation for radial wavefunction:

$$\left(-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right\} + V(r)\right)R_{El}(r) = ER_{El}(r)$$

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Using eigenfunctions of orbital angular momentum to analyze spherically symmetric systems -- continued

Example for free particle -- $V(r) = 0$

Equation for radial wavefunction:

$$\left(-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right\}\right)R_{El}(r) = ER_{El}(r)$$

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right)R_{El}(r) = 0 \qquad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

Spherical Bessel functions

$$\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + 1\right)f(\rho) = 0$$

Bessel functions

$$j_0(\rho) = \frac{\sin\rho}{\rho},$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho},$$

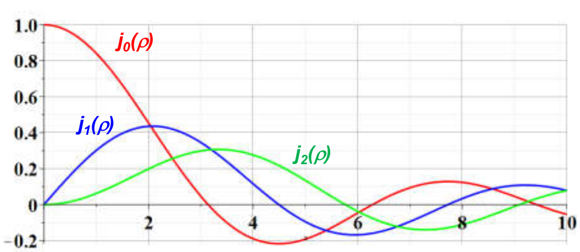
$$j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3\cos\rho}{\rho^2},$$

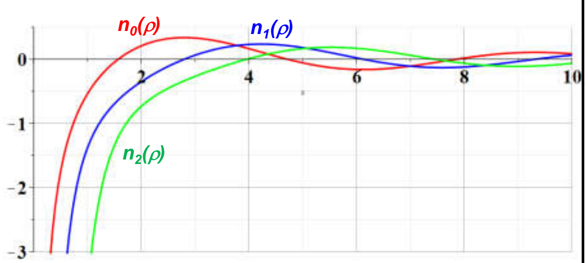
Neumann functions

$$n_0(\rho) = \frac{-\cos\rho}{\rho}$$

$$n_1(\rho) = \frac{-\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$$

$$n_2(\rho) = -\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\cos\rho - \frac{3\sin\rho}{\rho^2}$$





Solution for free particle using spherical symmetry -- continued

Example for free particle -- $V(r) = 0$

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 \right) R_{El}(r) = 0 \qquad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

$$R_{El}(r) = C_{El} j_l(kr)$$

(Note that Neumann function diverges for $r \to 0$)

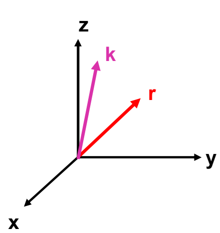
$$\text{Full solution: } \Psi(\mathbf{r}) = \sum_{lm} R_{El}(r) Y_{lm}(\theta,\phi)$$

$$= \sum_{lm} C_{El} j_l(kr) Y_{lm}(\theta,\phi)$$

Other solution forms for free particle:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r) \right) \Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Plane wave solution: $\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \qquad k^2 = \frac{2mE}{\hbar^2}$



$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos(\theta)}$$

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos(\theta)}$$

$$=1 + i\mathbf{k}\cdot\mathbf{r} + \frac{1}{2}\left(i\mathbf{k}\cdot\mathbf{r}\right)^2 + \ldots$$

It can be shown that these terms can be regrouped as a sum over Legendre polynomials and spherical Bessel functions:

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

Angular momentum sum rule:

$$P_l(\cos\theta) = P_l\left(\hat{\mathbf{r}}\cdot\hat{\mathbf{k}}\right) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}\left(\hat{\mathbf{r}}\right) Y_{lm}^*\left(\hat{\mathbf{k}}\right)$$

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \sum_{m=-l}^{l} Y_{lm}\left(\hat{\mathbf{r}}\right) Y_{lm}^*\left(\hat{\mathbf{k}}\right)$$

Connection between the spherical wave and plane representations of the free particle --

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$= \sum_{lm} 4\pi i^l Y_{lm}^*(\hat{\mathbf{k}}) j_l(kr) Y_{lm}(\hat{\mathbf{r}})$$

Other examples of spherically symmetric potentials – isotropic harmonic oscillator in three dimensions:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

For $V(r) = \frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right)$

Solution in cartesian coordinates:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2}m\omega^2 y^2 - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{1}{2}m\omega^2 z^2\right)\Psi(x,y,z)$$
$$= E\Psi(x,y,z)$$

$$\Psi(x,y,z) = X(x)Y(y)Z(z)$$

$$E = \hbar\omega\left(\frac{3}{2} + n_x + n_y + n_z\right) \qquad \text{for} \quad n_x, n_y, n_z = 0,1,2,3,\ldots$$

Other examples of spherically symmetric potentials – isotropic harmonic oscillator in three dimensions -- continued

$$E = \hbar\omega\left(\frac{3}{2} + n_x + n_y + n_z\right) \qquad \text{for} \quad n_x, n_y, n_z = 0,1,2,3,...$$

n_x	n_y	n_z	E
0	0	0	$\frac{3}{2}\hbar\omega$
1	0	0	$\frac{5}{2}\hbar\omega$
0	1	0	
0	0	1	

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Other examples of spherically symmetric potentials – isotropic harmonic oscillator in three dimensions -- continued

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

$$\Psi(\mathbf{r}) = R_{El}(r)Y_{lm}(\hat{\mathbf{r}})$$

Equation for radial wavefunction:

$$\left(-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right\} + \frac{1}{2}m\omega^2 r^2\right)R_{El}(r) = ER_{El}(r)$$

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} - \lambda^2 r^2 + k^2\right)R_{El}(r) = 0 \qquad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

$$\lambda = \frac{m\omega}{\hbar}$$

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Other examples of spherically symmetric potentials – isotropic harmonic oscillator in three dimensions -- continued

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} - \lambda^2 r^2 + k^2\right)R_{El}(r) = 0$$

$$\Rightarrow R_{El}(r) = r^l e^{-\lambda r^2/2} F(-n_r, l + \tfrac{3}{2}, \lambda r^2)$$

where confluent hypergeometric function is defined

$$F(-n_r,, l + \tfrac{3}{2}, \lambda r^2) = 1 + \frac{-n_r}{l + \frac{3}{2}}\lambda r^2 + \frac{-n_r(1-n_r)}{2!\left(l+\frac{3}{2}\right)\left(l+\frac{5}{2}\right)}\left(\lambda r^2\right)^2 + ..$$

with $E = \hbar\omega\left(\dfrac{3}{2} + 2n_r + l\right)$

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