Central Potential (continued)
PHY 314
Fall 2002

The wave function of a single particle with definite energy satisfies the differential equation:

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

In the case of a central potential: $V(\vec{r}) = V(r)$ we found that we could separate variables to yield: $y_{E\ell m}(r, q, f) = R_{E\ell}(r)\,\Theta_{\ell m}(q)\,\Phi_m(f)$.

Points of note:

a) We found that $\Phi_m(f) = e^{imf}$. For the wave function to be single valued under the substitution $f \rightarrow f + 2p$ (i.e. same point in space), *m* must be an integer.

b) For the wave function to be normalizable it turns out that the only possibilities are that ℓ =0, 1, 2, … and $m = -\ell, -\ell+1 \ldots \ell$. This is shown in PHY 302and we will rederive in a very elegant algebraic way next semester).

c) To clean up the notation, one usually collects the q and f dependence in a single function: $Y_{\ell m}(q, f) = N_{\ell m}\,\Theta_{\ell m}(q)\,\Phi_m(f)$ (spherical harmonics) where the coefficient is chosen such that the function is normalized to 1 over the unit sphere. That is, $\oiint Y_{\ell m}^{*} Y_{\ell m}\, d\Omega = 1$ where $d\Omega = df \sin q\, dq$ (where $q = 0 \rightarrow p$) or $d\Omega = df\, d(\cos q)$ (where $\cos q = -1 \rightarrow +1$).

d) The functions $Y_{\ell m}(q, f)$ are independent of the potential and *E*, and so may be solved for once and for all.

e) Because $R_{E\ell}(r)$ independent of *m* and this is the only factor that depends on *E*, there are always (at least) $2\ell + 1$ independent wave functions with this energy. (There could be other solutions of the same *E* but with different values of ℓ, but this would result from a special feature of the potential, and is not in general expected. This does happen for the hydrogen atom, it turns out.)

f) We derived $L_z = \frac{\hbar}{i}\frac{\partial}{\partial f}$ which leads directly to $L_z y_{E\ell m} = m\hbar y_{E\ell m}$. In accord with our postulates of quantum mechanics, if a system is in state $y_{E\ell m}(r, q, f)$, a measurement of L_z will lead to the result $m\hbar$ 100% of the time.

g) From the last set of notes on the central potential, we have

$$-\hbar^2\left[\frac{1}{\sin q}\frac{\partial}{\partial q}\left(\sin q\frac{\partial}{\partial q}\right)+\frac{1}{\sin^2 q}\frac{\partial^2}{\partial f^2}\right]Y_{\ell m}(q,f)=\ell(\ell+1)\hbar^2\, Y_{\ell m}(q,f)\,.$$

Beginning with the expressions for the angular momentum operators worked out in the last set of notes (central.doc), and solving the last homework set you will find that the differential operator in this equation is simply $\vec{L}^2$, the square of the angular momentum. Since the operator is independent of *r*, we have

$$\vec{L}^2 y_{E\ell m} = \ell(\ell+1)\hbar^2 y_{E\ell m}\,.$$

We now have the physical interpretation of the separated wave function. It is a state of definite energy *E*, definite total angular momentum squared $\ell(\ell+1)\hbar^2$, and definite z-component of angular momentum $m\hbar$. You can read more about this function in the PHY 302 tutorial SPH.

h) The function $\Theta_{\ell m}(q)$ that meets these conditions is known as the associated Legendre function (see tutorial ALF). It is related to the standard Legendre polynomials by $\Theta_{\ell m}(q) = P_{\ell m}(m) = (1-m^2)^{m/2}\frac{d^m}{dm^m}P_\ell(m)$ where $m = \cos q$ in the case m and ℓ are non-negative integers satisfying $0 \le m \le \ell$. Notice that $(1-m^2)^{m/2} = \sin^m q$ and that $\Theta_{\ell m}(q)$ is real for real angles. We will not need negative values because of result in j) below.

i) Orthogonality relations: For any value of *m* it works out that

$$\int_0^p \Theta_{\ell m}(q)\ \Theta_{\ell' m}(q)\sin q\, dq = 0$$

if $\ell \neq \ell'$. When this is combined with the similar expression for $\Phi_m(\phi)$ and with the normalization convention, it follows that

$$\oiint Y_{\ell m}(\theta,\phi)^* \, Y_{\ell' m'}(\theta,\phi)\, d\Omega = \delta_{\ell\ell'}\,\delta_{mm'}$$

The integral, as before, is over the unit sphere.

j) I'll also tell you, without proof, that the spherical harmonic satisfies the relation $Y_{\ell,-m}(\theta,\phi) = (-1)^m Y_{\ell m}(\theta,\phi)^*$. This expression is useful, because once we have the spherical harmonics for $m \geq 0$, we can easily get the ones with negative values of *m* by complex conjugation and (possibly) a sign flip.

k) The spherical harmonics are used in many different areas of physics, not just in quantum theory. For example: scattering of EM or acoustic waves from a raindrop, the multipole electric and magnetic moments of charge distributions, gravitational field problems of stars, the shape of the Earth, etc.

l) Now let's look at the spherical harmonics with the lowest three values of ℓ. You may also look at the Maple program that I have put on the class web site (ysh.mw) which will calculate for you – analytically – any spherical harmonic that you choose.

$$Y_{00} = \sqrt{\frac{1}{4\pi}}$$

$$Y_{11} = -\sqrt{\frac{3}{8\pi}}\,\sin\theta\; e^{i\phi}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}}\,\cos\theta$$

$$Y_{22} = \sqrt{\frac{15}{32\pi}}\,\sin^2\theta\; e^{2i\phi}$$

$$Y_{21} = -\sqrt{\frac{15}{8\pi}}\,\sin\theta\,\cos\theta\; e^{i\phi}$$

$$Y_{20} = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right) = \sqrt{\frac{5}{4\pi}}\,P_2(\cos\theta)$$

m) These examples show a general pattern: For the highest value of *m*, i.e. $m = \ell$ it turns out that $Y_{\ell\ell}(\theta,\phi) \propto \sin^\ell\theta\; e^{i\ell\phi}$. All of the "wiggles" are in the ϕ

dependence. If m =0, we have $Y_{\ell 0}(\theta,\phi)=\sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta)$ -- a normalized Legendre polynomial. In this case all of the wiggles are in the θ dependence. In between, both dependences wiggle, but the closer m is to ℓ, the more wiggling is in ϕ, and the closer m is to 0, the more wiggling is in the θ.

n) I'll draw some sketches of examples of $|Y_{\ell m}(\theta,\phi)|^2$ on the board…

o) Semi-classical pictures. Since the wave functions have only definite values of $\vec{L}^2 \to \ell(\ell+1)\hbar^2$ and $L_z \to m\hbar$ all we can specify quantum-mechanically is the length of the angular momentum vector and its z-component. Semi-classically, the angular momentum is determined only up to directions on a cone with definite $|\vec{L}|$ and L_z. For example, if $\ell = 3$ the length of $\vec{L}$ is $\sqrt{7}\,\hbar$ and there are 7 (=2 x 3 + 1) different orientations (or cones) with $L_z = -3\hbar, -2\hbar, \ldots 3\hbar$.

o) *Reminder about Legendre Polynomials.*
Things that you should know by heart (except perhaps 2). See tutorial LP from PHY 302 or your E&M book for more details.

1) Memorize: $P_0(x)=1 \quad P_1(x)=x \quad P_2(x)=\frac{1}{2}\left(3x^2-1\right) \ \ldots$

2) All the rest can be obtained from the recursion relation

$$(n+1)\,P_{n+1}(x)=(2n+1)\,x\,P_n(x)-n\,P_n(x)$$

For example if n = 1: $2\,P_2(x)=3x\,P_1(x)-P_0(x)=3x^2-1$ which checks with the P_2(x) in part a).

3) $P_n(1)=1$ for all values of n.

4) P_n(x) is a polynomial of order n.

5) P_n(x) is even if n is an even number and is odd if n is an odd number.

6) All the roots of P_n(x) lie in the interval (–1,1).

7) The roots of P_n(x) and P_{n+1}(x) interlace.

8) Orthogonality $\int_{-1}^{1} P_n(x)P_m(x)dx = d_{nm}\frac{2}{2n+1}$

9) Associated Legendre: $P_{nm}(x) = (1-x^2)^{m/2}\frac{d^m P_n(x)}{dx^m}$ where $m \geq 0$. The terms with m < 0 are not needed because of j) above. (Sometimes an extra factor of $(-1)^m$ is included in this definition, and is compensated for in the definition of Y. The definition of Y seems to be very stable.