8	Wed.10/22 Thurs 10/23 Fri.10/24	**4.1.2-.3** Schrodinger in Spherical: Angular & Radial(Q9.1) Computational: Spherical Schrodinger's 4.2 Hydrogen Atom (Q9.1)	**Daily 8.W** **Weekly 8** **Daily 8.F**
9	Mon., 10/27 Tues. 10/28 Wed., 10/29 Fri., 10/31	**4.3** Angular Momentum **4.4.1-.2** Spin ½ & Magnetic Fields (Q5.5,6.1-.2, 8.5) **4.4.3** Addition of Angular Momenta	**Daily 9.M** **Weekly 9** **Daily 9.W** **Daily 9.F**

Equipment

- Griffith's text
- Printout of roster with what pictures I have
- Spherical Schrodinger handout
- P plot.py

Check dailies

Announcements:

Math-physics research presentations today 4pm AHoN 116

4.1 Schrödinger Equation in Spherical Coordinates

4.1.1 Separation of Variables

Central Potential and Spherical Coordinates

If we're interested in a "central potential", that is, one that only depends upon how far the particle is from something (for example, an electron is from a proton), then the potential has spherical symmetry, and so we want to phrase the Schrodinger equation in spherical coordinates.

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right) + V(r)\Psi$$

Then we can hope for separability:

$$\Psi(r,\theta,\phi,t) = R(r)Y(\theta,\phi)\phi(t)$$

Indeed, multiplying by r^2, plugging in and dividing by the wavefunction gets us an equality between terms that clearly don't depend on theta or phi and terms that clearly don't depend on r, so these terms must equal a constant:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-r^2\frac{2m}{\hbar^2}[V(r)-E]\equiv l(l+1)\equiv -\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right)$$

4.1.2 The Angular Equation

Griffiths goes after the angular equation first.

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}=-l(l+1)Y$$

Heck, now that we've got a taste for separability, you probably recognize that the θ and ϕ dependence is separable.

$$Y=\Theta(\theta)\Phi(\phi)$$

Plugging this in and dividing by it, we have

$$\frac{1}{\Theta(\theta)}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right)+l(l+1)\sin^2\theta\equiv m^2\equiv-\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2}$$

ϕ dependence

$$\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2}=-m^2 \text{ or } \frac{\partial^2\Phi(\phi)}{\partial\phi^2}=-m^2\Phi(\phi)$$

Since we don't have a reason to believe that the wavefunction is simply 0 at a particular angle, guessing cosines or sines may not be the best, so we'll go with exponentials.

$$\Phi(\phi)=e^{im\phi}$$

does the job, and it's already normalized!

If we require that the wavefunction be single valued in space, then this needs to have the property that

$$\Phi(\phi)=\Phi(\phi+2\pi)$$

You may remember from last week's homework that this is easily satisfied if

$$m=0,\pm1,\pm2,\ldots$$

θ Dependence

Now, the θ equation's not so simple. Griffiths doesn't even pretend to lead us through a *derivation* of that solution; instead he names it and gets us familiar with it.
I'll back up at least one step to motivate it a little. The equation is

$$\frac{1}{\Theta(\theta)}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right)+l(l+1)\sin^2\theta=m^2$$

At the end of last time, I showed that this could be rewritten as

$$\left(1-\xi^2\right)\frac{\partial}{\partial\xi}\left(\left(1-\xi^2\right)\frac{\partial\Theta(\xi)}{\partial\xi}\right)=\left(m^2+l(l+1)\left(\xi^2-1\right)\right)\Theta(\xi)$$

Where $\xi\equiv\cos\theta$

Finally, just quoting Griffiths (who's just quoting someone else), and putting together equations 4.27 and 4.28, we have

$$\Theta(\xi)=AP_l^m(\xi)=A\frac{\left(1-\xi^2\right)^{|m|/2}}{2^l\,l!}\frac{\partial^{l+|m|}}{\partial\xi^{l+|m|}}\left(\xi^2-1\right)^l$$

No, that wasn't self-evident, but looking at the form of the differential equation, it's certainly gets points for plausibility.

"This is a more simple question about the Rodrigues formula (eqn 4.28 p. 136 U.S. book): the factorial only applies to l not 2^l, correct?" Gigja

Yeah, from the looks of it, that factorial is only being applied to the L Jeremy

Let's look at it (see Python program P.py)

Why must $|m|\le l$?

Well,

$$\left(\xi^2-1\right)^l=\xi^{2l}+a_{l-1}\xi^{2(l-1)}+a_{l-2}\xi^{2(l-2)}+\ldots+1$$

So $\frac{\partial^{l+|m|}}{\partial\xi^{l+|m|}}\left(\xi^2-1\right)^l$ is 0 for $l+|m|>2l$, thus $|m|\le l$.

So, we are one massive step nearer to having our solution,

$$\Psi(r,\theta,\phi,t)=R(r)Y(\theta,\phi)\phi(t)=R(r)\Theta(\theta)\Phi(\phi)\phi(t)=R(r)AP_l^m(\cos\theta)e^{im\phi}e^{-iEt/\hbar}$$

Normalization of Y

Though he doesn't yet have the full expression in hand, at this point, Griffiths begins addressing the question of normalization.

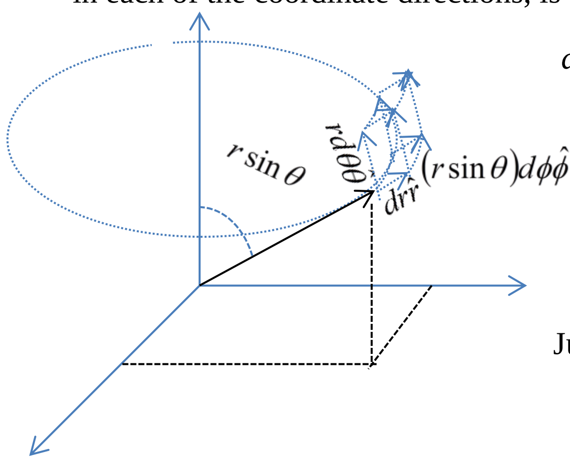
Remember, our approach to normalizing has its origin in the notion that summing the probabilities over all possibilities should result in certainty: a probability of 1. Where, in 3-space, $|\Psi|^2 = \Pr(r,\theta,\phi,t)/dVol$

So

$$1 = \int_{all.space} |\Psi|^2 dVol$$

1. *Math*: Where does equation 4.30 come from? Explain.

Now, in spherical coordinates, the differential block of volume, the product of differential steps in each of the coordinate directions, is



$$dVol = r^2 dr \sin\theta\, d\theta\, d\phi$$

so $$1 = \int_{all.space} |\Psi|^2 r^2 dr \sin\theta d\theta d\phi$$

$$1 = \int_{all.space} |R(r)|^2 |Y(\theta,\phi)|^2 r^2 dr \sin\theta d\theta d\phi$$

Just as the solution is separable, so is this integral:

$$1 = \int_{r=0}^{\infty} |R(r)|^2 r^2 dr \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} |Y(\theta,\phi)|^2 \sin\theta d\theta d\phi$$

Now, you could look at these two integrals as the probabilities of finding the particle at any distance and the probability of finding it in any direction, each of which should be 1.

$$1 = \int_{r=0}^{\infty} |R(r)|^2 r^2 dr \quad \text{and} \quad 1 = \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} |Y(\theta,\phi)|^2 \sin\theta d\theta d\phi$$

Griffiths just quotes the resulting normalization factor for the angular integral

$$Y(\theta,\phi) = AP_l^m(\cos\theta)e^{im\phi} = \varepsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}P_l^m(\cos\theta)e^{im\phi} \text{ where}$$

$$\varepsilon = \begin{cases} 1 & m \le 0 \\ (-1)^m & m > 0 \end{cases}$$

1. *Conceptual*: Is this expression valid if *V* is a function of θ? Explain.

Note that we have just found the possible angular dependences of the wavefunction for *any* central potential. It could be 1/r like the electric potential, it could be r^2 like a harmonic oscillator, or it could be (as we'll look at in a moment) the infinite spherical potential. All that we've required thus far is that the potential only depend upon *r*, but not *how* it depends upon *r*.

2. *Starting Weekly HW*: Use equations 4.27, 4.28, and 4.32 to construct $Y_1^0, Y_2^0,$ and Y_2^{-2}. Show that they are normalized and orthogonal. Show that they satisfy the differential equation 4.18.

4.1.3 the Radial Equation

Now it's time to think about that radial dependence. When last we left *r*, it was in this equation:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-r^2\frac{2m}{\hbar^2}\left[V(r)-E\right]\equiv l(l+1)\equiv-\frac{1}{Y}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right)$$

We'd looked at the *right* hand side of the equation to dig into the angular dependence, but now it's time to look at the *left* hand side of the equation:

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)-r^2\frac{2m}{\hbar^2}\left[V(r)-E\right]\equiv l(l+1)$$

Or rewriting it in a suggestive way,

$$ERr^2\equiv-\frac{\hbar^2}{2m}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\left(V(r)+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)Rr^2$$

As Griffiths shows, if we define $u\equiv rR$, so $R=\frac{u}{r}$, then the derivatives we have become

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)=\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\left(\frac{u}{r}\right)\right)=\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}-u\right)=\frac{\partial u}{\partial r}+r\frac{\partial^2 u}{\partial r^2}-\frac{\partial u}{\partial r}=r\frac{\partial^2 u}{\partial r^2}$$

So, in terms of *u*, this relation looks pretty familiar

$$Eur=-\frac{\hbar^2}{2m}r\frac{\partial^2}{\partial r^2}u+\left(V(r)+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)ur$$

$$Eu=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u+V_{eff}(r)u$$

Where

$$V_{eff}(r) = \left(V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \right)$$

"Why is there an additional term for the effective potential? What causes this centrifugal term?" Spencer

Very ~~Quantum~~ Classical

I should pause here and note that, since most of you've not yet taken Classical Mechanics yet, you might get the impression that this funny business about defining an effective potential and defining a new function that incorporates *r* is quantum-specific, but it's not. It's exactly what you'll do for a central potential in *classical* mechanics too. In that case, the function that's getting dealt with is the angular position of an orbiting body as a function of its distance. In *classical,* the effective potential takes the form of

$$V_{eff}(r) = \left(V(r) + \frac{L^2}{2mr^2} \right)$$

Where *L* is the angular momentum associated with the orbit. Keep an eye out; it won't be long before we make the same identification here.

It's worth taking a moment to think about what this potential looks like and why. To keep things nice and tangible, say we're considering a planet orbiting the sun.

$$E = \frac{p^2}{2m} + V(r)$$

Spherical coordinates are best since there's a central potential, so we convert the expression for momentum over to spherical coordinates. That means we ask what's the rate of change of position along each of the orthogonal coordinate directions:

$$\vec{p} = m\vec{v} = m\left(\frac{dr}{dt}\hat{r} + \frac{rd\theta}{dt}\hat{\theta} + \frac{r\sin\theta d\phi}{dt}\hat{\phi} \right), \text{ so } p^2 = m^2\left(\frac{dr}{dt}\right)^2 + m^2\left(\frac{rd\theta}{dt}\right)^2 + m^2\left(r\sin\theta\frac{d\phi}{dt}\right)^2$$

Now, as you know, a planet orbits in a plane, so if we define the plane of the orbit to be x-y, then θ is a constant 0, so

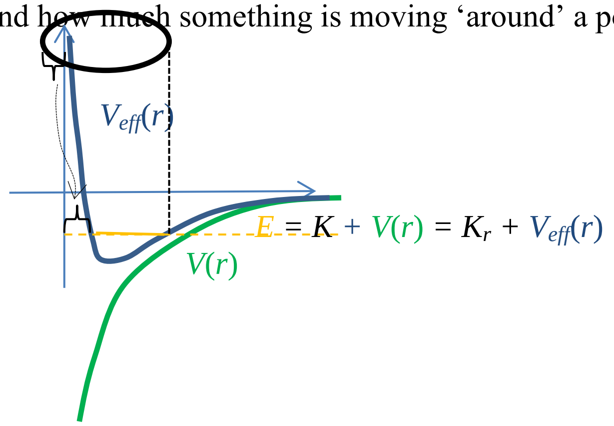
$$p^2 = m^2\left(\frac{dr}{dt}\right)^2 + m^2\left(r\frac{d\phi}{dt}\right)^2 = m^2 v_r^2 + (mr\omega)^2 = p_r^2 + \frac{(mr^2\omega)^2}{r^2} = p_r^2 + \frac{L^2}{r^2}$$

Or

$$E = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r) = \frac{p_r^2}{2m} + V_{eff}(r) \text{ with } V_{eff}(r) \equiv \frac{L^2}{2mr^2} + V(r)$$

It's worth recalling from Phys 231 that, for a central potential, the angular momentum is a constant so L^2 is a constant– okay, it's not $\hbar^2 l(l+1)$, but a constant none the less.

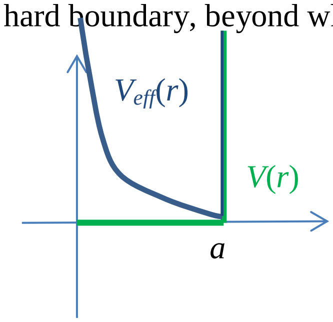
Now, what does it mean to have this effective potential? Well, think about what orbits look like: big ellipses. The distance between Haley's comet and the sun vary but, in spite of having an attractive gravitational potential, the comet never crashes into the sun, rather it whips around the sun, and how much something is moving 'around' a point is quantified in its angular momentum.



Now, be it classical or quantum mechanical, we can't go much further with the radial term unless we know the actual form of the potential. Of course, we're headed for a 1/r potential (classically, that's of great interest for the gravitational interactions, but for us, it'll be the electric interaction that interests us.)

Infinite Spherical Well (Example 4.1)

A simpler potential to initially consider initially is the infinite spherical potential: there's some hard boundary, beyond which the particle simply cannot go.



So, inside this well, the equation to solve is

$$Eu = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}u$$

Or

$$\left(\frac{l(l+1)}{r^2} - \frac{2mE}{\hbar^2}\right)u = \frac{\partial^2 u}{\partial r^2}$$

Special case: *l* = 0

Obviously, if we had $l = 0$, it would be the exact same equation as for a particle in a 1-D infinite square well, and we'd get sines.

$$-\frac{2mE}{\hbar^2}u = \frac{\partial^2 u}{\partial r^2} \text{ so}$$

$$u = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}r\right)$$

where it must be that $\frac{2mE}{\hbar^2} = \left(\frac{n\pi}{a}\right)^2 \Rightarrow E = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$

And the radial wavefunction would then be

$$R_{n,l=0}(r) = \frac{u}{r} = \sqrt{\frac{2}{a}}\frac{\sin\left(\frac{n\pi}{a}r\right)}{r}$$

Then

$$\Psi = R_{n,0}(r)Y_0^0 e^{-iEt/\hbar} = \sqrt{\frac{2}{a}}\frac{\sin\left(\frac{n\pi}{a}r\right)}{r}\frac{1}{\sqrt{4\pi}}e^{-iEt/\hbar} = \frac{1}{\sqrt{2\pi a}}\frac{\sin\left(\frac{n\pi}{a}r\right)}{r}e^{-iEt/\hbar}$$

General Case

Again, Griffiths merely quotes the result: there are two linearly independent solutions for this second-order differential equation, spherical Bessel functions and spherical Neumann functions.

1. *Conceptual*: The solution to the infinite spherical well potential consists of Bessel functions (eq. 4.47). What happened to the Neumann functions?

Same reason we dismiss cosine: it doesn't match the boundary conditions, in particular, it blows up at r = 0.

"Can we take a peek at the derivation of the bessel functions?" Casey P

P. 465 of Liboff, problem 10.66 defines creation and annihilation operators for them and then you can see that, once you've got one, you can generate the rest.

$$\hat{b}_l^{\pm} \equiv -\frac{i}{x}\frac{d}{dx}x \pm i\frac{l}{x} \quad \text{where } x = kr$$

Then $\left(\frac{l(l+1)}{r^2}-\frac{2mE}{\hbar^2}\right)u=\frac{\partial^2 u}{\partial r^2}$ becomes $\left(\hat{b}_l^+\hat{b}_l^- -1\right)R_l(x)=0$

And you can show that $\hat{b}_l^+ R_l = R_{l+1}$

So once you've got one (which we have, the *l* = 0 case), you can generate them all.

$$R_{n,l}(r)=Aj_l(k_{nl}r)=A(-k_{nl}r)^l\left(\frac{1}{k_{nl}r}\frac{d}{d(k_{nl}r)}\right)^l\frac{\sin(k_{nl}r)}{k_{nl}r}$$

Note: $\left(\frac{1}{kr}\frac{d}{d(kr)}\right)^l=\left(\frac{1}{kr}\frac{d}{d(kr)}\right)\left(\frac{1}{kr}\frac{d}{d(kr)}\right)\left(\frac{1}{kr}\frac{d}{d(kr)}\right)$... so the derivative acts upon the next factor's 1/(kr).

"Can we go over what beta_nl represents. I'm still a little confused about what it means." Jessica

i am confused on this as well Kyle B,

I am also unsure on how the beta_nl suddenly appeared in equations 4.49 & 4.50 Jeremy,

Imposing the boundary condition that this must go to 0 at r = a,

$$R_{n,l}(a)=Aj_l(k_n a)=0$$

Leads to determining what k_n must be (just as matching that boundary condition got $k_n = n\pi/a$ when the function was sine.)

Practically, how do you find *k* for a given Bessel function?

Since they're transindental, you have to plot and zero-find.

For example, looking at Figure 4.2 (where "x" is *ka*),

$R_{1,0}(a)=Aj_o(k_1 a)=0$, that is the 1st time that Bessel function goes to 0 is about $k_n a$=3.2.

2. *Conceptual*: What is meant by β_{nl}?

The *nth* value of its argument for which the *lth* Bessel function goes to zero is denoted β_{nl}

That is $\beta_{nl} = k_n a$. that is $k_{n,l} = \frac{\beta_{n,l}}{a}$. So it's akin to the $n\pi$ for sines.

Griffiths notes, but you'll show

$$\frac{2mE}{\hbar^2} = \left(\frac{\beta_{nl}}{a}\right)^2 \Rightarrow E = \frac{\hbar^2}{2m}\left(\frac{\beta_{nl}}{a}\right)^2$$

3. *Conceptual*: Mathematically, why doesn't the energy depend on *m*?

Better yet, *conceptually*, why doesn't the energy depend on *m?*

Classically, implicit in our choice of coordinate systems, the orbiting is happening *about* the z axis. Meanwhile, the wavefunctions are describing the *shape* of the orbitter where *l* describes how it varies as you move down the Z axis and m describes how it varies as you look *around* the Z axis. The angular momentum of an object about the Z axis wouldn't depend upon how it was distributed around the Z axis (in and out, yes, but not around).

4. *Starting Weekly HW*: Consider $u(r) = Arj_2(kr)$.
   a. Show that it satisfies the differential equation 4.41 with l=2.
   b. Make a plot of this function.
   c. Where is the first place the function goes to zero where x>0?
   d. What is n? What does this mean for k? What is the energy in terms of $\hbar$, m, and a?
5. Starting Weekly HW: Computational: Create a version of your Discrete, time-independent program to find the Angular components of the wave function in spherical coordinates and modify it to find the Radial components of the wave function for an infinite spherical well. See Handout.