Central potential problem and angular momentum

- What is a central potential?
- Separating the Angular and Radial wave equations
- Asymptotics of the radial equation
- Example 1: Free Particle
- Example 2: 3-d QHO

Next chapter is also a central potential problem…the Hydrogen atom.

Central field problem and angular momentum

As usual, we wish to solve Schroedinger's equation,

$$H\Psi_E = E\Psi_E$$

But limit ourselves to cases in which the

$$[H, L_i] = 0$$

This means that we can look for solutions which simultaneously diagonalize not just H but L^2 and L_z as well.

Note also that it will be most convenient to talk almost entirely in terms of spherical coordinates, for example,

$$\Psi_E(r, \theta, \phi)$$

Note also that one simple way to arrange for $[H, L_i] = 0$

Is for the potential, V, to depend on the radial co-ordinate only;

$$V(r, \theta, \phi) = V(r)$$

Now, since L_z and L^2 depend only on the angular co-ordinates

and since the wave functionals can be taken to diagonalize these operators, it must be that

$$\Psi_E(r, \theta, \phi) = R_{Elm}(r) Y_l^m(\theta, \phi)$$

And plugging this into the Schroedinger equation for a particle of mass μ

We have....

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) + V(r)\right]R_{El}(r) = E\, R_{El}$$

Where we have dropped the 'm' from R_{Elm}

since the resulting equation is independent of m. This means that there is always (atleast) a 2l+1 degeneracy (same energies, different states) in the energy eigenvectors in all these central field problems. From our discussion of the spherical harmonics in the preceeding we see that this degeneracy is a direct result of the spatial isotropy of the problem... the quantization axis 'z' can point in any direction.

And note also that for a two-body problem, our μ is really the reduced mass,

$$\mu = \frac{M m_1}{M + m_1}$$

We now proceed to discuss the asymptotics and solutions of this radial schroedinger equation.

It is useful to define a function U via;

$$R_{El}(r) = U_{El}/r$$

Before we go onto to solve the radial Schroedinger equation in U, etc. we note what has transpired with the norm; it started as

$$\delta_{ij} = \int \mathrm{d}^3\vec{x}\Psi_i(\vec{x})\Psi_j(\vec{x})$$

i,j are some multiindex. Specializing to spherical coordinates we can write this as

$$\delta_{ij} = (\text{spherical}) \int \mathrm{d}r \;\; r^2 R_i(r) R_j(r)$$

Where '(spherical)' are the angular integrals (also just products of delta functions in angular quantum numbers, but we focus here on the radial part).

Finally, in terms of U,

$$\delta_{ij} = (\text{spherical}) \int \mathrm{d}r U_i(r) U_j(r)$$

Now note what has happened in this variable change to the Schroed eqn; in U the radial schroedinger equation has become a 1-d problem with the usual norm BUT on the domain, 0 to ∞

Some Asymptotics

Ex: take V=0. Then, the Schroedinger equation reads,

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) + V(r)\right]R_{El}(r) \quad = E \quad R_{Elm}$$

With V=0 can be cast as

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2}\right]U_{El} = 0$$

And with the variable change $\rho = kr$ with $k = \sqrt{\frac{2\mu E}{\hbar^2}}$

This becomes,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{l(l+1)}{\rho^2}\right]U_{El} = U_{El}$$

We now investigate the asymptotics of this solution, just the free particle in 3-d in spherical co-ordinates.

At $r \sim \infty$ We can ignore the l-terms, so find wave-like solutions for U

So,

$$R_{El}(r) = A_+ \frac{e^{ikr}}{r} - A_- \frac{e^{-ikr}}{r} \qquad E > 0$$

These are inward traveling spherical waves. Here $k = \sqrt{\frac{2\mu E}{\hbar^2}}$

If the $E < 0$ then in analogy with the 1-d case of bound state, there are exponentially decreasing and increasing solutions. We are only interested in the decreasing exponential case,

$$U_{El} \rightarrow Ae^{-\kappa r} + Be^{\kappa r} \qquad E < 0$$

So must take B/A = 0. Note that here $\kappa = \sqrt{\frac{2\mu |E|}{\hbar^2}}$

At $r \longrightarrow 0$ The l-terms we ignored at large r start to dominate and searching for power law solutions,

$$U_{El} \sim r^{\alpha}$$

We find,

$$\alpha(\alpha - 1) = l(l+1)$$

So that

$$\alpha = l + 1$$

$$U_{El}(r) \sim r^{l+1}$$

non-sing

$$\alpha = -l$$

$$U_{El}(r) \sim r^{-l}$$

sing

Not just any large r solution will limit to a non-singular solution at r=0….this leads to discrete E, i.,e. A Quantization Condition.

As an example, note that for a coulomb potential,

$$V(r) = -\frac{e^2}{r}$$

We find, at large r, a joint power-exponential solution,

$$U_{El}(r) \sim r^{\frac{\mu e^2}{\kappa \hbar^2}} e^{-\kappa r} \qquad E < 0$$

With $$\kappa = \sqrt{\frac{2\mu |E|}{\hbar^2}}$$

We will see that the Hydrogen WF is of this form….more later.

A deeper look at the asymptotics

These asymptotics described above hold as long as

$$rV(r) \longrightarrow 0 \qquad \text{As r} \sim \infty$$

Thus the reason the Coulomb case was a joint power-exponential can be traced to the fact that it is a boundary case of this limit

Hermiticity also requires that

$$\left(U_1^* \frac{\mathrm{d}U_2}{\mathrm{d}r} - U_2 \frac{\mathrm{d}U_1^*}{\mathrm{d}r} \right) \Big|_0^\infty = 0$$

For bound states at large r this expression must vanish for all U_1 U_2 by normalizability. Thus, this is essentailly a condition at $r \longrightarrow 0$

Physically, we can think of computing the particle number current in a mixed state of U_1 and U_2 It is proportional to the above expresion.

Thus, hermiticity in this case is essentially the same as requiring that solutions do not correspond to creating or annihilating particles at $r = 0$

Note for example that V ~ $1/r^2$ Is too singular...this case will arise later...

The Free Particle in Spherical co-ordinates

We can compare this formulation of QM with the known solution for a free particle,

$$\psi_E(\vec{x}) = \frac{1}{h^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

Infeld: has a nice way of realizing these solutions in terms of spherical co-ordinates. First note that we are solving

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{l(l+1)}{\rho^2}\right] U_{El} = U_{El}$$

Write this as $$d_l d_l^\dagger U_{El} = U_{El}$$

With
$$d_l^\dagger = -\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{l+1}{\rho}$$

$$d_l = \frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{l+1}{\rho}$$

Note the identity,

$$d_l^\dagger d_l = d_{l+1} d_{l+1}^\dagger$$

So that

$$d_{l+1} d_{l+1}^\dagger (d_l^\dagger U_{El}) = d_l^\dagger U_{El}$$

indicating...

$$U_{E,l+1} = d_l^\dagger U_{El}$$

Thus a solution at *l=0* can be used to create a solution at all *l* . To do so note that the *U* for the *l=0* solution is (here written in terms of *R*) R_0 has two solns

$$R_0^A = \frac{\sin \rho}{\rho} \qquad R_0^B = \frac{-\cos \rho}{\rho}$$

Two solutions since still solving the full *l=0* D.E...not like the QHO case where it was a 1'st order equation for the ground state !

There will thus be two solution for each *l*

The are generated by putting the appropriate R_0 in the formula,

$$R_l = (-)^l \rho^l \left(\frac{\partial}{\rho \partial \rho} \right)^l R_0$$

This is just a telescoped version of the product of the d_l

The $R_0^A = \frac{\sin \rho}{\rho}$ lead to the spherical bessel functions (non-singular at *r=0*)

The $R_0^B = \frac{-\cos \rho}{\rho}$ lead to the spherical Neumann functions (singular at *r=0*)

The text has more detail for these functions to those interested….but we focus now on the upshot of this case for the free particle.

The Free Particle in Spherical co-ordinates

Note that for $\psi_E(\vec{x}) = \frac{1}{h^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar}$ In co-ordinates where the Z-axis is along the momentum vector, one may expand this plane wave interms of spherical harmonics directly. In that case the wave function has no ϕ dependence.

$$\vec{p}\cdot\vec{x}/\hbar = kz = kr\cos\theta$$

Then use the fact that

$$e^{i\vec{p}\cdot\vec{x}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_l^m J_l(kr) Y_l^m(\theta,\phi)$$

Combined with no ϕ dependence means that only the *m=0* spherical harmonics can contribute to the sum;

$$Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$$

Thus, $$e^{i\vec{p}\cdot\vec{x}} = \sum_{l=0}^{\infty} i^l (2l+1) J_l^0(kr) P_l(\cos\theta)$$

Where the coefficients in the expansion can be found, for example, by integration. This form of a plane wave will be quite useful later when we talk about the 3-d scattering of waves off a potential. It is called the partial wave decomposition of the plane wave.

Application: You have all had a direct experience of this equation without perhaps knowing it. When you are stopped at a stop light and listening to weak FM broadcast you can often find that inching the car up a fraction of a wavelength or so can improve the reception. This is due to reflections of the FM signal (all at the same frequency, so at fixed k) at various angles into your receiver. If there are many scattering centers or if you average over many experiences of the FM signal dropping out at different stoplights you will find that the mean distance between adjacent signal zeros are given by 2.4/k, where 2.4 is the first zero of the J_0 bessel function, which, we see is the only term that survives angular averaging in the expression above.

The Spherical (3-d) QHO

Another useful example is the 3-d isotropic harmonic oscillator: Its Hamiltonian is

$$H = \frac{1}{2\mu}(p_x^2 + p_y^2 + p_z^2) + \frac{\mu\omega^2}{2}(x^2 + y^2 + z^2)$$

Isotropy (*H* commutes with each L_i) allows us to once again search for solutions of the form

$$\psi_{Elm} = \frac{1}{r} U_{El}(r) Y_l^m(\theta, \phi)$$

It is convenient to take the dimensionless co-ordinate (as was done in the 1-d QHO case...remember?)

$$y = \sqrt{\frac{\mu\omega}{\hbar}} r$$

Then our ansatz for finding a solution is

$$U_{El}(r) = e^{-y^2/2} \nu(y)$$

With that ansatz, the radial equation can be written as a D.E. In *v* as,

$$\nu'' - 2y\nu' + \left[2\lambda - 1 - \frac{l(l+1)}{y^2}\right]\nu = 0$$

Where $\lambda = \frac{E}{\hbar\omega}$

We can again employ power series to search for a solution of this equation. Again, we will learn if we do so that the power series solutions do not truncate unless $\lambda = \frac{E}{\hbar\omega}$ Is actually a half-odd integer. That is,

$$E = (2k + l + 3/2)\hbar\omega$$

With $k = 0, 1, 2, \ldots$

We note that this spectrum thus has a larger degeneracy than just *2l+1*

At each *E*. This is due to what is termed a dynamical symmetry. It is the same dynamical symmetry that we will confront in the Hydrogen spectrum. Levels of different *l*'s will have the same energy.

The point is, that the algebra of observables formed from *p* and *x* will in rare instances contain a larger set of commuting operators than just

$$H \qquad L^2 \qquad L_z$$

The L_i's together form a group called *so(3)*, the group of rotation in 3-d. It will turn out that for special cases of *V(r)* there are additional operators that commute with *H*. In both this case and in the Hydrogen atom we will see that they lead to a group so(4), a rank 2 group which has an additional operator that commutes will the three above! More on that later....

$$[\quad]$$ $$[H, L_i] = 0$$ $$H \quad L^2$$

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

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

$$\mu = \frac{Mm_1}{M+m_1}$$

$$V(r, \theta, \phi) = V(r)$$

$$R_{El}(r) = U_{El}/r$$

$$\psi_E(r, \theta\phi) = R_{Elm}(r)Y_l^m(\theta, \phi)$$

R_{El} R_{Elm}

$$H\psi_E(r, \theta, \phi) = E\psi_E(r, \theta\phi)$$

$$R_{El}(r) = U_{El}/r$$

$$1/r^2$$

$$H = \frac{1}{2\mu}(p_x^2 + p_y^2 + p_z^2) + \frac{\mu\omega^2}{2}(x^2 + y^2 + z^2)$$

$$\alpha(\alpha - 1) = l(l+1)$$

$$\left(U_1^* \frac{\mathrm{d}U_2}{\mathrm{d}r} - U_2 \frac{\mathrm{d}U_1^*}{\mathrm{d}r} \right) \Big|_0^\infty = 0$$

$$\alpha = l + 1 \quad \alpha = -l$$

$$d_l^\dagger = -\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{l+1}{\rho} \qquad d_l d_l^\dagger U_{El} = U_{El} \qquad d_l^\dagger \qquad B = 0$$

$$B/A$$

$$d_l = \frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{l+1}{\rho} \qquad \infty \qquad d_l^\dagger d_l = d_{l+1} d_{l+1}^\dagger \qquad E > 0$$

$$E = (2k + l + 3/2)\hbar\omega$$

$$d_{l+1} d_{l+1}^\dagger (d_l^\dagger U_{El}) = d_l^\dagger U_{El}$$

$$E < 0$$

$$U_{E,l+1} = d_l^\dagger U_{El} \qquad k^2 = \frac{2\mu E}{\hbar^2} \qquad l = n - 2k$$

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

$$E = \frac{\hbar^2 k^2}{2\mu} \qquad k = \sqrt{\frac{2\mu E}{\hbar^2}}$$

$$m = 0$$

$$k = 0, 1, 2, \ldots$$

$$U_{El} \to Ae^{-\kappa r} + Be^{\kappa r}$$

$$\delta_{ij} = \int \mathrm{d}^3\vec{x}\, \Psi_i(\vec{x}) \Psi_j(\vec{x}) \qquad \delta_{ij} = (\text{spherical}) \int \mathrm{d}r \quad r^2 R_i(r) R_j(r)$$

$$\delta_{ij} = \text{spherical)} \int \mathrm{d}r U_i(r) U_j(r)$$

$$R \sim \frac{U}{r}$$

$$r = 0$$

$$\nu'' - 2y\nu' + \left[2\lambda - 1 - \frac{l(l+1)}{y^2}\right]\nu = 0$$

$$R_0$$

$$R_0^B = \frac{-\cos\rho}{\rho}$$

$$\psi_E(\vec{x}) = \frac{1}{h^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

$$R_0^A = \frac{\sin\rho}{\rho}$$

$$\psi_{Elm} = \frac{1}{r} U_{El}(r) Y_l^m(\theta, \phi)$$

$$R_l = (-)^l \rho^l \left(\frac{\partial}{\rho \partial \rho}\right)^l R_0$$

$$\psi_{Elm}(\mathrm{x}) = R_{El}(r) Y_l^m(\theta, \phi)$$

$$r \to 0$$

$$R_{El}(r) = A_+ \frac{e^{ikr}}{r} - A_- \frac{e^{-ikr}}{r}$$

$$U_{El}$$

$$rV(r) \to 0$$

$$\frac{\mathrm{d}^2 U_{El}(r)}{\mathrm{d}r^2} = -\frac{2\mu E}{\hbar^2} U_{El}(r)$$

$$U_{El} \to 0$$

$$U_{El} \to e^{ikr}$$

$$U_{El}(r) = e^{-y^2/2} \nu(y)$$

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2}\right] U_{El} = 0$$

$$U_{El}(r) \sim r^{\frac{\mu e^2}{\kappa \hbar^2}} e^{-\kappa r}$$

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{l(l+1)}{r^2}\right] U_{El} = U_{El}$$

$$U_{El}(r) \sim r^{l+1}$$

$U_{El}(r) \sim r^{-l}$ $U_{El} \sim r^{\alpha}$

$U_{El} \to 0$ U_1 U_2 $V(r) = -\frac{e^2}{r}$

$$Y_l^0(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta) \quad y = \sqrt{\frac{\mu\omega}{\hbar}} r$$