Lec 41: 12/04/2009

## Free Particle in Spherical Harmonics:

The equation for the radial part of the wavefunction in this case becomes:

$$-\frac{\hbar^2}{2\mu}\frac{d^2 U_{El}}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} U_{El} = E\, U_{El}$$

After defining:

$$k^2 = \frac{2\mu E}{\hbar^2}, \qquad \rho = rk$$

We find:

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

First, lets consider the case where $l=0$. The equation becomes quite simple and the solution is:

$$U_0(\rho) \propto \sin\rho,\ -\cos\rho$$

The negative sign is chosen to be in accordance with the convention for spherical Neumann function (which we will see shortly).

Next, consider $\ell \neq 0$. The solutions can be found from $U_0$ by introducing the following operators:

$$d_\ell = \frac{d}{d\rho} + \frac{\ell+1}{\rho} \quad , \quad d_\ell^\dagger = \frac{-d}{d\rho} + \frac{\ell+1}{\rho}$$

We note that:

$$(d_\ell d_\ell^\dagger) U_\ell = U_\ell \Rightarrow d_\ell^\dagger d_\ell (d_\ell^\dagger U_\ell) = d_\ell^\dagger U_\ell$$

It is easy to verify that:

$$d_\ell^\dagger d_\ell = d_{\ell+1} d_{\ell+1}^\dagger$$

This implies that:

$$d_{\ell+1} d_{\ell+1}^\dagger (d_\ell^\dagger U_\ell) = d_\ell^\dagger U_\ell \Rightarrow d_\ell^\dagger U_\ell = c_\ell U_{\ell+1}$$

Therefore, we can find $U_\ell$ from $U_0$ by operating $d_\ell^\dagger$ on the latter $\ell$ times. As a result:

$$R_0 \propto \frac{U_0}{\rho} = \frac{\sin\rho}{\rho} , \frac{-\cos\rho}{\rho}$$

$$R_\ell \propto \frac{U_\ell}{\rho} = (-\rho)^\ell \left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^\ell R_0$$

For $R_0 = \frac{\sin\rho}{\rho}$ we have:

$$R_\ell^A \equiv j_\ell = (-\rho)^\ell \left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^\ell \left(\frac{\sin\rho}{\rho}\right)$$

These are called the spherical Bessel functions. For

$R_0 = \frac{-\cos\rho}{\rho}$ we have:

$$R_\ell^B \equiv n_\ell = (-\rho)^\ell \left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\right)^\ell \left(\frac{-\cos\rho}{\rho}\right)$$

These are called spherical Neumann functions. We can form spherical Hankel functions $h_\ell$ from $j_\ell$ and $n_\ell$:

$$h_\ell = j_\ell + i n_\ell$$

It can be shown that:

$$j_\ell(\rho) \to \frac{\rho^\ell}{(2\ell+1)!!} \propto \rho^\ell \qquad \rho \to 0$$

$$n_\ell(\rho) \to -\frac{(2\ell-1)!!}{\rho^{\ell+1}} \propto \rho^{-(\ell+1)} \qquad \rho \to 0$$

These are the expected behavior of the radial part of the wave function that we derived in a general case (for potentials where $r^2 V(r) \to 0$ as $r \to 0$).

Similarly, we find that:

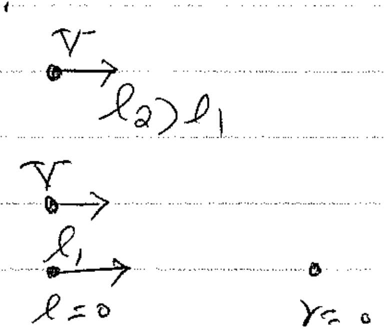
$$j_\ell(\rho) \longrightarrow \frac{1}{\rho}\sin\left(\rho - \frac{\ell\pi}{2}\right) \qquad \rho \to \infty$$

$$n_\ell(\rho) \to -\frac{1}{\rho}\cos\left(\rho - \frac{\ell\pi}{2}\right) \qquad \rho \to \infty$$

This is also compatible with the general behavior at large distances for potentials where $rV_{(r)} \to 0$ as $r \to \infty$.

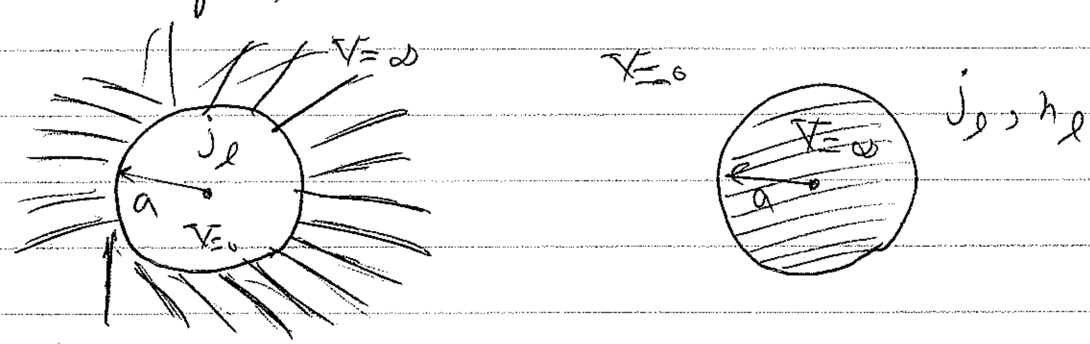
Some important points to note:

1) For a given $E>0$ (the spectrum is continuous, as expected for a free particle), we can have all values of $\ell \geq 0$. This is easy to understand intuitively. A free particle with a given energy (hence velocity) can have an arbitrary large angular momentum depending on its normal distance from the center $r=0$:



Here quantum mechanics tells us that angular momentum eigenvalues are quantized.

2) Depending on the boundary condition one or both of the $j_\ell$ and $n_\ell$ are acceptable solutions. If we are interested in a region that contains the center (like a particle in a spherical box), then only $j_\ell$ is acceptable. As mentioned earlier, the choice of $n_\ell$ leads to a singularity at $r=0$. On the other hand, if we are interested in a region that does not contain $r=0$, then both $j_\ell$ and $n_\ell$ are acceptable (and so is $h_\ell$). This happens, for example, when there is an infinite barrier at $r<a$.



3) Only for $l=0$ the wavefunction does not vanish at $r=0$:

$$j_l(\rho) \propto \rho^{l+1} \Rightarrow R_l(r) \propto r^l \qquad r \to 0$$

For $l>0$, we have $R(0)=0$. $l=0$ is called the S-wave in the partial wave expansion of a freely moving particle. This has important consequences when discussing scattering of a particle off a potential that is localized around $r=0$.

Let us finish by a quick example.

Example: Find the energy eigenvalues of a free particle of mass $\mu$ in a spherical box with radius $a$. Consider only $l=0$ case.

Since we are interested in a region that contains $r=0$, then only $j_l$ is acceptable. For $l=0$, we have:

$R_0(r) \propto \frac{\sin \rho}{\rho}$

Because of the hard wall at $r=a$, we must have $R_0(a)=0$. This requires that:

$\sin(ka)=0 \Rightarrow \frac{2\mu}{\hbar^2} E_n a^2 = n^2\pi^2 \qquad n=1,2,\ldots$

$$\boxed{\Rightarrow E_n = \frac{\hbar^2 \pi^2 n^2}{2\mu a^2}}$$

As expected, the spectrum is quantized due to the boundary condition.