Lec 40: 12/02/2009

Energy Eigenstates for Central Potentials

A rotationally invariant system has a central potential:

$$[H, L_x] = [H, L_y] = [H, L_z] = 0 \Leftrightarrow V(x,y,z) = V(r)$$

In the coordinate basis Schrodinger equation reads:

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi_E(r,\theta,\varphi)$$

$$+ V(r)\,\psi_E(r,\theta,\varphi) = E\,\psi_E(r,\theta,\varphi)$$

This is a separable problem and we have:

$$\psi(r,\theta,\varphi) = R(r)\,\Theta(\theta)\,\Phi(\varphi)$$

The three ordinary differential equation for R, Θ, Φ are:

(periodicity with respect to φ)

$$\frac{d^2}{d\varphi^2}\Phi(\varphi) = -m^2\,\Phi(\varphi) \qquad m = 0, \pm 1, \pm 2, \ldots$$

$(\ell = 0, 1, 2, \ldots)$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta}\Theta(\theta) - \frac{m^2}{\sin^2\theta}\Theta(\theta) = \ell(\ell+1)\,\Theta(\theta)$$

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr} r^2\frac{d}{dr}R(r) - \frac{\ell(\ell+1)}{r^2}R(r)\right] + V(r)\,R(r) = E\,R(r)$$

The first two equations are just eigenvalue problems for L_z and L^2 because (in the coordinate basis):

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$L^2 = (-\hbar^2)\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Note that $\Phi(\phi)$ depends on one integer m, $\Theta(\theta)$ depends on two integers m, ℓ, and $R(r)$ depends on three parameters. We therefore show them as:

$$\Phi_m(\phi), \quad \Theta_{\ell m}(\theta), \quad R_{E\ell}(r)$$

The two integers ℓ, m (related to the total orbital angular momentum and its z component) are used to uniquely specify degenerate energy eigenstates.

$\Phi_m(\phi)$ is simply $e^{im\phi}$. $\Theta_{\ell m}(\theta)$ are the so called "associated Legendre polynomials":

$\Theta_{lm}(\theta) \propto P_{lm}(\cos\theta)$

These are obtained from Legendre polynomials P_l.

Recall that P_l are orthonormal polynomials such that:

$$\int_{-1}^{+1} P_l(x) P_{l'}(x) (1-x^2)\, dx = 0$$

$$P_l(-x) = (-1)^l P_l(x)$$

The associated polynomials are obtained according to:

$$P_{lm}(x) = (1-x^2)^{m/2} \frac{d^m P_l(x)}{dx^m} \qquad m \geq 0$$

$$P_{lm}(x) = (-1)^m P_{l\,-m}(x) \qquad m < 0$$

The product of $\Theta_{lm}(\theta)$ and $\Phi_m(\varphi)$ is nothing but the "spherical harmonics $Y_{lm}(\theta,\varphi)$". They satisfy the orthonormality condition:

$$\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_{lm}(\theta,\varphi) Y_{l'm'}(\theta,\varphi) \sin\theta\, d\theta\, d\varphi = \delta_{ll'}\, \delta_{mm'}$$

They are given by:

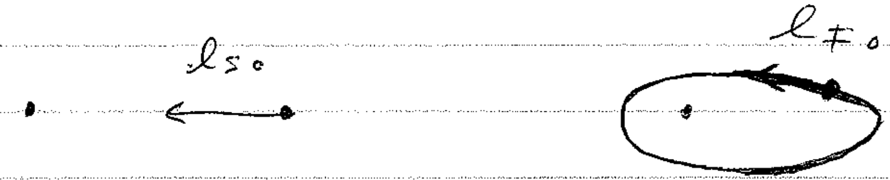
$$Y_{lm}(\theta,\varphi) = \left[\frac{(2l+1)\,(l-m)!}{4\pi\,(l+m)!}\right]^{\frac{1}{2}} (-1)^m e^{im\varphi} P_{lm}(\cos\theta)$$

Next we consider $R_{E\ell}(r)$. The relevant differentia[l] equation is;

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

Note that for $\ell\neq 0$ (non-zero total angular momentum) there exists a term $+\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}R_{E\ell}$, in the equation. This amounts to an effective repulsive potential.

It can be understood physically. For an attractive potential $V(r)$ the particles falls to the center if it has no angular momentum. The angular momentu[m] will change the trajectory from radial to elliptical, and hence the particles will miss the center.



The differential equation looks much simpler by making a re-definition $R_{E\ell}(r) = \frac{U_{E\ell}(r)}{r}$. Then we find:

$$-\frac{\hbar^2}{2\mu}\frac{d^2 U_{E\ell}}{dr^2} + \underbrace{\left[\frac{\ell(\ell+1)\hbar^2}{r^2} + V(r)\right]}_{\text{effective potential}} U_{E\ell} = E\, U_{E\ell}$$

This is just a one-dimensional Schrodinger equation ($0 \leq r < +\infty$) with an effective potential that includes a $\frac{1}{r^2}$ term for non-zero angular momentum.

Before discussing solutions for given $V(r)$, let us examine the asymptotic behavior of the solutions. The operator on the left-hand side of the above equation is Hermitian. This results in a requirement that (U_1 and U_2 two solutions):

$$\left(U_1^* \frac{dU_2}{dr} - U_2^* \frac{dU_1}{dr}\right)\Big|_0^{+\infty} = 0$$

We notice that $U \to 0$ as $r \to \infty$, or $U \to e^{\pm ikr}$ as

$r \to \infty$, is required by the normalization condition:

$$\int_0^\infty |R_{E\ell}|^2 r^2 dr = \int_0^\infty |U_{E\ell}|^2 dr = \begin{cases} 1 & \text{bound states} \\ \delta\text{-function} & \text{unbound states} \end{cases}$$

This already fines the asymptotic behavior of $R_{E\ell}(r)$ as $r \to \infty$:

$$\boxed{R_{E\ell}(r) \to \frac{e^{\pm ikr}}{r} \quad \text{or} \quad 0 \qquad r \to \infty}$$

Once we have this, the Hermiticity requires that:

$U_{(r)} = \text{Const.} \qquad r \to 0$

This constant must be zero. Otherwise we will have sigularities in the equation for $R_{E\ell}(r)$. Thus:

$$\boxed{U_{E\ell}(0) = 0}$$

So far, we have not made any specification of the potential. More information about $U_{(r)}$ at small and large distances can be found if we know the asymptotic behavior of $V_{(r)}$.

1- $r^2 V_{(r)} \to 0$ as $r \to 0$. For this class of potentials, $V_{(r)}$ is shallower than $\frac{1}{r^2}$ at small distances. In the equation:

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

We can drop the $V_{(r)} U$ and EU terms as $r \to 0$.

This results in a simple equation:

$$-\frac{\hbar^2}{2\mu}\frac{d^2 U}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} U = 0 \Rightarrow U \propto r^{\ell+1} \text{ or } r^{-\ell},$$

Note that $r^{-(\ell+1)}$ is not acceptable because it blows up at $r=0$. As we saw, $U_{(0)} = 0$, and hence we find:

$$\boxed{U_{(r)} \to r^{\ell+1} \qquad r \to 0}$$

2- $r\, V_{(r)} \to 0$ as $r \to \infty$. For this class of potentials, We can simply neglect the $\frac{\hbar^2 l(l+1)}{r^2} U$ and $V_{(r)} U$ terms, hence finding:

$$-\frac{\hbar^2}{2\nu}\frac{d^2U}{dr^2} = EU$$

The solutions are:

$$\boxed{\begin{array}{lll} U_{(r)} \rightarrow e^{\pm ikr} & k = \frac{\sqrt{2\nu E}}{\hbar} & E > 0 \\ U_{(r)} \rightarrow e^{-kr} & k = \frac{\sqrt{-2\nu E}}{\hbar} & E < 0 \end{array}}$$

Note that e^{+kr} in the case $E<0$ is not acceptable because of the general behavior expected at large distances.

These are the same solutions that one finds for $V_{(r)} = 0$. However, the condition $rV_{(r)} \rightarrow 0$ as $r \rightarrow \infty$ is necessary for the solutions to be effectively the same as that for $V = 0$ at large distances.

To understand this better, lets consider the case with $E>0$. Since V_{eff} falls off rapidly, we can use the WKB approximation at sufficiently large distance:

$$U(r) \simeq \frac{1}{\sqrt{P(r)}} \exp\left[\pm \frac{i}{\hbar} \int_{r_0}^{r} \sqrt{2\nu(E - V_{eff})}\, dr'\right]$$

Note that $P(r) = \sqrt{2m(E - V_{ff})} \simeq \sqrt{2mE}$ at large distances. The integral in the exponent becomes:

$$\int_{r_0}^{r} \sqrt{2\nu(E - V_{ff})}\, dr' \simeq \int_{r_0}^{r} \sqrt{2\nu E}\, dr' - \int_{r_0}^{r} \frac{\sqrt{2\nu E}\; V_{eff}}{2E}\, dr'$$

$$= \sqrt{2\nu E}\,(r - r_0) - \int_{r_0}^{r} \sqrt{\frac{\nu}{2E}}\; V_{eff}\, dr'$$

$$V_{eff} = \frac{\hbar^2 \ell(\ell+1)}{2\nu r^2} + V(r)$$

The integral of the first term is convergent $\text{as } r \to \infty$ and amounts to an overall phase. Now, if $V(r) \propto \frac{1}{r}$, the integral will be divergent $\propto \ln r$:

$$-\int_{r_0}^{r} \sqrt{\frac{\nu}{2E}}\, \frac{1}{r}\, dr' = -\sqrt{\frac{\nu}{2E}}\, \ln\left(\frac{r}{r_0}\right)$$

There fore, the exponential function will be:

$$U(r) \rightarrow e^{\pm ikr}\, e^{\mp\frac{i}{\hbar}\sqrt{\frac{\nu}{2E}}\ \ln r}$$

This implies that the particle will never become completely free. This happens for a Coulomb potential and any potential shallower than $\frac{1}{r}$.

For example, the fact that a charged particle feels the Coulomb force no matter how far it is from the center ($r=0$) is the physical reason why the cross-section for Rutherford scattering of electrons of a proton is ∞.