Centeral force field

§: Angular momentum conservation and radial equation

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r),$$

$$\vec{l} = \vec{r}\times\vec{p}, \qquad [l_i, r_j] = i\epsilon_{ijk} r_k \hbar \quad [l_i, P_j] = i\epsilon_{ijk} P_k \hbar$$

$$[l_i, r^2] = [l_i, r_j r_j] = \hbar\left[r_j[l_i, r_j] + [l_i, r_j] r_j\right] = (i\epsilon_{ijk} r_j r_k + i\epsilon_{ijk} r_k r_j)\hbar$$

$$= i[\epsilon_{ijk} + \epsilon_{ikj}] r_j r_k \hbar = 0$$

$$[l_i, P^2] = 0, \qquad [l_i, l^2] = 0,$$

$$r = \sqrt{r^2} \quad\rightarrow\quad [l_i, V(r)] = 0.$$

$$\Rightarrow [l_i, H] = 0,$$

$$l^2 = l_x^2 + l_y^2 + l_z^2 \Rightarrow [l_i^2, H] = 0$$

Complete set of compatible obeservables (H, l^2, l_z).

We will use spherical coordinate:

Ex: prove

$$\hat{l}_x = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{l}_y = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

$$\hat{l}_z = -i\hbar\frac{\partial}{\partial\varphi}$$

and

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

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r} r^2\frac{\partial}{\partial r} + \frac{\hat{l}^2}{2mr^2}$$

$$= -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\hat{l}^2}{2mr^2} \leftarrow \text{centrifugal potential}$$

★ eigenstates of ℓ^2: spherical harmonics $Y_{\ell m}(\theta, \varphi)$

$$\hat{\ell}^2 \, Y_{\ell m}(\theta, \varphi) = \ell(\ell+1)\hbar^2 \, Y_{\ell m}(\theta, \varphi)$$

$$Y_{\ell m}(\theta, \varphi) = (-)^m \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{\frac{(\ell-m)!}{(\ell+m)!}} \, P_\ell^m(\cos\theta) e^{im\varphi}$$

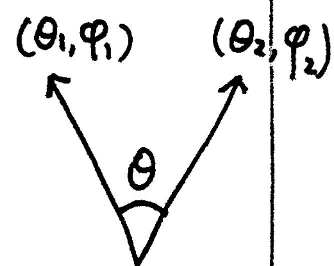
$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} (x^2-1)^\ell \longleftarrow \frac{1}{(1-2xt+t^2)^{1/2}} = \sum_{\ell=0}^{\infty} t^\ell P_\ell(x)$$

generation function

$$P_\ell^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x) = \frac{1}{2^\ell \ell!} (1-x^2)^{m/2} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell \quad (m \geq 0)$$

$$P_\ell^{-m}(x) = (-)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(x)$$

$$P_\ell(\cos\theta) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}^*(\theta_1, \varphi_1) \, Y_{\ell m}(\theta_2, \varphi_2)$$



$$\frac{1}{|\vec{r}-\vec{r}'|} = \frac{1}{r_<} \sum_{\ell=0}^{\infty} \left(\frac{r_<}{r_>}\right)^\ell P_\ell(\cos\theta)$$

☆ the asymptoic behavior at $r \to 0$.

We assume that $r^2 V(r) \to 0$ as $r \to 0$, othewise if $V(r) \to -\infty$, then the Hamiltonian is not bound from below. Suppose we put particle at a distance Δr, then the kinetic energy $\sim \frac{\hbar^2}{2m(\Delta r)^2}$ but $V(r) \sim \frac{-k}{(\Delta r)^3}$, $E \simeq \frac{\hbar^2}{2m(\Delta r)^2} - \frac{k}{(\Delta r)^3} \longrightarrow -\infty$, thus the ground state energy $\to -\infty$. We will not consider this subtle situation in this lecture. But this kind of interaction does exist, say, the dipolar interaction $V = -\frac{d^2}{r^3} \frac{3\cos^2\theta - 1}{2}$. We need regularization for this case.

For the potentials, say, $V \sim r^2,\ r,\ \ln r,\ \frac{1}{r},\ \frac{1}{r}e^{-r/\lambda}, \ldots,$

all of them satisfies $r^2 V(r) \xrightarrow{r\to\infty} 0$.

Now we separate variables $\psi(r,\Omega) = R(r)\, Y_{lm}(\theta,\varphi)$ $(l=0,1,2,\cdots)$

$$H = -\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\right) + \frac{\hat{l}^2}{2mr^2}$$

$\longrightarrow$

$$\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[\frac{2m}{\hbar^2}(E-V(r)) - \frac{l(l+1)}{r^2}\right]R = 0$$

as $r\to 0$, $\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2}R = 0$, try $R \sim r^s$

$\Rightarrow$ $s(s-1) + 2s - l(l+1) = 0 \Rightarrow s = l$, or $s = -(l+1)$.

Shall we keep both? No!

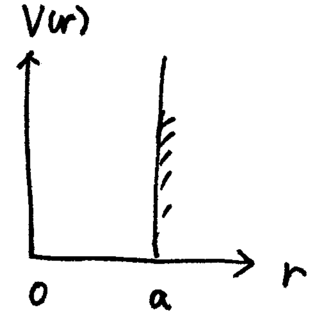
① for a bound state, $\int r^2 dr\, |\psi(r)|^2$ should converge, thus the $r^{-(l+1)}$ is unacceptable for $l \geq 1$. How about the solution at $l=0$? $\overline{\psi_0 \sim \frac{1}{r}}$. Plug in $\psi_0 \sim \frac{1}{r}$, directly into $H = -\frac{\hbar^2\nabla^2}{2m} + V(r)$,

$-\nabla^2 \frac{1}{r} = 4\pi\delta(\vec{r})$, thus $(H-E)\psi_0 \sim \frac{2\pi\hbar^2}{m}\delta(r)$, which cannot satisfy the Schrödinger Eq either.

② we can only keep the regular solution $R \sim r^l$.

1) Application: Spherical potential well

$$V(r) = \begin{cases} 0 & r<a \\ \infty & r>a \end{cases}$$



$$\psi_{lm}(r,\Omega) = R_l(r)\, Y_{lm}(\theta,\varphi)$$

$$\frac{d^2}{dr^2}R_l + \frac{2}{r}\frac{d}{dr}R_l + \left[\frac{2m}{\hbar^2}(E-V(r)) - \frac{l(l+1)}{r^2}\right]R_l = 0$$

in the case $l=0$, and define $\chi_0 = r R_0(r)$,

$$\frac{1}{r}\frac{d^2}{dr^2}(r R_0(r)) = \frac{2}{r}\frac{d}{dr}R(r) + r\frac{d^2}{dr^2}R(r) \Rightarrow$$

$$\chi'' + \frac{2m}{\hbar^2}(E-V(r))\chi = 0, \quad \text{define } k = \frac{\sqrt{2mE}}{\hbar}$$

$\rightarrow \chi'' + k^2\chi = 0$ with boundary condition $\begin{cases} \chi(0)=0 \\ \chi(a)=0 \end{cases}$

$\chi(r) = \sin kr$ and $\begin{cases} ka = (n_r+1)\pi, \quad n_r = 0,1,2,\cdots \\ E_{n_r,0} = \dfrac{\pi^2\hbar^2(n_r+1)^2}{2ma^2} \end{cases}$

normalization: $\displaystyle\int_0^{+\infty} r^2 dr\, |R(r)|^2 = \int_0^{+\infty} dr\, |rR(r)|^2 = \int_0^{+\infty} dr\, |\chi(r)|^2 = 1.$

$\rightarrow$ normalization $\chi(r) = \sqrt{\frac{2}{a}}\sin\frac{(n_r+1)\pi}{a}r$,

or $\boxed{R_{l=0}(r) = \sqrt{\frac{2}{a}}\,\frac{1}{r}\sin\frac{(n_r+1)\pi}{a}r.}$

how about $l\neq 0$?, $\boxed{\frac{d^2}{dr^2}R_l + \frac{2}{r}\frac{d}{dr}R_l + \left[\frac{2m}{\hbar^2}E - \frac{l(l+1)}{r^2}\right]R_l = 0,}$

introducing $\rho = kr$, and $R = u(\rho)/\sqrt{\rho}$,

spherical Bessel Eq.

$$\Rightarrow \frac{d^2u}{d\rho^2} + \frac{1}{\rho}\frac{du}{d\rho} + \left[1 - \frac{(l+1/2)^2}{\rho^2}\right]u = 0, \quad \text{for } V=0.$$

Bessel equation at $l+1/2$-order $\quad J_{l+1/2}(\rho), \; J_{-(l+1/2)}(\rho)$

$$R_l \sim \begin{cases} \frac{1}{\sqrt{\rho}} J_{l+1/2}(\rho) \\ \frac{1}{\sqrt{\rho}} J_{-(l+1/2)}(\rho) \end{cases}$$

define spherical Bessel function $\begin{cases} j_l(\rho) = \sqrt{\frac{\pi}{2\rho}}\, J_{l+1/2}(\rho) \\ n_l(\rho) = (-)^{l+1}\sqrt{\frac{\pi}{2\rho}}\, J_{-l-1/2}(\rho) \end{cases}$

as $\rho \to 0$, $\begin{cases} j_l(\rho) \to \dfrac{\rho^l}{(2l+1)!!} \\ n_l(\rho) \to -(2l-1)!!\,\rho^{-(l+1)} \end{cases}$.

For the spherical well problem, we only take $j_l(\rho)$, which is regular at $\rho=0$

$R_l(r) = C_l\, j_l(kr)$.

At boundary $r=a$, $R_l(a) = 0 \Rightarrow j_l(ka) = 0$

ka take the ~~roots of~~ value of $j_l(x)=0$, i.e $k_{n_r,l} = \dfrac{x_{n_r,l}}{a}$.

(n_r the radial quantum number).

$l \backslash n_r$	0	1
0	π	2π
1	4.49	..
2	5.76	..
3	6.988	..

energy level

0f

1s

0d

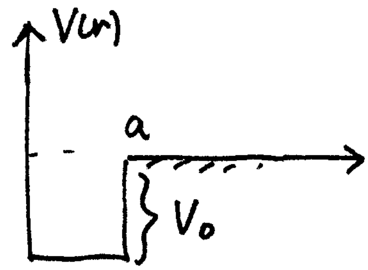
0p

0s

normalization: we need to use $\int j_\ell^2 x^2 dx = \frac{x^3}{2}\left(j_\ell^2 - j_{\ell-1} j_{\ell+1}\right)$

$$\Rightarrow \text{for} \begin{cases} R_{n_r,\ell}(r) = C\, j_\ell(k_{n_r\ell}\, r), \quad k_{n_r\ell} = \dfrac{\chi_{n_r,\ell}}{a} \\ C = \left[-2/a^3 \big/ j_{\ell-1}(ka)\, j_{\ell+1}(ka)\right]^{1/2} \quad \text{for } \ell \geq 1. \end{cases}$$

*) finite depth spherical well (bound state)



$$k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}, \quad \beta = \sqrt{\frac{2m|E|}{\hbar^2}}$$

$$\Rightarrow \begin{cases} R'' + \frac{2}{r} R' + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right] R = 0 & (r<a) \\ R'' + \frac{2}{r} R' + \left[(ik')^2 - \frac{\ell(\ell+1)}{r^2}\right] R = 0 & (r>a) \end{cases}$$

For $r<a \Rightarrow R(r) = A\, j_\ell(kr)$

$r>a$: imaginary variable – Hankel function

$$h_\ell(x) = j_\ell(x) + i n_\ell(x) \xrightarrow{x\to\infty} -\frac{i}{x} e^{i(x-\ell\pi/2)}$$

set $x = ik'r \Rightarrow h_\ell(ik'r) \xrightarrow{x\to\infty} \frac{1}{k'r} e^{-k'r}$ (bound state)

thus $R(r) = B\, h_\ell(ik'r)$.

$R(r)$ and $R'(r)$ need to be continuous at $x=a \Rightarrow \left.\frac{R'(r)}{R(r)}\right|_{x=a^-} = \left.\frac{R'(r)}{R}\right|_{x=a^+}$

$$\Rightarrow \boxed{\frac{k\, j_\ell'(ka)}{j_\ell(ka)} = \frac{ik'\, h_\ell'(ik'a)}{h_\ell(ik'a)}} \longleftarrow \text{spectrum}$$