

§: Angular momentum conservation and radial equation

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

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

$$[l_i, r^2] = [l_i, r_j r_j] = \hbar [r_j [l_i, r_j] + [l_i, r_j] r_j] = (i\epsilon_{ijk} r_j r_k + i\epsilon_{ijk} r_k r_j) \hbar \\ = i(\epsilon_{ijk} + \epsilon_{ikj}) r_j r_k \hbar = 0$$

$$[l_i, p^2] = 0, \quad [l_i, l^2] = 0,$$

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

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

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

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

We will use spherical coordinate:

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

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

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

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

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

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

* eigenstates of $\hat{L}^2$: spherical harmonics $Y_{lm}(\theta, \varphi)$

(2)

$$\hat{L}^2 Y_{lm}(\theta, \varphi) = l(l+1)\hbar^2 Y_{lm}(\theta, \varphi)$$

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

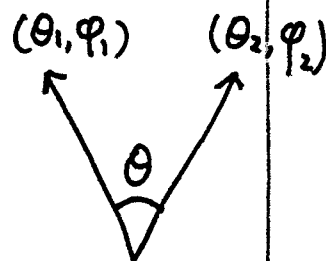
$$P_l(x) = \frac{1}{2^l l!} \frac{d^l}{dx^l} (x^2-1)^l \quad \leftarrow \text{generation function} \quad \frac{1}{(1-2xt+t^2)^{1/2}} = \sum_{l=0}^{\infty} t^l P_l(x)$$

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

$$P_l^{-m}(x) = (-)^m \frac{(l-m)!}{(l+m)!} P_l^m(x)$$

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

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



* the asymptotic behavior at $r \rightarrow 0$.

We assume that $r^2 V(r) \rightarrow 0$ as $r \rightarrow 0$, otherwise if $V(r) \rightarrow -\infty$, 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

$$V(r) \sim \frac{-k}{(\Delta r)^3} \cdot E \sim \frac{\hbar^2}{2m(\Delta r)^2} - \frac{k}{(\Delta r)^3} \longrightarrow -\infty, \text{ thus the ground}$$

state energy $\rightarrow -\infty$. 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, $V \sim r^2, r, \ln r, \frac{1}{r}, \frac{1}{r} e^{-r/\lambda}, \dots$,

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

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

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

→

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

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

$$\Rightarrow S(S-1) + 2S - l(l+1) = 0 \Rightarrow S = l, \text{ or } S = -(l+1).$$

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

$l=0$? Plug in $\psi_0 \sim \frac{1}{r}$, directly into $H = -\frac{\hbar^2}{2m} \nabla^2 + V(r)$, $\psi_0 \sim \frac{1}{r}$

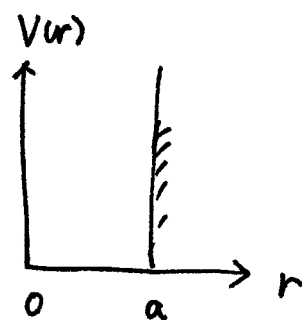
$$-\nabla^2 \frac{1}{r} = 4\pi \delta(\vec{r}), \text{ thus } (H-E) \psi_0 \sim \frac{2\pi\hbar^2}{m} \delta(\vec{r}), \text{ which}$$

cannot satisfy the Schrödinger Eq either.

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

1) Application: Spherical potential well

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



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

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

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

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

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

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

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

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

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

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

how about $l \neq 0$?

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

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

↑ spherical Bessel Eq.

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

→ Bessel equation at $l+1/2$ -order $J_{l+1/2}(p), J_{-(l+1/2)}(p)$

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

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

$$\text{as } p \rightarrow 0, \begin{cases} j_l(p) \rightarrow \frac{p^l}{(2l+1)!!} \\ n_l(p) \rightarrow -(2l-1)!! p^{-(l+1)} \end{cases}$$

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

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

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

ka take the roots of $j_l(x)=0$, i.e. $k_{nr,l} = \frac{\chi_{nr,l}}{a}$.
value of

(n_r the radial quantum number).

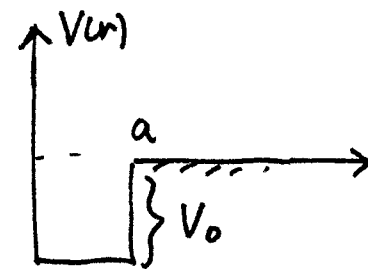
$l \backslash n_r$	0	1
0	π	2π
1	4.49	..
2	5.76	..
3	6.988	..

energy level

_____ of
 _____ 1s
 _____ 0d
 _____ 0p
 _____ 0s

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

$$\Rightarrow \text{for } \begin{cases} R_{n,l}(r) = C j_l(kr) \\ c = \left[-2/a^3 / j_{l-1}(ka) j_{l+1}(ka) \right]^{1/2} \end{cases} \quad k_{n,l} = \frac{\chi_{n,l}}{a} \quad \text{for } l \geq 1.$$



* finite depth spherical well
(bound state)

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

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

$$\text{For } r < a \Rightarrow R(r) = A j_l(kr)$$

$r > a$: imaginary variable - Hankel function

$$h_l(x) = j_l(x) + i n_l(x) \xrightarrow{x \rightarrow \infty} -\frac{i}{x} e^{i(x - l\pi/2)}$$

$$\text{set } x = ik'r \Rightarrow h_l(ik'r) \xrightarrow{x \rightarrow \infty} \frac{1}{kr} e^{-kr} \quad (\text{bound state})$$

$$\text{thus } R(r) = B h_l(ik'r).$$

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

$$\Rightarrow \boxed{\frac{k j'_l(ka)}{j_l(ka)} = \frac{ik' h'_l(ik'a)}{h_l(ik'a)}} \quad \leftarrow \text{spectrum}$$