Tues 8 May 07

QM - week 6

Ch 12 - Rotational Invariance & Angular Momentum

Recall that LINEAR MOMENTUM OPERATORS GENERATE TRANSLATIONS

$$P_x \longrightarrow -i\hbar \frac{\partial}{\partial x}$$

Generator of small translation $T(\varepsilon) = I - \frac{i\varepsilon}{\hbar} P = I + \varepsilon \frac{\partial}{\partial x}$

$\Delta x = \varepsilon$

2.29) Generator of finite translation $T(a) = e^{-iaP/\hbar} = e^{a\partial/\partial x}$

$\Delta x = a$

TRANSLATIONAL INVARIANCE $\longleftrightarrow$ LINEAR MOMENTUM CONSERVATION

(11.2.21) $T^{\dagger}(\varepsilon) H T(\varepsilon) = H \longrightarrow [H, P] = 0 \longrightarrow \langle \dot{P} \rangle = 0$

(11.2.24) & Ehrenfest Thm

Similarly, ANGULAR MOMENTUM OPERATORS GENERATE ROTATIONS

2.2.19) $L_z \longrightarrow -i\hbar \frac{\partial}{\partial \varphi}$ $\quad z\uparrow \circlearrowright \varphi$

Generator of small rotation $U(\varepsilon) = I - \frac{i\varepsilon}{\hbar} L_z = I + \varepsilon \frac{\partial}{\partial \varphi}$

$\Delta\varphi = \varepsilon$

2.2.18) Generator of finite rotation $U(\varphi_0) = e^{-i\varphi_0 L_z/\hbar} = e^{\varphi_0 \partial/\partial\varphi}$

$\Delta\varphi = \varphi_0$

ROTATIONAL INVARIANCE $\longleftrightarrow$ ANGULAR MOMENTUM CONSERVATION

(12.2.21) $U^{+} H U = H$ $\qquad [L_z, H] = 0$

If H is rotationally invariant, L_z & H have a common basis & simultaneous eigenvalues *

(spherical symmetry)

,4.17) If H is invariant under ARBITRARY rotations, then $[L^2, H] = 0$ also.

translational $\quad\quad$ momentum

INVARIANCE $\longleftrightarrow$ CONSERVATION

$T^\dagger H T = H \qquad\qquad [H, P] = 0$

$$H = T^\dagger(a) H T(a) = e^{iaP/\hbar} H e^{-iaP/\hbar}$$

$$= \left[I + \left(\frac{iaP}{\hbar}\right) + \frac{1}{2}\left(\frac{iaP}{\hbar}\right)^2 + \cdots\right] H \left[I + \left(-\frac{iaP}{\hbar}\right) + \frac{1}{2}\left(-\frac{iaP}{\hbar}\right)^2 + \cdots\right]$$

$$= \left[H + \frac{iaPH}{\hbar} - \frac{1}{2}\frac{P^2H}{\hbar^2} - \cdots\right]\left[I - \frac{iaP}{\hbar} - \frac{1}{2}\frac{a^2P^2}{\hbar^2} + \cdots\right]$$

$$= H - \frac{iaHP}{\hbar} - \frac{1}{2}\frac{a^2HP^2}{\hbar} + \frac{iaPH}{\hbar} + \frac{a^2PHP}{\hbar^2} - \frac{1}{2}\frac{ia^3PHP^2}{\hbar^3}$$

$$- \frac{1}{2}\frac{a^2P^2H}{\hbar^2} \qquad + \frac{1}{2}\frac{ia^3P^2HP}{\hbar^2} + \frac{1}{4}\frac{a^4P^2HP^2}{\hbar^2} \cdots$$

$$= H + \frac{ia}{\hbar}[HP - PH] - \frac{1}{2}\frac{a^2}{\hbar^2}\left(HP^2 - 2PHP + P^2H\right) + \cdots$$

$$= H + \frac{ia}{\hbar}[H, P] - \frac{1}{2}\frac{a^2}{\hbar^2}\left[(HP - PH)P + P(PH - HP)\right] + \cdots$$

$$H = H + \frac{ia}{\hbar}[H, P] - \frac{1}{2}\frac{a^2}{\hbar^2}[H, P]P - \frac{1}{2}\frac{a^2}{\hbar^2}P[P, H] + \cdots$$

If this is to be true for arbitrary a,
each coefficient must vanish,
therefore $[H, P] = 0$,

therefore, by Ehrenfest's theorem, $\langle\dot{P}\rangle = 0$
and momentum is conserved.

SPHERICAL SYMMETRY

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

(2) $L_z \to -i\hbar \frac{\partial}{\partial\phi}$

(3) $\nabla^2 \to \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{r^2} \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}$

General defn- not just for SS.

Sph. Sym. : $\to$ $[H, L^2] = [H, L_z] = 0$

since also $[L^2, L_z] = 0 \to$ Eigenstates of H are also Estates of L_z,

can find simultaneous Eigenbasis for H, L^2, L_z.

These Estates are $|lm\rangle$ where (4) $L^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle$ ← $l = 0, 1, 2, 3, \ldots$

and (5) $L_z |lm\rangle = \hbar m |lm\rangle$ ← $m = 0, \ldots, \pm(l-1), \pm l$

$-l, -l+1, \ldots, l-1, l$

In the coordinate basis, kets $|lm\rangle$ are (angular momentum e-fxn)

(6) $\Psi_{lm}(\vec{r}) = \langle r\theta\phi | lm\rangle = R(r)\, Y_l^m(\theta, \phi)$

where the functions $Y_l^m(\theta,\phi)$ = SPHERICAL HARMONICS; $1 = \int_0^{4\pi} |Y_l^m(\theta,\phi)|^2 d\Omega$

$(\sin\theta\, d\theta\, d\phi)$

$R(r)$ arbitrary since operation by L^2 doesn't change it. Hamiltonian matters.

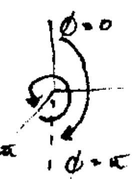
Normalization condition on R? (Y_l^m part integrates to 1...)

$1 = \int_0^\infty \int_0^{4\pi} |\Psi_{lm}|^2 r^2\, dr\, d\Omega = \int_0^\infty |R(r)|^2 r^2\, dr \ast \int_0^{4\pi} |Y_m^l(\theta,\phi)|^2 d\Omega$

$(dV = r^2 \sin\theta\, dr\, d\theta\, d\phi)$

$= \int_0^\infty |R(r)|^2 r^2\, dr$

Why 4π? $r^2 \int_0^\pi \int_0^{2\pi} \overbrace{\sin\theta\, d\theta\, d\phi}^{d\Omega}$



$= \int_0^{4\pi} d\Omega = 4\pi r^2$

differential AREA patches

$r^2 \int d\Omega = r^2 \int_0^\pi \left[-\cos\theta\right]_0^{2\pi} d\phi$

$= r^2 \int [-1-1]\, d\phi$

$= -2r^2 \int_0^\pi d\phi = 2\pi r^2$

Ψ_{lm} : $\theta\phi$ dependence fixed; r dependence arbitrary

Ψ_{Elm} : also fixes r-dependence.

Now solve Schrödinger eqn. In position basis: $H\Psi_{Elm}(\vec{r}) = E\Psi_{Elm}(\vec{r})$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E\right]\Psi_{Elm}(\vec{r}) = 0$$

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} \underbrace{-\frac{\hbar^2}{2mr^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)}_{(1)\ \frac{L^2}{2mr}} + V(r) - E\right]\Psi_{Elm} = 0$$

, and $\underset{(4)}{L^2\Psi_{Elm}} = \hbar^2 l(l+1)\Psi_{Elm}$

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - E\right]\underbrace{\Psi_{Elm}}_{R_{Elm}(r)Y_l^m(\theta,\phi)} = 0$$

can divide both sides by Y_l^m and get purely

* RADIAL EQUATION for r-dependence. Doesn't depend on (m) any longer (m-states all have same energy - degenerate for spher. sym.)

pseudo-repulsion or centrifugal potential.

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2mr^2}\right]R_{Elm}(r) = 0$$

To get the Ultimate Radial equation, define $U_{El}(r) = rR_{El}(r)$

$$(7)\quad \left\{\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2mr^2}\right]\right\}U_{El}(r) = 0$$

(middle steps in exercise)

Normalization: $1 = \int_0^\infty |R(r)|^2 r^2\,dr = \int_0^\infty |R(r)\,r|^2\,dr = \int_0^\infty |U_{El}(r)|^2\,dr$

Now find some boundary conditions with U:

(i) $\boxed{r\to 0}$ dominant terms $\frac{d^2}{dr^2}$ and $-\frac{\hbar^2 l(l+1)}{2mr^2}$. $\boxed{U_{El}\to r^{l+1}}$ (if $V(r)\to r^\alpha$, $\alpha > -2$)

r^{-l} would work except it blows up

eg V constant at origin. Many such potential

V "singular" at origin: goes to infinity. So is E term here

But eg HO pot. not sing. at. or. Coul pot / Grav pot s.a.o. only at $\frac{1}{r}$

(ii) $\boxed{r\to\infty}$ $U_{El}(r) \longrightarrow 0$

$\longrightarrow Ae^{ikr}$ wave

free particles if far enough apart

if $rV(r)\to 0$ as $r\to\infty$. Eg for particle-in-spherical-box, Pot = 0 inside, ∞ outside? ... happens for weak nuke force.

* Rae does it all by separation of variables, but you get no physical sense from it.

ISOTROPIC OSCILLATOR

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

SAME FOR HYDROGEN ATOM p. 364

find U_{El}, reconstruct total wave fcn.

1. Look at asymptotic behavior. $r \to \infty$? no, never free particle, Dominant term $\frac{1}{2}m\omega^2 r^2$

$\xrightarrow[r\to\infty]{} \left[\frac{d^2}{dr^2} - \frac{1}{2}m\omega^2 r^2\right] U_{El} = 0$ same as ordinary HO in this limit: Same potential except for centrifugal term, which vanishes in this limit.

for HO: $U_{El} = y^m e^{-y^2/2}$ where $y = \sqrt{\frac{m\omega}{\hbar}}\, r$ (maximum power k)

At zero, $V(r) \to r^2$ $(\alpha > -2)$! (i) so

$\xrightarrow[r\to 0]{} U_{El} \to y^{l+1}$ (minimum power)

cf 13.1.10 p. 364

So, putting these together, $\underline{U_{El} = v(y)\, e^{-y^2/2}}$, where $\underline{v(y) = y^{l+1}\sum_{k=0} c_k y^k}$

2. Write out eqn for $v(y)$: again same as HO except for extra term.
Diffeq becomes (see 7.3.11, p. 203) $u'' - 2yu' + (2\varepsilon - 1)u = 0$

$$v'' - 2yv' + \left[2\lambda - 1 - \frac{l(l+1)}{y^2}\right] v = 0 \qquad (\lambda = E/\hbar\omega, \text{ same as for HO})$$

Try power series solution: claims $v(y) = \sum_{k=0} c_k y^{l+1+k}$

$v'' = (l+k+1)(l+k)c_k y^{l+k-1}$

$v' = (l+k+1)\, y^{l+k}$

$$0 = \sum_{k=0}\left\{(l+k+1)(l+k)c_k y^{l+k-1} - 2c_k(l+k+1)y^{l+k+1} + [2\lambda-1]c_k y^{l+k+1} - l(l+1)c_k y^{l+k-1}\right\}$$

$$= \sum_{k=0}\left\{\underset{(l+k+3)(l+k+2)}{(l+k+1)(l+k)} - l(l+1)\right\} \underset{y^{l+k+1}}{y^{l+k-1}}\, \underset{c_{k+2}}{c_k} + \left\{-2(l+k+1) + 2\lambda - 1\right\} c_k y^{l+k+1}$$

$$c_{k+2} = \frac{2\lambda + 2(l+k+1) - 1}{(l+3+k)(l+2+k) + l(l+1)}\, c_k$$

particular energy values - must have some where $0 = 2\lambda - 2l - 2k - 3 \to$

QUANTIZATION $\lambda = \frac{E}{\hbar\omega} = \underbrace{l + k}_{n} + 3/2$ (integer)

note also k must always be even. odd power series doesn't go to zero in correct way.

HYDROGEN ATOM $\left\{\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left[E + \frac{e^2}{r} - \frac{\ell(\ell+1)}{2mr^2}\right]\right\} u_{E\ell} = 0$

$\left(u_{E\ell} \underset{r\to\infty}{\to} \rho^n e^{-\rho}\right)\left(u_{E\ell} \underset{r\to 0}{\to} \rho^{\ell+1}\right) \Rightarrow u_{E\ell} = e^{-\rho} v_{E\ell}(\rho)$

$E_n = \frac{-me^4}{2\hbar^2 n^2} = -\frac{R_y}{n^2}$ where $n = 1, 2, 3, \ldots$ $\ell = n-1, n-2, n-3, \ldots, 0$

$m = -\ell, \ldots, +\ell$

bump in prob dist : $n-\ell$

$\rho = 0$

possibility distribution for energy level $n=2, \ell=0$, depending on radius