Phys 522 **Lec. 1** Spring 2024

Units

CGS - Gaussian

cetimeter, gram, second

charge esu $= \sqrt{\text{dyne}} \cdot \text{cm} = \sqrt{g}\,(\text{cm})^{3/2}/s$

$$\text{dyne} = g\left(\frac{\text{cm}}{s}\right)^2 \cdot \text{cm}$$

electron charge $= 4.8 \times 10^{-10}$ esu

So that Coulomb potential is

$$V_c = \frac{q_1 q_2}{r} = -\frac{Ze^2}{r} = -Z\frac{\alpha\hbar c}{r}$$

nuclear charge $\quad q_1 = Ze \;,\; q_2 = -e \quad$ and $\quad \frac{e^2}{\hbar c} = \alpha = \frac{1}{137.036}$

with $\hbar c = 197 \text{ eV}\cdot\text{nm} = 197 \text{ MeV}\cdot\text{fm}$

texts: Sakurai

Shankar

Comm~~ins~~ atomic, p191.

Convenient to convert mass to

$$\frac{1\,\text{eV}}{c^2} = 1.78 \times 10^{-33}\,g \quad \text{so that}$$

$$m_e = \frac{9.1 \times 10^{-28}\,g}{1.78 \times 10^{-33}\,g / \frac{\text{eV}}{c^2}} = \frac{1}{2} \times 10^6 \frac{\text{eV}}{c^2} = \frac{1}{2}\,\text{MeV}/c^2$$

atomic physics derived

Bohr radius $a_0 = \frac{\hbar^2}{m_e e^2} = \left(\frac{\hbar c}{mc^2}\right)\left(\frac{\hbar c}{e^2}\right)$

$= \frac{197\ \text{eV}\cdot\text{nm}}{0.51\times10^6\ \text{eV}}\left(\frac{1}{\alpha}\right) = 0.053\ \text{nm}$

Ionization of hydrogen R_y

$R_y = \frac{me^4}{2\hbar^2} = \frac{m_e c^2}{2}\left(\frac{e^2}{\hbar c}\right)^2$

$= \frac{1}{2}\left(\frac{1}{2}\times10^6\ \text{eV}\right)\alpha^2 = 13.3\ \text{eV}$

electron Compton wavelength $/2\pi \equiv ƛ_c$

$ƛ_c = \alpha a_0 = \frac{\hbar^2}{m_e c^2}\left(\frac{e^2}{\hbar c}\right) = \frac{\hbar c}{m_e c^2} = 3.9\times10^{-4}\ \text{nm}$

some atomic units: value = 1 unit

m_e
a_0
speed $\langle v\rangle = \alpha c$
charge e
action $\hbar$
energy $e^2/a_0 = \frac{e^2}{\hbar^2/m_e e^2} = \frac{e^4 m_e}{\hbar^2}$

$V_c = -\frac{Z}{r}$

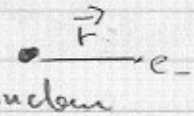
$\frac{e^2}{a_0} = \frac{e^2}{\hbar^2/(m_e e^2)} = \frac{m_e e^4}{\hbar^2} = 2R_y$

I will not use atomic units

hydrogen atom $\quad V = -\frac{e^2}{r} = -\frac{\hbar c \alpha}{r}$

In Galilean fram where atom is at rest;

$$\vec{r} = \vec{r}_n - \vec{r}_e$$



reduced mass

$$\mathcal{L} = \frac{1}{2}\mu|\dot{\vec{r}}|^2 - V(\vec{r}) \qquad \mu = \frac{m_p m_e}{m_e + m_p}$$

$$m_p/m_e = 1836 \qquad \mu = \frac{m_e}{1 + \frac{m_e}{m_p}} = \frac{m_e}{1.0005447}$$

$$= m_e \times (0.999455)$$

$$V(r) = -e^2/r$$

$$\hat{H} = \underbrace{\frac{p_r^2}{2\mu}}_{\text{radial}} + \underbrace{\frac{\hat{L}^2}{2\mu r^2}}_{\text{rotational}} + V(r)$$

KE

$$\hat{p}_r = \frac{\hbar}{i}\left(\frac{1}{r}\frac{\partial}{\partial r} r\right)$$

$$\frac{\hat{p}_r^2}{2\mu} = -\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial}{\partial r} r\right)\left(\frac{1}{r}\frac{\partial}{\partial r} r\right)$$

$$\frac{p_r^2}{2\mu} f(r) = -\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2} r f\right)$$

$$= -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial}{\partial r}\left(r f' + f\right)$$

$$= -\frac{\hbar^2}{2\mu}\frac{1}{r}\left(r f'' + 2f'\right)$$

$$= -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) f$$

with $\psi = R(r)\, Y_{em}(\theta, \phi)$,

$$\hat{L}^2 Y_{em} = \hbar^2 \ell(\ell+1)$$

radial equation is

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial R^2} + 2\frac{\partial}{\partial R}\right)R + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1)R - \frac{e^2}{r}R = ER.$$

define $u = rR$

$$P_r^2 R = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r}\left(\frac{\partial}{\partial r} r\right)\right]\left[\frac{1}{r}\frac{\partial}{\partial r} r\right]$$

$$= -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}U = -\frac{\hbar^2}{2\mu}\frac{1}{r}u''$$

so

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}u'' + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1)\left(\frac{u}{r}\right) - \frac{e^2}{r}\left(\frac{U}{r}\right) = ER$$

multiply by r,

$$-\frac{\hbar^2}{2\mu}u'' + \frac{\hbar^2}{2\mu r^2}\ell(\ell+1)u - \frac{e^2}{r}u = Eu$$

$$U'' - \frac{\ell(\ell+1)}{r^2}u + \frac{e^2 2\mu}{\hbar^2}\frac{u}{r} = -\frac{2\mu E}{\hbar^2}U$$

in general, U depends on E, ℓ

E depends on ℓ

$$U''_{E,\ell} - \frac{\ell(\ell+1)}{r^2}U_{E,\ell} + \frac{e^2 2\mu}{\hbar^2 r}U_{E,\ell} = -\frac{2\mu E}{\hbar^2}u$$

must have $u_{E,l} \underset{r\to\infty}{\longrightarrow} 0$

as $r \to \infty$, eq. becomes   bound state $E < 0$

$$u''_\infty = \left(-\frac{2\mu}{\hbar^2} E_l\right) u_\infty = \frac{2\mu}{\hbar^2}|E|\, u_\infty$$

define $\rho = r\left(\frac{2\mu|E|}{\hbar^2}\right)^{1/2}$

let prime mean $\frac{\partial}{\partial \rho}$,

$$u''_\infty = +u_\infty \qquad \underset{r\to\infty}{u} = e^{-\rho}$$

then $u_{El} = e^{-\rho}\, v_{e,l}$

radial equation is:

$$\frac{\partial}{\partial r} = \sqrt{\frac{2\mu|E|}{\hbar^2}}\frac{\partial}{\partial \rho}$$

$$\frac{2\mu|E|}{\hbar^2} u'' - \frac{l(l+1)}{\rho^2}\left(\frac{2\mu|E|}{\hbar^2}\right) + \frac{e^2 2\mu}{\hbar^2}\sqrt{\frac{\hbar^2}{2\mu|E|}}\frac{u}{\rho} = +\frac{|E|2\mu}{\hbar^2} u$$

$$u'' - \frac{l(l+1)}{\rho}u + e^2 \underbrace{\sqrt{\frac{2\mu}{\hbar^2|E|}}}_{\equiv\ \boxed{\lambda = \sqrt{\frac{2\mu}{\hbar^2|E|}}}} \frac{u}{\rho} = +u$$

$$u'' - \frac{l(l+1)}{\rho^2}u + \lambda e^2 \frac{u}{\rho} - u = 0$$

as $\rho \to 0$,

$$U'' - \frac{\ell(\ell+1)}{\rho^2}u - u = 0$$

then $U \xrightarrow[\rho \to 0]{} c\rho^{\ell+1}$ c = constant

$$u' = c(\ell+1)\rho^{\ell}$$
$$u'' = c\ell(\ell+1)\rho^{\ell-1}$$

gives $c\rho^{\ell+1} = 0$

true for all ℓ.

radial equation in u equivalent to 1D schrodinger with $\rho = 0$ at origin boundary condition.

$$R = \frac{u}{r} \xrightarrow[r \to 0]{} c\, r^{\ell}$$

$\Rightarrow$ $\ell = 0$ is finite at $r = 0$ $\Rightarrow$

Positronium e^+e^- bound state

decay rate
$$\Gamma \propto |\psi_{100}(0)|^2$$

cascade to $\ell = 0$ state to annihilate

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in terms of $u = e^{-\rho} V$

$$u'' = u - 2e^{-\rho}V' + e^{-\rho}V''$$

cancel overall $e^{-\rho}$ factor

$$V'' - 2V' + \left[\frac{\lambda e^2}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right]V = 0$$

now we have

$$U(\rho) = \rho^{\ell+1} e^{-\rho} F(\rho)$$

power series solution

$$V(\rho) = \rho^{\ell+1} F(\rho)$$

$F = \sum C_k \rho^k$ gives recursion

$$\frac{C_{k+1}}{C_k} = \frac{-e^2\lambda + 2(k+\ell+1)}{(k+\ell+2)(k+\ell+1) - \ell(\ell+1)}$$

$$\frac{C_{k+1}}{C_k} \xrightarrow[k\to\infty]{} \frac{2}{k+\ell+2} \to \frac{2}{k}$$

since $e^{2x} = \sum_{k=0}^{\infty} \frac{(2x)^k}{k!}$

$$\frac{C_{k+1}}{C_k} \text{ is } \frac{k!}{(k+1)!} \cdot \frac{2^{k+1}}{2^k} = \frac{2}{k}$$

then $V(\rho) \xrightarrow[\infty]{} \rho^{\ell+1} e^{-\rho} e^{\rho} \to \infty$

series must terminate to satisfy

boundary condition at ∞.

Condition is

$$-e^2\lambda_k + 2(k+l+1) = 0$$

quatized energy levels are

$$\lambda_k = \frac{2(k+l+1)}{e^2}$$

$$E_k = -\frac{2\mu}{\hbar^2\lambda_k^2} = \frac{-2\mu e^4}{4(k+l+1)^2\hbar^2}$$

$$= -\frac{\mu e^4}{2\hbar^2}\frac{1}{(k+l+1)^2}$$

where $k = 0, 1, 2, \dots \infty$

define $n = k+l+1$

$$n = 1, 2, 3, \dots \infty$$

$$E_n = \frac{-\mu e^4}{2\hbar^2}\frac{1}{n^2}$$

$e^2 = \hbar c \alpha$ $\quad E_n = \frac{-\mu \hbar^2 c^2 \alpha^2}{2\hbar^2}\frac{1}{n^2} = -R_y \frac{1}{n^2}$

$$\boxed{E_n = -\frac{(\mu c^2)\alpha^2}{2}\frac{1}{n^2}}$$

allowed l for each n,

$$l = n-k-1 = n-1, n-2, \dots 0$$

or $l = 0, \ldots, n-1$

for each l, Y_{lm} are degenerate

$(2l+1)$ state for each l,

$$\sum_{n=0}^{n-1} (2l+1) = n^2$$

E_n independent of l with n^2 degeneracy

wave function

$$\psi_{nlm} = R_{nl} Y_{lm} = \frac{U_{nl}}{r} Y_{lm}$$

$$U_{nl} = \rho^{l+1} e^{-\rho} F(\rho)$$ F polynomial degree $n-l-1$

$$F(\rho) = L_{n-l-1}^{2l+1} (2\rho)$$

known a associated Laguerre polynomial.

$$\rho = \sqrt{\frac{2\mu |E|}{\hbar^2}} = \frac{me^2}{\hbar^2 n} r = \left(\frac{r}{a_0}\right)\frac{1}{n}$$

when $a_0 = \dfrac{\hbar^2}{me^2}$

$$R_{nl} \xrightarrow[r \to \infty]{} r^{n-1} e^{-r/a_0}$$

independent of l

normalized wave functions,

$$\psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}$$

$$\psi_{200} = \left(\frac{1}{32\pi a_0^3}\right)^{1/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$$

$$\psi_{210} = \left(\frac{1}{32\pi a_0^3}\right)^{1/2} \frac{r}{a_0} e^{-r/2a_0} \cos\theta$$

$$\psi_{21,\pm1} = \mp \left(\frac{1}{64\pi a_0^3}\right)^{1/2} \frac{r}{a_0} e^{-r/2a_0} \sin\theta \, e^{\pm i\phi}$$

and $\langle r \rangle_{n\ell m} = \frac{a_0}{2}\left[3n^2 - \ell(\ell+1)\right]$

n^2 degeneracy is result of dynamical symmetry.

Classical orbits are closed for $1/r$, r^2 potentials.

Dynamical Symmetry

note $(\vec{P}\times\vec{L})^{\dagger}_i = (\varepsilon_{ijk} P_j L_k)^{\dagger} = \varepsilon_{ijk} L_k P_j$

$= \varepsilon_{ijk} L_k P_j = -\varepsilon_{ikj} L_k P_j$

$= -(L\times P)_i$

$(P\times L)^{\dagger} = -(L\times P)$ not Hermitian

$[L_k, P_j] = \varepsilon_{kmn}[r_m P_n, P_j]$

$= \varepsilon_{kmn}[r_m P_n P_j - P_j r_m P_n]$

$\hookrightarrow r_m P_j P_n$

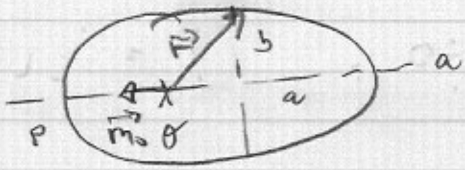
$[r_m, P_j] = i\hbar\,\delta_{mj}$

$(P_j \cancel{r_m} + i\hbar\,\delta_{mj})P_n - P_j \cancel{r_m P_n}$

$= \varepsilon_{kmn}\, i\hbar\,\delta_{mj} P_n = i\hbar\,\varepsilon_{kjn} P_n \neq 0$

Dynamical Symmetry

ref. Schiff Q.M.



eccentricity ε

$$\varepsilon = \sqrt{a^2-b^2}\,/\,a$$

$$H = \frac{p^2}{2\mu} - \frac{e^2}{r}$$

classical, $H = E$ const. in time

rotational symmetry $\vec{L} = \vec{r}\times\vec{p}$ const. orbit in plane

$$E = -\frac{e^2}{2a} \qquad L^2 = \mu e^2 a(1-\varepsilon^2)$$

Closed for $\frac{1}{r}$ potential $\Rightarrow$ another constant

Runge-Lenz

$$\vec{m}_0 = \frac{\vec{p}\times\vec{L}}{\mu} - \frac{e^2}{r}\vec{r} \qquad |\vec{m}_0| = e^2\varepsilon$$

$$\vec{L}\cdot\vec{m}_0 = 0 \qquad m_0^2 = \frac{2H}{\mu}L^2 + e^4$$

Q.M.

$$\vec{m}_0 = \frac{1}{2\mu}\underbrace{\left(\vec{p}\times\vec{L} - \vec{L}\times\vec{p}\right)}_{\text{Hermitian}} - \frac{e^2}{r}\vec{r}$$

$$[m_{o_i}, H] = 0$$

$$\vec{L} \cdot \vec{m}_o = \vec{m}_o \cdot \vec{L} \qquad \vec{L} \perp \vec{m}_o$$

$$m_o^2 = \frac{2H}{\mu}(L^2 + \hbar^2) + e^4 \qquad \text{Pauli, 1926}$$

$\vec{m}_o$ generates rotations just like $\vec{L}$

$6!/2!4! = 15$ combinations

$$[L_i, L_j] = i\hbar \, \varepsilon_{ijk} L_k \qquad 3$$

$$[m_i, L_j] = i\hbar \, \varepsilon_{ijk} m_k \qquad 3 \times 3 = 9$$

last three harder,

$$[m_i, m_j] = -\frac{2i\hbar}{\mu} H \, \varepsilon_{ijk} L_k \qquad 3$$

Hamiltonian

Algebra of 6 generators does not close.

Work in subspace of Hilbert space

with $\hat{H}\psi_E = E\psi_E$ $\underline{\underline{E<0}}$ bound state

Scale, $\vec{m} \equiv \left(-\frac{\mu}{2E}\right)^{1/2} \vec{m}_0$

then last 3 commutators are

$[m_i, m_j] = i\hbar\, \varepsilon_{ijk} L_k$ $\underline{\text{closes}}$.

Identify with $SO(4)$ orthogonal, $\in$ det $=1$ 4x4 real matrices

invent fictitious 4th r_4, p_4 with

$$\boxed{[x_i, p_j] = i\hbar\,\delta_{ij}} \quad i,j = 1, \ldots 4$$

$\underline{\text{define}}$

$$m_1 \equiv x_1 p_4 - x_4 p_1$$
$$m_2 \equiv x_2 p_4 - x_4 p_2$$
$$m_3 \equiv x_3 p_4 - x_4 p_3$$

4th phase space dimension is fictitious,
hence dynamical symmetry

Rank 2 group 2 Casimir operator

define

$$I_i = \tfrac{1}{2}(L_i + M_i) \qquad K_i = \tfrac{1}{2}[L_i - M_i]$$

get

$$[I_i, I_j] = i\hbar\,\varepsilon_{ijk} I_k$$

$$[K_i, K_j] = i\hbar\,\varepsilon_{ijk} K_k$$

$$[I_i, K_j] = 0 \qquad [I_i, H] = 0 \qquad [K_i, H] = 0$$

follows that 2 Casimir operators are

$$\vec{I}^2 = \tfrac{1}{4}(\vec{L} + \vec{m})^2$$

$$\vec{K}^2 = \tfrac{1}{4}(\vec{L} - \vec{m})^2$$

I_i, K_i are each su(2) algebras,

They commute. simultaneous eigenvalues

$$I^2 \psi_{jk} = j(j+1)\hbar^2 \psi_{jk} \;;\; K^2 \psi_{jk} = k(k+1)\hbar^2 \psi_{jk}$$

where $j, k = 0, \tfrac{1}{2}, 1, \ldots$ just

as for rep. of su(2)

lec 1-16

We could have chosen two Casimirs as

$$C = (I^2 + K^2)\ ;\ C' = I^2 - K^2 = \frac{1}{2}(\vec{L}\cdot\vec{M} + \vec{M}\cdot\vec{L}) = 0$$

since $C' = 0$, must have $j = k$
eigenvalues of C are

adding i, j terms

$$C\psi_k = 2k(k+1)\hbar^2\psi_k \qquad k = 0, \frac{1}{2}, 1, \ldots$$

But $C = \frac{1}{2}\left(L^2 - \frac{\mu}{2E}M_0^2\right)$ (E < 0 in both)

$$M_0^2 = \frac{2E}{\mu}(L^2 + \hbar^2) + e^4$$

<u>L^2 terms cancel</u>, giving

$$C = -\frac{\mu e^4}{4E} - \frac{1}{2}\hbar^2$$ and eigenvalue equation

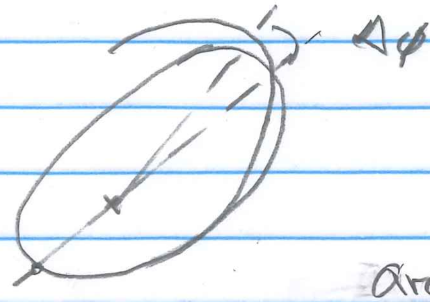
gives

$$2k(k+1)\hbar^2 = -\frac{\mu e^4}{4E} - \frac{1}{2}\hbar^2$$

$2k(k+1) + \frac{1}{2} = \frac{1}{2}(2k+1)^2 \qquad 2k+1 = 1, 2, 3, \ldots$ integer

$$E_k = \frac{-\mu e^4}{2\hbar^2(2k+1)^2}$$

Note on precession of Mercury



eccentricity of ellipse greatly exaggerated

Perihelion	Arc-sec/century (wikipedia)
mercury observed	574
planet perturbation	532
G.R.	43
oblate sun	0.03

but G.R., oblate both give correction to potential $V \sim \frac{1}{r^3}$

See Baierlein Newton Dynamics