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DARA CORR

ID: 18483836

QM II HW 1

Q1 Solve 3-d Schrödinger Eqn

$$V(x,y,z) = \begin{cases} 0, & 0 \le x \le a,\ 0 \le y \le b,\ 0 \le z \le c \\ \infty, & \text{otherwise} \end{cases}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = E\psi$$

$\psi = 0$ outside box

$E \geq V_{min} = 0$ inside box

Find soln using separation of variables:

Let $\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$

eqn becomes

$$-\frac{\hbar^2}{2m} \nabla^2 (X(x)\,Y(y)\,Z(z)) = E\,X(x)\,Y(y)\,Z(z)$$

$$-\frac{\hbar^2}{2m}(X''YZ + XY''Z + XYZ'') = EXYZ$$

$$(X''YZ + XY''Z + XYZ'') = \frac{-2mE}{\hbar}XYZ$$

$$\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = -\frac{2mE}{\hbar^2}$$

$$\frac{X''}{X} = -\frac{2mE}{\hbar^2} - \frac{Y''}{Y} - \frac{Z''}{Z}$$

$$f(x) = g(y) + h(z) \iff f(x) = g(y) + h(z) = \text{Const.}$$

$$\frac{X''}{X} = -k_x^2 = \text{Const.} \rightarrow \boxed{X'' + k_x^2 X = 0}$$

$$\frac{Y''}{Y} + \frac{Z''}{Z} = \frac{-2mE}{\hbar^2} - k_x^2$$

$$\frac{Y''}{Y} = \frac{-2mE}{\hbar^2} - \frac{Z''}{Z} + k_x^2 = \text{Const.} - k_y^2$$

$$\frac{Y''}{Y} = -k_y^2 = \frac{2mE}{\hbar^2} - \frac{Z''}{Z} + k_x^2$$

$$\boxed{Y'' + k_y^2 Y = 0}$$

$$-k_y^2 = -\frac{2mE}{\hbar^2} - \frac{Z''}{Z} + k_x^2$$

$$\frac{Z''}{Z} = \frac{-2mE}{\hbar^2} + k_x^2 + k_y^2$$

Let $-k_z^2 = \frac{-2mE}{\hbar^2} + k_x^2 + k_y^2$

$$\frac{Z''}{Z} = -k_z^2$$

$$\boxed{Z'' + k_z^2 Z = 0}$$

$X'' + k_x^2 X = 0 \rightarrow$ ① $X = A\cos k_x x + B\sin k_x x$
$Y'' + k_y^2 Y = 0 \rightarrow$ ② $Y = C\cos k_y y + D\sin k_y y$
$Z'' + k_z^2 Z = 0 \rightarrow$ ③ $Z = E\cos k_z z + F\sin k_z z$

① $\Psi = 0$ inside box $0 \le x \le a$ $X(0) = X(a) = 0$
$A\cos(0) + B\sin(0) = A + B(0) = 0$
$\rightarrow A = 0$
$B\sin(k_x a) = 0$, $B > 0 \rightarrow \sin(k_x a) = 0$
$k_x a = p\pi$

$\boxed{k_x = \frac{p\pi}{a}}$ $\boxed{B\sin\left(\frac{p\pi}{a}x\right)}$

e-value e-function.

② $0 \le y \le b$ $Y(0) = Y(a) = 0$
$C(1) + D(0) = 0 \rightarrow C = 0$
$D\sin(k_y b) = 0 \rightarrow k_y b = q\pi$.

$\boxed{k_y = \frac{q\pi}{b}}$ $\boxed{D\sin\left(\frac{q\pi}{b}y\right)}$

e-value e-function

③ $0 \leq Z \leq c \quad Z(0) = Z(c) = 0$

$E(1) + F(0) = 0 \rightarrow E = 0$

$F\sin(k_z c) = 0 \rightarrow k_z c = r\pi$

e-value $\boxed{k_z = \frac{r\pi}{c}}$ $\boxed{F\sin\left(\frac{r\pi}{c}z\right)}$ e-function

$\psi(x,y,z) = X(x)Y(y)Z(z) = B\sin\left(\frac{p\pi}{a}x\right)D\sin\left(\frac{q\pi}{b}y\right)F\sin\left(\frac{r\pi}{c}z\right)$

normalise: $\langle \psi_{pqr} | \psi_{pqr} \rangle = 1 = \iiint A^2 |\psi_{pqr}|^2 \, dx\,dy\,dz$

$\psi^* = \psi$ here since ψ is real.

call BDF, constant A.

$$1 = \int_0^{z=c}\int_0^{y=b}\int_0^{x=a} A^2 \sin^2\left(\frac{p\pi x}{a}\right)\sin^2\left(\frac{q\pi y}{b}\right)\sin^2\left(\frac{r\pi z}{c}\right)dx\,dy\,dz$$

$$= A^2\int_0^a \sin^2\left(\frac{p\pi x}{a}\right)dx\int_0^b \sin^2\left(\frac{q\pi y}{b}\right)dy\int_0^c \sin^2\left(\frac{r\pi z}{c}\right)dz$$

$$= A^2\int_0^a \tfrac{1}{2}\left(1-\cos\left(\frac{2p\pi x}{a}\right)\right)dx\int_0^b \tfrac{1}{2}\left(1-\cos\left(\frac{2q\pi y}{b}\right)\right)dy\int_0^c \tfrac{1}{2}\left(1-\cos\left(\frac{2r\pi z}{c}\right)\right)dz$$

$$1 = A^2\left(\tfrac{1}{2}a \cdot \tfrac{1}{2}b \cdot \tfrac{1}{2}c\right)$$

$$A^2 = \frac{8}{abc}$$

$$A = \left(\frac{8}{abc}\right)^{1/2}$$

$$\psi_{pqr}(x,y,z) = \left(\frac{8}{abc}\right)^{1/2}\sin\left(\frac{p\pi x}{a}\right)\sin\left(\frac{q\pi y}{b}\right)\sin\left(\frac{r\pi z}{c}\right)$$

for $p, q, r = 1, 2, \ldots$

eigenvalues: $k_x^2 = \left(\frac{p\pi}{a}\right)^2$ $k_y^2 = \left(\frac{q\pi}{b}\right)^2$ $k_z^2 = \left(\frac{r\pi}{c}\right)^2$

recall: $$-k_z^2 = \frac{-2mE}{\hbar^2} + k_x^2 + k_y^2$$

$$\frac{2mE}{\hbar^2} = k_x^2 + k_y^2 + k_z^2$$

$$E = \frac{\hbar^2}{2m}\left(\left(\frac{p\pi}{a}\right)^2 + \left(\frac{q\pi}{b}\right)^2 + \left(\frac{r\pi}{c}\right)^2\right)$$

$$E_{pqr} = \frac{\hbar^2\pi^2}{2m}\left(\frac{p^2}{a^2} + \frac{q^2}{b^2} + \frac{r^2}{c^2}\right)$$

for $p, q, r = 1, 2, \ldots$

Q2 ground & first excited states of the Hydrogen atom:

$$\psi_{100}(r,\theta,\phi) = A\exp(-r/a)$$

$$\psi_{200}(r,\theta,\phi) = B(1-r/2a)\exp(-r/2a)$$

$a = 4\pi\varepsilon_0 \hbar^2/me^2$, A, B constants

(a) Find A & B for normalised ψ_{100} & ψ_{200}

$$1 = \iiint |\psi|^2 dV \qquad dV = r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$1 = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} A^2 e^{-\frac{2r}{a}} r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$1 = A^2 \int_0^{\infty} r^2 e^{-\frac{2r}{a}} \int_0^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\phi$$

$$1 = A^2\, 2\pi \underbrace{(-\cos\pi - \cos(0))}_{=2} \int_0^{\infty} r^2 e^{-\frac{2r}{a}} dr$$

$$1 = A^2\, 4\pi \int_0^{\infty} r^2 e^{-2r/a} dr$$

$$\Gamma(n+1) = \int_0^{\infty} e^{-x} x^n dx = n!$$

$x = \frac{2r}{a}$

$r = \frac{ax}{2}$

$n=2$

$\frac{dr}{dx} = a/2$

$dr = a/2\, dx$

$r^2 = \frac{a^2 x^2}{4}$

$$1 = A^2 4\pi \int_0^{\infty} e^{-x} x^2 \frac{a^2}{4} \cdot a/2\, dx$$

$$1 = A^2 \frac{a^3\pi}{2} \int_0^{\infty} e^{-x} x^2 dx = 2! = 2$$

$$1 = A^2 a^3 \pi$$

$$A = \frac{1}{\sqrt{a^3\pi}}$$

note $\int_0^{2\pi}\int_0^{\pi} \sin\theta \, d\theta \, d\phi = 4\pi$

Find B: $1 = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |B|^2 \left(1 - \frac{r}{2a}\right)^2 e^{-r/a} \, r^2 \sin\theta \, dr \, d\theta \, d\phi$

$$1 = B^2 4\pi \int_0^{\infty} \left(1 - \frac{r}{2a}\right)^2 e^{-r/a} \, r^2 \, dr$$

$$r^2\left(1 - \frac{r}{a}\right)^2 = r^2\left(1 - \frac{r}{2a}\right)\left(1 - \frac{r}{2a}\right)$$

$$= r^2\left(1 - \frac{r}{a} + \frac{r^2}{4a^2}\right)$$

$$= r^2 - \frac{r^3}{a} + \frac{r^4}{4a^2}$$

$$1 = B^2 4\pi \left[\int_0^{\infty} r^2 e^{-r/a} - \frac{r^3}{a} e^{-r/a} + \frac{r^4}{4a^2} e^{-r/a} \, dr\right]$$

$$= B^2 4\pi \left[\int_0^{\infty} r^2 e^{-r/a} \, dr - \frac{1}{a}\int_0^{\infty} r^3 e^{-r/a} \, dr + \frac{1}{4a^2}\int_0^{\infty} r^4 e^{-r/a} \, dr\right]$$

$$\Gamma(n+1) = \int_0^{\infty} e^{-x} x^n \, dx = n!$$

$$\frac{r}{a} = x \qquad \frac{dr}{dx} = a$$

$$r^2 = x^2 a^2 \qquad r = xa \qquad dr = a\,dx$$

$$1 = B^2 4\pi \left[\int_0^{\infty} e^{-x} x^2 a^2 a \, dx - \frac{1}{a}\int_0^{\infty} e^{-x} x^3 a^3 a \, dx + \frac{1}{4a^2}\int_0^{\infty} e^{-x} x^4 a^4 a \, dx\right]$$

$$1 = B^2 4\pi \left[a^3 2! - a^3 3! + \frac{1}{4a^2} \cdot a^5 \cdot 4!\right]$$

$$1 = B^2 4\pi \left[2a^3 - \cancel{6a^3} + \cancel{6a^3}\right]$$

$$1 = B^2 4\pi \, 2a^3$$

$$B^2 = \frac{1}{8\pi a^3} \qquad B = \frac{1}{\sqrt{8\pi a^3}}$$

orthogonality condition

(b) Check orthogonality $\boxed{\iiint \psi_{100}\psi_{200}\, dr\, d\theta\, d\phi = 0}$

$$\frac{1}{\sqrt{a^3\pi}}\cdot\frac{1}{\sqrt{8\pi a^3}}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} e^{-r/a}\cdot e^{-r/2a}\cdot\left(1-\frac{r}{2a}\right)\cdot \underset{\sin\theta}{r^2}\, dr\, d\theta\, d\phi$$

$$\frac{4\pi}{a^3\pi\sqrt{8}}\int_0^{\infty} e^{-r/a}\cdot e^{-r/2a}\cdot\left(1-r/2a\right) r^2\, dr$$

$$\frac{4}{\sqrt{8}}\cdot 1/a^3\int_0^{\infty} e^{-\frac{3r}{2a}}\cdot\left(r^2-\frac{r^3}{2a}\right) dr$$

$$4/\sqrt{8}\cdot 1/a^3\left(\int_0^{\infty} r^2 e^{-3r/2a} dr - \int_0^{\infty}\frac{r^3}{2a}e^{-3r/2a} dr\right)$$

$$4/\sqrt{8}\cdot 1/a^3\left(\int_0^{\infty} r^2 e^{-3r/2a} dr - \frac{1}{2a}\int_0^{\infty} r^3 e^{-3r/2a} dr\right)$$

$x = 3r/2a$

$r = \frac{2a}{3}x$ $\qquad \frac{dr}{dx} = 2a/3$

$r^2 = 4a^2/9\, x^2 \quad r^3 = 8/27\, a^3 x^3 \qquad dx\cdot 2a/3 = dr$

$$\left(\int_0^{\infty}\frac{4a^2}{9}x^2 e^{-x}\cdot\frac{2a}{3}dx - \frac{1}{2a}\int_0^{\infty}\frac{8}{27}a^3x^3e^{-x}\cdot\frac{2a}{3}dx\right)$$

$$\left(8/27\, a^3\int_0^{\infty}x^2e^{-x}dx - 1/2a\left(\frac{16}{81}a^4\right)\int_0^{\infty}x^3e^{-x}dx\right)$$

$$4/\sqrt{8}\cdot 1/a^3\left(8/27\, a^3\cdot 2! \quad - \quad \frac{8}{81}a^3\cdot 3!\right)$$

$$4/\sqrt{8}\cdot 1/a^3\left(16/27\, a^3 - 16/27\, a^3\right)$$

$= 0$

$\therefore$ the eigenstates are orthogonal

(c) $\langle r \rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{100}\, r\, \psi_{100}^{*}\, r^2 \sin\theta \, dr\, d\theta\, d\phi$

$$\langle r \rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \frac{1}{a^3\pi} e^{-2r/a} r^3 \sin\theta \, dr\, d\theta\, d\phi$$

$$\langle r \rangle = \frac{4\pi}{a^3\pi}\int_0^{\infty} e^{-2r/a} r^3 \, dr$$

$x = +\frac{2r}{a}$ $\quad \frac{dr}{dx} = \frac{a}{2}$ $\quad \langle r \rangle = \frac{4\cancel{\pi}}{a^3\cancel{\pi}}\int_0^{\infty} e^{-x} \frac{a^3}{8} x^3 \cdot \frac{a}{2} dx$

$r = \frac{a}{2}x$ $\quad dr = \frac{a}{2}dx$

$r^3 = \frac{a^3}{8}x^3$

$$\langle r \rangle = \frac{4}{a^3}\cdot\frac{a^4}{16}\int_0^{\infty} e^{-x} \cdot x^3$$

$$\langle r \rangle = \frac{a}{4}\cdot 3! = \frac{6}{4}a$$

$$\langle r \rangle = \frac{3}{2}a$$

$$\langle r^2 \rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{100}\, r^2\, \psi_{100}^{*}\, r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$= \frac{4\pi}{a^3\pi}\int_0^{\infty} e^{-2r/a} r^4 \, dr$$

$x = 2r/a$ $\quad r = a/2\, x$ $\quad r^4 = \frac{a^4}{16}x^4$ $\quad \langle r^2 \rangle = \frac{4}{a^3}\int_0^{\infty} e^{-x} \frac{a^4}{16} x^4 \cdot \frac{a}{2} dx$

$dr/dx = a/2$ $\quad dr = a/2\, dx$

$$\langle r^2 \rangle = \frac{4}{a^3}\frac{a^5}{32}\int_0^{\infty} e^{-x} x^4$$

$$\langle r^2 \rangle \frac{a^2}{8}\cdot 4! = 3a^2$$

$$\sigma_r^2 = \langle r^2 \rangle - \langle r \rangle^2 = 3a^2 - \frac{9}{4}a^2 = \frac{3}{4}$$

$$\sigma_r = \sqrt{\frac{3}{4}}a = \frac{\sqrt{3}}{2}a$$

$$\text{for } \psi_{200} \quad \langle r \rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{200}\, r\, \psi_{200}^{*}\, r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$\langle r \rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \frac{1}{8\pi a^3}\left(1-\frac{r}{2a}\right)^2 e^{-2r/2a}\, r^3 \sin\theta \, dr\, d\theta\, d\phi$$

$$\frac{4\pi}{8\pi a^3}\int_0^{\infty} r^3\left(1-\frac{r}{a}+\frac{r^2}{4a^2}\right) e^{-r/a}\, dr$$

$$\langle r \rangle = \frac{4\pi}{8\pi a^3} = \frac{1}{2a^3}\int_0^{\infty}\left(r^3-\frac{r^4}{a}+\frac{r^5}{4a^2}\right)e^{-r/a}\, dr$$

$$= \frac{1}{2a^3}\left[\int_0^{\infty} e^{-r/a} r^3\, dr - \frac{1}{a}\int_0^{\infty} e^{-r/a} r^4\, dr + \frac{1}{4a^2}\int_0^{\infty} e^{-r/a} r^5\, dr\right]$$

$$x = r/a \qquad r = ax$$

$$dr/dx = a \qquad dr = a\,dx$$

$$\langle r \rangle = \frac{1}{2a^3}\left[\int_0^{\infty} e^{-x} a^3x^3\, a\,dx - \frac{1}{a}\int_0^{\infty} e^{-x} a^4x^4\, a\,dx + \frac{1}{4a^2}\int_0^{\infty} e^{-x} a^5x^5\, a\,dx\right]$$

$$= \frac{1}{2a^3}\left[a^4\int_0^{\infty} e^{-x}x^3\,dx - \frac{1}{a}\cdot a^5\int_0^{\infty} e^{-x}x^4\,dx + \frac{a^6}{4a^2}\int_0^{\infty} e^{-x}x^5\,dX\right]$$

$$\frac{1}{2}\left[a\cdot 3! - a\cdot 4! + \frac{a}{4}\cdot 5!\right]$$

$$\langle r \rangle = \left[3a - 12a + 15a\right]$$

$$\langle r \rangle = 6a$$

$$\langle r^2\rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi_{200}\, r^2\, \psi_{200}^{*}\, r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$\langle r^2\rangle = \frac{4\pi}{8\pi a^3}\int_0^{\infty}(1-r/2a)^2\cdot r^4\cdot e^{-2r/2a}\,dr$$

$$\langle r^2\rangle = \frac{1}{2a^3}\int_0^{\infty} r^4\left(1-r/a+\frac{r^2}{4a^2}\right)e^{-r/a}\,dr$$

$$\langle r^2\rangle = 1/2a^3\left[\int_0^{\infty} e^{-r/a} r^4 dr - 1/a\int_0^{\infty} e^{-r/a} r^5 dr + 1/4a^2\int_0^{\infty} e^{-r/a} r^6 dr\right]$$

$x = r/a$

$r = ax$, $dr/dx = a$

$a\,dx = dr$

$$\langle r^2\rangle = 1/2a^3\left[\int_0^{\infty} e^{-x} a^4 x^4 a\,dx - 1/a\int_0^{\infty} e^{-x} a^5 x^5 a\,dx + 1/4a^2\int_0^{\infty} e^{-x} a^6 x^6 a\,dx\right]$$

$$\langle r^2\rangle = 1/2a^3\left[a^5\int_0^{\infty} e^{-x} x^4 dx - a^5\int_0^{\infty} e^{-x} x^5 dx + \frac{a^5}{4}\int_0^{\infty} e^{-x} x^6 dx\right]$$

$$\langle r^2\rangle = 1/2\left[a^2\cdot 4! - a^2\cdot 5! + \frac{a^2}{4}\cdot 6!\right]$$

$$\langle r^2\rangle = [12a^2 - 60a^2 + 90a^2]$$

$$\langle r^2\rangle = 42a^2$$

$$\sigma_r^2 = \langle r^2\rangle - \langle r\rangle^2 = 42a^2 - 36a^2$$

$$\sigma_r^2 = 6a^2$$

$$\sigma_r = \sqrt{6}a \simeq 2.45a$$

Q3 $\underline{r} = r\sin\theta\cos\phi\,\underline{\hat{i}} + r\sin\theta\sin\phi\,\underline{\hat{j}}$
$+ r\cos\theta\,\underline{\hat{k}}$

$$\underline{\hat{e}_r} = \frac{1}{|\partial_r \underline{r}|}\partial_r \underline{r}$$

$$\underline{\hat{e}_\theta} = \frac{1}{|\partial_\theta \underline{r}|}\partial_\theta \underline{r}$$

$$\underline{\hat{e}_\phi} = \frac{1}{|\partial_\phi \underline{r}|}\partial_\phi \underline{r}$$

(a) $\hat{e}_r$ $\frac{\partial \underline{r}}{\partial r} = \sin\theta\cos\phi\,\underline{\hat{i}} + \sin\theta\sin\phi\,\underline{\hat{j}}$
$+ \cos\theta\,\underline{\hat{k}}$

$$|\partial_r \underline{r}| = \left|\frac{\partial \underline{r}}{\partial r}\right| = \sqrt{(\sin\theta\cos\phi)^2 + (\sin\theta\sin\phi)^2 + (\cos\theta)^2}$$

$$= (\sin^2\theta\cos^2\phi + \sin^2\theta\sin^2\phi + \cos^2\theta)^{1/2}$$

$\div$ accross by $\sin^2\theta$

$$\left(\cos^2\phi + \sin^2\phi + \frac{\cos^2\theta}{\sin^2\theta}\right)^{1/2}$$

but $\cos^2\phi + \sin^2\phi = 1$

$$\left(1 + \frac{\cos^2\theta}{\sin^2\theta}\right)^{1/2}$$

multiply accross by $\sin^2\theta$ to undo division

$$= (\sin^2\theta + \cos^2\theta)^{1/2}$$

$|\partial_r \underline{r}| = (1)^{1/2} = 1$

so $\hat{e}_r = \frac{1}{|\partial_r \underline{r}|}\partial_r \underline{r} = \sin\theta\cos\phi\,\underline{\hat{i}} + \sin\theta\sin\phi\,\underline{\hat{j}}$
$+ \cos\theta\,\underline{\hat{k}}$

$$\underline{r} = r\sin\theta\cos\phi\,\hat{\underline{i}} + r\sin\theta\sin\phi\,\hat{\underline{j}} + r\cos\theta\,\hat{\underline{k}}$$

$$\hat{e}_\theta : \partial_\theta \underline{r} = \frac{\partial \underline{r}}{\partial\theta} = +r\cos\theta\cos\phi\,\hat{\underline{i}} + r\cos\theta\sin\phi\,\hat{\underline{j}}$$
$$- r\sin\theta\,\hat{\underline{k}}$$

$$|\partial_\theta \underline{r}| = \sqrt{(r\cos\theta\cos\phi)^2 + (r\cos\theta\sin\phi)^2 + (-r\sin\theta)^2}$$

$$= \left(r^2\cos^2\theta\cos^2\phi + r^2\cos^2\theta\sin^2\phi + (r^2\sin^2\theta)\right)^{1/2}$$

$$= \left(r^2 (\cos^2\theta\cos^2\phi + \cos^2\theta\sin^2\phi + \sin^2\theta\right)^{1/2}$$

$\div$ accross by $\cos^2\theta$ inside brackets

$$= \left(r^2\left(\cos^2\phi + \sin^2\phi + \frac{\sin^2\theta}{\cos^2\theta}\right)\right)^{1/2}$$

$$= \left(r^2\left(1 + \frac{\sin^2\theta}{\cos^2\theta}\right)\right)^{1/2} \times \cos^2\theta$$

$$= \left(r^2(\cos^2\theta + \sin^2\theta)\right)^{1/2}$$

$$|\partial_\theta \underline{r}| = (r^2 \cdot 1)^{1/2} = (r^2)^{1/2} = r$$

$$\hat{\underline{e}}_\theta = \frac{1}{r}\left[r\cos\theta\cos\phi\,\hat{\underline{i}} + r\cos\theta\sin\phi\,\hat{\underline{j}} - r\sin\theta\,\hat{\underline{k}}\right]$$

$$\hat{\underline{e}}_\theta = \cos\theta\cos\phi\,\hat{\underline{i}} + \cos\theta\sin\phi\,\hat{\underline{j}} - \sin\theta\,\hat{\underline{k}}$$

$$\hat{e}_\phi : \partial_\phi \underline{r} = -r\sin\theta\sin\phi\,\underline{\hat{i}} + r\sin\theta\cos\phi\,\underline{\hat{j}} + 0\underline{\hat{k}}$$

$$|\partial_\phi \underline{r}| = \left((-r\sin\theta\sin\phi)^2 + (r\sin\theta\cos\phi)^2\right)^{1/2}$$

$$= \left(r^2(\sin^2\theta\sin^2\phi + \sin^2\theta\cos^2\phi)\right)^{1/2}$$

$\div$ by $\sin^2\theta$ inside brackets

$$= \left(r^2(\sin^2\phi + \cos^2\phi)\right)^{1/2}$$

$$= \left(r^2(1)\right)^{1/2}$$

multiply inside by $\sin^2\theta$

$$= \left(r^2(\sin^2\theta)\right)^{1/2}$$

$$|\partial_\phi \underline{r}| = r\sin\theta$$

$$\underline{\hat{e}_\phi} = \frac{1}{r\sin\theta}\left(-r\sin\theta\sin\phi\,\hat{i} + r\sin\theta\cos\phi\,\hat{j}\right)$$

$$\underline{\hat{e}_\phi} = -\sin\phi\,\underline{\hat{i}} + \cos\phi\,\underline{\hat{j}}$$

(b) Show $\hat{\underline{e}}_r$, $\hat{\underline{e}}_\theta$ and $\hat{\underline{e}}_\phi$ are mutually orthogonal

orthogonality condition: if two vectors a, b are orthogonal then $a \cdot b = 0$

- $\hat{\underline{e}}_r \cdot \hat{\underline{e}}_\theta = \sin\theta\cos\phi \cdot \cos\theta\cos\phi + \sin\theta\sin\phi \cdot \cos\theta\sin\phi + \cos\theta \cdot -\sin\theta$

$= \sin\theta\cos\theta \cdot \cos^2\phi + \sin\theta\cos\theta \cdot \sin^2\phi - \sin\theta\cos\theta$

$= \sin\theta\cos\theta\left((\cos^2\phi + \sin^2\phi\right) - \sin\theta\cos\theta$

$= \sin\theta\cos\theta(1) - \sin\theta\cos\theta = 0$

$\therefore$ $\hat{\underline{e}}_r$ & $\hat{\underline{e}}_\theta$ are orthogonal

- $\hat{\underline{e}}_r \cdot \hat{\underline{e}}_\phi = \sin\theta\cos\phi \cdot -\sin\phi + \sin\theta\sin\phi \cdot \cos\phi + \cos\theta \cdot 0$

$= \sin\theta(-\sin\phi\cos\phi + \sin\phi\cos\phi)$

$\hat{\underline{e}}_r \cdot \hat{\underline{e}}_\phi = \sin\theta(0) = 0$

$\therefore$ $\hat{\underline{e}}_r$ & $\hat{\underline{e}}_\phi$ are orthogonal

- $\hat{\underline{e}}_\theta \cdot \hat{\underline{e}}_\phi = \cos\theta\cos\phi \cdot -\sin\phi + \cos\theta\sin\phi \cdot \cos\phi - \sin\theta \cdot 0$

$= \cos\theta(-\sin\phi\cos\phi + \sin\phi\cos\phi)$

$\hat{\underline{e}}_\theta \cdot \hat{\underline{e}}_\phi = \cos\theta(0) = 0$

$\therefore$ $\hat{\underline{e}}_\theta$ & $\hat{e}_\phi$ are orthogonal recall $\hat{i} \times \hat{j} = \hat{k}$

$\hat{j} \times \hat{k} = \hat{i}$

$\hat{k} \times \hat{i} = \hat{j}$

$$\begin{tikzcd} & \hat{i} \arrow[dr] & \\ \hat{k} \arrow[ur] & & \hat{j} \arrow[ll] \end{tikzcd}$$

$$\underline{\hat{e}}_r \times \underline{\hat{e}}_\theta = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \underline{\hat{e}_{r1}} & \underline{\hat{e}_{r2}} & \underline{\hat{e}_{r3}} \\ \underline{e_{\theta 1}} & \underline{e_{\theta 2}} & \underline{e_{\theta 3}} \end{vmatrix} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \end{vmatrix}$$

$$= (-\sin^2\theta\sin\phi - \cos^2\theta\sin\phi)\hat{i}$$
$$- (-\sin^2\theta\cos\phi - \cos^2\theta\cos\phi)\hat{j}$$
$$+ (\underbrace{\sin\theta\cos\theta\cos\phi\sin\phi - \sin\theta\cos\theta\cos\phi\sin\phi}_{=0})\underline{\hat{k}}$$

$$= (-\sin^2\theta\sin\phi - \cos^2\theta\sin\phi)\underline{\hat{i}}$$
$$+ (\sin^2\theta\cos\phi + \cos^2\theta\cos\phi)\underline{\hat{j}}$$
$$= -\sin\phi(+\sin^2\theta + \cos^2\theta)\underline{\hat{i}} + \cos\phi(\sin^2\theta + \cos^2\theta)\underline{\hat{j}}$$
$$= -\sin\phi\,\underline{\hat{i}} + \cos\phi\,\underline{\hat{j}} = \underline{\hat{e}}_\phi$$
$$\therefore \underline{\hat{e}}_r \times \underline{\hat{e}}_\theta = \hat{e}_\phi$$

$$\hat{e}_\theta \times \hat{e}_\phi = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \end{vmatrix}$$

$$= (0 + \sin\theta\cos\phi)\hat{i}$$
$$- (0 - \sin\theta\sin\phi)\hat{j}$$
$$+ (\cos^2\phi\cos\theta + \sin^2\phi\cos\theta)\underline{\hat{k}}$$

$$= \sin\theta\cos\phi\,\hat{i} + \sin\theta\cos\phi\,\underline{\hat{j}} + \cos\theta(\cos^2\phi + \sin^2\phi)\underline{\hat{k}}$$
$$= \sin\theta\cos\phi\,\hat{i} + \sin\theta\cos\phi\,\underline{\hat{j}} + \cos\theta\,\hat{k}$$
$$= \underline{\hat{e}}_r$$

$$\therefore \underline{\hat{e}}_\theta \times \underline{\hat{e}}_\phi = \underline{\hat{e}}_r$$

$$\underline{\hat{e}}_\phi \times \underline{\hat{e}}_r = \begin{vmatrix} \hat{\imath} & \hat{\jmath} & \hat{k} \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{vmatrix}$$

$$= (\cos\theta\cos\phi - 0)\hat{\imath}$$
$$- (-\cos\theta\sin\phi - 0)\hat{\jmath}$$
$$+ (-\sin^2\phi \cdot \sin\theta - \cos^2\phi \cdot \sin\theta)$$

$$= \cos\theta\cos\phi\,\hat{\imath} + \cos\theta\sin\phi\,\hat{\jmath} - \sin\theta(\cos^2\phi + \sin^2\phi)\hat{k}$$
$$= \cos\theta\cos\phi\,\underline{\hat{\imath}} + \cos\theta\sin\phi\,\underline{\hat{\jmath}} - \sin\theta\,\underline{\hat{k}}$$
$$= \hat{e}_\theta$$

$$\therefore \underline{\hat{e}}_\phi \times \underline{\hat{e}}_r = \underline{\hat{e}}_\theta$$

(c) $\underline{p} = p_r \underline{\hat{e}_r} + p_\theta \underline{\hat{e}_\theta} + p_\phi \hat{e}_\phi$

$\underline{r} = r\sin\theta\cos\phi\,\underline{\hat{i}} + r\sin\theta\sin\phi\,\underline{\hat{j}} + r\cos\theta\,\underline{\hat{k}}$

$\underline{r} = r\underline{\hat{e}}_r$

$\underline{L} = \underline{r} \times \underline{p}$

$\underline{L} = (r\underline{\hat{e}}_r \times p_r \underline{\hat{e}}_r) + (r\underline{\hat{e}}_r \times p_\theta \underline{\hat{e}_\theta})$
$+ (r\underline{\hat{e}}_r \times p_\phi \underline{\hat{e}}_\phi)$

Recall $\underline{\hat{e}}_r \times \underline{\hat{e}}_\theta = \underline{\hat{e}}_\phi$

$\underline{\hat{e}}_\phi \times \underline{\hat{e}}_r = \underline{\hat{e}}_\theta \rightarrow \underline{\hat{e}}_r \times \underline{\hat{e}}_\phi = -\hat{e}_\theta$

$\underline{\hat{e}}_r \times \underline{\hat{e}}_r = 0$

$\underline{L} = rp_r(\underline{\hat{e}_r} \times \underline{\hat{e}_r}) + rp_\theta(\underline{\hat{e}_r} \times \underline{\hat{e}_\theta})$
$+ rp_\phi(\underline{\hat{e}}_r \times \underline{\hat{e}}_\phi)$

$\underline{L} = rp_\theta \underline{\hat{e}}_\phi - rp_\phi \underline{\hat{e}_\theta}$

$|L|^2 = L \cdot L = (rp_\theta \hat{e}_\phi) \cdot (rp_\theta \hat{e}_\phi) + (-rp_\phi \underline{\hat{e}_\theta}) \cdot (-rp_\phi \underline{\hat{e}}_\theta)$

$= r^2 p_\theta^2 (1) + r^2 p_\phi (1)$

Since $\underline{\hat{e}_\phi} \cdot \underline{\hat{e}_\phi} = \underline{\hat{e}_\theta} \cdot \underline{\hat{e}_\theta} = 1$

$L^2 = r^2(p_\theta^2 + p_\phi^2)$

(d) $H = \frac{p^2}{2m} + V(r)$

$$\underline{p} = p_r \hat{\underline{e}}_r + p_\theta \hat{\underline{e}}_\theta + p_\phi \hat{\underline{e}}_\phi$$

$$p^2 = \underline{p} \cdot \underline{p} = p_r^2 + p_\theta^2 + p_\phi^2$$

$$H = \frac{p_r^2 + p_\theta^2 + p_\phi^2}{2m} + V(r)$$

$$V_{eff}(r) = V(r) + \frac{L^2}{2mr^2}$$

$$= V(r) + \frac{r^2(p_\theta^2 + p_\phi^2)}{2mr^2}$$

$$= V(r) + \frac{p_\theta^2 + p_\phi^2}{2m}$$

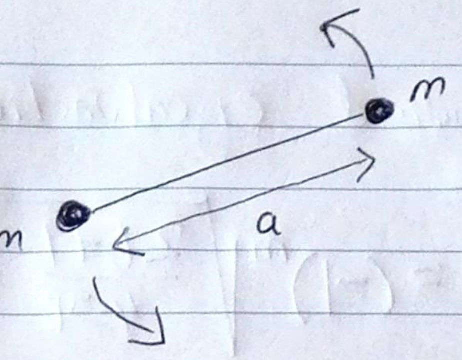
$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2 + p_\phi^2}{2m} + V(r)$$

so that the Hamiltonian can be expressed as:

$$H = \frac{p_r^2}{2m} + V_{eff}(r)$$

$$V_{eff}(r) = \frac{p_\theta^2 + p_\phi^2}{2m} + V(r)$$

Q4 (a)



$$L = I\omega$$

$$I = m\left(\frac{a}{2}\right)^2 + m\left(\frac{a}{2}\right)^2$$

$$= m\frac{a^2}{4} + m\frac{a^2}{4}$$

$$= \frac{ma^2}{2}$$

$$L = \frac{ma^2}{2}\omega \qquad \omega = \frac{2L}{ma^2}$$

$$E = \frac{1}{2} I \omega^2 = \frac{1}{2} \cdot \frac{ma^2}{2} \cdot \left(\frac{2L}{ma^2}\right)^2$$

$$E = \frac{1}{2} \cdot \frac{ma^2}{2} \cdot \frac{4L^2}{m^2a^4}$$

$$E = \frac{ma^2}{4} \cdot \frac{4L^2}{m^2a^4}$$

$$E = \frac{L^2}{ma^2}$$

(b) recall $L^2 f = \hbar^2 l(l+1) f$

$$\rightarrow L^2 = \hbar^2 l(l+1)$$

$\therefore$ Energy Eigenvalues are given by

$$E_l = \frac{\hbar^2 l(l+1)}{ma^2}$$

for $l = 0, 1, 2, \ldots$

(c) The normalised eigenfunctions of the system are

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

(d) Since Energy E_l only depends on l, degeneracy occurs in this system for different values of m for the same value of l

We find there are $2l+1$ degenerate states in the system as the Energy depends on l and for each choice in l there are $2l+1$ possible choices in m (i.e. $l=1$, $m=-1,0,1$) and thus the system has $2l+1$ degenerate states.