Chap 6

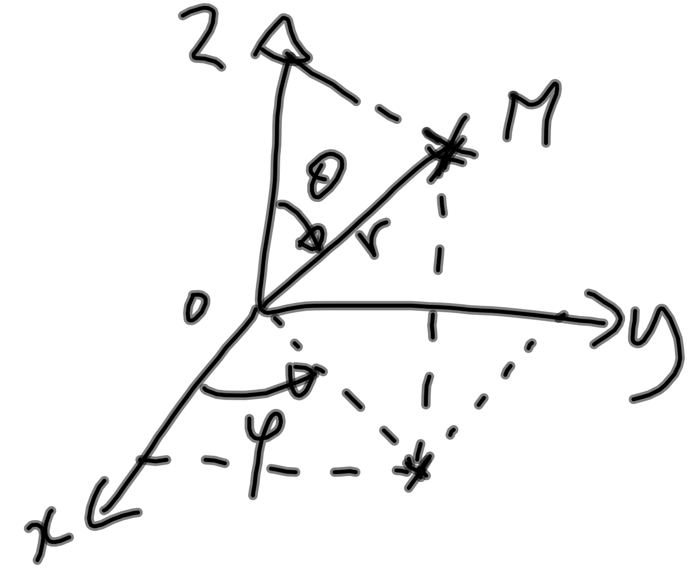
HYDROGEN ATOM

The potential is:

$$V(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$$

The S eq can be written as:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi + \left(-\frac{e^2}{4\pi\varepsilon r}\right)\Psi = E\Psi$$



cartesian coord. (x, y, z)

Spherical coord (r, θ, φ)

$$\Psi(x, y, z) \to \Psi(r, \theta, \varphi)$$

we have:

$$\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$$

we assume that

$$\Psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi)$$

R: Rarial function

Y: Angular function

Solving the S eq, we find:

$$R(r) = R_{nl}(r) = C_{nl} F_{nl}\left(\frac{2r}{n a_0}\right)$$

a_0: is the Bohr radius

n: principal quantum number

The constant C_{nl} is:

$$C_{nl} = \frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[a_0(n+l)!]^3}}$$

ℓ is the secondary quantum number
(ℓ takes n values)
$\ell = 0, 1, 2, \dots n-1$

and

$$F_{n\ell}(x) = x^{\ell} e^{-\frac{x}{2}} L^{2\ell+1}_{n-\ell-1}(x)$$

where:

$$L^{k}_{p}(x) = (-1)^{k} \frac{d^{k}}{dx^{k}} L^{0}_{k+p}(x)$$

= Associate polynomials of Laguerre.

and

$$L^{0}_{p}(x) = L_{p}(x) \cdot e^{x} \frac{d^{p}}{dx^{p}} \left(e^{-x} x^{p}\right)$$

is the Laguerre polyn.

$\cancel{R_{1210} \neq R_{1210}}$!!
$\cancel{n=121, \ell=0 \quad n=12, \ell=10}$

So we use for
$\ell = 0, 1, 2, 3, 4, \dots$
state s, p, d, f, g, h ...

Ex $R_{2s}(x)$; $R_{3p}(x)$

we have for example:

$$R_{2s}(r) = \frac{1}{\sqrt{2a_0^3}}\left(1 - \frac{r}{2a_0}\right) e^{-\frac{r}{2a_0}}$$

and

$$R_{2p}(r) = \frac{1}{\sqrt{24a_0^3}} \frac{r}{a_0} e^{-\frac{r}{2a_0}}$$

$\overline{\text{Expectation}}$ values of r^s:

$$\langle r^s \rangle = \int_0^\infty R_{nl}^2(r)\, r^{s+2}\, dr$$

There are two recurrence formula

$$\langle r^{-(p+2)} \rangle = \left\langle \frac{1}{r^{p+2}} \right\rangle = \left(\frac{2}{n a_0} \right)^{2p+1} \frac{(2l-p)!}{(2l+p+1)!} \langle r^{p-1} \rangle$$

for $l \geq \frac{p}{2}$

$$\frac{p+1}{n^2} \langle r^p \rangle - (2p+1) a_0 \langle r^{p-1} \rangle + \frac{p}{4} a_0^2 \left[(2l+1)^2 - p^2 \right] \langle p^{p-2} \rangle = 0$$

for $p + 2l + 1 > 0$

chap 7

ANGULAR MOMENTUM

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$$\vec{L} = \vec{r} \times \vec{p}, \text{ where}$$

$$\vec{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \text{ and } \vec{p} = \frac{\hbar}{i}\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}$$

So:

$$L_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$L_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

using the spherical coordinates:

$$L_x = \frac{\hbar}{i}\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)$$

$$L_y = \frac{\hbar}{i}\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)$$

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

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

The action on ψ is:

$$L^2|\psi\rangle = \ell(\ell+1)\hbar^2|\psi\rangle$$

$$L_z|\psi\rangle = m\hbar|\psi\rangle$$

ℓ · ndary q.n.

m gnetic q.n.

$\ell = 0, 1, 2, \dots n-1$ (n values)

$m = -\ell, \dots -1, 0, 1, \dots +\ell$ (2ℓ+1 values)

$-\ell \leq m \leq \ell$

or

$$L^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle$$

$$L_z|\ell,m\rangle = m\hbar|\ell,m\rangle$$

or

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

$$L_z Y_{\ell,m}(\theta,\varphi) = m\hbar Y_{\ell,m}(\theta,\varphi)$$

Ex:
Show that:

$$[L_x, L_y] = i\hbar L_z$$