LECTURE 15/36 OCT-9-02

PARTICLE IN A BOX

HYDROGEN ATOM

ORBITAL

MULTI ELECTRON ATOMS

BACKGROUND: OXTOBY CH 15

READ: TODAY'S LEC GRAY CH1 p21-28

NEXT LEC GRAY CH2 p42-56

PS #4 PROBLEM 9

DUE OCTOBER 18

$$V(x) = \begin{cases} 0 & \text{IF } 0 < x < L \\ \infty & \text{IF } x \leq 0 \\ & \phantom{\text{IF }} x \geq L \end{cases}$$

$$\hat{H}\Psi = E\Psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi$$

$$\frac{d^2\Psi}{dx^2} = -\frac{2mE}{\hbar^2}\Psi \equiv -k^2\Psi$$

<u>KNOWN SOLUTION</u> FROM THE CLASSICAL WAVE EQ.

$$\Psi(x) = A\sin(kx) + B\cos(kx)$$

WE WANT THE electron IN THE BOX

$\Rightarrow \quad \Psi(0) = \Psi(L) = 0$

$$0 = \Psi(0) = A\sin(0) + B\cos(0)$$

$$0 = B$$

$$\Psi(L) = 0 = A\sin(kL)$$

$\Rightarrow \quad kL = n\pi \qquad n = 1, 2, 3, \ldots$

$$k = \frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi(x) = A \sin\left(\frac{n\pi}{L} x\right)$$

RECALL

$$1 = \int_0^L A^2 \sin\left(\frac{n\pi}{L}x\right)^2 dx$$

$$1 = A^2 \int_0^L \sin\left(\frac{n\pi}{L}x\right)^2 dx$$

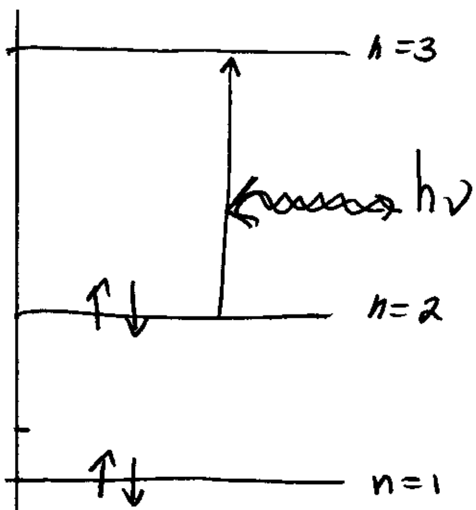
$$= A^2 \frac{L}{2}$$

$$\Rightarrow \quad A = \sqrt{\frac{2}{L}}$$

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$$

$$\boxed{E_n = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2} n^2} \boxed{= \frac{h^2}{8mL^2} n^2}$$

FOR BUTADINE WE HAVE 4 π-e



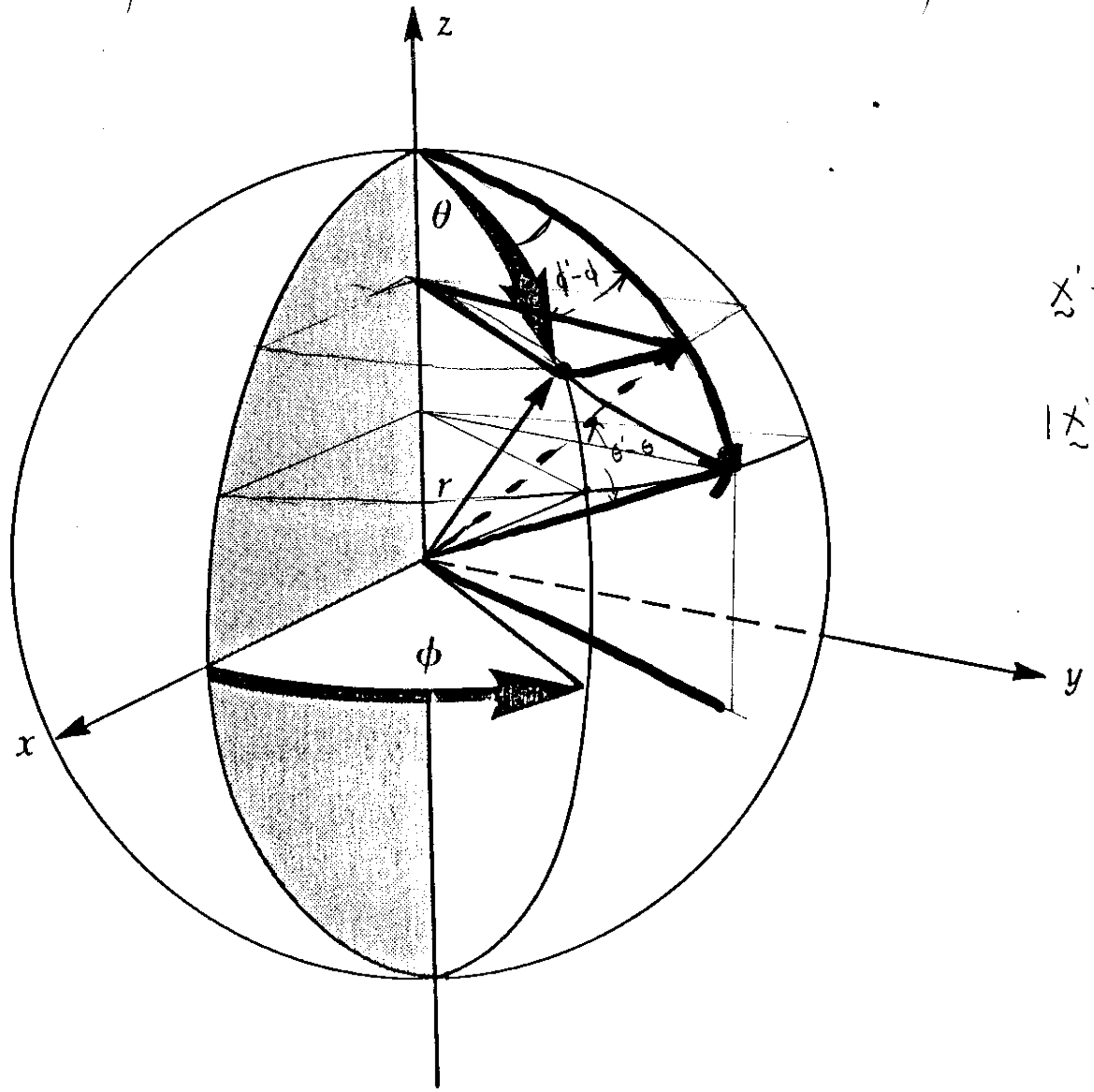
FIRS EXCITATION

$n=2 \longrightarrow n=3$

$$\Delta E = E_3 - E_2 = \frac{h^2}{8mL}\left(3^2-2^2\right) = \frac{h^2 5}{8mL}$$

$$\Delta E = 9.02 \times 10^{-19}\,J = h\nu \frac{\lambda}{\lambda} = \frac{hc}{\lambda}$$

$$\frac{1}{\lambda} \equiv \bar{\nu} = \frac{\Delta E}{hc} = 4.54 \times 10^{4}\,cm^{-1}$$



$$\underset{\sim}{x}' - \underset{\sim}{x} = r \sin\theta (\varphi' - \varphi)\, \hat{\varphi} + r(\theta' - \theta)\, \hat{\theta}$$

$$|\underset{\sim}{x}' - \underset{\sim}{x}| = r\gamma$$

$$= r \cos^{-1}\left\{ \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\varphi' - \varphi) \right\}$$

$\varphi' = 0$, $\theta = 0$ || $\varphi' = \pi/2$, $\theta = \pi/2$

FIGURE 5.26 Relation between rectilinear (or cartesian) coordinates (x, y, z) and spherical polar coordinates (r, θ, ϕ). Here r is the radius, θ the polar angle or colatitude, and ϕ the azimuthal angle or longitude. The trigonometric relations between the two sets of coordinates are: $x = r \sin \theta \cos \phi$, $y = r \sin \theta \sin \phi$, $z = r \cos \theta$, and $r^2 = x^2 + y^2 + z^2$. In the application to the hydrogen atom, the nucleus is at the origin ($r = 0$) and the electron at the surface of a sphere of radius r.

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HYDROGEN ATOM

FOR THE HYDROGEN-LIKE ATOMS, WE CONSIDER A NUCLEUS WITH CHARGE $+Z|e|$ AND AN ELECTRON ORBITING AROUND. THE POTENTIAL ENERGY FOR THIS SYSTEM IS

$$V(r) = -\frac{Z|e|^2}{4\pi\epsilon_0 r}.$$

ONCE WE KNOW THE POTENTIAL ENERGY, WE CAN WRITE THE SCHRÖDINGER EQ.

$$\hat{H}\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Z|e|^2}{4\pi\epsilon_0 r}\right]\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

WHERE

$$\mu = \frac{m_e m_N}{m_e + m_N} = \text{REDUCED MASS}$$

THE SOLUTION OF THE SCHRÖDINGER EQ IS THE PRODUCT OF TWO FUNCTIONS AND HAS 3 QUATUM NUMBERS, n, l, AND m.

$$\psi \longrightarrow \psi_{n,l,m}(r,\theta,\varphi) = R_{n,l}(r)\, Y_l^m(\theta,\varphi)$$

$n = 1, 2, 3, \ldots$ PRINCIPAL QUANTUM NUMBER

$l = 0, 1, 2, 3, \ldots, n-1$ AZIMUTHAL QUANTUM NUMBER

$m = 0, \pm 1, \pm 2, \ldots \pm l$ MAGNETIC QUANTUM NUMBER

THE ENERGY IS QUANTIZED AND GIVEN BY

$$E_n = -\frac{\mu Z^2 |e|^4}{8 \epsilon_0^2 h^2} \frac{1}{n^2}$$

ENERGY ONLY DEPENDS ON n !

FOR A GIVEN n WE HAVE THE SAME ENERGY FOR DIFFERENT l AND m.

$n=3$ $l=0,\ m=0$ (9)
$l=1 \quad m=-1,\ 0,\ +1$
$l=2 \quad m=-2,\ -1,\ 0,\ +1,\ +2$

$n=2$ $l=0,\ m=0$ (4)
$l=1,\ m=-1,\ 0,\ +1$

$n=1$ (1)

NUMBER OF WAVE FUNCTIONS

$E_1 \longrightarrow \psi_{1,0,0}$

$E_2 \longrightarrow \psi_{2,0,0}\ \psi_{2,1,-1}\ \psi_{2,1,0}\ \psi_{2,1,1}$

$E_3 \longrightarrow \psi_{3,0,0}\ \psi_{3,1,-1}\ \psi_{3,1,0}\ \psi_{3,1,1}\ \psi_{3,2,-2}\ \psi_{3,2,-1}\ \psi_{3,2,0}\ \psi_{3,2,1}\ \psi_{3,2,2}$