LECTURE # 3

Note Title 9/5/2007

$\boxed{\text{MON SEPT } 10^{th} \text{ NO CLASS}}$

Makeup → NOV 9 FRI 1:40 – 2:55 (NOV 14 II MIDTERM) ←

HW 1

Hydrogen $\boxed{\text{Scaling}}$

$$a_B = \frac{\hbar^2}{\mu e^2} = .5\,\text{Å} \quad (\text{define size } H)$$

$$Ry = \frac{e^2}{2a_B} = \frac{\mu e^4}{2\hbar^2} \nearrow 13.6\ eV \quad (\text{Binding E of H ground state})$$

$$\text{Hartree} = 2\,Ry$$

excitons, donor, ... hydrogenic systems

Rescale μ and e^2 EXCITON.

Separation of variables

3D

$$\left(-\frac{\hbar^2}{2\mu}\vec{\nabla}_r^2 - \frac{e^2}{r}\right)\psi(\vec{r}) = E\,\psi(\vec{r})$$

Make ANSATZ $\psi(\vec{r}) = \boxed{R(r)\,Y(\theta,\phi)}$

$$\vec{\nabla}_r^2 = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\hat{\ell}^2}{r^2}$$

$$V(r) = -\frac{e^2}{r}$$

$$\hat{\ell}^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin\theta^2}\frac{\partial^2}{\partial\phi^2}$$

$$\left[\underbrace{\boxed{-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right.} + \frac{\hat{\ell}^2}{r^2}\Bigg)}_{Y \text{ pass through}} + \overbrace{V(r)}^{R \text{ pass through}}\right] R(r)\,Y(\theta,\phi) = E\,R(r)\,Y(\theta,\phi)$$

Divide by $R(r)\,Y(\theta,\phi)$ Multiply by $-\frac{2\mu r^2}{\hbar^2}$

$$\underbrace{\boxed{\frac{1}{R}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R - \frac{2\mu r^2}{\hbar^2}\left(V(r)-E\right)}}_{F(r)} + \underbrace{\boxed{\frac{1}{Y(\theta,\phi)}\hat{\ell}^2\,Y(\theta,\phi)}}_{G(\theta,\phi)} = 0$$

$$F(r) + G(\theta,\phi) = 0$$

$$\frac{1}{R(r)\cancel{Y(\theta,\phi)}}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R(r)\cancel{Y(\theta,\phi)} = \frac{1}{\cancel{R(r)}\cancel{Y(\theta,\phi)}}E\,\cancel{R(r)}\cancel{Y(\theta,\phi)}$$

$\forall r$
$\forall \theta$
$\forall \phi$

$$f(x) + g(y) = 0$$

$$\left.\begin{aligned} G(\theta,\phi) &= \text{CONSTANT} = c \\ F(r) &= -\text{CONSTANT} \end{aligned}\right\}$$

No other solutions !

Eq. *

$$\boxed{\hat{\ell}^2 Y(\theta,\phi) = c\, Y(\theta,\phi)}$$

We know how to solve

$\hat{\ell}$ = total angular momentum

$$\hat{\ell} = r \times \hat{p} = \hat{r} \times -i\hbar \vec{\nabla}_r$$

$$\hat{\ell}^2 = \hat{\ell} \cdot \hat{\ell}$$

$Y(\theta, \phi)$ are Spherical Harmonics (Eigenstates)

c <u>has</u> to be $l(l+1)$ $\quad l = 0, 1, 2, 3$

$c = 0 \quad 2 \quad 6 \ldots$ ONLY Possible

values of c for which $\exists$ solution

of Eq. $*$

$\downarrow$

$F(r) = 0$

$$\boxed{\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}R - \frac{e^2}{r} + \frac{\overset{c}{\downarrow}}{} \frac{l(l+1)}{r^2}\right]R(r) = E\,R(r)}$$

Make substitutions

$$R(r) = r^{l} e^{-r/2} w(r)$$

Eq. for $w(r)$ that is solvable $\boxed{\text{Solutions Known}}$

$$w(r) = L^{2l+1}_{n+l}(r) \rightarrow \text{Laguerre polinomials}$$

Only meaningful solutions for $w(r)$ are those in which

$$\boxed{n - l \quad \text{INTEGER} > 1}$$ Otherwise it diverges

$$\boxed{E = -\frac{1}{n^2} Ry}$$

$\boxed{E = -\frac{1}{n^2} Ry}$; n - ℓ integer > 1

n: principal quantum number

ℓ: angular momentum

$\rightarrow n = 1$ $\quad \boxed{\ell = 0} \rightarrow$ s orbitals

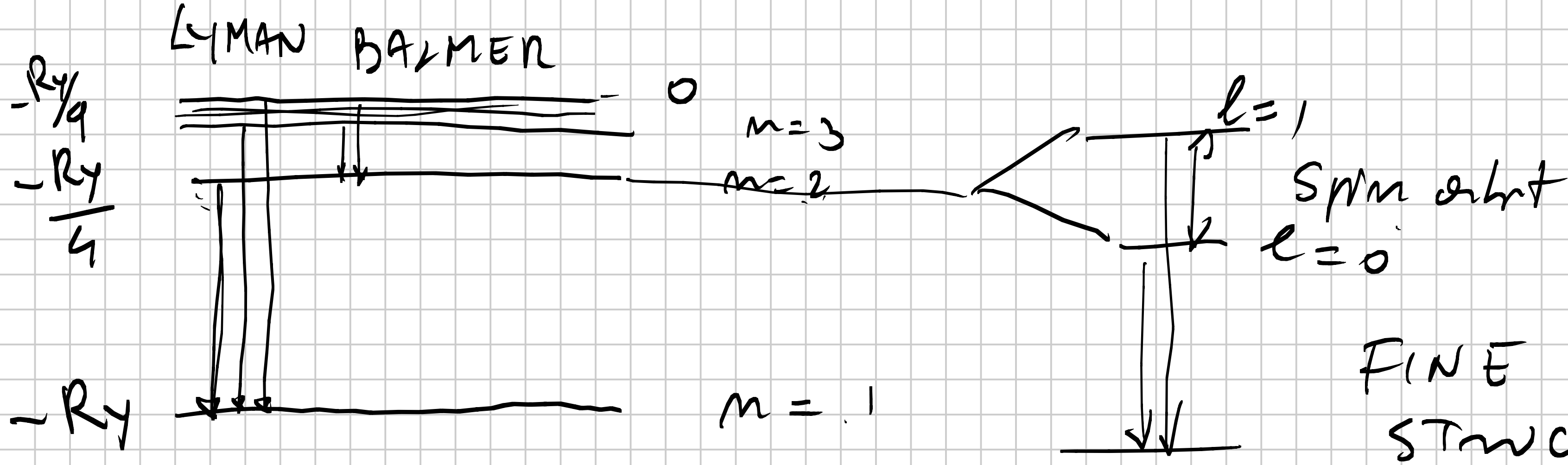
$n = 2$ $\quad \ell = 0 \quad \boxed{\ell = 1} \rightarrow$ p orbital

$n = 3$ $\quad \ell = 0, \ \ell = 1, \ \ell = 2 \rightarrow$ d orbital

f

g

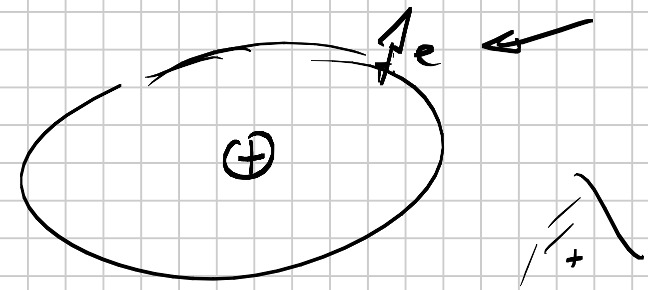
h



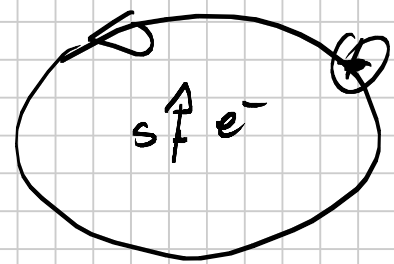
FINE STRUCTURE

- RELATIVISTIC EFFECTS DUE TO SPIN ELECTRON

→ Spin-Orbit effects



From e^- frame



current due to proton

$s \cdot \underline{\underline{B}}_{eff}$

$I \sim \vec{L}$

$$\boxed{H_{SO} = \alpha \vec{S} \cdot \vec{e}}$$

Eliminate p-degeneracy → Fine-structure of atom

SPIN e spin p

Hyperfine coupling.

$H = \alpha \vec{S}_e \cdot \vec{S}_p$ → Hyperfine-structure much smaller