Hydrogenlike Atoms

$$\Psi_{n\ell m}(r,\theta,\varphi) = R_{n\ell}(r)\, Y_\ell^m(\theta,\varphi)$$

$$Y_\ell^m(\theta,\varphi) = (-1)^m \sqrt{\frac{(2\ell+1)(\ell-|m|)!}{4\pi(\ell+|m|)!}}\; P_\ell^{|m|}(\cos\theta)\, e^{im\varphi}$$

$$\int_0^{2\pi}\int_0^{\pi} Y_{\ell'}^{m'*}(\theta,\varphi)\, Y_\ell^m(\theta,\varphi)\sin\theta\, d\theta\, d\varphi = \delta_{\ell,\ell'}\,\delta_{m,m'}$$

FOR A GIVEN $n \rightarrow \ell = 0, 1, 2, \ldots, n-1$ AND $m = 0, \pm 1, \ldots, \pm \ell$

(Arfken)

$$R_{n\ell}(r) = \sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]}}\;(\alpha r)^\ell e^{-\alpha r/2}\, L_{n-\ell-1}^{2\ell+1}(\alpha r)$$

$$\alpha = \frac{2Z}{na_0}$$

$$\int_0^\infty e^{-x} x^k L_n^k(x)\, L_m^k(x)\, dx = \frac{(n+k)!}{n!}\,\delta_{m,n}$$

$$\int_0^\infty e^{-x} x^{k+1} L_n^k(x)\, L_n^k(x) = \frac{(n+k)!}{n!}(2n+k+1)$$

$$E_n = -\frac{\mu Z^2 |e|^4}{8\epsilon_0^2 h^2}\frac{1}{n^2} \qquad n = 1, 2, 3, \ldots$$

$m = 0, \pm 1, \pm 2, \ldots \pm J$

ANGULAR PART

$Y_J^m(\theta, \varphi)$

$J =$	0	1	2	3	4	5
	s	p	d	f	g	h

GROUND STATE

$n = 1$

$l = 0$

$m = 0$

$$\Psi_{1,0,0}(r, \theta, \varphi) = R_{1,0}(r)\, Y_0^0(\theta, \varphi)$$

$$\Psi_{1,0,0}(r, \theta, \varphi) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a}\right)^{3/2} e^{-\frac{Zr}{a}}$$

$\cancel{a = \frac{\mu}{m_e} a_0}$

$$E_1 = -\frac{\mu}{m_e} Z^2\, 13.6\, eV$$

$$a = \frac{m_e}{\mu} a_0$$

$$\text{PROB}\{\underset{\sim}{r},\ \underset{\sim}{r}+d\underset{\sim}{r}\} = \underbrace{|\Psi_{1,0,0}(r,\theta,\varphi)|^2}_{\text{PROBABILITY DENSITY}}\, d\underset{\sim}{r}$$

$$d\underset{\sim}{r} \equiv dV = r^2 \sin(\theta)\, dr\, d\theta\, d\varphi$$

INTEGRATE OVER φ AND θ

$$P_{1s}(r) = 4\left(\frac{Z}{a}\right)^3 e^{-\frac{2Zr}{a}}\, \underline{\underline{r^2}}$$

RADIAL DISTRIBUTION FUNCTION

$$\langle r\rangle = \langle 1s|r|1s\rangle = \int_0^\infty r\, P_{1s}(r)\, dr$$

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

MAX OF $P_{1s}(r)$ is $\frac{a}{Z}$

$$\boxed{r_0 = \frac{a}{Z} = \frac{1}{Z}\frac{m_e}{\mu}a_0} \qquad \mu = \frac{Zm_p\, m_e}{Zm_p + m_e}$$

HYDROGEN $r_0 = 1.00055\, a_0$

$$a_0 = 52.9 \text{ pm}$$

$$r_0 \sim \frac{a_0}{Z}$$

$$\left.\frac{dP_{1s}}{dr}\right|_{r_{max}} = 0$$

$$\frac{dP_{1s}}{dr} = 4\left(\frac{Z}{a}\right)^3 \left\{ 2r - r^2 \frac{2Z}{a} \right\} e^{-\frac{2Zr}{a}}$$

$$= 4\left(\frac{Z}{a}\right)^3 \left\{ 1 - \frac{Zr}{a} \right\} 2r\, e^{-\frac{2Zr}{a}}$$

$$\frac{Z r_{max}}{a} = 1$$

$$r_{max} = \frac{a}{Z} \equiv r_0$$

$$\Psi_{2,0,0}(r,\theta,\varphi) \equiv \Psi_{2s}(r)$$

$$= \frac{1}{\sqrt{32\pi r_0^3}}\left[2 - \frac{r}{r_0}\right] e^{-\frac{r}{2r_0}}$$

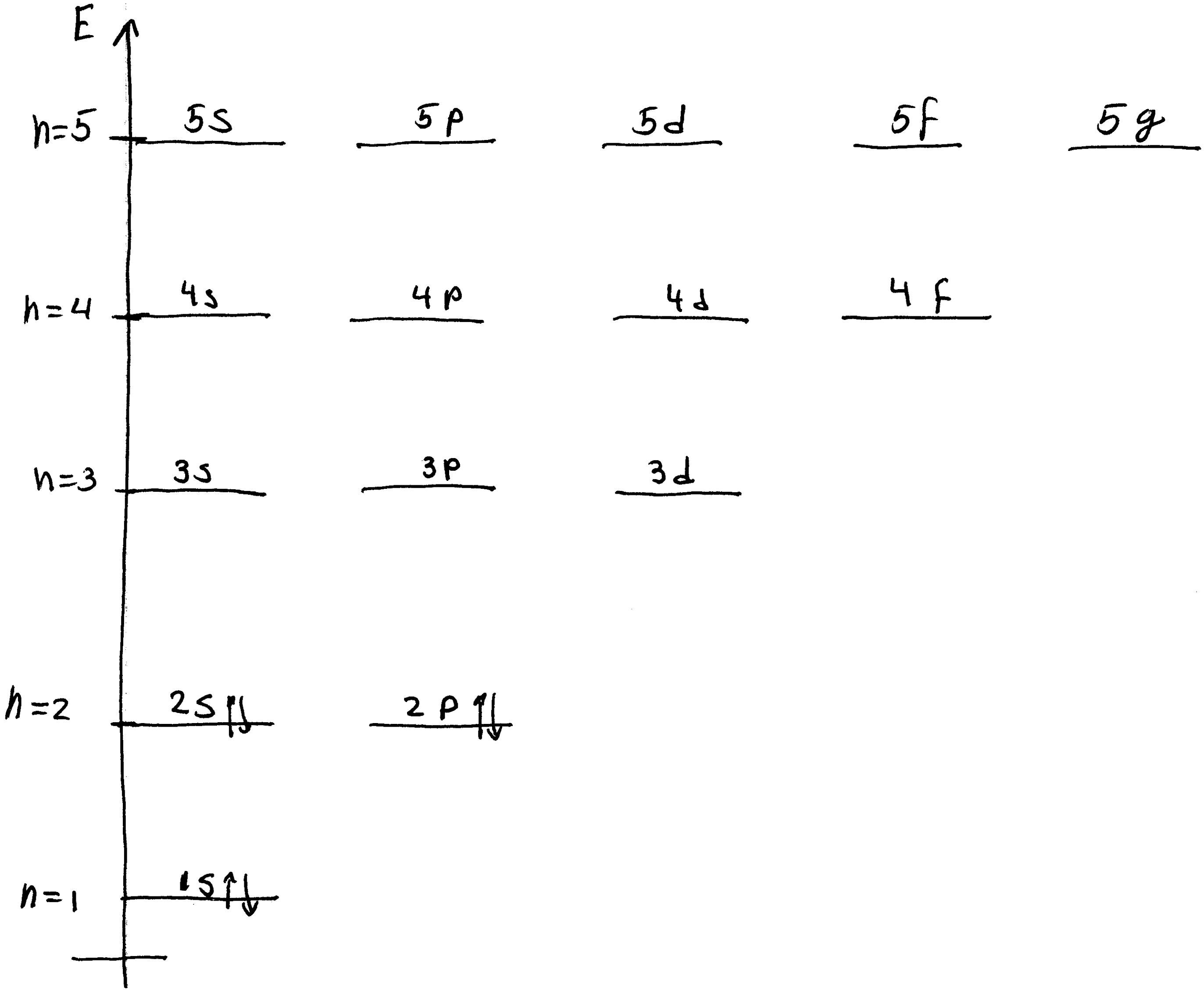
PROBABILITY DENSITY $\quad \frac{1}{32\pi r_0^3}\left(2 - \frac{r}{r_0}\right)^2 e^{-\frac{r}{r_0}}$

RADIAL DISTRIBUTION FUNCTION $\quad P_{2s}(r) = \int_0^{\pi}\int_0^{2\pi} |\Psi_{2s}(r)|^2 r^2 \sin\theta \, d\theta \, d\varphi$

$$P_{2s}(r) = \frac{r^2}{8r_0^3}\left(2 - \frac{r}{r_0}\right)^2 e^{-\frac{r}{r_0}}$$

$$\langle 2s|r|2s\rangle = \int_0^{\infty} r P_{2s}(r)\, dr = 6\frac{a}{Z}$$

FOR A HYDROGEN-LIKE ATOM



$$l = 0, 1, 2, 3, 4, 5$$
s p d f g, h

WE ADD SPIN OR INTERNAL ANGULAR MOMENTUM TO THE ELECTRON $S = \frac{1}{2}$

WITH TWO PROJECTIONS $\pm 1/2$ $(\uparrow, \downarrow)$

$$m_s = \pm \frac{1}{2}$$

$$S = 1/2$$

NOTICE THE SIMILARITY BETWEEN

$$m = 0, \pm 1, \pm 2, \cdots \pm J$$

$$J = 0, 1, 2, \cdots, n-1$$

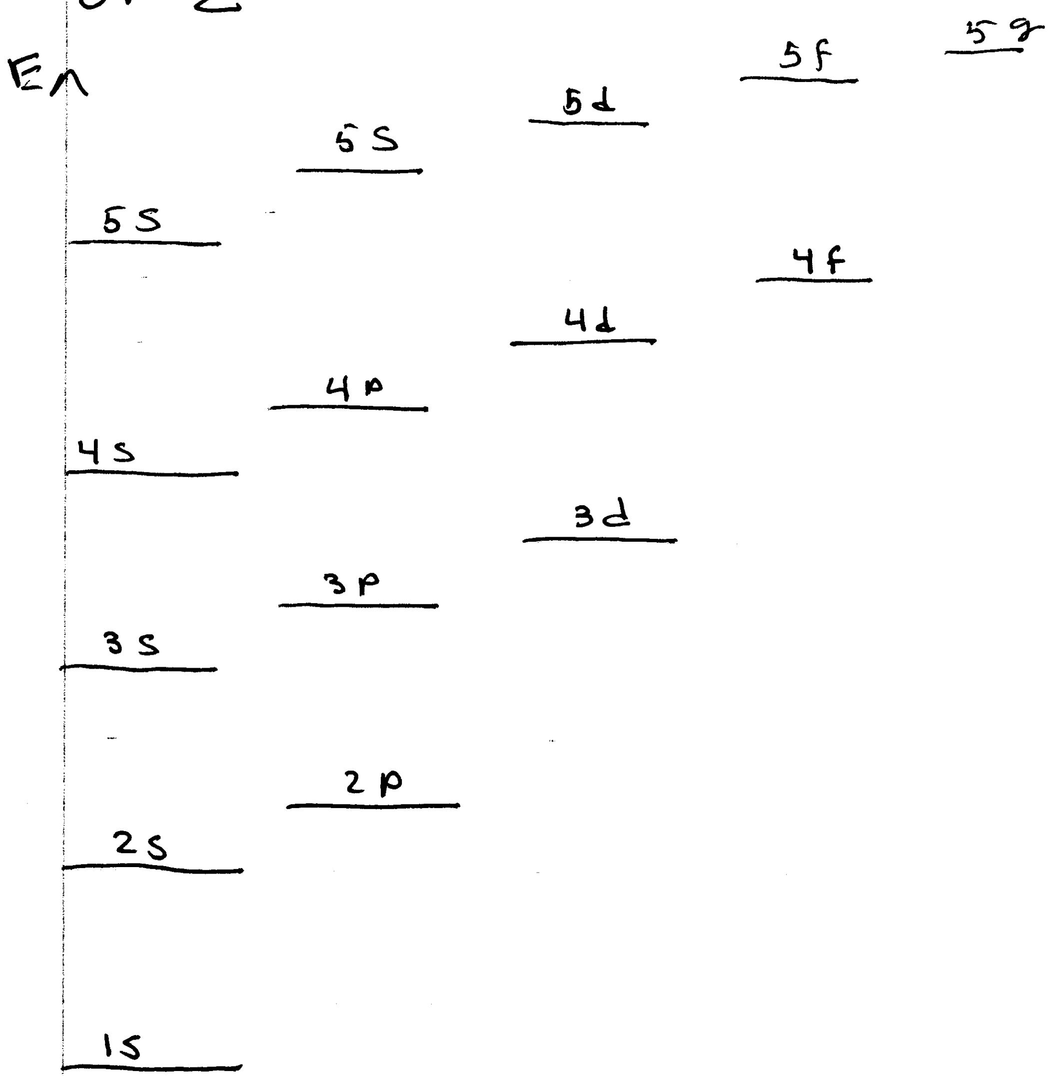
ELECTRON HAVE 5 QUANTUM NUMBERS

$$n, J, m, S, m_s$$

AND NO 2 e^- CAN HAVE THE SAME

QUATUM NUMBERS

FOR OTHER ATOM, WE HAVE TO INCLUDE e-e INTERACTIONS AND NUMERICAL SOLUTIONS SHOW SPLITTING IN THE ENERGY LEVELS AS FUNCTION OF Z

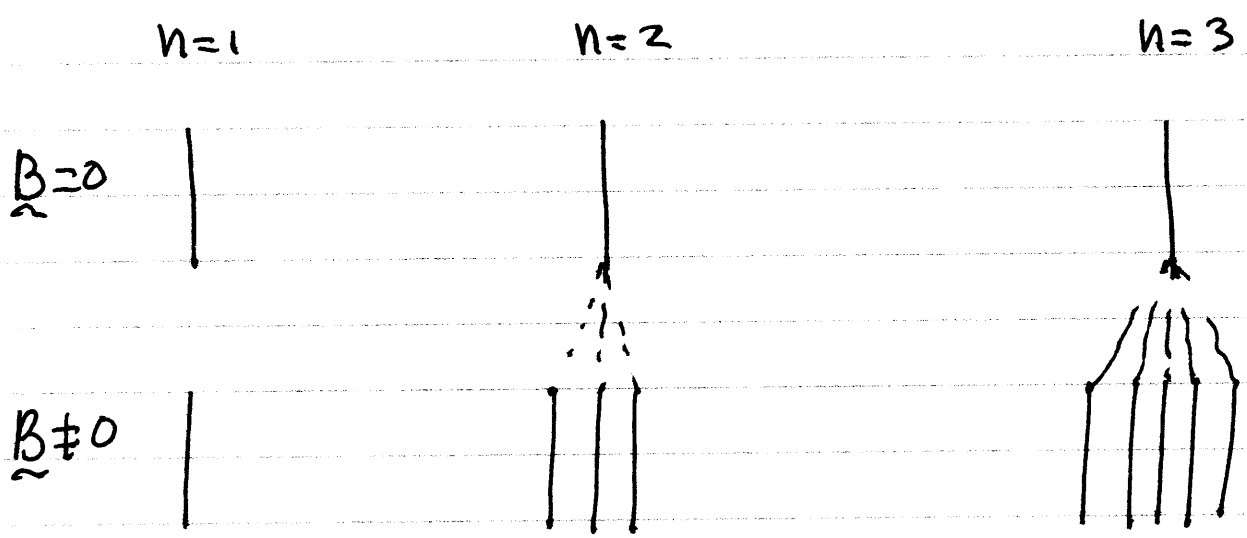


Hydrogen Atom in an External Magnetic Field

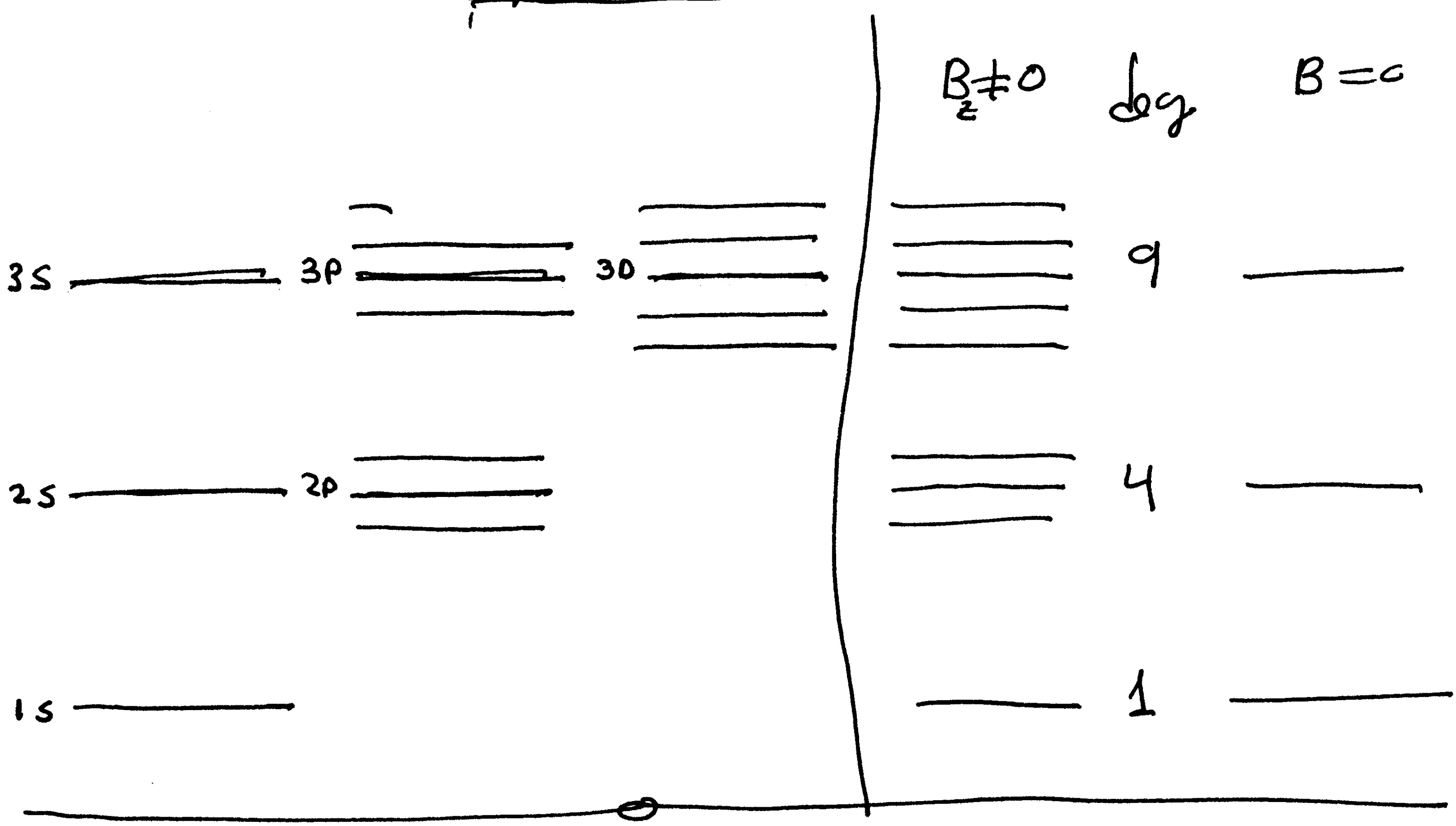
$$\hat{H} = \hat{H}_0 + \beta_e \frac{B_z}{\hbar} \hat{L}_z$$

$$\Rightarrow \quad E = E_n^{(0)} + \beta_e B_z m$$

Degeneracy $\rightarrow n^2$



HYDROGEN ATOM IN A MAGNETIC FIELD



Multielectron Atoms