

Problem 1

$$E_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{2m_e} \left( \frac{n_1^2 + n_2^2}{L^2} + \frac{n_3^2}{L_3^2} \right)$$

$L = 4 \text{ \AA}$ . For example, assume the triply degenerate states are:

$(1, 2, 1)$ ;  $(2, 1, 1)$ ;  $(1, 1, 3)$ . The condition is:

$$\frac{2^2 + 1^2}{L^2} + \frac{1^2}{L_3^2} = \frac{1^2 + 1^2}{L^2} + \frac{9}{L_3^2} \Rightarrow \frac{5}{L^2} + \frac{1}{L_3^2} = \frac{2}{L^2} + \frac{9}{L_3^2} \Rightarrow$$

$$\Rightarrow \frac{3}{L^2} = \frac{8}{L_3^2} \Rightarrow \frac{L_3^2}{L^2} = \frac{8}{3} \Rightarrow \boxed{L_3 = \sqrt{\frac{8}{3}} L = 6.532 \text{ \AA}} \quad (a)$$

So  $\frac{1}{L_3^2} = \frac{3}{8} \frac{1}{L^2} = \frac{0.375}{L^2} \Rightarrow$  energies are:

$$E_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{2m_e L^2} (n_1^2 + n_2^2 + 0.375 n_3^2)$$

the quantum numbers for the lowest 6 energy states are:

$n_1$	$n_2$	$n_3$	$n_1^2 + n_2^2 + 0.375 n_3^2$	degeneracy
2	2	1	6.5375	2
2	1	1	5.375	3
1	1	3	5.375	1
1	1	2	3.5	1
1	1	1	2.375	1

(c)  $E_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{2m_e L^2} \left( n_1^2 + n_2^2 + \frac{n_3^2}{100^2} \right)$  since  $L_3 = 100L$

Since the last term is so small, lowest 6 states are (111)(112)(113)(114)(115)(116)

All energies are approximately same, since last term is at most  $\frac{36}{10,000} = 0.0036$  compared with  $1^2 + 1^2 = 2$  for first 2 terms.

$$E = \frac{\hbar^2}{2m_e} \left( \frac{\pi}{L} \right)^2 (2) = 3.81 \text{ eV} \left( \frac{\pi}{4} \right)^2 \cdot 2 = \boxed{4.70 \text{ eV}} \quad (c)$$

## Problem 2

$$\Psi(r, \theta, \phi) = C r e^{-2r/a_0} \sin \theta g(\phi)$$

From  $(\sin \theta)$  we infer  $l=1, m=\pm 1 \Rightarrow g(\phi) = e^{i\phi}$  or  $g(\phi) = e^{-i\phi}$

Then,  $n \geq 2$ . From the  $r$ -dependence (no nodes)  $\Rightarrow n=2$

(b) The exponential is  $e^{-2r/na_0}$ ,  $n=2 \Rightarrow z=4$

energy  $E = -E_0 \frac{z^2}{n^2} = -E_0 \frac{4^2}{2^2} = -4E_0 = -54.4 \text{ eV}$

(c) Radial probability:

$$P(r) \propto r^2 R(r)^2 = r^2 \cdot r^2 \cdot e^{-4r/a_0} = r^4 e^{-4r/a_0}$$

$$\langle r \rangle = \frac{\int_0^\infty dr r P(r)}{\int_0^\infty dr P(r)} = \frac{\int_0^\infty dr r^5 e^{-4r/a_0}}{\int_0^\infty dr r^4 e^{-4r/a_0}} = \frac{5! \cdot a_0^6 \cdot 4^5}{4^6 \cdot 4! \cdot a_0^5} = \frac{5}{4} a_0$$

So  $\langle r \rangle = \frac{5}{4} a_0 = 1.25 a_0$

$$\langle \frac{1}{r} \rangle = \frac{\int_0^\infty dr \frac{1}{r} P(r)}{\int_0^\infty dr P(r)} = \frac{\int_0^\infty dr r^3 e^{-4r/a_0}}{\int_0^\infty dr r^4 e^{-4r/a_0}} = \frac{3! \cdot a_0^4 \cdot 4^5}{4^4 \cdot 4! \cdot a_0^5} = \frac{1}{a_0}$$

$\Rightarrow \langle \frac{1}{r} \rangle = \frac{1}{a_0}$

(d) Maximize  $P(r)$ :  $0 = P'(r_m) = 4r_m^3 - \frac{4}{a_0} r_m^4 = 0 \Rightarrow r_m = a_0$

Most probable radius for electron is  $r_m = a_0$

Note that  $\langle \frac{1}{r} \rangle = \frac{1}{r_m}$  that is so for all states with  $l = n-1$

And  $r_m = n^2 \frac{a_0}{z}$  as in the Bohr atom

### Problem 3

Orbital magnetic moment:  $\vec{\mu}_L = -\frac{e}{2m_e} \vec{L}$

Spin magnetic moment:  $\vec{\mu}_S = -\frac{e}{2m_e} g_s \vec{S}$ ,  $g_s = 2$

Total magnetic moment:  $\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S = -\frac{e}{2m_e} (\vec{L} + 2\vec{S})$

z component:  $\mu_z = -\frac{e\hbar}{2m_e} (m + 2m_s) = -\mu_B (m + 2m_s)$

Energy in magnetic field:  $\Delta E = -\vec{\mu} \cdot \vec{B} = -\mu_z B = \mu_B (m + 2s) B$

$\mu_B = 5.79 \times 10^{-5} \text{ eV/T}$ ,  $B = 69.1 \text{ T} \Rightarrow \mu_B B = 4.00 \times 10^{-3} \text{ eV}$

$l=1$ :  $m = 1, 0, -1$ ,  $2s = \pm 1 \Rightarrow m + 2s = 2, 1, 0, -1, -2 \Rightarrow$

$\Delta E =$	{	$2\mu_B B = 8 \times 10^{-3} \text{ eV}$	$m$	$m_s$	}	6 states
		$\mu_B B = 4 \times 10^{-3} \text{ eV}$	1	1/2		
		$0$	0	1/2		
		$-\mu_B B = -4 \times 10^{-3} \text{ eV}$	1	-1/2 or -1 1/2		
		$-2\mu_B B = -8 \times 10^{-3} \text{ eV}$	0	-1/2		

total = 6 states

$l=0$ :  $m = 0$ ,  $2s = \pm 1$

$\Delta E =$	{	$\mu_B B = 4 \times 10^{-3} \text{ eV}$	$m$	$m_s$	}	2 states
		$-\mu_B B = -4 \times 10^{-3} \text{ eV}$	0	1/2		
			0	-1/2		

(b) With spin-orbit coupling, quantum numbers are  $l, j, m_j$  with  $|l-s| \leq j \leq l+s$ ;  $-j \leq m_j \leq j$ ; energy depends on  $l$  and  $j$ , not  $m, m_j$  (if no magnetic field applied)

$l=0 \Rightarrow |l-s| = |l+s| = 1/2 = j$ .  $l=1 \Rightarrow j = 1/2$  or  $3/2$

all the energies  $E_{l,j}$

$\underline{\underline{E_{0,1/2}}}$ $l=0, j=1/2, m_j=1/2$ $l=0, j=1/2, m_j=-1/2$ <div style="border: 1px solid black; padding: 5px; display: inline-block;">2 states</div>	$\underline{\underline{E_{1,1/2}}}$ $l=1, j=1/2, m_j=1/2$ $l=1, j=1/2, m_j=-1/2$ <div style="border: 1px solid black; padding: 5px; display: inline-block;">2 states</div>	$\underline{\underline{\underline{E_{1,3/2}}}}$ $l=1, j=3/2, m_j=3/2$ $l=1, j=3/2, m_j=1/2$ <div style="border: 1px solid black; padding: 5px; display: inline-block;">4 states</div> 3 different energies $E_{l,j}$ <div style="border: 1px solid black; padding: 5px; display: inline-block;"><math>E_{1,1/2} &lt; E_{0,1/2} &lt; E_{1,3/2}</math></div>
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8 states