PH206 — First MidTerm Exam Solution — March 4, 2002

1(a)
$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{32\pi a_0^3} \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) \int_0^\infty \frac{r^2 dr}{r^3} \left(\frac{r}{a_0}\right)^2 e^{-r/a_0} \times \cos^2\theta$$

$$= \frac{2\pi}{32\pi a_0^3} \cdot \underbrace{\frac{2}{3}}_{\int_{-1}^{1} x^2 dx} \cdot \frac{1}{a_0^2} \underbrace{\int_0^\infty r\, e^{-r/a_0}\, dr}_{a_0^2} = \boxed{\frac{1}{24 a_0^3}}$$

(b)
$$\vec{L}\cdot\vec{S} = \frac{1}{2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right)$$

$L = 1 \Rightarrow \vec{L}^2 = L(L+1) = 2$ (in units where $\hbar = 1$)

$S = 1/2 \Rightarrow \vec{S}^2 = S(S+1) = 3/4$

$J = 1/2$ or $3/2 \Rightarrow \vec{J}^2 = \frac{3}{4}$ or $\frac{15}{4}$

So
$$\boxed{\vec{L}\cdot\vec{S} = \begin{cases} -\hbar^2, & J = 1/2, \quad \text{dgen} = 2 \\ \hbar^2/2, & J = 3/2, \quad \text{dgen} = 4 \end{cases}}$$

Check: $2(-\hbar^2) + 4(\hbar^2/2) = 0$ ✓. Average vanishes as it must. ✓

(c) $(\vec{L}\cdot\vec{S})_{J=3/2} - (\vec{L}\cdot\vec{S})_{J=1/2} = \frac{3}{2}\hbar^2$

So, $\Delta E = \frac{e^2}{2m_e^2 c^2} \cdot \frac{1}{24} \cdot \left(\frac{m_e e^2}{\hbar^2}\right)^3 \cdot \frac{3}{2}\hbar^2$

$$= \frac{e^8 m_e}{32 c^2 \hbar^4} = \frac{1}{32}\left(\frac{e^2}{\hbar c}\right)^4 \cdot (m_e c^2)$$

$$\boxed{\Delta E = \frac{1}{32}\alpha^4 m_e c^2} \quad O(\alpha^4).$$

(d) Numerically evaluate ΔE.

$\alpha \cong \frac{1}{137}$. $\quad m_e c^2 = 0.51 \times 10^6 \, eV$

$$\Rightarrow \boxed{\Delta E \cong 4.5 \times 10^{-5} \, eV}$$

2 (a) 1. $\langle n,1,1 | z | n,1,1 \rangle = 0$ because

Zero

$z \to -z$ under parity, but $|Y_1^1(\theta,\phi)|^2$ is invariant. (Looks like it could be non-zero, though, since $\Delta m = 0$)

2. $\langle n,1,1 | z | n,1,0 \rangle = 0$ because m

Zero

Changes from 0 to 1, but $\hat{z}$ can't change m.

3. $\langle n,1,1 | x | n,1,1 \rangle = 0$ because x

Zero

has $\Delta m = \pm 1$, but the two states have the same m $(=1)$. Also, $x \to -x$ under parity

4. $\langle n,2,2 | y | n,1,1 \rangle \neq 0$ in general

Non-Zero

because $\langle 2,2 | \left(|1,1\rangle \otimes |1,1\rangle \right) \neq 0$.

5. $\langle n+2,1,0 | z | n,1,0 \rangle = 0$. Clebsch-Gordan

Coefficient $\langle 1,0 | \left(|1,0\rangle \otimes |1,0\rangle \right) = 0$. Also,

$z \to -z$ under parity, but $|Y_1^0(\theta,\phi)|^2$ is even.

Zero

Note that the change in the principle quantum number, $n \to n+2$, is irrelevant in this problem. (In any case, we didn't specify the radial problem. Is it a hydrogen atom? Particle in spherical box? Something else?)

2. (a) 6. $\langle n,2,0|\hat{x}\hat{z}|n,0,0\rangle = 0$ because

Zero Operators $\hat{x}\hat{z}$ Change m by ± 1.

(b) 1. Phosphorus $^4S_{3/2}$. Maximize S $|\uparrow\uparrow\uparrow\rangle$

$\Rightarrow$ put each of 3 valent electrons into different p-orbital (p_x, p_y, p_z)

$\Rightarrow L=0 \Rightarrow J = 3/2 = S$.

2. Chlorine : 1 hole in 3p shell $\Rightarrow S = 1/2$, $L = 1$

$^2P_{3/2}$ $J = L+S = 3/2$

3. Iron $^5D_4$ 6 3d electrons.

put 5 $\uparrow$ into each of the 5 3d orbitals. $\Rightarrow L=0$

put one $\downarrow$ into one of the 3d orbitals $\Rightarrow L=2$

4 remaining (unpaired) up electrons $\Rightarrow S=2$.

$J = L+S = 2+2 = 4$.

4. Copper $^3S_{1/2}$ Just one 4s electron

$\Downarrow$

(3d shell is full! Ignore!) $S = 1/2$, $L=0$

$J = 1/2$.

c) Bohr Theory of Helium atom.

Force balance : $\dfrac{m_e v^2}{r} = \dfrac{2e^2}{r^2} - \dfrac{e^2}{(2r)^2} = \dfrac{7}{4}\dfrac{e^2}{r^2}$

attracted to $Z=2$ nucleus

repelled by other electron.

Virial thm

So, $E = \left(-\frac{1}{2} m_e v^2\right) \times 2 = -m_e v^2 = \boxed{-\frac{7}{4}\frac{e^2}{r}}$

2 electrons

But what does $r = ?$ Quantize $L = mvr = \hbar$ (n=1

$$\frac{mv^2}{r} = \frac{\hbar^2}{mr^3} = \frac{7}{4}\frac{e^2}{r} \Rightarrow r = \frac{4}{7}\frac{\hbar^2}{me^2} = \frac{4}{7} a_0$$

(Note : $r = a_0/2$ if we ignore e-e interaction.) Other electron increases r. ✓

$\Rightarrow$ Screening of nucleus by other electron

So, $E = -\dfrac{7}{4}\dfrac{e^2}{r} = -\dfrac{7}{4} \cdot \dfrac{7}{4} \cdot e^2 \cdot \dfrac{me^2}{\hbar^2}$

$$= -\frac{49}{16}\frac{me^4}{\hbar^2} = -\frac{49}{8} R_y = \boxed{-83.3\,\text{eV}}$$

Not bad compared to exact answer -78.975 eV, but our variational calculation, using real quantum mechanics, did ~~much~~ better ($E_0 \cong -77.5$ eV)

d) Use Clebsch-Gordan coefficient table to get $-\frac{1}{\sqrt{4}} = -1/2$