SOLUTIONS TO HOMEWORK 4

1) (a) $n = 4$; the statistical weight is $n^2 = 16.$ **[5]**

(b) *l=0 m=0*

l=1 m=-1,0,1

l=2 m=-2,-1,0,1,2

l=3 m=-3,-2,-1,0,1,2,3 **[5]**

2(a) The probability distribution for the full quantum state, in 3 dimensions is: $|\psi|^2 d\tau = R_{nl}^2(r)\,|Y_{lm}(\theta,\phi)|^2 r^2\, dr \sin\theta\, d\theta\, d\phi$ (note that R_{nl} is real so we can write a simple square, while the spherical harmonic is complex, so we have $|Y_{lm}|^2$. Notice that the spherical harmonic does not depend on Z.)

The radial part of the probability is $P(r) = r^2 R_{nl}^2(r)$. This has a maximum

If $$\frac{dP}{dr} = \frac{Z^5}{24}\left(-Z r^4 e^{-Zr} + 4r^3 e^{-Zr}\right) = 0$$

$\Rightarrow -Zr + 4 = 0$ so $r = 2$, since $Z = 2$. You can verify with a sketch that this is a maximum, not a minimum. Note that for hydrogen ($Z = 1$) we'd have $r = 4$. The helium atom in this sense is 'half the size' of hydrogen. **[5]**

(b) $\langle r \rangle = \int_0^\infty R_{2p}(r)\, r\, R_{2p}(r)\, dr$.

$$= \frac{Z^5}{24}\int r^5 e^{-Zr}\, dr = \frac{1}{24}\int (Zr)^5 e^{-Zr}\, dr$$

substituting $u = Zr$, we get:

$$\langle r \rangle = \frac{1}{24}\int_0^\infty u^5 e^{-u}\frac{du}{Z} = 2.5 \text{ atomic units}$$ **[5]**

(check that for hydrogen you would get twice the value, Z=5 au)

(c)

$E_n = -Z^2/2n^2$ so $E_{n=2}(Z=2) = -1/2$ a.u. **[5]**

3)Initially the extranuclear electron of tritium's wavefunction equals the ground state of a hydrogen atom . It is undisturbed by the decay, so initially its wavefunction is unchanged $= \phi_{1s}^{H}(\underline{r})$. We have a superposition of states.

$$\Psi(\underline{r}) = \sum_i c_i \psi_i^{He^+}(\underline{r}) = \phi_{1s}^{H}(\underline{r})$$

However if a measurement of the energy is carried out on the He+ ion, we will find the electron in one of the eigenstates of the He ion. The probability of finding the i-th state is given by $|c_i|^2$.

$$c_i = \int \psi_i^{*He^+}\, \Psi(\underline{r})\, d\underline{r}$$

$$= \int \psi_{1s}^{*\,He^+}(\underline{r})\, \phi_{1s}^{H}(\underline{r})\, d\underline{r}$$

The *1s* state of an atom of charge Z is $= 2Z^{3/2} e^{-Zr} Y_{00}(\theta,\phi)$

$$\Rightarrow C_{1s} = \int_0^\infty 4\sqrt{8}\, e^{-3r} r^2 dr \int_0^{2\pi} d\phi \int_0^{\pi} |Y_{00}|^2 \sin\theta\, d\theta$$

since the spherical harmonics are normalised, the angular integral=1.

The radial part of the integral $\int 4\sqrt{8}\, r^2 e^{-3r} dr = 8\sqrt{8}/3^3 = C_{1s}$.

Hence the probability $|C_{1s}|^2 = 2^9/3^6$. **[10]**

b) $C_{2p} = 0$ since the angular integral is zero, ie

$\int Y_{2m}^* Y_{00} \sin\theta\, d\theta\, d\phi = 0$. **[2]**

4)a) $\hat{L}_z Y_{10}(\theta,\phi) = \sqrt{3/4\pi} \cdot \hbar/i \cdot \partial/\partial\phi\,(\cos\theta) = 0 \times Y_{10}$ **[3]**

NB note that in this solution we include the normalisation constant $(Y_{10} = \sqrt{3/4\pi}\cos\theta)$ whereas in the original question we use the unnormalised spherical harmonic $(Y_{10}(\theta,\phi) = \cos\theta)$. The eigenvalues are unaffected.

b) $\hat{L}_x Y_{10} = \sqrt{3/4\pi}\, i\hbar \left(\sin\phi \frac{\partial(\cos\theta)}{\partial\theta} + \cot\theta \cos\phi \frac{\partial(\cos\theta)}{\partial\phi}\right) = -i\hbar \sqrt{3/4\pi}\, \sin\phi \sin\theta$

$$\hat{L}_y Y_{10} = i\hbar \cos\phi \sin\theta \,.\, \sqrt{3/4\pi}$$

Hence, $-\frac{1}{\sqrt{2}\hbar}(\hat{L}_x + i\hat{L}_y) Y_{10} = \sqrt{\frac{3}{8\pi}} \sin\theta(\cos\phi + i\sin\phi)$

$$= \sqrt{3/8\pi}\, \sin\theta\, e^{i\phi}$$ **[5]**

$$\hat{L}_z Y_{11} = \sqrt{\frac{3}{8\pi}} \sin\theta\, \hbar/i\, \frac{\partial}{\partial\phi}(e^{i\phi}) = \hbar \sqrt{\frac{3}{8\pi}} \sin\theta\, e^{i\phi}$$

$$\Rightarrow \hat{L}_z Y_{11}(\theta,\phi) = \hbar Y_{11}(\theta,\phi)$$

Hence the eigenvalue is $= \hbar$.

[5]

(NB remember that $\hat{L}_z Y_{lm} = m\hbar Y_{lm}$).