Química Física I
Grado en Química

UNIVERSIDAD DE MURCIA

Lesson: HIDROGENIC ATOMS

PROBLEM SHEET: QUESTIONS

1. (♦◇◇) The radial $1s$ function is $R_{1,0} = N\, e^{-Zr/a_o}$. Find the value of r that maximizes the radial distribution function and calculate the normalization constant N.

2. (♦◇◇) Calculate $\langle r \rangle_{1s}$. Compare the result with that provided by the general expression $\langle r \rangle_{n,l} = \frac{a_o}{2Z}(3n^2 - l(l+1))$.

3. (♦♦◇) Consider the following function to describe the angular part for an electron in a hydrogen atom:

$$\psi(\theta, \phi) = N e^{i\,A\,\phi} \cos\theta$$

where N and A are constants.

   a) Is $\psi(\theta, \phi)$, in general, eigenfunction of $\hat{L}_z$?
   b) Calculate the value of A so that $\psi(\theta, \phi)$ is eigenfunction of $\hat{L}^2$ and find the corresponding values of the quantum numbers l and m_l.

4. (♦♦◇) Let us consider two spherical harmonics which $\hat{L}^2$ and $\hat{L}_z$ eigenvalues are $6\hbar^2$ and $\pm 2\hbar$ respectively.

   a) Prove that they are orthogonal.
   b) Obtain a real spherical harmonic expressed as a linear combination of them.

5. (♦♦◇) Calculate the extremes of the $2s$ radial distribution function for a hidrogenic atom. Identify them as maximun or minimun taking into account that the function is always positive.

6. (♦♦◇) Calculate the probability of finding an $1s$ electron at distances smaller than a_0 for a hidrogenic atom with atomic number Z. Prove that the probability always increases with Z.

7. (♦♦◇) Calculate the probability of finding the $1s$ or $2s$ electrons in the classically forbidden region.

Dificulty level: (♦◇◇) Easy, (♦♦◇) Normal, (♦♦♦) To think a bit.

PROBLEM SHEET: SOLUTIONS

Question 1 ⇒ $r_{\mathrm{max}} = \frac{a_0}{Z}$, $N = 2\left(\frac{Z}{a_0}\right)^{3/2}$

Question 2 ⇒ $\langle \hat{r} \rangle = \frac{3}{2}\frac{a_o}{Z}$

Question 3 ⇒ (a) It is eigenfunction because $\hat{l}_z\psi = \hbar A\psi$

(b) $A = 0$, l=1 and m_l =0.

Question 4 ⇒ $\psi_{\text{real}}(\theta,\phi) = \frac{\sqrt{15}}{4\sqrt{\pi}}\sin^2\theta\cos 2\phi$

Question 5 ⇒ $r_{\mathrm{min}} = \frac{2a_0}{Z}$, $r_{\mathrm{max}} = 0.76\frac{a_0}{Z}$, $r_{\mathrm{max}} = 5.23\frac{a_0}{Z}$

Question 6 ⇒ $P(r \leq a_0) = 1 - e^{-2Z}(1 + 2Z + 2Z^2)$

Question 7 ⇒ $P_{1s} = 0.238$, $P_{2s} = 0.186$