Quiz #2 Chem 1410

1a. avg. of r^2 for a $2p_0$ orbital of the H atom?

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

1b) avg. of z for a $2p_0$ orbital of H?

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

using $z = r\cos\theta$

1c) The probability that an electron in the 3s orbital is within $2a_0$ of the nucleus?

$$\text{Prob} = \frac{4\pi}{(81)^2(3\pi)} \int_0^{2a_0} r^2 \left(27 - 18\frac{r}{a_0} + 2\left(\frac{r}{a_0}\right)^2\right) e^{-2r/3a_0}\, dr$$

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2. How would you find the values of r that maximize the probability density.

$$\text{Prob} \sim (2-\sigma)^2 \sigma^2 e^{-\sigma} = (4\sigma^2 - 4\sigma^3 + \sigma^4) e^{-\sigma}$$

$$\frac{d\,\text{Prob}}{d\sigma} = 0 = (8\sigma - 12\sigma^2 + 4\sigma^3) e^{-\sigma} - (4\sigma^2 - 4\sigma^3 + \sigma^4) e^{-\sigma}$$

$$= (8\sigma - 16\sigma^2 + 8\sigma^3 - \sigma^4) e^{-\sigma} = 0$$

$$\Rightarrow \sigma = 0 \quad \text{and} \quad (8 - 16\sigma + 8\sigma^2 - \sigma^3) = 0$$

we know $\sigma = 2$ is a root and can factor this out, giving $\sigma^2 - 6\sigma + 4 = 0$. Need to solve for the two roots of this equation.

3. What is the extent of the degeneracy of the $n=4$ level of the H atom.

$$n=4 \Rightarrow \begin{array}{ll} \ell=3 & 2\ell+1=7 \\ \ell=2 & 2\ell+1=5 \\ \ell=1 & 2\ell+1=3 \\ \ell=0 & 2\ell+1=1 \\ \hline & 16 \leftarrow \text{levels} \end{array}$$