Answers: HW #4, Chem 1410

1. radial part of ψ_{2p_z} (in a.u.) $= r e^{-r/2}$
(Note that if we just want to find the maximum, we don't need to normalize)

$P_{radial} \propto r^2 \psi^2 = r^4 e^{-r}$ $\qquad \frac{dP}{dr} = (4r^2 - r^3) e^{-r}$

$\Rightarrow r_{max} = 4$ a.u.

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2. $\psi = 1/\sqrt{2}\,(\psi_{2s} + \psi_{2p_z})$: What is the probability of finding the electron between $\theta = 0$ and $\theta = \pi/2$. By symmetry it is $1/2$. Do you see this?

$$\psi^2 = 1/2 \, \frac{1}{32\pi}\left((2-r)^2 + r^2\cos^2\theta + 2r(2-r)\cos\theta\right)e^{-r}$$

$$\int_0^\infty r^2(2-r)^2 e^{-r}\,dr = 8, \quad \int_0^\infty r^4 e^{-r}\,dr = 24, \quad \int_0^\infty 2r^3(2-r)e^{-r}\,dr = -24$$

$$\int_0^{\pi/2} \sin\theta\,d\theta = 1, \quad \int_0^{\pi/2} \cos\theta\sin\theta\,d\theta = 1/2, \quad \int_0^{\pi/2} \cos^2\theta\sin\theta\,d\theta = 1/3$$

$$\frac{2\pi}{64\pi}\int \psi^2 r^2 \sin\theta\,dr\,d\theta = \frac{1}{32}\left[8 + 24/3 - 24/2\right] = \frac{1}{32}\left[8+8-12\right] = 1/8$$

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3. $$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} - \frac{1}{r} + \frac{\hat{\ell}^2}{2r^2}\right]\psi = E\psi$$

$\psi = r e^{-r/2}$ | radial part only. $\hat{\ell}^2$ on angular part gives 1(2) since this is a p orbital

$$\psi' = \left(1 - \frac{r}{2}\right)e^{-r/2}; \quad \psi'' = \left(-\frac{1}{2} - \frac{1}{2} + \frac{r}{4}\right)e^{-r/2} = \left(-1 + \frac{r}{4}\right)e^{-r/2}$$

$$-\frac{1}{2}\left[-1 + \frac{r}{4}\right] - \frac{1}{r}\left(1 - \frac{r}{2}\right) - \frac{r}{r} + \frac{2}{2r} = Er$$

$$\Rightarrow \left(-1/2 + 1/2\right) + \left(-\frac{r}{8} - Er\right) + \left(-\frac{1}{r} + \frac{1}{r}\right) = 0, \Rightarrow E = -\frac{1}{8} \text{ a.u.}$$

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4. $$\frac{4\pi}{\pi}\int_0^{1.9\times10^{-5}} r^2 e^{-2r}\,dr = 4(228 \times 10^{-15}) \text{ a.u.}$$