# Homework Solutions #7 (McIntyre Chapter 8)

**7** The classically forbidden region is where $E < V(r)$. The boundary is where

$$-\frac{1}{2\,2^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{1}{a_0} = -\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{1}{r} \qquad \Rightarrow \qquad r = 8a_0$$

Therefore, for energy eigenstates,

$$\mathcal{P}_{r>8a_0} = \int_{8a_0}^{\infty} dr\, r^2 |R_{nl}(r)|^2 \int d\Omega\, Y_l^{m*} Y_l^m = \int_{8a_0}^{\infty} dr\, r^2 R_{nl}^2$$

For $n = 2, l = 0$:

$$\int_{8a_0}^{\infty} dr\, r^2 R_{20}^2 = \int_{8a_0}^{\infty} dr\, r^2 \left[2\left(\frac{1}{2a_0}\right)^{\frac{3}{2}}\left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0}\right]^2$$

$$= \frac{1}{2}\int_8^{\infty} d\rho\,\left(\rho^2 - \rho^3 + \frac{\rho^4}{4}\right)e^{-\rho} = 0.186$$

For $n = 2, l = 1$:

$$\int_{8a_0}^{\infty} dr\, r^2 R_{21}^2 = \int_{8a_0}^{\infty} dr\, r^2 \left[\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{\frac{3}{2}}\frac{r}{a_0}e^{-r/2a_0}\right]^2$$

$$= \frac{1}{24}\int_8^{\infty} d\rho\, \rho^4 e^{-\rho} = 0.100$$

**8** In the ground state, $n = 1, l = 0, m = 0$.

$$\langle r^2 \rangle = \frac{4}{a_0^3}\int_0^{\infty} dr\, r^2 r^2 e^{-2r/a_0} = 3a_0^2 = \frac{a_0^2}{2}\left[5 \cdot 1^2 + 1\right]$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{4}{a_0^3}\int_0^{\infty} dr\, r^2 \frac{1}{r} e^{-2r/a_0} = \frac{1}{a_0} = \frac{1}{a_0 1^2}$$

$$\left\langle \frac{p^2}{2m} \right\rangle = \langle H \rangle + \left\langle \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} \right\rangle = E_1 + \frac{e^2}{4\pi\varepsilon_0}\left\langle \frac{1}{r} \right\rangle = \frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{1}{a_0} = 13.6\text{ eV}$$

**11** The $\beta$-decay changes the nucleus from $Z = 1$ to $Z = 2$. The probability we want is the magnitude squared of the overlap integral of the two different ground states:

$$\mathcal{P} = \left| \int dr\, r^2\, 2\left(\frac{1}{a_0}\right)^{\frac{3}{2}} e^{-r/a_0} 2\left(\frac{2}{a_0}\right)^{\frac{3}{2}} e^{-2r/a_0} \int d\Omega\, Y_0^{0*} Y_0^0 \right|^2 = 0.702$$

**13**$^*$ Using cylindrical coordinates will be easiest, with $r = \sqrt{\rho^2 + z^2}$ and $rdr = \rho d\rho$. Neither $\psi_1$ nor $\psi_2$ depend on $\phi$, so the angular integrals will just contribute a factor of $\int_0^{2\pi} d\phi = 2\pi$.

Start with $\psi_1$:

$$\mathcal{P}_1(z) = \frac{1}{a_0^3} \int_0^\infty d\rho\, \rho \left( e^{-r/a_0} + \frac{z}{4\sqrt{2}a_0} e^{-r/2a_0} \right)^2 =$$

$$\frac{1}{a_0^3} \int_{|z|}^\infty dr\, r \left( e^{-2r/a_0} + \frac{z}{2\sqrt{2}a_0} e^{-3r/2a_0} + \frac{z^2}{32a_0^2} e^{-r/a_0} \right) =$$

$$\frac{1}{4a_0} e^{-2|z|/a_0} \left( \frac{2|z|}{a_0} + 1 \right) + \frac{z\sqrt{2}}{9a_0^2} e^{-3|z|/2a_0} \left( \frac{3|z|}{2a_0} + 1 \right) + \frac{z^2}{32a_0^3} e^{-|z|/a_0} \left( \frac{|z|}{a_0} + 1 \right)$$

Then $\psi_2$:

$$\mathcal{P}_2(z) = \frac{1}{8a_0^3} \int_0^\infty d\rho\, \rho \left[ \left( 1 - \frac{r}{2a_0} \right) e^{-r/2a_0} + \frac{z}{4a_0} e^{-r/2a_0} \right]^2 =$$

$$\frac{1}{8a_0^3} \int_{|z|}^\infty dr\, r \left( 1 - \frac{r}{2a_0} + \frac{z}{2a_0} \right) e^{-r/a_0} = \frac{e^{-|z|/a_0}}{16a_0^4} \left( a_0^3 + a_0^2|z| + |z|^3 - z^3 \right)$$

Now, for the dipole moment,

$$\langle \mathbf{r} \rangle = \langle x \rangle \mathbf{i} + \langle y \rangle \mathbf{j} + \langle z \rangle \mathbf{k} = \langle \rho \cos\phi \rangle \mathbf{i} + \langle \rho \cos\phi \rangle \mathbf{j} + \langle z \rangle \mathbf{k} = \langle z \rangle \mathbf{k}$$

Here, $\langle x \rangle = \langle y \rangle = 0$ because $\int d\phi \cos\phi = \int d\phi \sin\phi = 0$. In other words, the symmetry of the states with respect to rotations about the $z$ axis means that only $\langle z \rangle$ can be nonzero.

We get $\langle z \rangle$ by using $\mathcal{P}(z)$, and simplifying matters by paying attention to whether the integrated terms are even or odd functions.

$$\langle z \rangle = \int_{-\infty}^\infty dz\, P(z) z$$

$$\langle z \rangle_1 = \frac{2\sqrt{2}}{9a_0^2} \int_0^\infty dz\, z^2 e^{-3z/2a_0} \left( \frac{3z}{2a_0} + 1 \right) = \frac{2^{15/2}}{3^5} a_0 = 0.745 a_0$$

$$\langle z \rangle_2 = -\frac{1}{8a_0^4} \int_0^\infty dz\, z^4 e^{-z/a_0} = -\frac{4!}{8} a_0 = -3a_0$$

With $q = -e$, the electronic dipole moments are

$$\mathbf{d}_1 = -0.745 e a_0 \mathbf{k} \qquad \mathbf{d}_2 = 3 e a_0 \mathbf{k}$$