Phys 201 F'09 Problem Set 12 Solutions

8.42 $$P_{1s}(r) = \frac{4}{a_B^3} r^2 e^{-2r/a_B}$$

$$\langle r \rangle = \int_0^\infty r P_{1s}(r)\, dr$$

$$= \frac{4}{a_B^3} \int_0^\infty r^3 e^{-2r/a_B}\, dr$$

Integrate by parts three times:

$u = r^3$, $dv = e^{-2r/a_B} dr$

$$\langle r \rangle = \frac{4}{a_B^3}\left[\cancelto{0}{r^3 e^{-2r/a_B}\left(-\frac{a_B}{2}\right)}\Big|_0^\infty - \int_0^\infty \left(-\frac{3a_B}{2}\right) r^2 e^{-2r/a_B}\, dr \right]$$

$u = r^2$, $dv = e^{-2r/a_B} dr$

$$= \frac{6}{a_B^2}\left[\cancelto{0}{r^2 e^{-2r/a_B}\left(-\frac{a_B}{2}\right)}\Big|_0^\infty - \int_0^\infty \left(-\frac{2a_B}{2}\right) r e^{-2r/a_B}\, dr \right]$$

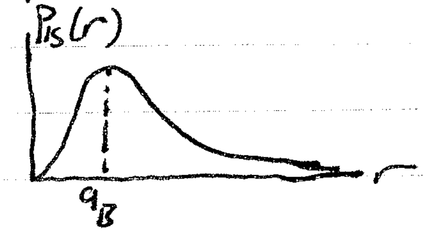
$u = r$, $dv = e^{-2r/a_B} dr$

$$= \frac{6}{a_B}\left[\cancelto{0}{r\left(-\frac{a_B}{2}\right) e^{-2r/a_B}}\Big|_0^\infty - \int_0^\infty \left(-\frac{a_B}{2}\right) e^{-2r/a_B}\, dr \right]$$

$$= 3\left(-\frac{a_B}{2}\right) e^{-2r/a_B}\Big|_0^\infty = -\frac{3a_B}{2}(0-1)$$

$$= \boxed{\frac{3}{2} a_B}$$

Note that this is larger than the most probable radius $r_{mp} = a_B$ because of the tail in the radial probability distribution $P_{1s}(r)$.



8.50 Max $P_{2s}(r) \longrightarrow \frac{d}{dr} P_{2s}(r)\Big|_{r_{mp}} = 0$

$$\frac{d}{dr}\sqrt{P_{2s}(r)}\Big|_{r_{mp}} = \frac{1}{2\sqrt{P_{2s}(r)}} \frac{d}{dr} P_{2s}(r)\Big|_{r_{mp}} = 0$$

(as long as $P_{2s}(r_{mp}) \neq 0$.)

$$\sqrt{P_{2s}(r)} = \sqrt{4\pi}\, A_{2s}\, r\left(2 - \frac{r}{a_B}\right)e^{-r/2a_B}$$

normalization const.

$$\frac{d}{dr}\sqrt{P_{2s}(r)} = \sqrt{4\pi}\,A_{2s}\left[\left(2-\frac{2r}{a_B}\right)e^{-r/2a_B} - \frac{1}{2a_B}\left(2r - \frac{r^2}{a_B}\right)e^{-r/2a_B}\right]$$

$$= \sqrt{4\pi}\,A_{2s}\left(\frac{r^2}{2a_B^2} - \frac{3r}{a_B} + 2\right)e^{-r/2a_B} = 0 \text{ @ } r = r_{mp}.$$

$$\Longrightarrow r_{mp}^2 - 6a_B r_{mp} + 4a_B^2 = 0$$

$$r_{mp} = \frac{6a_B \pm \sqrt{36a_B^2 - 16a_B^2}}{2} = (3 \pm \sqrt{5})\,a_B = (3 \pm 2.2)\,a_B$$

At $r = (3+\sqrt{5})a_B$, $P_{2s}(r) = 4\pi |A_{2s}|^2 (1.5\, a_B^2)$

At $r = (3-\sqrt{5})a_B$, $P_{2s}(r) = 4\pi |A_{2s}|^2 (0.4\, a_B^2)$

Hence, $r_{mp} = (3+\sqrt{5})\,a_B = \boxed{5.2\, a_B}$

$$P_{2p}(r) = 4\pi |A_{2p}|^2 r^4 e^{-r/a_B}$$

$$\frac{d}{dr} P_{2p}(r) = 4\pi |A_{2p}|^2 \left(4r^3 e^{-r/a_B} - \frac{1}{a_B} r^4 e^{-r/a_B}\right) = 0 \text{ @ } r = r_{mp}$$

$$r_{mp}^4/a_B - 4 r_{mp}^3 = 0 \longrightarrow r_{mp} = 0 \text{ or } r_{mp} = 4a_B$$

At $r=0$, $P_{2p}(r) = 0$.
At $r = 4a_B$, $P_{2p}(r) = 4\pi |A_{2p}|^2 \cdot 256\, a_B^4 e^{-4} > 0$

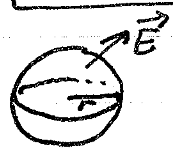
Hence, $\boxed{r_{mp} = 4a_B}$

10.2 a) $\int_0^\infty \rho(r)\, 4\pi r^2 dr = -(Z-1)|e|$

$$= \int_0^\infty \rho_0\, e^{-r/R} 4\pi r^2 dr$$

$$= 4\pi\rho_0 \cdot 2R^3 \quad \left(\text{using } \int_0^\infty x^2 e^{-x/b} dx = 2b^3 \text{ from Appendix B}\right)$$

$$\Rightarrow \boxed{\rho_0 = \frac{-(Z-1)|e|}{8\pi R^3}}$$

b) 

$$\int \vec{E}\cdot d\vec{A} = |\vec{E}|\cdot 4\pi r^2 = \frac{1}{\varepsilon_0}\left[\int_0^r \rho(r')\, 4\pi r'^2 dr' + Z|e|\right]$$

by Gauss' Law — electron charge in sphere of radius r — proton charge

$$|\vec{E}| 4\pi r^2 = \frac{1}{\varepsilon_0}\left(4\pi\rho_0 \int_0^r r'^2 e^{-r'/R} dr' + Z|e|\right)$$

$$= \frac{1}{\varepsilon_0}\left(4\pi\rho_0 \left[-(2R^3 + 2R^2 r' + Rr'^2) e^{-r'/R}\right]_0^r + Z|e|\right) \quad \text{from Appendix B.}$$

$$= \frac{1}{\varepsilon_0}\left(4\pi \frac{(Z-1)|e|}{8\pi R^3}\left[(2R^3 + 2R^2 r + Rr^2)e^{-r/R} - 2R^3\right] + Z|e|\right)$$

$$\boxed{|\vec{E}| = \frac{|e|}{4\pi\varepsilon_0 r^2}\left(1 + (Z-1)\left(1 + \frac{r}{R} + \frac{r^2}{2R^2}\right)e^{-r/R}\right)}$$

(Note $\frac{1}{4\pi\varepsilon_0} = K$ Coulomb constant)

c) As $r \to \infty$ the term multiplying $e^{-r/R}$ is negligible, so $|\vec{E}(r)| \to \frac{k|e|}{r^2}$, which is the electric field due to the one net unit of charge from Z protons and $(Z-1)$ electrons.

As $r \to 0$, $|\vec{E}(r)| \to \frac{k|e|}{r^2}\left(1 + (Z-1)\right)$

$$= \frac{Zk|e|}{r^2},$$

which is the electric field due to the Z protons in the nucleus.

D.19 Ca $4s^2$ closed shell + 2 electrons
S $3s^2 3p^4$ closed shell −2 electrons
$\boxed{CaS}$

Ca $4s^2$ closed shell + 2
Cl $3s^2 3p^5$ closed shell −1
$\boxed{CaCl_2}$

Li $2s^1$ closed shell + 1
O $2s^2 2p^4$ closed shell −2
$\boxed{Li_2O}$

Na $3s^1$ closed shell + 1
P $3s^2 3p^3$ closed shell − 3
$\boxed{Na_3P}$

12.23 O $\underset{2s}{\uparrow\downarrow}$ $\underset{2p}{\uparrow\downarrow\ \uparrow\ \uparrow}$ 2 unpaired electrons
F $\underset{2s}{\uparrow\downarrow}$ $\underset{2p}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow}$ 1 unpaired electron
$\boxed{OF_2}$

N $\underset{2s}{\uparrow\downarrow}$ $\underset{2p}{\uparrow\ \uparrow\ \uparrow}$ 3 unpaired electrons
$\boxed{NF_3}$