8. Calculate $\langle \frac{1}{r} \rangle$ for 3p and 3d orbitals of a hydrogenic atom.

$$R_{3p}(r) = \frac{8}{27\sqrt{6}} Z^{3/2} \left(Zr - \frac{Z^2 r^2}{6}\right) e^{-Zr/3}$$

$$\left\langle \frac{1}{r} \right\rangle_{3p} = \int_0^\infty \frac{8^2}{27^2 \times 6} Z^3 \left(Zr - \frac{Z^2 r^2}{6}\right)^2 e^{-2Zr/3}\, r\, dr = \frac{Z^3 8^2}{27^2 \times 6} I$$

$$I = \int_0^\infty \left(Z^2 r^2 + \frac{Z^4 r^4}{6^2} - \frac{2Zr Z^2 r^2}{6}\right) e^{-2Zr/3}\, r\, dr = I_1 + I_2 + I_3$$

$$I_1 = Z^2 \frac{3!}{\left(\frac{2Z}{3}\right)^4} = \frac{6 \times 81}{16 Z^2} \quad : \quad Z^2 \int_0^\infty r^3 e^{-2Zr/3} dr$$

$$I_2 = \frac{Z^4}{6^2} \frac{5!}{\left(\frac{2Z}{3}\right)^6} = \frac{15 \times 81}{32 Z^2} \quad : \quad \frac{Z^4}{6^2} \int_0^\infty r^5 e^{-2Zr/3} dr$$

$$I_3 = -\frac{Z^3}{3} \frac{4!}{\left(\frac{2Z}{3}\right)^5} = -\frac{3 \times 81}{4 Z^2} \quad : \quad -\frac{Z^3}{3} \int_0^\infty r^4 e^{-2Zr/3} dr$$

$$\therefore I = \frac{3 \times 81}{32 Z^2} \qquad \therefore \left\langle \frac{1}{r} \right\rangle_{3p} = \frac{\cancel{Z^3}\, \cancel{8} \times 8}{\underset{3}{\cancel{27}} \times \underset{3}{\cancel{27}} \times \underset{2}{\cancel{6}}} \times \frac{\cancel{3} \times \cancel{81}}{\cancel{32}\, \cancel{Z^2}} = \frac{Z}{9} \text{ a.u.}$$

$$\left\langle \frac{1}{r} \right\rangle_{3d} = \frac{4^2}{81^2 \times 30} Z^7 \int_0^\infty r^5 e^{-2Zr/3} dr = \frac{16 \times Z^7}{81 \times 81 \times 30} \times \frac{5!\, 3^6}{2^6 Z^6}$$

$$= \frac{\cancel{16} \times \cancel{Z^7}}{\cancel{81} \times \underset{9}{\cancel{81}} \times \underset{2}{\cancel{30}}} \times \frac{\cancel{15} \times \cancel{81} \times \cancel{9}}{\cancel{8}\, \cancel{Z^6}} = \frac{Z}{9} \text{ a.u.}$$

The two integrals are equal. Is this expected?

How is the energy related to $\langle \frac{1}{r} \rangle$?