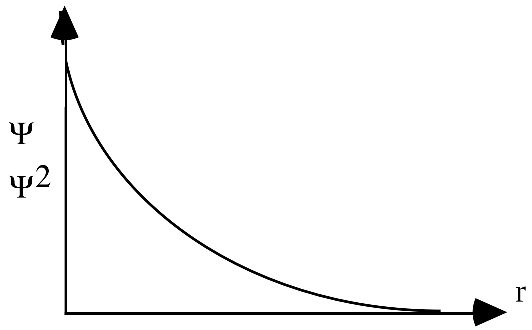
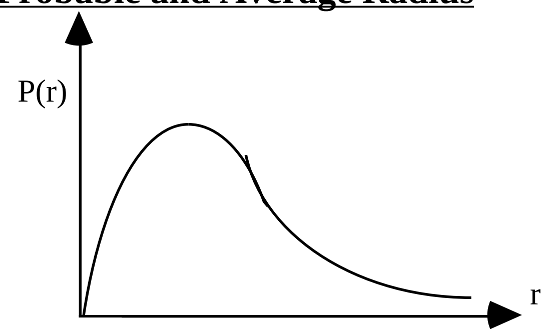
How Big is an Atom?: Most Probable and Average Radius





$$\Psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_o}\right)^{3/2} e^{-Zr/a_o}$$

radial probability distribution function:

$$P(r) = \int_o^{\pi}\int_o^{2\pi} \Psi^2\, r^2 \sin\theta\, d\theta\, d\phi = 4\pi r^2 \Psi^2$$

$$\text{volume of annular ring} = \int_o^{\pi}\int_o^{2\pi} r^2 \sin\theta\, dr\, d\theta\, d\phi = 4\pi r^2\, dr$$

most probable radius:

$$\frac{dP(r)}{dr} = 0 \qquad 4\pi\,\frac{1}{\pi}\left(\frac{Z}{a_o}\right)^3 \frac{d\, r^2 e^{-2Zr/a_o}}{dr} = 0$$

$$4\pi\,\frac{1}{\pi}\left(\frac{Z}{a_o}\right)^3 \left(2r - \frac{2r^2 Z}{a_o}\right) e^{-2Zr/a_o} = 0$$

$$\left(1 - \frac{r\,Z}{a_o}\right) = 0 \qquad r_{mp} = \frac{a_o}{Z} \qquad a_o = 0.529\text{Å}$$

expectation value of r: $\langle r\rangle = \int \Psi^* r\, \Psi\, d\tau \,/\, \int \Psi^*\Psi\, d\tau$

$$\langle r\rangle = 4\pi\,\frac{1}{\pi}\left(\frac{Z}{a_o}\right)^3 \int_o^{\infty} r^3 e^{-2Zr/a_o}\, dr$$

why r^3?

$$\int_0^{\infty} x^n e^{-ax}\, dx = \frac{n!}{a^{n+1}} = \frac{3!}{(2Z/a_o)^4}$$

$$\langle r\rangle = 4\pi\,\frac{1}{\pi}\left(\frac{Z}{a_o}\right)^3 \frac{6a_o^4}{16Z^4} = \frac{3}{2}\,\frac{a_o}{Z}$$