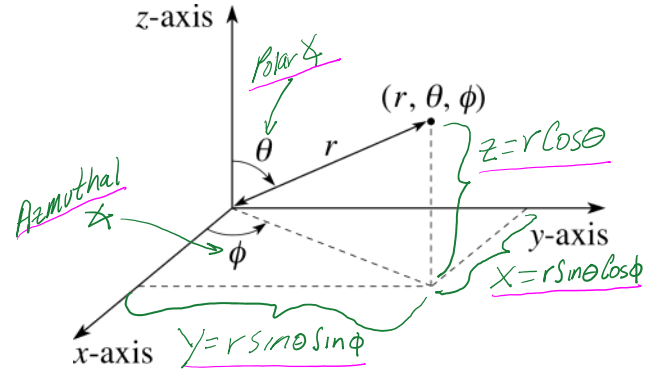


Normalizing WFs

Sunday, September 18, 2016 2:33 PM

$$\psi(r) = e^{-r/a_0}$$

Hydrogen atom
 r = radial distance
 a_0 = Bohr radius



$$dV = dr d\theta d\phi$$

$$dV = r^2 dr \sin\theta d\theta d\phi$$

$$\int dV = \int_0^\infty r^2 dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi$$

Normalizing a WF

$$\langle N\psi | N\psi \rangle = 1$$

$$\int N^* \psi^* N \psi dV = 1$$

$$|N|^2 \int \psi^* \psi dV = 1$$

$$\psi(r) = e^{-r/a_0}$$

$$|\psi(r)|^2 = e^{-2r/a_0}$$

$$|N|^2 \int_0^\infty r^2 e^{-2r/a_0} dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi = 1$$

$$\int_0^\infty r^2 e^{-ar} dr = \frac{2!}{a^3}$$

$$-[\cos\pi - \cos 0]$$

$$-[-1 - 1]$$

$$-(-2) = 2$$

$$= \frac{2}{\left(\frac{2}{a_0}\right)^3}$$

$$= \frac{a_0^3}{4}$$

$$|N|^2 \frac{a_0^3}{4} \cdot 2 \cdot 2\pi = 1$$

$$\frac{\pi |N|^2 a_0^3}{2} = 1 \quad \text{assume } N^* = N$$

Maxwell-Boltzmann Integral

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$\cdot ax \quad \text{let } a = \frac{2}{a_0}$$

...

$$N^2 = \frac{1}{\pi a_0^3}$$

$$N = \frac{1}{\sqrt{\pi a_0^3}}$$

$$\psi_n(r) = N \psi(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$