

9.21: Numerical Solutions for the Hydrogen Atom Radial Equation

Reduced mass: $\mu = 1$

Angular momentum: $L = 0$

Integration limit: $r_{\max} = 18$

Nuclear charge: $Z = 1$

Solve Schrödinger's equation numerically. Use Mathcad's ODE solve block:

Given

$$\frac{-1}{2\mu} \frac{d^2}{dr^2} \psi(r) - \frac{1}{r\mu} \frac{d}{dr} \psi(r) + \left[\frac{L(L+1)}{2\mu r^2} + \frac{1}{2} k r^2 \right] \psi(r) = E \psi(r) \quad \psi(.0001) = .1 \quad \psi'(.0001) = 0.1$$

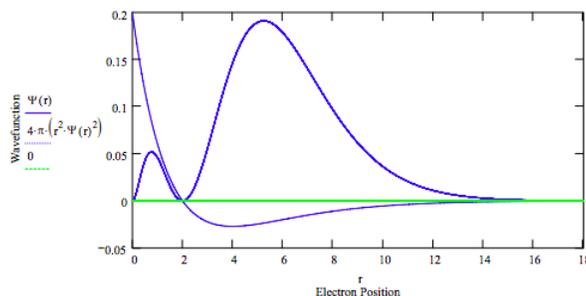
$$\psi = \text{Odesolve}(r, r_{\max})$$

Normalize wave function:

$$\psi(r) = \left(\int_0^{r_{\max}} \psi(r)^2 4\pi r^2 dr \right)^{-\frac{1}{2}} \psi(r)$$

Energy guess:

$E = -.125$ $r = 0, .001 \dots r_{\max}$



Calculate average position:

$$\int_0^{r_{\max}} \psi(r) r \psi(r) 4\pi r^2 dr = 5.997$$

Calculate kinetic energy:

$$\int_0^{r_{\max}} \psi(r) \left[\frac{-1}{2\mu} \frac{d^2}{dr^2} \psi(r) - \frac{1}{r\mu} \frac{d}{dr} \psi(r) + \left[\frac{L(L+1)}{2\mu r^2} \right] \psi(r) \right] 4\pi r^2 dr = 0.125$$

Calculate potential energy:

$$\int_0^{r_{\max}} \psi(r) \frac{-Z}{r} \psi(r) 4\pi r^2 dr = -0.25$$

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