9.21: Numerical Solutions for the Hydrogen Atom Radial Equation

Reduced mass: μ = 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

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

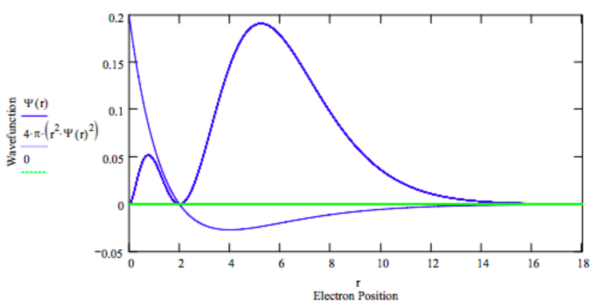
$$\psi = Odesolve(r, r_{max})$$

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 .. 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:

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