

Numerical Solutions for the Radial Equation of the Hydrogen Atom

Reduced mass: $\mu := 1$ Angular momentum: $L := 0$ Integration limit: $r_{\max} := 18$

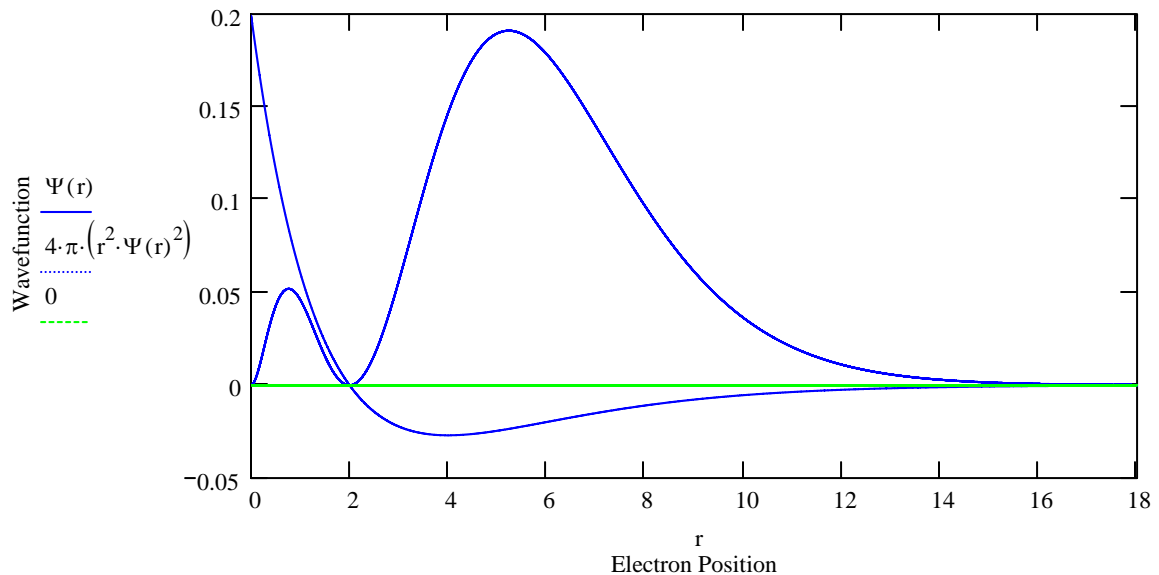
Nuclear charge: $Z := 1$

Solve Schrodinger's equation numerically use Mathcad's ODE solve block:

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

$\Psi := \text{Odesolve}(r, r_{\max})$ Normalize the wavefunction:
$$\Psi(r) := \left(\int_0^{r_{\max}} \Psi(r)^2 \cdot 4 \cdot \pi \cdot r^2 \, dr \right)^{\frac{-1}{2}} \cdot \Psi(r)$$

Energy guess: $E \equiv -.125$ $r := 0, .001 .. r_{\max}$



Calculate average position:
$$\int_0^{r_{\max}} \Psi(r) \cdot r \cdot \Psi(r) \cdot 4 \cdot \pi \cdot r^2 \, dr = 5.997$$

Calculate kinetic energy:
$$\int_0^{r_{\max}} \Psi(r) \cdot \left[\frac{-1}{2 \cdot \mu} \cdot \frac{d^2}{dr^2} \Psi(r) - \frac{1}{r \cdot \mu} \cdot \frac{d}{dr} \Psi(r) + \left[\frac{L \cdot (L + 1)}{2 \cdot \mu \cdot r^2} \right] \cdot \Psi(r) \right] \cdot 4 \cdot \pi \cdot r^2 \, dr = 0.125$$

Calculate potential energy:
$$\int_0^{r_{\max}} \Psi(r) \cdot \frac{-Z}{r} \cdot \Psi(r) \cdot 4 \cdot \pi \cdot r^2 \, dr = -0.25$$