

# Hydrogen Atom Calculation Assuming the Electron is a Particle in a Sphere of Radius R

Trial wave function:  $\Phi(r, R) := \frac{1}{\sqrt{2 \cdot \pi \cdot R}} \cdot \frac{\sin\left(\frac{\pi \cdot r}{R}\right)}{r}$       Integral:  $\int_0^{\infty} 4 \cdot \pi \cdot r^2 dr$

Kinetic energy operator:  $T = -\frac{1}{2 \cdot r} \cdot \frac{d^2}{dr^2}(r \cdot \Phi)$       Potential energy operator:  $V = -\frac{1}{r}$

Demonstrate the wave function is normalized.  $\int_0^R \Phi(r, R)^2 \cdot 4 \cdot \pi \cdot r^2 dr \rightarrow 1$

Set up the variational energy integral.

$$E(R) := \int_0^R \Phi(r, R) \cdot \left[ -\frac{1}{2 \cdot r} \cdot \frac{d^2}{dr^2}(r \cdot \Phi(r, R)) \right] \cdot 4 \cdot \pi \cdot r^2 dr + \int_0^R \Phi(r, R) \cdot \left[ -\frac{1}{r} \cdot \Phi(r, R) \right] \cdot 4 \cdot \pi \cdot r^2 dr$$

Minimize the energy with respect to the variational parameter R.

$R := 1$        $R := \text{Minimize}(E, R)$        $R = 4.049$        $E(R) = -0.301$

The exact ground state energy for the hydrogen atom is  $-0.5 E_h$ .

Calculate the percent error.

$$\frac{-0.5 - E(R)}{-0.5} = 39.793\%$$

Compare optimized trial wave function with the exact solution by plotting the radial distribution functions.

$S(r) := \frac{1}{\sqrt{\pi}} \cdot \exp(-r)$        $r := 0, .02.. 4.2$

