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

Trial wave function:

$$\Phi(r, R) := \frac{1}{\sqrt{2\pi R}} \frac{\sin(\frac{\pi r}{R})}{r}$$

Integral:

$$\int_0^\infty \blacksquare 4\pi r^2 dr$$

Kinetic energy operator:

$$T = \frac{1}{2r} \frac{d^2}{dr^2}(r\blacksquare)$$

Potential energy operator:

$$V = \frac{1}{r}$$

Demonstrate the wave function is normalized.

Set up the variational energy integral.

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

Minimize the energy with respect to the variational parameter R.

R := 1 R := Minimize(E, R) R = 4.049 E(R) = -0.301

The exact ground state energy for the hydrogen atom is -.5 E_h. Calculate the percent error.

$$\frac{-.5 - E(R)}{-.5} = 39.793$$

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

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