

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

Trial wave function:

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

Integral:

$$\int_0^{\infty} 4\pi r^2 dr$$

Kinetic energy operator:

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

Potential energy operator:

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

Demonstrate the wave function is normalized.

Set up the variational energy integral.

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

Minimize the energy with respect to the variational parameter R.

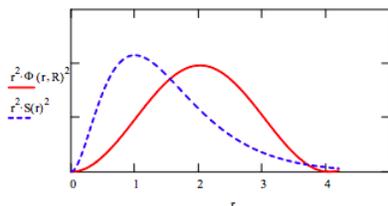
$$R := 1 \quad R := \text{Minimize}(E, R) \quad R = 4.049 \quad E(R) = -0.301$$

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.

$$S(r) := \frac{1}{\sqrt{\pi}} \exp(-r) \quad r := 0, .02, .4, 2$$



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