10.22: Variation Calculation on the 1D Hydrogen Atom Using a Gaussian Trial Wavefunction

The energy operator for this problem is:

$$\frac{-1}{2}\frac{d^2}{dx^2}\blacksquare - \frac{1}{x}\blacksquare$$

The trial wave function is:

$$\psi(x,\alpha) = 2(\frac{2\alpha}{\pi^{\frac{1}{3}}})(x)exp(-\alpha x^2)$$

Evaluate the energy integral.

$$E(\alpha) = \int_x^\alpha -\frac{1}{2}\frac{d^2}{dx^2}\psi(x,\alpha)dx + \int_0^\infty \frac{-1}{x}\psi(x,\alpha)^2 dx|_{simplify}^{assume,\,\alpha>0} \rightarrow \frac{-1}{2\pi^{\frac{1}{2}}}[(-3)\pi^{\frac{1}{2}}\alpha + (4)2^{\frac{1}{2}}\alpha^{\frac{1}{2}}]$$

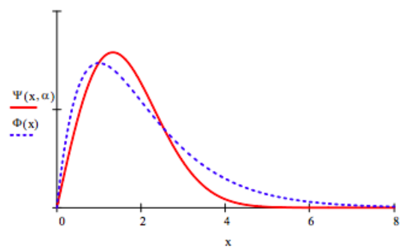
Minimize the energy with respect to the variational parameter α and report its optimum value and the ground-state energy.

α = 1 α = Minimize (E, α) α = 0.2829 E (α) = -0.4244

The exact ground state energy for the hydrogen atom is -0.5 E_h. Calculate the percent error.

$$\left|\frac{-0.5 - E(\alpha)}{-0.5}\right| = 15.1174$$

Plot the optimized trial wave function and the exact solution, $\Phi(x) = 2(x)exp(-x)$.



Find the distance from the nucleus within which there is a 95% probability of finding the electron.

α = 1. Given:

$$\int_0^a \psi(x,\alpha)^2 dx = .95$$

Find (a) = 2.6277

Find the most probable value of the position of the electron from the nucleus.

$$\alpha = 0.2829\frac{d}{dx}|\psi(x,\alpha)| = 0|_{float,\,3}^{solve,\,x} \rightarrow \begin{pmatrix} -1.33 \\ 1.33 \end{pmatrix}$$

Calculate the probability that the electron will be found between the nucleus and the most probable distance from the nucleus.

$$\int_0^{1.33} \psi(\alpha,x)^2 dx = 0.3584$$

Break the energy down into kinetic and potential energy contributions. Is the *virial theorem* obeyed?

$$T = \int_0^\infty \psi(x,\alpha)\frac{1}{2}\frac{d^2}{dx^2}\psi(x,\alpha)dx$$
$$= 0.4244$$

$$V = \int_0^\infty \frac{-1}{x}\psi(x,\alpha)^2 dx$$
$$= -0.8488$$
$$|\frac{V}{T}| = 2.00$$

Calculate the probability that tunneling is occurring.

Classical turning point:

$$E(\alpha) = \frac{-1}{x}|^{solve,\,x}_{float,\,3} \rightarrow 2.36$$

Tunneling probability:

$$\int_{2.36}^{\infty} \psi(x,\alpha)^2 dx = 0.0978$$