10.21: Variation Calculation on the 1D Hydrogen Atom Using a Trigonometric Trial Wave Function

The energy operator for this problem is:

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

The trial wave function:

$$\Psi(\alpha, x) := \frac{\sqrt{12\alpha^3}}{\pi}(x)sech(\alpha, x)$$

Evaluate the variational energy integral.

$$E(\alpha) := \int_0^\infty \Psi(\alpha, x) - \frac{1}{2}\frac{d^2}{dx^2}\Psi(\alpha, x)dx + \int_0^\infty \frac{-1}{x}\Psi(\alpha, x)^2 dx |_{simplify}^{assume,\ \alpha>0} \rightarrow \frac{1}{6}\alpha\frac{12\alpha_\alpha\pi^2 - 72ln(2)}{\pi^2}$$

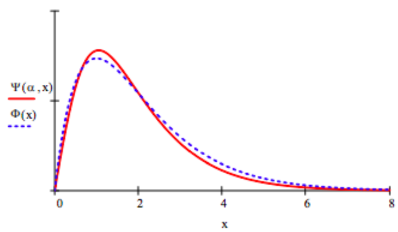
Minimize the energy with respect to the variational parameter α and report its optimum value and the ground-state energy.

α := 1 α := Minimize (E, α) α = 1.1410 E(α) = -0.4808

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

$$|\frac{-.5 - E(\alpha)}{-.5}| = 3.8401$$

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:

$$\int_0^a \Psi(\alpha, x)^2 dx = 0.95$$

Find (a) = 2.8754

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

$$\alpha := 1.1410 \quad \frac{d}{dx}|\frac{\sqrt{12\alpha^3}}{\pi}(x)sech(\alpha, x)| = 0 |_{float,\ 3}^{solve,\ x} \rightarrow 1.05$$

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

$$\int_0^{1.05} \Psi(\alpha, x)^2 dx = 0.3464$$

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

$$T := \int_0^\infty \Psi(\alpha, x)\frac{-1}{2}\frac{d^2}{dx^2}\Psi(\alpha, x)dx \quad T = 0.4808$$

$$V := \int_0^\infty \frac{-1}{x}\Psi(\alpha, x)^2 dx \quad V = -0.9616$$

$$|\frac{V}{T}| = 2.0000$$

Use the exact result to discuss the weakness of this trial function.

E_{exact} := -0.5

Using the virial theorem we know: T_{exact} := 0.500 V_{exact} := -1.00

Calculate the difference between the variational results and the exact calculation:

$E(\alpha) - E_{exact} = 0.0192$

$T - T_{exact} = -0.0192$

$V - V_{exact} = 0.0384$

The variational wave function yields a lower kinetic energy, but at the expense of a potential energy that is twice as unfavorable as the kinetic energy result is favorable.

Calculate the probability that tunneling is occurring.

Classical turning point:

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

Tunneling probability:

$$\int_{2.08}^{\infty} \Psi(\alpha, x)^2 dx = 0.1783$$