

Variation Method Calculation on a One-dimensional Model for the Hydrogen Atom Using a Gaussian Trial Wavefunction

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The energy operator for this problem is: $-\frac{1}{2} \cdot \frac{d^2}{dx^2} - \frac{1}{x}$

The trial wave function is: $\Psi(x, \alpha) := 2 \cdot \left(\frac{2 \cdot \alpha}{\pi} \right)^{\frac{3}{4}} \cdot x \cdot \exp(-\alpha \cdot x^2)$

Evaluate the variational energy integral.

$$E(\alpha) := \int_0^{\infty} \Psi(x, \alpha) \cdot \left[-\frac{1}{2} \cdot \frac{d^2}{dx^2} \Psi(x, \alpha) - \frac{1}{x} \cdot \Psi(x, \alpha) \right] dx + \int_0^{\infty} \frac{1}{x} \cdot \Psi(x, \alpha)^2 dx \quad \left| \begin{array}{l} \text{assume, } \alpha > 0 \\ \text{simplify} \end{array} \right. \rightarrow \frac{-1}{2 \cdot \pi^{\frac{1}{2}}} \cdot \left[(-3) \cdot \pi^{\frac{1}{2}} \cdot \alpha + 4 \cdot 2 \cdot \alpha^{\frac{1}{2}} \cdot \frac{1}{2} \right]$$

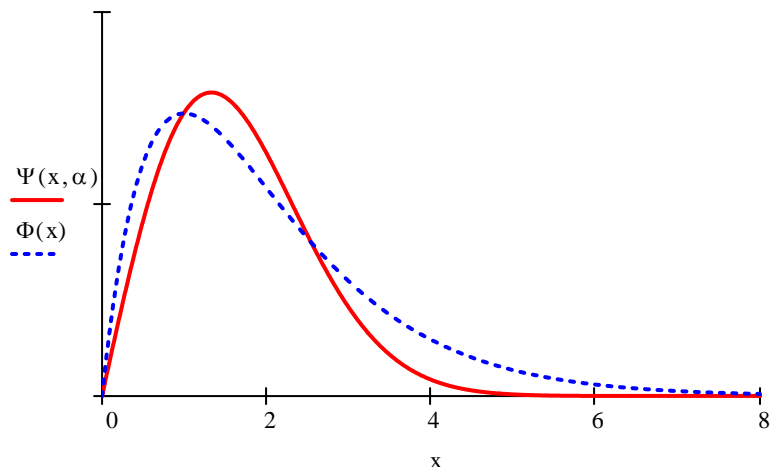
Minimize the energy with respect to the variational parameter α and report its optimum value and the ground-state energy.

$$\alpha := 1 \quad \alpha := \text{Minimize}(E, \alpha) \quad \alpha = 0.2829 \quad E(\alpha) = -0.4244$$

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, $\Phi(x) := 2 \cdot x \cdot \exp(-x)$.



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

$$a := 1 \quad \text{Given} \quad \int_0^a \Psi(x, \alpha)^2 dx = .95 \quad \text{Find}(a) = 2.6277$$

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

$$\alpha := 0.2829 \quad \frac{d}{dx} |\Psi(x, \alpha)| = 0 \quad \left| \begin{array}{l} \text{solve, } x \\ \text{float, } 3 \end{array} \right. \rightarrow \begin{pmatrix} 1.33 \\ -1.33 \end{pmatrix}$$

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?

$$T := \int_0^{\infty} \Psi(x, \alpha) \cdot \frac{1}{2} \cdot \frac{d^2}{dx^2} \Psi(x, \alpha) dx \quad T = 0.4244 \quad V := \int_0^{\infty} \frac{-1}{x} \cdot \Psi(x, \alpha)^2 dx \quad V = -0.8488$$

$$\left| \frac{V}{T} \right| = 2.00$$

Calculate the probability that tunneling is occurring.

Classical turning point: $E(\alpha) = \frac{-1}{x} \quad \left| \begin{array}{l} \text{solve, } x \\ \text{float, } 3 \end{array} \right. \rightarrow 2.36$ Tunneling probability: $\int_{2.36}^{\infty} \Psi(x, \alpha)^2 dx = 0.0978$

