

Variation Method Calculation on a One-dimensional Model for the Hydrogen Atom Using a Trigonometric 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: $\Psi(\alpha, x) := \frac{\sqrt{12 \cdot \alpha^3}}{\pi} \cdot x \cdot \operatorname{sech}(\alpha \cdot x)$

Evaluate the variational energy integral.

$$E(\alpha) := \int_0^{\infty} \Psi(\alpha, x) \cdot \left(-\frac{1}{2} \cdot \frac{d^2}{dx^2} \right) \Psi(\alpha, x) dx \dots \left| \begin{array}{l} \text{assume, } \alpha > 0 \\ \text{simplify} \end{array} \right. \rightarrow \frac{1}{6} \cdot \alpha \cdot \frac{12 \cdot \alpha + \alpha \cdot \pi^2 - 72 \cdot \ln(2)}{\pi^2}$$

$$+ \int_0^{\infty} \frac{-1}{x} \cdot \Psi(\alpha, x)^2 dx$$

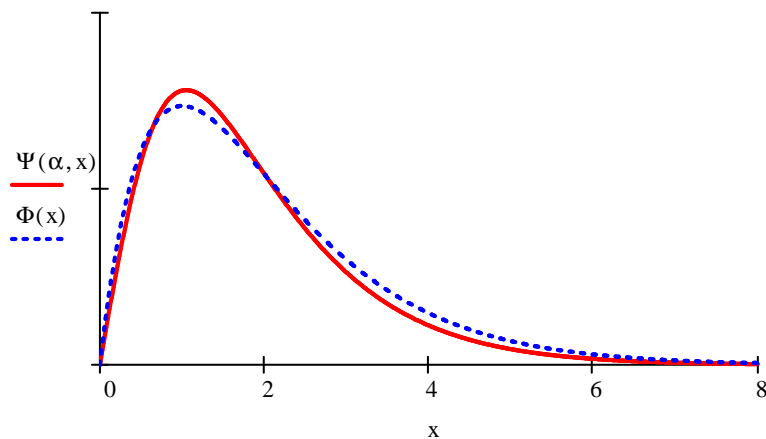
Minimize the energy with respect to the variational parameter α and report its optimum value and the ground-state energy.

$$\alpha := 1 \quad \alpha := \operatorname{Minimize}(E, \alpha) \quad \alpha = 1.1410 \quad E(\alpha) = -0.4808$$

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

$$\left| \frac{-0.5 - E(\alpha)}{-0.5} \right| = 3.8401 \%$$

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.

$$a := 1 \quad \text{Given} \quad \int_0^a \Psi(\alpha, x)^2 dx = .95 \quad \text{Find}(a) = 2.8746$$

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

$$\alpha := 1.1410 \quad \frac{d}{dx} \left| \frac{\sqrt{12 \cdot \alpha^3}}{\pi} \cdot x \cdot \operatorname{sech}(\alpha \cdot x) \right| = 0 \quad \left. \begin{array}{l} \text{solve, } x \\ \text{float, } 3 \end{array} \right\} \rightarrow 1.05$$

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?

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

$$V := \int_0^\infty \frac{-1}{x} \cdot \Psi(\alpha, x)^2 dx \quad V = -0.9616 \quad \left| \frac{V}{T} \right| = 2.0000$$

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

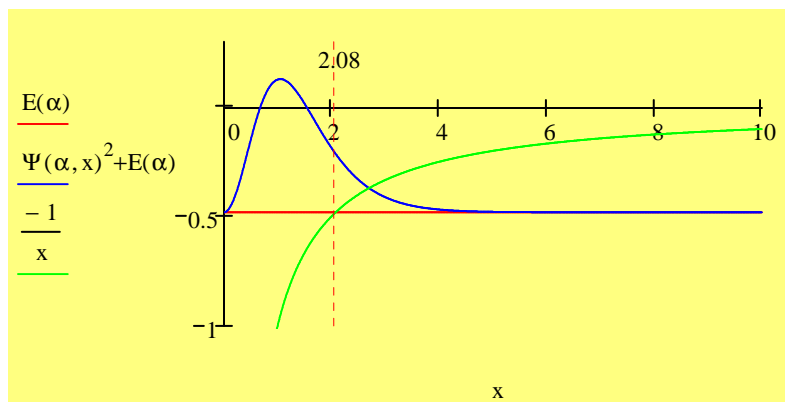
$$E_{\text{exact}} := -0.5 \quad \text{Using the virial theorem we know:} \quad T_{\text{exact}} := 0.500 \quad V_{\text{exact}} := -1.00$$

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

$$E(\alpha) - E_{\text{exact}} = 0.0192 \quad T - T_{\text{exact}} = -0.0192 \quad V - V_{\text{exact}} = 0.0384$$

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: $E(\alpha) = \frac{-1}{x} \left| \begin{array}{l} \text{solve, } x \\ \text{float, } 3 \end{array} \right. \rightarrow 2.08$ Tunneling probability: $\int_{2.08}^{\infty} \Psi(\alpha, x)^2 dx = 0.1783$