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:  
\[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{x}\]

The trial wave function is:  
\[\Psi(\alpha, x) := \sqrt{\frac{12 \alpha^3}{\pi}} x \cdot \text{sech}(\alpha \cdot x)\]

Evaluate the variational energy integral.

\[E(\alpha) := \int_{0}^{\infty} \Psi(\alpha, x) \left(\frac{1}{2} \frac{d^2}{dx^2} \Psi(\alpha, x)\right) dx + \int_{0}^{\infty} \frac{-1}{x} \cdot \Psi(\alpha, x)^2 dx \]

\[\text{assume, } \alpha > 0 \rightarrow \text{simplify} \rightarrow \frac{1}{6} \alpha ^2 - \frac{12 \cdot \alpha}{\pi^2} - \frac{72 \cdot \ln(2)}{\pi^2}\]

Minimize the energy with respect to the variational parameter \(\alpha\) and report its optimum value and the ground-state energy.

\[\alpha := 1 \quad \alpha := \text{Minimize}(E, \alpha) \quad \alpha = 1.1410 \quad E(\alpha) = -0.4808\]

The exact ground state energy for the hydrogen atom is \(-.5 E_h\). 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.

\[ a := 1 \quad \text{Given} \quad \int_{0}^{a} \Psi(\alpha, x)^{2} \, dx = 0.95 \quad \text{Find}(a) = 2.8746 \]

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

\[ \alpha := 1.1410 \quad \frac{d}{dx} \left| \frac{\sqrt{12} \cdot \alpha^3}{\pi} \cdot x \cdot \text{sech}(\alpha \cdot x) \right| = 0 \quad \text{solve}, x \quad \text{float}, 3 \rightarrow 1.05 \]

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?

\[ T := \int_{0}^{\infty} \Psi(\alpha, x) \cdot \frac{1}{2} \left( \frac{d^{2}}{dx^{2}} \Psi(\alpha, x) \right) \, dx \quad \text{T} = 0.4808 \]

\[ V := \int_{0}^{\infty} \frac{-1}{x} \Psi(\alpha, x)^{2} \, dx \quad \text{V} = -0.9616 \quad \frac{|V|}{T} = 2.0000 \]

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: \[ E(\alpha) = \frac{-1}{x} \quad \text{solve}, x \quad \text{float}, 3 \rightarrow 2.08 \quad \text{Tunneling probability:} \quad \int_{2.08}^{\infty} \Psi(\alpha, x)^{2} \, dx = 0.1783 \]
\[
\Psi(\alpha, x)^2 + E(\alpha) - \frac{1}{x}
\]