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

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

Evaluate the variational energy integral.

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

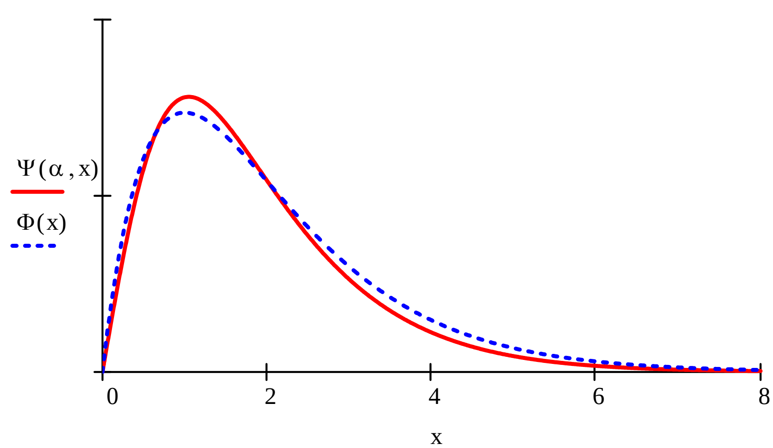
Minimize the energy with respect to the variational parameter $\alpha$ and report its optimum value and the ground-state energy.

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

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

$$\left|\frac{-.5 - E(\alpha)}{-.5}\right| = 3.8401\,\%$$

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.

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

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

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

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?

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

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

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

$E_{exact} := -0.5$ Using the virial theorm we know: $T_{exact} := 0.500$ $V_{exact} := -1.00$

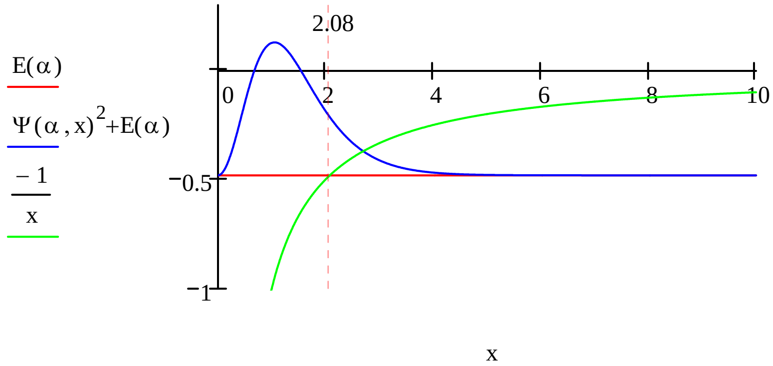
Calculate the difference between the variational results and the exact calculation:

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

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 occuring.

Classical turning point: $E(\alpha) = \frac{-1}{x} \ \Big|\begin{matrix}\text{solve}, x\\ \text{float}, 3\end{matrix} \rightarrow 2.08$ Tunneling probability: $\int_{2.08}^{\infty} \Psi(\alpha, x)^2\, dx = 0.1783$


E(α)
Ψ(α, x)^2+E(α)
−1/x
2.08
0
2
4
6
8
10
−0.5
−1
x