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

The trial wave function is: $\Psi(x,\alpha) := 2\cdot\left(\frac{2\cdot\alpha}{\pi^{\frac{1}{3}}}\right)^{\frac{3}{4}}\cdot x\cdot \exp\left(-\alpha\cdot x^2\right)$

Evaluate the variational energy integral.

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

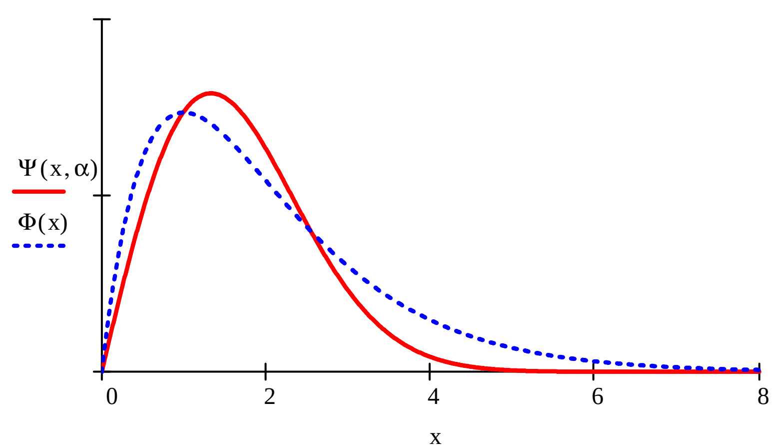
Minimize the energy with respect to the variational parameter α and report its optimum value and the ground-state energy.

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

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

$$\left|\frac{-.5 - E(\alpha)}{-.5}\right| = 15.1174\,\%$$

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.

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

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

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

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

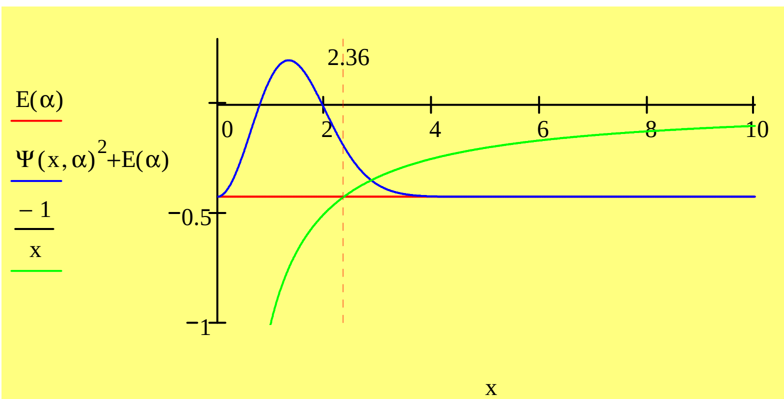
$$\int_0^{1.33} \Psi(\alpha, x)^2\,dx = 0.3584$$

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

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

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

Calculate the probability that tunneling is occuring.



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