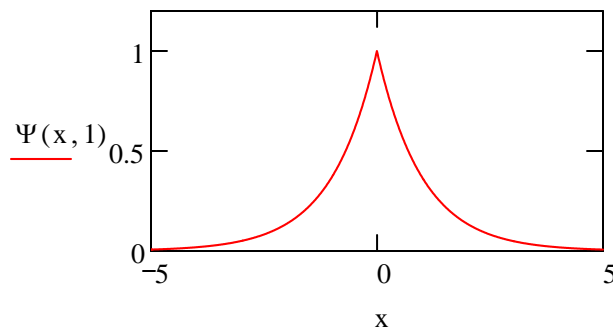


The One-dimensional Hydrogen Atom with a Delta Function Potential Energy Interaction Between the Proton and Electron

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The following normalized trial wave function is suggested for a variational calculation for the energy of a one-dimensional model of the hydrogen atom that postulates a delta-function potential energy interaction between the electron and the proton.

$$\Psi(x, \alpha) := \sqrt{\alpha} \cdot \exp(-\alpha \cdot |x|) \quad \int_{-\infty}^{\infty} \Psi(x, \alpha)^2 dx \text{ assume, } \alpha > 0 \rightarrow 1$$



The Hamiltonian energy operator in coordinate space is:

$$H = -\frac{1}{2} \cdot \frac{d^2}{dx^2} + \Delta(x)$$

The problem this tutorial seeks to solve is that it is obvious that the coordinate wave function is unsuitable for the calculation of the expectation value for kinetic energy because it is not well-behaved at $x = 0$. The wave function and its derivatives are discontinuous at $x = 0$. However, the expectation value for potential energy presents no problems in coordinate space.

Therefore the plan is to calculate the potential energy in coordinate space and then to Fourier transform the coordinate wave function into momentum space for the calculation of kinetic energy.

Calculation of Potential Energy in Coordinate Space

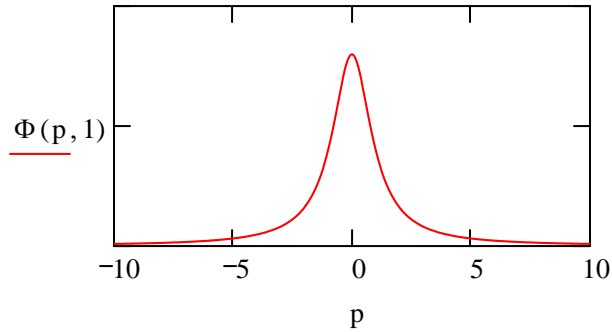
$$V(\alpha) := \int_{-\infty}^{\infty} \Psi(x, \alpha) \cdot \Delta(x) \cdot \Psi(x, \alpha) dx \rightarrow -\alpha$$

Fourier Transform of the Coordinate Space Wave Function into Momentum Space

$$\Phi(p, \alpha) := \int_{-\infty}^{\infty} \frac{\exp(-i \cdot p \cdot x)}{\sqrt{2 \cdot \pi}} \cdot \Psi(x, \alpha) dx \quad \left| \begin{array}{l} \text{assume, } \alpha > 0 \\ \text{simplify} \end{array} \right. \rightarrow \left(-\frac{1}{2} \right) \cdot \frac{\alpha^{\frac{3}{2}}}{(i \cdot p - \alpha) \cdot \pi^{\frac{1}{2}} \cdot (i \cdot p + \alpha)}$$

Before proceeding we demonstrate that the momentum space wave function is normalized and well-behaved.

$$\int_{-\infty}^{\infty} \Phi(p, \alpha)^2 dp \text{ assume, } \alpha > 0 \rightarrow 1$$



The kinetic energy operator in momentum space for an electron is: $\frac{p^2}{2}$

Therefore, the kinetic energy is:

$$T(\alpha) := \int_{-\infty}^{\infty} \Phi(p, \alpha) \cdot \frac{p^2}{2} \cdot \Phi(p, \alpha) dp \text{ assume, } \alpha > 0 \rightarrow \frac{1}{2} \cdot \alpha^2$$

Now the coordinate and momentum space calculations are combined and the total energy is minimized with respect to the variational parameter, α .

$$E(\alpha) := T(\alpha) + V(\alpha)$$

$$\alpha := .2 \quad \alpha := \text{Minimize}(E, \alpha) \quad \alpha = 1 \quad E(\alpha) = -0.5$$

The coordinate and momentum wave functions are compared below:

