

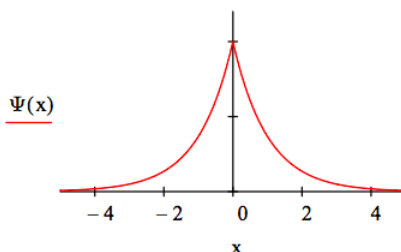
2.61: One-dimensional H-atom with Delta Function Potential

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

The energy Hamiltonian and a normalized wave function for the hydrogen atom with delta function interaction between the electron and proton is given below.

$$H = -\frac{1}{2} \frac{d^2}{dx^2} - \Delta(x) \quad \Psi(x) = \exp(-|x|) \quad \int_{-\infty}^{\infty} \Psi(x)^2 dx \rightarrow 1$$

The wave function is not well-behaved in coordinate space making the evaluation of kinetic energy tricky. However, the evaluation of potential energy is straight forward. So the strategy is to evaluate potential energy in coordinate space and kinetic energy in momentum space. The latter requires a Fourier transform of the coordinate space wave function.



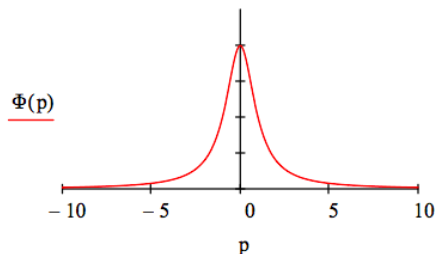
Calculation of Potential Energy in Coordinate Space

$$V = \int_{-\infty}^{\infty} \Psi(x) - \Delta(x) \Psi(x) dx \rightarrow -1$$

Fourier Transform of the Coordinate Wave Function into Momentum Space

$$\Psi(p) = \int_{-\infty}^{\infty} \frac{\exp(-i p x)}{\sqrt{2\pi}} \Psi(x) dx \text{ simplify } \rightarrow \frac{\sqrt{2}}{\sqrt{\pi} (p^2 + 1)}$$

Display the Momentum Wave Function to Show it is Well-behaved



Calculation of Kinetic Energy in Momentum Space

$$T = \int_{-\infty}^{\infty} \Phi(p) \frac{p^2}{2} \Phi(p) dp \text{ simplify } \rightarrow \frac{1}{2}$$

Calculation of Total Energy

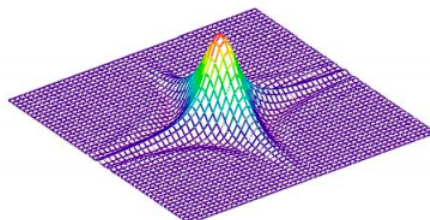
$$E = T + V \rightarrow E = -\frac{1}{2}$$

The Wigner Function

The Wigner phase-space distribution function is calculated using the momentum wave function.

$$W(x, p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \overline{\Phi\left(p + \frac{s}{2}\right)} \exp(-i s x) \Phi\left(p - \frac{s}{2}\right) ds$$

$$N = 50 \quad i = 0 \dots N \quad x_i = -4 + \frac{8i}{N} \quad j = 0 \dots N \quad p_j = -7 + \frac{14j}{N} \quad \text{Wigner}_{i,j} = W(x_i, p_j)$$



Wigner

Next we look at two variational calculations on the same system. The first involves a gaussian trial wave function, and the second a trigonometric trial wave function.

Gaussian Trial Wave Function

$$\Psi_1(x, \beta) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} \exp(-\beta x^2) \quad \int_{-\infty}^{\infty} \Psi_1(x, \beta)^2 dx \text{ assume, } \beta > 0 \rightarrow 1$$

Evaluation of Variational Energy Integral

$$E(\beta) = \int_{-\infty}^{\infty} \Psi_1(x, \beta) - \frac{1}{2} \frac{d^2}{dx^2} \Psi(x, \beta) dx \dots \text{assume, } \beta > 0 \rightarrow \frac{\beta}{2} - \frac{\sqrt{2}\sqrt{3}}{\sqrt{\pi}} + \int_{-\infty}^{\infty} -\Delta(x) \Psi_1(x, \beta)^2 dx$$

Energy Minimization With Respect to Variational Parameter

$$\frac{d}{d\beta} E(\beta) = 0 \text{ solve, } \beta \rightarrow \frac{2}{\pi} \quad E(\beta) \left| \begin{array}{l} \text{substitute, } \beta = \frac{2}{\pi} \\ \text{simplify} \end{array} \right. \rightarrow -\frac{1}{\pi} = -0.318$$

Error

$$\left| \frac{-0.318 + 0.5}{-0.5} \right| = 36.4\%$$

Trigonometric Trial Wave Function

$$\Psi_2(x, \beta) = \sqrt{\frac{\beta}{2}} \text{sech}(\beta x)$$

Evaluation of Variational Energy Integral

$$E(\beta) = \int_{-\infty}^{\infty} \Psi_2(x, \beta) - \frac{1}{2} \frac{d^2}{dx^2} \Psi_2(x, \beta) dx \dots \left| \begin{array}{l} \text{assume, } \beta > 0 \\ \text{simplify} \end{array} \right. \rightarrow \frac{\beta(\beta-3)}{6} + \int_{-\infty}^{\infty} -\Delta(x) \Psi_2(x, \beta)^2 dx$$

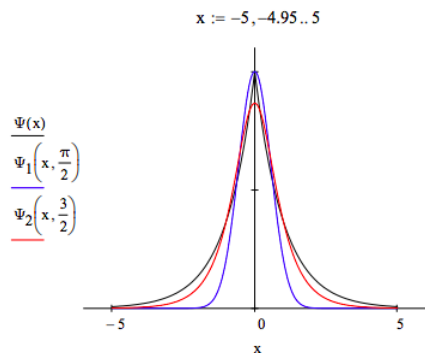
Energy Minimization With Respect to Variational Parameter

$$\frac{d}{d\beta} E(\beta) = 0 \text{ solve, } \beta \rightarrow \frac{3}{2} \quad E(\beta) \left| \begin{array}{l} \text{substitute, } \beta = \frac{3}{2} \\ \text{simplify} \end{array} \right. \rightarrow -\frac{3}{8} = -0.375$$

Error

$$\left| \frac{-0.375 + 0.5}{-0.5} \right| = 25\%$$

Graphical Comparison of Exact Wave Function with Trial Wave Function



This graphical comparison is consistent with the variational results presented above. The trigonometric trial function more closely resembles the exact wave function.

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