

Variational Methods: The ABS(X) Potential in Momentum Space

The energy operator in atomic units in coordinate space for a unit mass particle with potential energy $V = |x|$ is given below.

$$H = -\frac{1}{2} \cdot \frac{d^2}{dx^2} + |x| \quad \text{Suggested trial wave function: } \Psi(x, \beta) := \left(\frac{2 \cdot \beta}{\pi}\right)^{\frac{1}{4}} \cdot \exp(-\beta \cdot x^2)$$

Demonstrate that the wave function is normalized. $\int_{-\infty}^{\infty} \Psi(x, \beta)^2 dx$ assume, $\beta > 0 \rightarrow 1$

Carry out Fourier transform to get momentum wave function:

$$\Phi(p, \beta) := \frac{1}{\sqrt{2 \cdot \pi}} \cdot \int_{-\infty}^{\infty} \exp(-i \cdot p \cdot x) \cdot \Psi(x, \beta) dx \quad \left| \begin{array}{l} \text{assume, } \beta > 1 \\ \text{simplify} \end{array} \right. \rightarrow \frac{1}{2} \cdot \frac{2^{\frac{3}{4}}}{\pi^{\frac{1}{4}}} \cdot \frac{e^{-\frac{1}{4} \cdot \frac{p^2}{\beta}}}{\beta^{\frac{1}{4}}}$$

Demonstrate that the momentum wave function is normalized. $\int_{-\infty}^{\infty} \overline{\Phi(p, \beta)} \cdot \Phi(p, \beta) dp$ assume, $\beta > 0 \rightarrow 1$

The energy operator in momentum space is: $H = \frac{p^2}{2} + \left| i \cdot \frac{d}{dp} \right|$

Evaluate the variational energy integral.

$$E(\beta) := \int_{-\infty}^{\infty} \overline{\Phi(p, \beta)} \cdot \frac{p^2}{2} \cdot \Phi(p, \beta) dp + \int_{-\infty}^{\infty} \overline{\Phi(p, \beta)} \cdot \left| i \cdot \frac{d}{dp} \Phi(p, \beta) \right| dp \quad \left| \begin{array}{l} \text{assume, } \beta > 0 \\ \text{simplify} \end{array} \right. \rightarrow \frac{1}{2} \cdot \frac{\pi^{\frac{1}{2}} \cdot \beta^{\frac{3}{2}}}{\beta^2 \cdot \pi^2} + 2^{\frac{1}{2}}$$

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

$$\beta := 1 \quad \beta := \text{Minimize}(E, \beta) \quad \beta = 0.542 \quad E(\beta) = 0.813$$

Plot the coordinate and momentum wave functions and the potential energy on the same graph.

