Approximate Methods: The Quartic Oscillator

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For unit mass the quartic oscillator has the following energy operator in atomic units.

\[ H = -\frac{1}{2} \frac{d^2}{dx^2} + k \cdot x^4 \quad \int_{-\infty}^{\infty} \frac{1}{x} \, dx \]

Suggested trial wave function:

\[ \psi(x, \beta) := \left( \frac{2\beta}{\pi} \right)^{\frac{1}{4}} \cdot \exp\left(-\beta x^2\right) \]

Demonstrate that the wave function is normalized.

\[ \int_{-\infty}^{\infty} \psi(x, \beta)^2 \, dx \quad \text{assume,} \quad \beta > 0 \quad \rightarrow 1 \]

Evaluate the variational energy integral.

\[ E(\beta) := \int_{-\infty}^{\infty} \psi(x, \beta) \cdot \frac{1}{2} \frac{d^2}{dx^2} \psi(x, \beta) \, dx + \int_{-\infty}^{\infty} \psi(x, \beta) \cdot x^4 \cdot \psi(x, \beta) \, dx \quad \text{assume,} \quad \beta > 0 \quad \rightarrow \frac{1}{16} \frac{8\beta^3 + 3}{\beta^2} \]

Minimize the energy with respect to the variational parameter \( \beta \) and report its optimum value and the ground-state energy.

\[ \beta := 1 \quad \beta := \text{Minimize}(E, \beta) \quad \beta = 0.90856 \quad E(\beta) = 0.68142 \]

Plot the optimum wave function and the potential energy on the same graph.

Calculate the classical turning point and the probability that tunneling is occurring.

\[ x_{\text{ctp}} := 0.68142 \quad x_{\text{ctp}} = 0.90856 \quad 2 \int_{x_{\text{ctp}}}^{\infty} \psi(x, \beta)^2 \, dx = 0.083265 \]
Compare the variational result to energy obtained by numerically integrating Schrödinger's equation for the quartic oscillator by using the numerical integration algorithm provided below.

**Numerical Solutions for Schrödinger's Equation**

Integration limit: \( x_{\text{max}} := 3 \)

Effective mass: \( \mu := 1 \)

Force constant: \( k := 1 \)

Potential energy: \( V(x) := k \cdot x^4 \)

Numerical integration of Schrödinger's equation:

Given

\[
-\frac{1}{2 \mu} \frac{d^2 \Phi(x)}{dx^2} + V(x) \cdot \Phi(x) = \text{Energy} \cdot \Phi(x) \quad \Phi(-x_{\text{max}}) = 0 \quad \Phi'(-x_{\text{max}}) = 0.1
\]

\( \Phi := \text{Odesolve}(x, x_{\text{max}}) \)

Normalize wave function: \( \Phi(x) := \frac{\Phi(x)}{\sqrt{\int_{-x_{\text{max}}}^{x_{\text{max}}} \Phi(x)^2 \, dx}} \)

Enter energy guess: Energy = 0.6679864

Compare the variational and numerical solutions for the quartic oscillator by putting them on the same graph.

Also compare the energies for the two methods:

\[
\frac{E(\beta) - \text{Energy}}{E(\beta)} = 1.97\%
\]