Approximate Methods: The Quartic Oscillartor

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

$$H = -\frac{1}{2}\cdot\frac{d^2}{dx^2}\blacksquare + k\cdot x^4\cdot\blacksquare \qquad \int_{-\infty}^{\infty}\blacksquare\,dx$$

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

Demonstrate that the wave function is normalized.

$$\int_{-\infty}^{\infty}\Psi(x,\beta)^2\,dx \text{ assume}, \beta > 0 \;\rightarrow 1$$

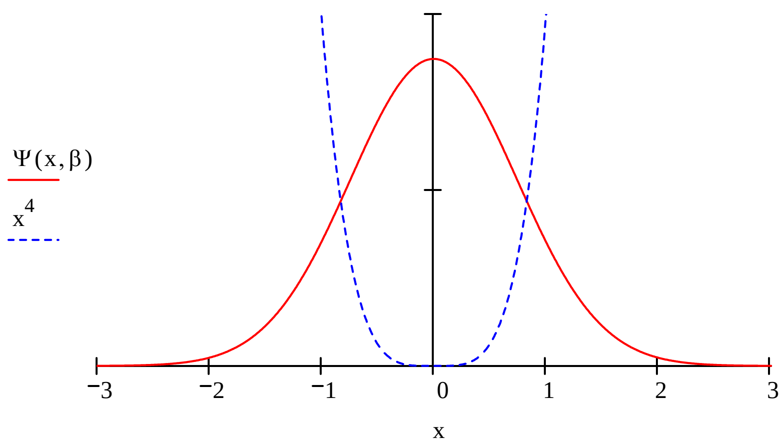
Evaluate the variational energy integral.

$$E(\beta) := \int_{-\infty}^{\infty}\Psi(x,\beta)\cdot-\frac{1}{2}\cdot\frac{d^2}{dx^2}\Psi(x,\beta)\,dx + \int_{-\infty}^{\infty}\Psi(x,\beta)\cdot x^4\cdot\Psi(x,\beta)\,dx \;\Bigg|\begin{array}{l}\text{assume}, \beta > 0\\ \text{simplify}\end{array} \rightarrow \frac{1}{16}\cdot\frac{8\cdot\beta^3 + 3}{\beta^2}$$

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

$\beta := 1 \qquad \beta := \text{Minimize}(E,\beta) \qquad \beta = 0.90856 \qquad E(\beta) = 0.68142$

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



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

$x_{ctp} := 0.68142^{\frac{1}{4}} \qquad x_{ctp} = 0.90856 \qquad 2\cdot\int_{x_{ctp}}^{\infty}\Psi(x,\beta)^2\,dx = 0.083265$

Compare the variational result to energy obtained by numerically integrating Schrodinger's equation for the quartic oscillator by using the numerical integration algorithm provided below.

Numerical Solutions for Schrodinger's Equation

Integration limit: $x_{max} := 3$ Effective mass: $\mu := 1$ Force constant: $k := 1$

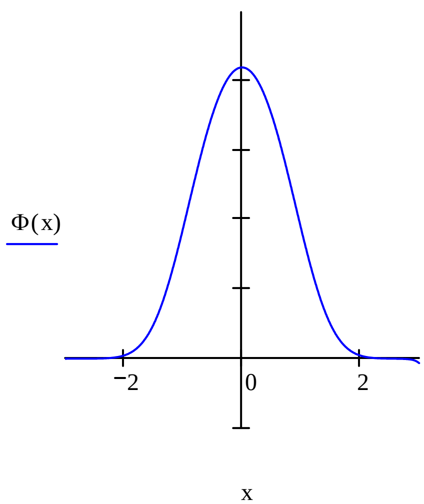
Potential energy: $V(x) := k \cdot x^4$

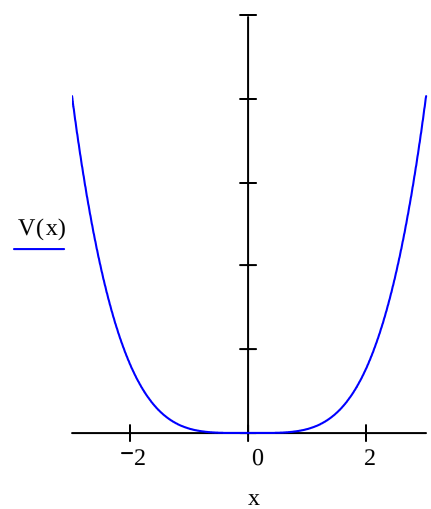
Numerical integration of Schrodinger's equation:

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

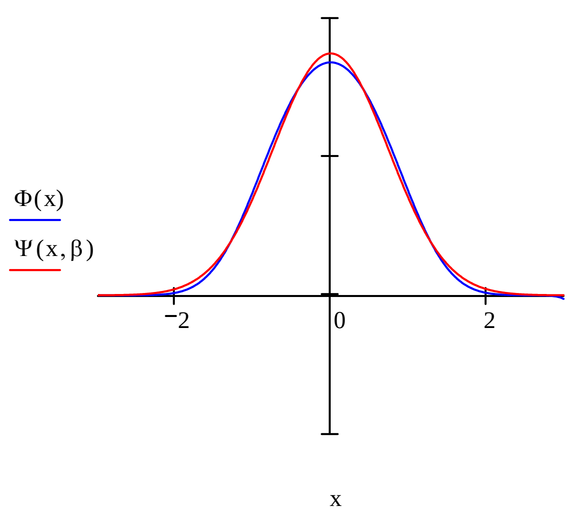
$\Phi := Odesolve(x, x_{max})$ Normalize wave function: $\Phi(x) := \frac{\Phi(x)}{\sqrt{\int_{-x_{max}}^{x_{max}} \Phi(x)^2 \, dx}}$

Enter energy guess: $Energy \equiv .6679864$





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:

$\frac{E(\beta) - Energy}{E(\beta)} = 1.97\,\%$