Variational Approach to the Harmonic Oscillator

This exercise deals with a variational treatment for the ground state of the simple harmonic oscillator which is, of course, an exactly soluble quantum mechanical problem.

The energy operator for a harmonic oscillator with unit effective mass and force constant is:

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

The following trial wave function is selected: $\Psi(x,\beta) := \frac{1}{1+\beta\cdot x^2}$

The variational energy integral is evaluated (because of the symmetry of the problem it is only necessary to integrate from 0 to ∞, rather than from -∞ to ∞:

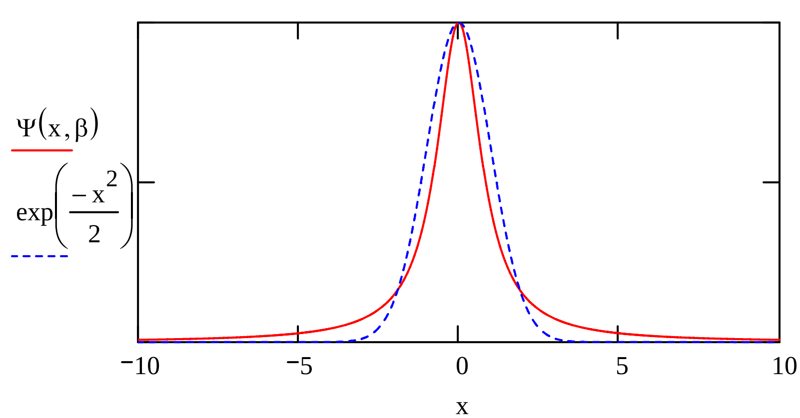
$$E(\beta) := \frac{\int_0^{\infty} \Psi(x,\beta)\cdot\frac{-1}{2}\cdot\frac{d^2}{dx^2}\Psi(x,\beta)\,dx + \int_0^{\infty} \Psi(x,\beta)\cdot\frac{x^2}{2}\cdot\Psi(x,\beta)\,dx}{\int_0^{\infty} \Psi(x,\beta)^2\,dx} \;\Bigg|\; \begin{array}{l}\text{assume}, \beta > 0 \\ \text{simplify}\end{array} \rightarrow \frac{1}{4}\cdot\frac{\beta^2+2}{\beta}$$

The energy integral is minimized with respect to the variational parameter:

$\beta := 1$ $\quad\beta := \text{Minimize}(E,\beta)$ $\quad\beta = 1.414$ $\quad E(\beta) = 0.707$

The % error is calculated given that the exact result is 0.50 E_h. $\quad \frac{E(\beta) - 0.5}{0.5} = 41.421\,\%$

The optimized trial wave function is compared with the SHO ground-state eigenfunction.



Now a second trial function is chosen:

$$\Psi(x,\beta) := \frac{1}{\left(1+\beta\cdot x^2\right)^2}$$

Evaluate the variational energy integral:

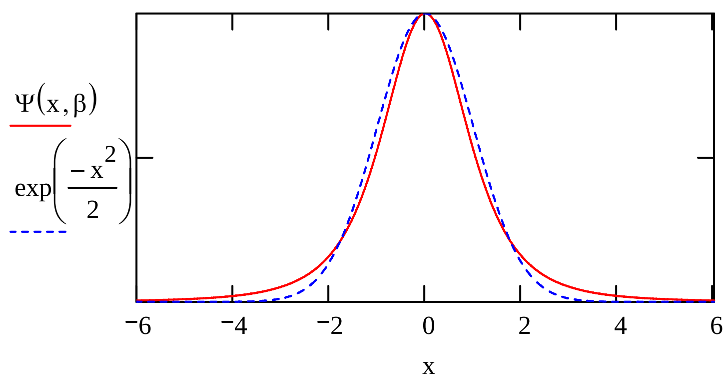
$$E(\beta) := \frac{\displaystyle\int_0^\infty \Psi(x,\beta)\cdot\frac{-1}{2}\cdot\frac{d^2}{dx^2}\Psi(x,\beta)\,dx + \int_0^\infty \Psi(x,\beta)\cdot\frac{x^2}{2}\cdot\Psi(x,\beta)\,dx}{\displaystyle\int_0^\infty \Psi(x,\beta)^2\,dx} \quad \begin{array}{|l} \text{assume}, \beta > 0 \\ \text{simplify} \end{array} \rightarrow \frac{1}{10}\cdot\frac{7\cdot\beta^2+1}{\beta}$$

Minimize the energy integral with respect to the variational parameter:

$\beta := 1$ $\beta := \text{Minimize}(E,\beta)$ $\beta = 0.378$ $E(\beta) = 0.529$

Calculate the % error given that the exact result is 0.50 E_h. $\frac{E(\beta)-0.5}{0.5} = 5.83\,\%$

The optimized trial wave function is compared with the SHO ground-state eigenfunction.



Suggestion: Continue this exercise with the following trial wave function and interpret the improved agreement with the exact solution.

$$\Psi(x,\beta) = \frac{1}{\left(1+\beta\cdot x^2\right)^n}$$

where n is an integer greater than 2.