10.17: Variation Method for 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:

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

The following trial wavefunction is selected:

$$\psi(x,\beta) = \frac{1}{1+\beta x^2}$$

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 ∞:

$$E(\beta) = \frac{\int_0^\infty \psi(x,\beta)\frac{-1}{2}\frac{d^2}{dx^2}\psi(x,\beta)dx + \int_0^\infty \psi(x,\beta)\frac{x^2}{2}\psi(x,\beta)dx}{\int_0^\infty \psi(x,\beta)^2 dx}\Big|_{simplify}^{assume,\ \beta>0} \rightarrow \frac{1}{4}\frac{\beta^2+2}{\beta}$$

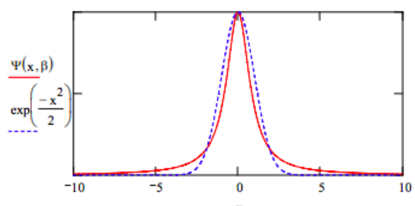
The energy integral is minimized with respect to the variational parameter:

β := 1 β := Minimize (E, β) β = 1.414 E(β) = 0.707

The % error is calculated given that the exact result is $0.50E_h$.

$$\frac{E(\beta)-0.5}{0.5} = 41.421\%$$

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



Now a second trial function is chosen:

$$\psi(x,\beta) := \frac{1}{(1+\beta x^2)^2}$$

Evaluate the variational energy integral:

$$E(\beta) := \frac{\int_0^\infty \psi(x,\beta)\frac{-1}{2}\frac{d^2}{dx^2}\psi(x,\beta)dx + \int_0^\infty \psi(x,\beta)\frac{x^2}{2}\psi(x,\beta)dx}{\int_0^\infty \psi(x,\beta)^2 dx}\Big|_{simplify}^{assume,\ \beta>0} \rightarrow \frac{1}{10}\frac{7\beta^2+1}{\beta}$$

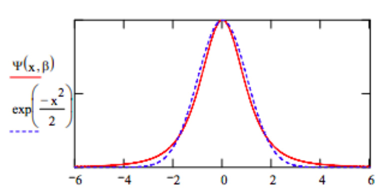
Minimize the energy integral with respect to the variational parameter:

β := 1 β := Minimize (E, β) β = 0.378 E(β) = 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 wavefunction is compared with the SHO ground-state eigenfunction.



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

$$\psi(x, \beta) - \frac{1}{(1+\beta x^2)^n}$$

where n is an integer greater than 2.
