

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:

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

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 $-\infty$ to ∞):

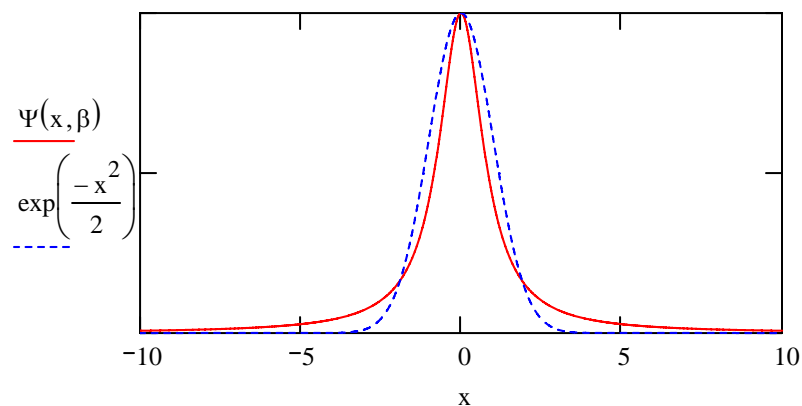
$$E(\beta) := \frac{\int_0^{\infty} \Psi(x, \beta) \cdot \frac{-1}{2} \cdot \frac{d^2}{dx^2} \Psi(x, \beta) dx + \int_0^{\infty} \Psi(x, \beta) \cdot \frac{x^2}{2} \cdot \Psi(x, \beta) dx}{\int_0^{\infty} \Psi(x, \beta)^2 dx} \quad \left| \begin{array}{l} \text{assume, } \beta > 0 \\ \text{simplify}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

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

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

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

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



Now a second trial function is chosen:

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

Evaluate the variational energy integral:

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

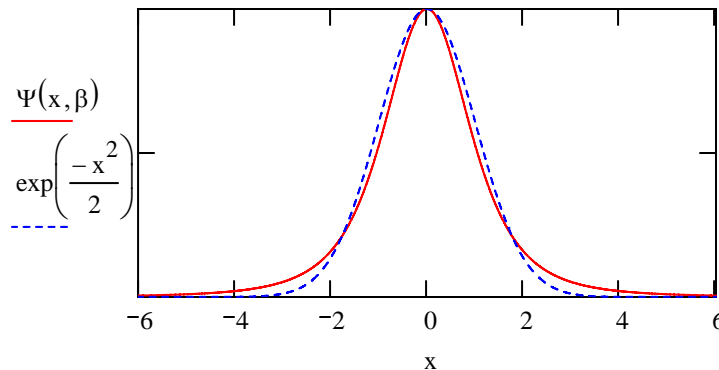
Minimize the energy integral with respect to the variational parameter:

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

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.

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

where n is an integer greater than 2.