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:

\[
H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{x^2}{2}
\]

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 ∞):

\[
E(\beta) = \frac{\int_0^{\infty} \psi(x, \beta) \frac{-1}{2} \frac{d^2}{dx^2} \psi(x, \beta) dx + \int_0^{\infty} \psi(x, \beta) \frac{x^2}{2} \psi(x, \beta) dx}{\int_0^{\infty} \psi(x, \beta)^2 dx} \bigg|_{\beta > 0} \rightarrow \frac{1}{4} \frac{\beta^2 + 2}{\beta}
\]

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

\[
\beta = 1.414 \quad E(\beta) = 0.707
\]

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

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

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:

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

Minimize the energy integral with respect to the variational parameter:

\[ \langle \beta \rangle := 1 \langle \beta \rangle := \text{Minimize} (E, \langle \beta \rangle) \langle \beta \rangle = 0.378 \quad E(\langle \beta \rangle) = 0.529 \]

Calculate the % error given that the exact result is 0.50 \( E_h \).

\[ \left( \frac{E(\beta) - 0.5}{0.5} \right) \times 100 = 5.83\% \]

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

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

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

\[ \langle \psi(x, \beta) - \frac{1}{(1 + \beta x^2)^n} \rangle \]

where \( n \) is an integer greater than 2.