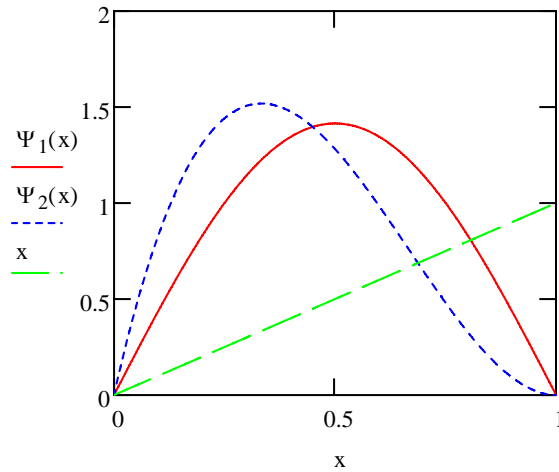


Trial Wave Function for Particle in Slanted Box

Trial wave functions: $\Psi_1(x) := \sqrt{2} \cdot \sin(\pi \cdot x)$ $\Psi_2(x) := \sqrt{105} \cdot x \cdot (1 - x)^2$

Plot trial wave functions and potential energy. x := 0, .005 .. 1



Evaluate matrix elements:

$$S_{11} := \int_0^1 \Psi_1(x)^2 dx \quad S_{11} = 1 \quad S_{12} := \int_0^1 \Psi_1(x) \cdot \Psi_2(x) dx \quad S_{12} = 0.9347 \quad S_{22} := \int_0^1 \Psi_2(x)^2 dx \quad S_{22} = 1$$

$$H_{11} := \int_0^1 \Psi_1(x) \cdot \left(-\frac{1}{2} \cdot \frac{d^2}{dx^2} \Psi_1(x) \right) dx + \int_0^1 \Psi_1(x) \cdot x \cdot \Psi_1(x) dx \quad H_{11} = 5.4348$$

$$H_{12} := \int_0^1 \Psi_1(x) \cdot \left(-\frac{1}{2} \cdot \frac{d^2}{dx^2} \Psi_2(x) \right) dx + \int_0^1 \Psi_1(x) \cdot x \cdot \Psi_2(x) dx \quad H_{12} = 5.0163$$

$$H_{22} := \int_0^1 \Psi_2(x) \cdot \left(-\frac{1}{2} \cdot \frac{d^2}{dx^2} \Psi_2(x) \right) dx + \int_0^1 \Psi_2(x) \cdot x \cdot \Psi_2(x) dx \quad H_{22} = 7.375$$

Solve the secular equations and normalization constraint for the energy and coefficients.

Seed values for energy and coefficients: $E := 5$ $c_1 := .5$ $c_2 := .5$

Given $(H_{11} - E \cdot S_{11}) \cdot c_1 + (H_{12} - E \cdot S_{12}) \cdot c_2 = 0$ $(H_{12} - E \cdot S_{12}) \cdot c_1 + (H_{22} - E \cdot S_{22}) \cdot c_2 = 0$

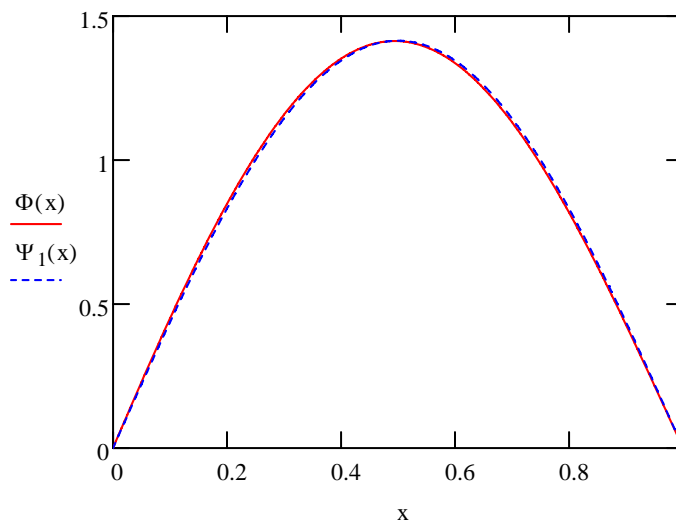
$$c_1^2 \cdot S_{11} + 2 \cdot c_1 \cdot c_2 \cdot S_{12} + c_2^2 \cdot S_{22} = 1$$

$$\begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} := \text{Find}(E, c_1, c_2)$$

$$\begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 5.4328 \\ 0.971 \\ 0.031 \end{pmatrix}$$

Compare variational ground state to PIB ground state:

$$\Phi(x) := c_1 \cdot \Psi_1(x) + c_2 \cdot \Psi_2(x)$$



Calculate average position of the particle in the box:

$$\int_0^1 x \cdot \Phi(x)^2 dx = 0.496$$

Calculate the probability that the particle is in the left half of the box:

$$\int_0^{.5} \Phi(x)^2 dx = 0.5088$$