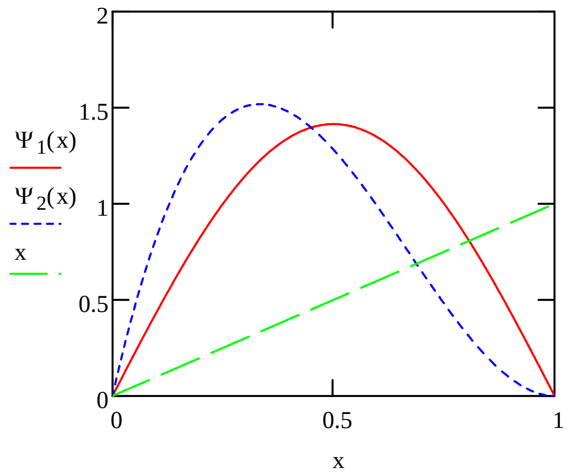
Trial Wave Function for Particle in Slanted Box

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:

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

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

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

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

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

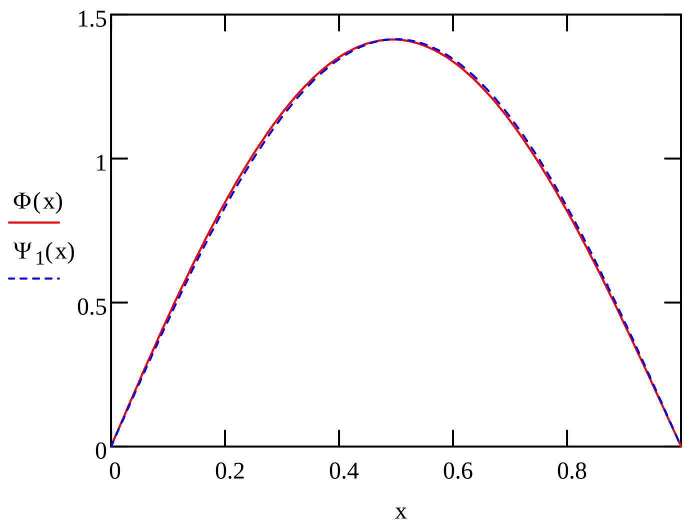
Seed values for energy and coefficients: $E := 5$ $c_1 := .5$ $c_2 := .5$

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

$c_1^2 \cdot S_{11} + 2 \cdot c_1 \cdot c_2 \cdot S_{12} + c_2^2 \cdot S_{22} = 1$ $\begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} := \mathrm{Find}(E, c_1, c_2)$ $\begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 5.4328 \\ 0.971 \\ 0.031 \end{pmatrix}$

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