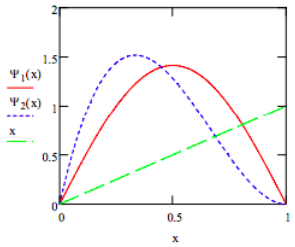
10.11: Linear Variational Method for a Particle in a Slanted 1D Box

Trial wavefunctions:

- $\psi_1(x) = \sqrt{2}\sin(\pi x)$
- $\psi_2(x) = \sqrt{105}x(1-x)^2$

Plot trial wavefunctions and potential energy. x = 0, .005 ... 1



Evaluate matrix elements:

$$S_{11} = \int_0^1 \psi_1(x)^2 dx \tag{10.11.1}$$

$$= 1 \tag{10.11.2}$$

$$S_{12} = \int_0^1 \psi_1(x)\psi_2(x) dx \tag{10.11.3}$$

$$= 0.9347 \tag{10.11.4}$$

$$S_{22} = \int_0^1 \psi_2(x)^2 dx \tag{10.11.5}$$

$$= 1 \tag{10.11.6}$$

$$H_{11} = \int_0^1 \psi_1(x)(-\tfrac{1}{2})\tfrac{d^2}{dx^2}\psi_1(x)dx + \int_0^1 \psi_1(x)\ x\ \psi_1(x)dx \quad H_{11} = 5.4348$$

$$H_{12} = \int_0^1 \psi_1(x)(-\tfrac{1}{2})\tfrac{d^2}{dx^2}\psi_2(x)dx + \int_0^1 \psi_1(x)\ x\ \psi_2(x)dx \quad H_{12} = 5.0163$$

$$H_{22} = \int_0^1 \psi_2(x)(-\tfrac{1}{2})\tfrac{d^2}{dx^2}\psi_2(x)dx + \int_0^1 \psi_2(x)\ x\ \psi_2(x)dx \quad H_{22} = 7.375$$

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

$$(H_{11} - ES_{11})c_1 + (H_{12} - ES_{12})c_2 = 0$$

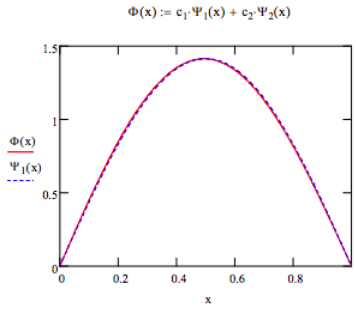
$$(H_{12} - ES_{12})c_1 + (H_{22} - ES_{22})c_2 = 0$$

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

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

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

Compare variational ground state to PIB ground state:



Calculate average position of the particle in the box:

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

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

$$\int_0^{0.5} \Phi(x)^2 dx = 0.5088$$

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