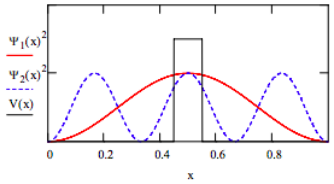
10.13: Variation Method for a Particle in a Box with an Internal Barrier

$$\psi_1(x) = \sqrt{2}\sin \pi x$$

$$\psi_2(x) = \sqrt{2}\sin 3\pi x$$

$$V(x) = if[(x \geq .45)(x \leq .55), 3, 0]$$

Plot trial wavefunctions and potential energy.



Evaluate matrix elements for $100 E_h$ internal barrier:

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

$$S_{12} = \int_0^1 \psi_1(x)\psi_2(x) dx \;\; S_{12} = 0$$

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

$$H_{11} = \int_0^1 \psi_1(x)(-\frac{1}{2})\frac{d^2}{dx^2}\psi_1(x)dx + \int_{.45}^{.55} \psi_1(x)\ 100\ \psi_1(x)dx \tag{10.13.1}$$

$$\approx 24.7711 \tag{10.13.2}$$

$$H_{12} = \int_0^1 \psi_1(x)(-\frac{1}{2})\frac{d^2}{dx^2}\psi_2(x)dx + \int_{.45}^{.55} \psi_1(x)\ 100\ \psi_2(x)dx \tag{10.13.3}$$

$$\approx -19.1912 \tag{10.13.4}$$

$$H_{22} = \int_0^1 \psi_2(x)(-\frac{1}{2})\frac{d^2}{dx^2}\psi_2(x)dx + \int_{.45}^{.55} \psi_2(x)\ 100\ \psi_2(x)dx \tag{10.13.5}$$

$$\approx 62.9972 \tag{10.13.6}$$

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

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

Given

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

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

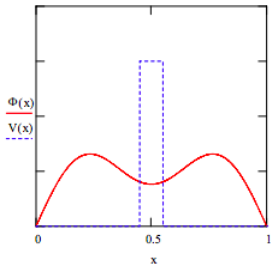
$$c_1^2 S_{11} + 2c_1 c_2 S_{12} + c_2^2 S_{22} = 1$$

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

$$\begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 16.7989 \\ 0.9235 \\ 0.3836 \end{pmatrix}$$

Plot variational results:

$$\Phi(x) = c_1\Phi_1(x) + c_2\psi_2(x)$$



Calculate the probability the particle is in the barrier:

$$\int_{0.45}^{0.55} \Phi(x)^2 dx = 0.0605$$

Calculate potential and kinetic energy:

$$V = 100 \int_{0.45}^{0.55} \Phi(x)^2 dx \; V = 6.0541$$

$$T = E - V$$

$$T = 10.7448$$
