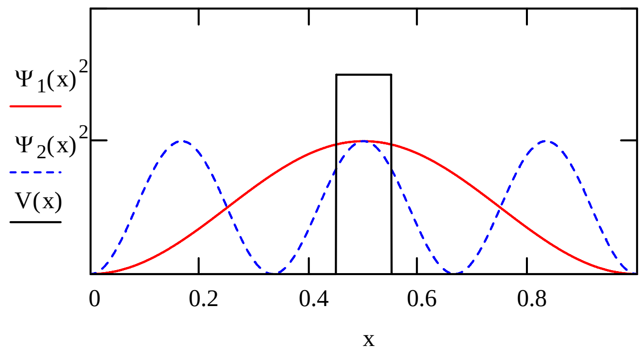
Variation Method for a Particle in a Box with an Internal Barrier

$\Psi_1(x) := \sqrt{2}\cdot\sin(\pi\cdot x)$ $\qquad$ $\Psi_2(x) := \sqrt{2}\cdot\sin(3\cdot\pi\cdot x)$ $\qquad$ $V(x) := \text{if}[(x \ge .45)\cdot(x \le .55), 3, 0]$

Plot trial wave functions and potential energy.



Evaluate matrix elements for 100 E_h internal barrier:

$S_{11} := \int_0^1 \Psi_1(x)^2\,dx$ $\quad S_{11} = 1$ $\qquad$ $S_{12} := \int_0^1 \Psi_1(x)\cdot\Psi_2(x)\,dx$ $\quad S_{12} = 0$ $\qquad$ $S_{22} := \int_0^1 \Psi_2(x)^2\,dx$ $\quad S_{22} = 1$

$$H_{11} := \int_0^1 \Psi_1(x)\cdot -\frac{1}{2}\cdot\frac{d^2}{dx^2}\Psi_1(x)\,dx + \int_{.45}^{.55} \Psi_1(x)\cdot 100\cdot\Psi_1(x)\,dx \qquad H_{11} = 24.7711$$

$$H_{12} := \int_0^1 \Psi_1(x)\cdot -\frac{1}{2}\cdot\frac{d^2}{dx^2}\Psi_2(x)\,dx + \int_{.45}^{.55} \Psi_1(x)\cdot 100\cdot\Psi_2(x)\,dx \qquad H_{12} = -19.1912$$

$$H_{22} := \int_0^1 \Psi_2(x)\cdot -\frac{1}{2}\cdot\frac{d^2}{dx^2}\Psi_2(x)\,dx + \int_{.45}^{.55} \Psi_2(x)\cdot 100\cdot\Psi_2(x)\,dx \qquad H_{22} = 62.9972$$

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

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

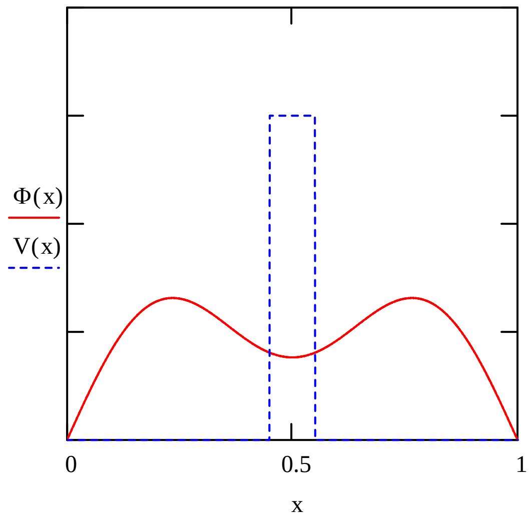
Given $\qquad (H_{11} - E\cdot S_{11})\cdot c_1 + (H_{12} - E\cdot S_{12})\cdot c_2 = 0$ $\qquad (H_{12} - E\cdot S_{12})\cdot c_1 + (H_{22} - E\cdot S_{22})\cdot c_2 = 0$

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

$$\begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} := \text{Find}(E, c_1, c_2) \qquad \begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 16.7989 \\ 0.9235 \\ 0.3836 \end{pmatrix}$$

Plot variational results:

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



Calculate the probability the particle is in the barrier: $\int_{.45}^{.55} \Phi(x)^2 \, dx = 0.0605$

Calculate potential and kinetic energy: $V := 100 \cdot \int_{.45}^{.55} \Phi(x)^2 \, dx \qquad V = 6.0541$

$$T := E - V \qquad T = 10.7448$$