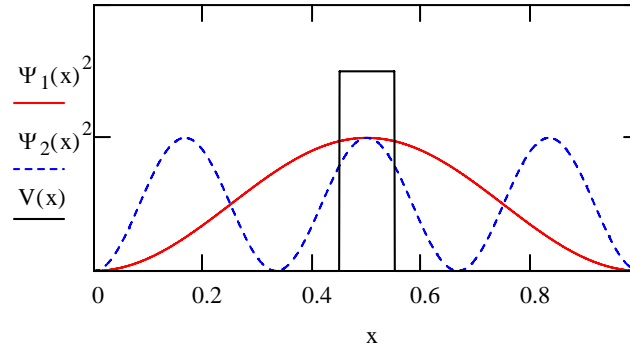


Variation Method for a Particle in a Box with an Internal Barrier

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

Plot trial wave functions and potential energy.



Evaluate matrix elements for 100 E_h internal barrier:

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

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

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

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

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

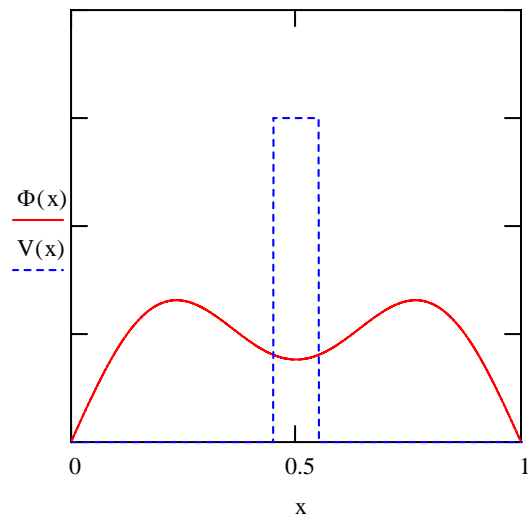
Seed values for energy and coefficients: $E := 5$ $c_1 := .5$ $c_2 := .5$

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

$$c_1^2 \cdot S_{11} + 2 \cdot c_1 \cdot c_2 \cdot S_{12} + c_2^2 \cdot S_{22} = 1 \quad \begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} := \text{Find}(E, c_1, c_2) \quad \begin{pmatrix} E \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 16.7989 \\ 0.9235 \\ 0.3836 \end{pmatrix}$$

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: $V := 100 \cdot \int_{.45}^{.55} \Phi(x)^2 dx \quad V = 6.0541$

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