

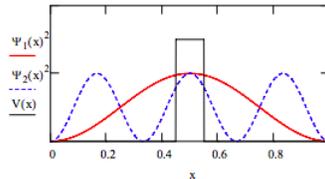
10.13: Variation Method for a Particle in a Box with an Internal Barrier

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

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

$$V(x) = \begin{cases} 0 & (x \leq .45) \\ 3 & (x \geq .55) \\ 0 & \text{elsewhere} \end{cases}$$

Plot trial wavefunctions and potential energy.



Evaluate matrix elements for 100E_n internal barrier:

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

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

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

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

$$\approx 24.7711 \quad (10.13.2)$$

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

$$\approx -19.1912 \quad (10.13.4)$$

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

$$\approx 62.9972 \quad (10.13.6)$$

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

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

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

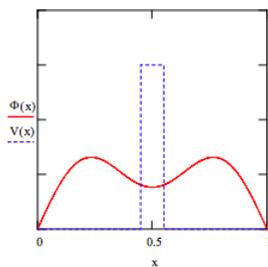
$$c_1^2 S_{11} + 2c_1 c_2 S_{12} + c_2^2 S_{22} = 1$$

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

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

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:

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

$$T = E - V$$

$$T = 10.7448$$

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