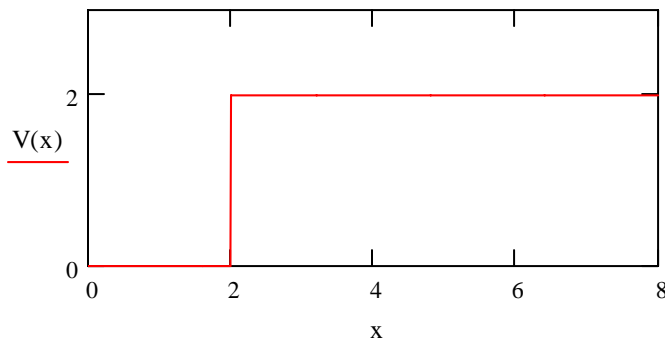


# Variation Method for a Particle in a Semi-infinite Potential Well

This problem deals with the variational approach to the particle in the semi-infinite potential well.

Kinetic energy operator:  $-\frac{1}{2} \cdot \frac{d^2}{dx^2}$       Integral:  $\int_0^{\infty} \blacksquare dx$

Potential energy:  $V(x) := \text{if}[(x \leq 2), 0, 2]$



Trial wave function:  $\Phi(x, \beta) := 2 \cdot \beta^{\frac{3}{2}} \cdot x \cdot \exp(-\beta \cdot x)$

If the trial wave function is not normalized, normalize it.

$$\int_0^{\infty} \Phi(x, \beta)^2 dx \text{ assume, } \beta > 0 \rightarrow 1$$

Evaluate the variational energy integral.

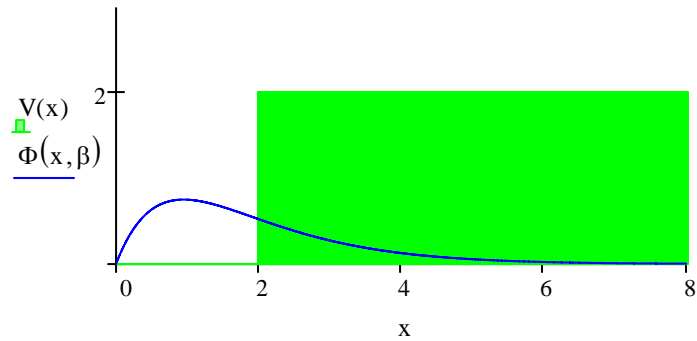
$$E(\beta) := \int_0^{\infty} \Phi(x, \beta) \cdot \left(-\frac{1}{2} \cdot \frac{d^2}{dx^2}\right) \Phi(x, \beta) dx \dots \left| \begin{array}{l} \text{assume, } \beta > 0 \\ \text{simplify} \end{array} \right. \rightarrow \frac{1}{2} \cdot \beta^2 + 16 \cdot \beta^2 \cdot e^{-4 \cdot \beta} + 8 \cdot \beta \cdot e^{-4 \cdot \beta} + 2 \cdot e^{-4 \cdot \beta}$$

$$+ \int_2^{\infty} 2 \cdot \Phi(x, \beta)^2 dx$$

Minimize the energy with respect to  $\beta$ :

$$\beta := .3 \quad \beta_{\text{opt}} := \text{Minimize}(E, \beta) \quad \beta = 1.053 \quad E(\beta) = 0.972$$

Display optimized trial wave function and potential energy:



Calculate average position and most probable position of the particle:

$$\int_0^{\infty} x \cdot \Phi(x, \beta)^2 dx = 1.425 \qquad \frac{d}{dx} \Phi(x, \beta) = 0 \quad \left| \begin{array}{l} \text{solve, } x \\ \text{float, 3} \end{array} \right. \rightarrow \frac{1}{\beta} = 0.95$$

Calculate the probability the particle is in the barrier.

$$\int_2^{\infty} \Phi(x, \beta)^2 dx = 20.891 \%$$

Calculate the potential energy, and the kinetic energy.

$$\underline{V} := \int_2^{\infty} 2 \cdot \Phi(x, \beta)^2 dx \qquad V = 0.418 \qquad \underline{T} := E(\beta) - V \qquad T = 0.554$$