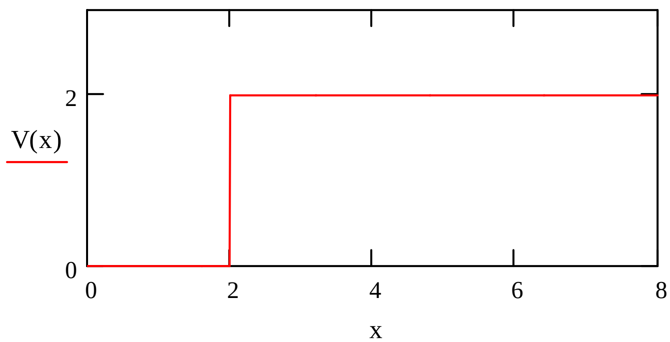
Variation Method for a Particle in a Semi-infinite Potential Well

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

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

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



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.

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

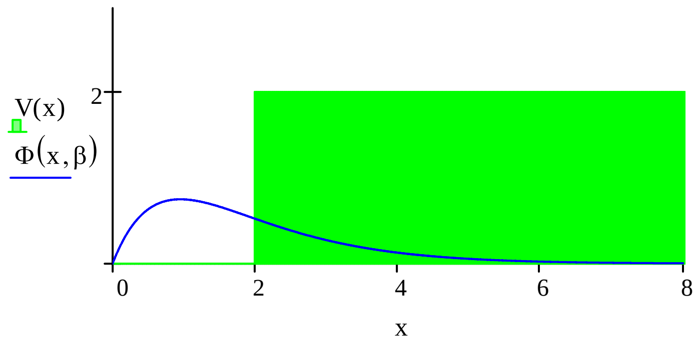
Evaluate the variational energy integral.

$$E(\beta) := \int_0^{\infty}\Phi(x,\beta)\cdot-\frac{1}{2}\cdot\frac{d^2}{dx^2}\Phi(x,\beta)\,dx\ ... + \int_2^{\infty}2\cdot\Phi(x,\beta)^2\,dx \ \Bigg|\ \begin{array}{l}\text{assume}, \beta > 0\\ \text{simplify}\end{array} \rightarrow \frac{1}{2}\cdot\beta^2 + 16\cdot\beta^2\cdot e^{-4\cdot\beta} + 8\cdot\beta\cdot e^{-4\cdot\beta} + 2\cdot e^{-4\cdot\beta}$$

Minimize the energy with respect to β:

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

Display optimized trial wave function and potential energy:



Calculate average position and most probable position of the particle:

$$\int_0^{\infty} x \cdot \Phi(x, \beta)^2 \, dx = 1.425 \qquad \frac{d}{dx}\Phi(x, \beta) = 0 \;\Bigg|\; \begin{matrix} \text{solve}, x \\ \text{float}, 3 \end{matrix} \rightarrow \frac{1}{\beta} = 0.95$$

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.

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