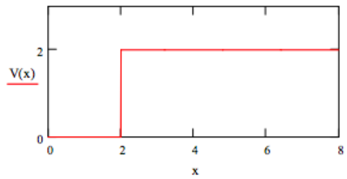
# 10.12: Variation Method for a Particle in a Semi-Infinite Potential Well

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

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

Integral: $\int_0^\infty \blacksquare dx$

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




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

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

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

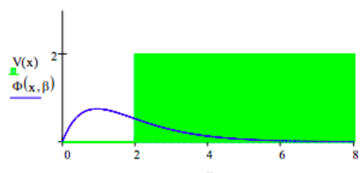
Evaluate the variational energy integral.

$$E(\beta) := \int_0^\infty \Phi(x,\beta)(-\frac{1}{2})\frac{d^2}{dx^2}\Phi(x,\beta)dx \ldots |_{simplify}^{assume,\ \beta>0} \rightarrow \frac{1}{2}\beta^2 + 16\beta^2 e^{-4\beta} + 8\beta e^{-4\beta} + 2e^{-4\beta} + \int_2^\infty 2\Phi(x,\beta)^2 dx$$

Minimize the energy with respect to $\beta$:

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

Display optimized trial wave function and potential energy:




Calculate average position and most probable position of the particle:

$$\int_0^\infty x\Phi(x,\beta)^2 dx = 1.425$$

$$\frac{d}{dx}\Phi(x,\beta) = 0|_{solve,\ x}^{float,\ 3} \rightarrow \frac{1}{\beta} = 0.95$$

Calculate the probability of the particle in the barrier.

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

Calculate the potential energy, and the kinetic energy.

$$V := \int_2^\infty 2\Phi(x,\beta)^2 dx\ V = 0.418$$

$$T := E(\beta) - V\ \ T = 0.554$$