

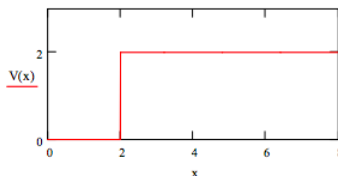
10.12: Variation Method for a Particle in a Semi-Infinite Potential Well

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

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

Integral: \int_0^∞ ■ 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.

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

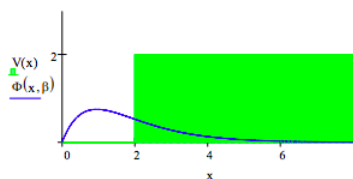
Evaluate the variational energy integral.

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

Minimize the energy with respect to β :

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

Display optimized trial wave function and potential energy:



Calculate average position and most probable position of the particle:

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

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

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.

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

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

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