

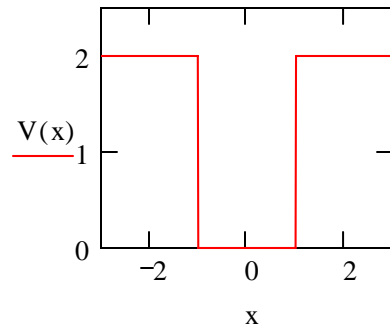
Approximate Quantum Mechanical Methods

Variation Method

Particle in a Finite Potential Well

Define potential energy: $V(x) := \text{if } [(x \geq -1) \cdot (x \leq 1)], 0, 2]$

Display potential energy:



Choose trial wave function: $\Psi(x, \beta) := \left(\frac{2 \cdot \beta}{\pi}\right)^{\frac{1}{4}} \cdot \exp(-\beta \cdot x^2)$

Demonstrate that the trial wave function is normalized.

$$\int_{-\infty}^{\infty} \Psi(x, \beta)^2 dx \text{ assume, } \beta > 0 \rightarrow 1$$

Evaluate the variational integral:

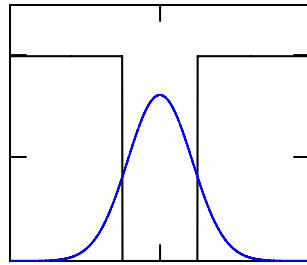
$$E(\beta) := \int_{-\infty}^{\infty} \Psi(x, \beta) \cdot \left(-\frac{1}{2} \cdot \frac{d^2}{dx^2}\right) \Psi(x, \beta) dx \dots \left| \begin{array}{l} \text{assume, } \beta > 0 \\ \text{simplify} \end{array} \right. \rightarrow \frac{1}{2} \cdot \beta + 2 - 2 \cdot \text{erf}\left(\frac{1}{2} \cdot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

$$+ 2 \cdot \int_{-1}^1 2 \cdot \Psi(x, \beta)^2 dx$$

Minimize the energy integral with respect to the variational parameter, β .

$$\beta := 1 \quad \beta_{\text{min}} := \text{Minimize}(E, \beta) \quad \beta = 0.678 \quad E(\beta) = 0.538$$

Display wave function in the potential well and compare result with the exact energy, $0.530 E_h$.



$$\frac{E(\beta) - 0.530}{0.530} = 1.546\%$$

x

Calculate the fraction of time tunneling is occurring.

$$2 \cdot \int_1^{\infty} \Psi(x, \beta)^2 dx = 0.1$$