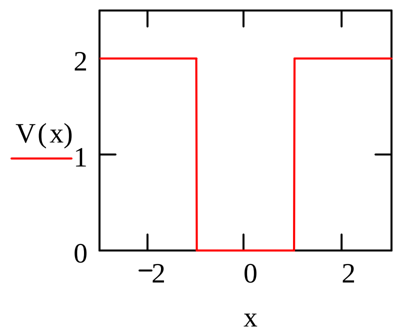
Approximate Quantum Mechanical Methods
Variation Method
Particle in a Finite Potential Well

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

Display potential energy:



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

Demonstrate that the trial wave function is normalized.

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

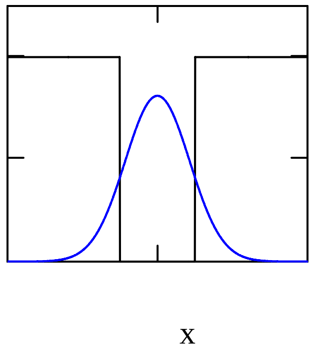
Evaluate the variational integral:

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

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

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

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



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

Calculate the fraction of time tunneling is occuring.

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