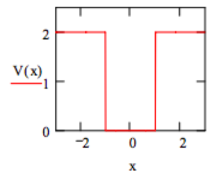
10.5: Variational Method for a Particle in a Finite Potential Well

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

Display potential energy:



Choose trial wavefunction: $\psi(x,\beta) := (\frac{2 \cdot \beta}{\pi})^{\frac{1}{4}} \cdot (-\beta \cdot x^2)$

Demonstrate that the trial wavefunction is normalized.

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

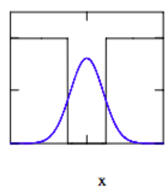
Evaluate the variational integral:

$$E(\beta) := \int_{-\infty}^{\infty} \psi(x,\beta) \cdot -\frac{1}{2} \cdot \frac{d^2}{dx^2} \psi(x,\beta) dx \ldots |_{simplify}^{assume,\, \beta>0} \rightarrow \frac{1}{2} \cdot \beta + 2 - 2 \cdot erf(2^{\frac{1}{2}} \cdot \beta^{\frac{1}{2}})$$

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 wavefunction 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 occurring.

$$2 \cdot \int_{1}^{\infty} \psi(x,\beta)^2 dx = 0.1$$