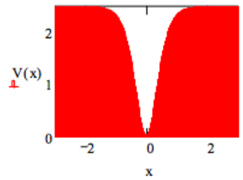
10.33: Variational Method for the Feshbach Potential

Define potential energy: V_0 = 2.5 d = 0.5 $V(x) = V_o \tanh\left(\frac{x}{d}\right)^2$

Display potential energy:



Choose Gaussian trial wavefunction:

$$\psi(x,\beta) = \left(\frac{2\beta}{\pi}\right)^{\frac{1}{4}} exp(-\beta x^2)$$

Demonstrate that the trial wavefunction is normalized.

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

Evaluate the variational integral.

$$E(\beta) = \int_{-\infty}^{\infty} \psi(x,\beta) \frac{-1}{2} \frac{d^2}{dx^2} \psi(x,\beta) dx + \int_{-\infty}^{\infty} V(x)\psi(x,\beta)^2 dx$$

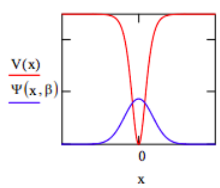
Minimize the energy integral with respect to the variational parameter, β.

β = 1 β = Minimize (E, β) β = 0.913 E(β) = 1.484

Calculate the % error given that numerical integration of Schrödinger′s equation (see next tutorial) yields E = 1.44949 E_h.

$$\frac{E(\beta) - 1.44949}{1.44949} \times 100 = 2.36$$

Display wavefunction in the potential well.



Calculate the probability that tunneling is occurring.

$$V(x) = 1.484 \Big|_{float,\ 3}^{solve,\ x} \rightarrow \begin{pmatrix} -1.511 \\ 0.511 \end{pmatrix}$$

$$2\int_{0.511}^{\infty} \psi(x,\beta)^2 dx = 0.329$$