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

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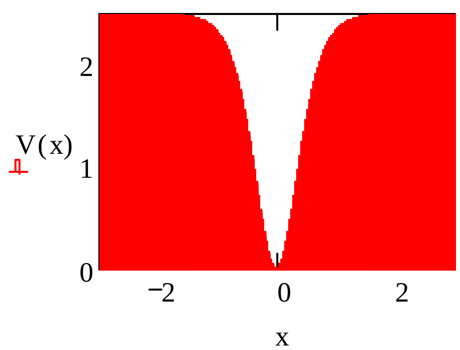
Define potential energy: $V_0 := 2.5$ $\quad d := 0.5$ $\quad V(x) := V_0 \cdot \tanh\left(\frac{x}{d}\right)^2$

Display potential energy:



Choose gaussian 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:

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

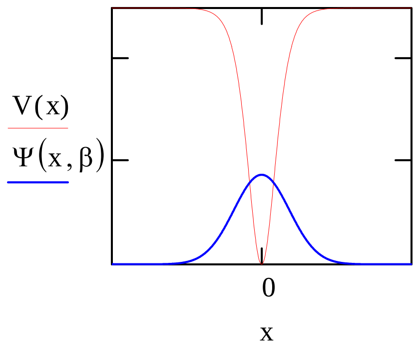
Minimize the energy integral with respect to the variational parameter, β.

$\beta := 1$ $\qquad \beta := \text{Minimize}(E,\beta)$ $\qquad \beta = 0.913$ $\qquad E(\beta) = 1.484$

Calculate the % error given that numerical integration of Schrodinger's equation (see next tutorial) yields $E = 1.44949\ E_h$.

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

Display wave function in the potential well.



Calculate the probability tunneling is occuring.

$$V(x) = 1.484 \;\Big|\; \begin{matrix} \text{solve}, x \\ \text{float}, 3 \end{matrix} \rightarrow \begin{pmatrix} -.511 \\ .511 \end{pmatrix}$$

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