

Numerical Solutions for a Modified Harmonic Potential

Frank Rioux
 Department of Chemistry
 College of St. Benedict | St. John's University

This tutorial deals with the following potential function:

$$V(x, d) = \begin{cases} \frac{1}{2} \cdot k \cdot (x - d)^2 & \text{if } x \geq 0 + d \geq 0 \\ \infty & \text{otherwise} \end{cases}$$

If $d = 0$ we have the harmonic oscillator on the half-line with eigenvalues 1.5, 3.5, 5.5, ... for $k = \mu = 1$. For large values of d we have the full harmonic oscillator problem displaced in the x -direction by d with eigenvalues 0.5, 1.5, 2.5, ... for $k = \mu = 1$. For small to intermediate values of d the potential can be used to model the interaction of an atom or molecule with a surface.

Integration limit: $x_{\max} := 10$ Effective mass: $\mu := 1$ Force constant: $k := 1$ Potential energy minimum: $d := 5$

Potential energy: $V(x, d) := \frac{k}{2} \cdot (x - d)^2$

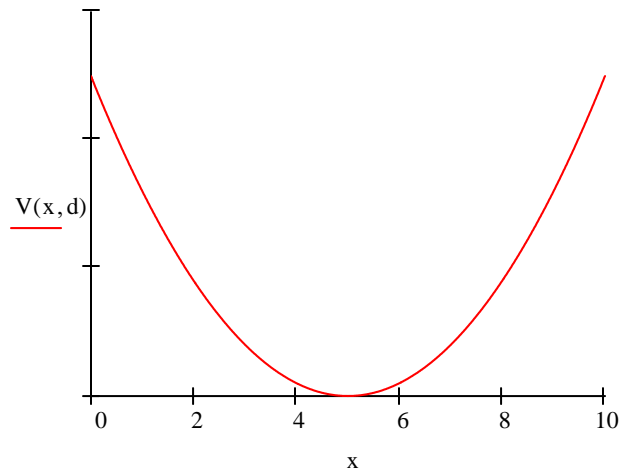
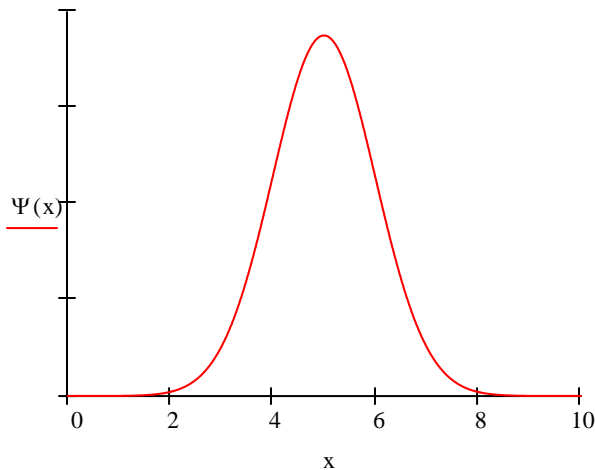
Integration algorithm: Given $\frac{-1}{2 \cdot \mu} \cdot \frac{d^2}{dx^2} \Psi(x) + V(x, d) \cdot \Psi(x) = E \cdot \Psi(x)$ $\Psi(0) = 0$ $\Psi'(0) = 0.1$

$\Psi := \text{Odesolve}(x, x_{\max})$

Normalize wavefunction:

$$\Psi(x) := \frac{\Psi(x)}{\sqrt{\int_0^{x_{\max}} \Psi(x)^2 dx}}$$

Energy guess: $E \equiv 0.5$



Calculate average position:

$$X_{\text{avg}} := \int_0^{x_{\max}} \Psi(x) \cdot x \cdot \Psi(x) dx \quad X_{\text{avg}} = 5$$

Calculate potential and kinetic energy:

$$V_{\text{avg}} := \int_0^{x_{\max}} \Psi(x) \cdot V(x, d) \cdot \Psi(x) dx \quad V_{\text{avg}} = 0.25$$

$$T_{\text{avg}} := E - V_{\text{avg}} \quad T_{\text{avg}} = 0.25$$

Exercises:

- For $d = 0$, $k = \mu = 1$ confirm that the first three energy eigenvalues are $1.5, 3.5$ and $5.5 E_h$. Start with $x_{\max} = 5$, but be prepared to adjust to larger values if necessary. x_{\max} is effectively infinity.
- For $d = 5$, $k = \mu = 1$ confirm that the first three energy eigenvalues are $0.5, 1.5$ and $2.5 E_h$. Start with $x_{\max} = 10$, but be prepared to adjust to larger values if necessary.
- Determine and compare the virial theorem for the exercises above.
- Calculate the probability that tunneling is occurring for the ground state for the first two exercises. (Answers: 0.112, 0.157)