Numerical Solutions for a Modified Harmonic Potential

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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 = μ = 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 = μ = 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.

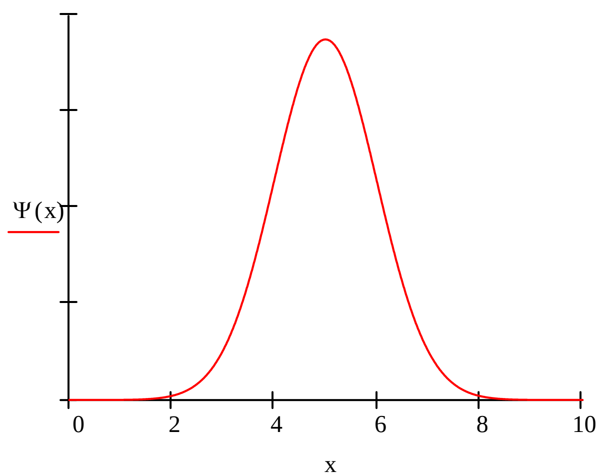
Integration limit: $x_{max} := 10$ Effective mass: $\mu := 1$ Force constant: $k := 1$ Potential energy minimum: $d := 5$

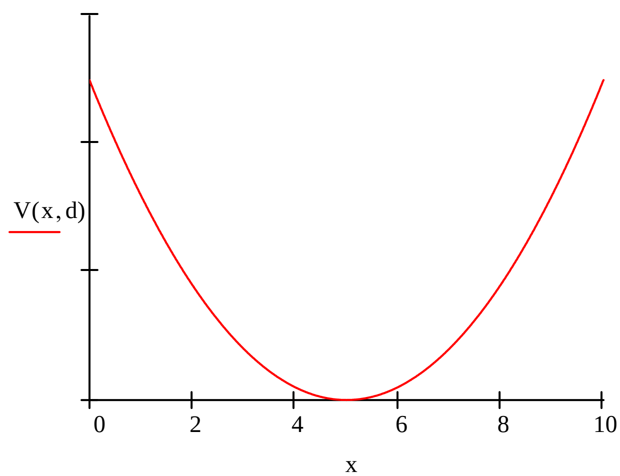
Potential energy: $V(x,d) := \frac{k}{2}\cdot(x-d)^2$

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:

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

Calculate potential and kinetic energy:

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

$T_{avg} := E - V_{avg}$ $T_{avg} = 0.25$

Exercises:

- For d = 0, k = μ = 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 = μ = 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 occuring for the ground state for the first two exercises. (Answers: 0.112, 0.157)