9.22: Numerical Solutions for a Modified Harmonic Potential

This tutorial deals with the following potential function:

$$V(x, d) = \left| \begin{array}{l} \frac{1}{2}k(x-d)^2 \; if \; x \geq 0 + d \leq 0 \\ \\ \infty \; otherwise \end{array} \right.$$

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: μ = 1

Force constant: k = 1

Potential energy minimum: d = 5

Potential energy:

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

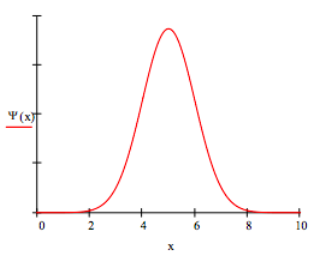
Integration algorithm:

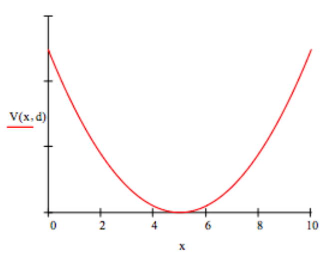
Given

Normalize wavefunction:

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

Energy guess: E = 0.5





Calculate average position:

$$X_{avg} = \int_0^{x_{max}} \psi(x) x \psi(x) dx = 5$$

Calculate potential and kinetic energy:

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

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

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. xmax is effectively infinity.
- For d = 5, k = μ = 1 confirm that the first three energy eigenvalues are 0.5, 1.5 and 2.5 Eh. 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)
