Numerical Solutions for a Modified Harmonic Potential

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This tutorial deals with the following potential function:

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

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: \( x_{\text{max}} := 10 \)  
Effective mass: \( \mu := 1 \)  
Force constant: \( k := 1 \)  
Potential energy minimum: \( d := 5 \)

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

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

\( \psi := \text{Odesolve}(x, x_{\text{max}}) \)  
Normalize wavefunction: \( \psi(x) := \frac{\psi(x)}{\sqrt{\int_0^{x_{\text{max}}} \psi(x)^2 \, dx}} \)

Energy guess: \( E = 0.5 \)

Calculate average position:

\[
X_{\text{avg}} := \int_0^{x_{\text{max}}} \psi(x) \cdot x \cdot \psi(x) \, dx \quad X_{\text{avg}} = 5
\]

Calculate potential and kinetic energy:

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

\[
T_{\text{avg}} := E - V_{\text{avg}} \quad T_{\text{avg}} = 0.25
\]
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 $x_{\text{max}} = 5$, but be prepared to adjust to larger values if necessary. $x_{\text{max}}$ 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 $x_{\text{max}} = 10$, 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)