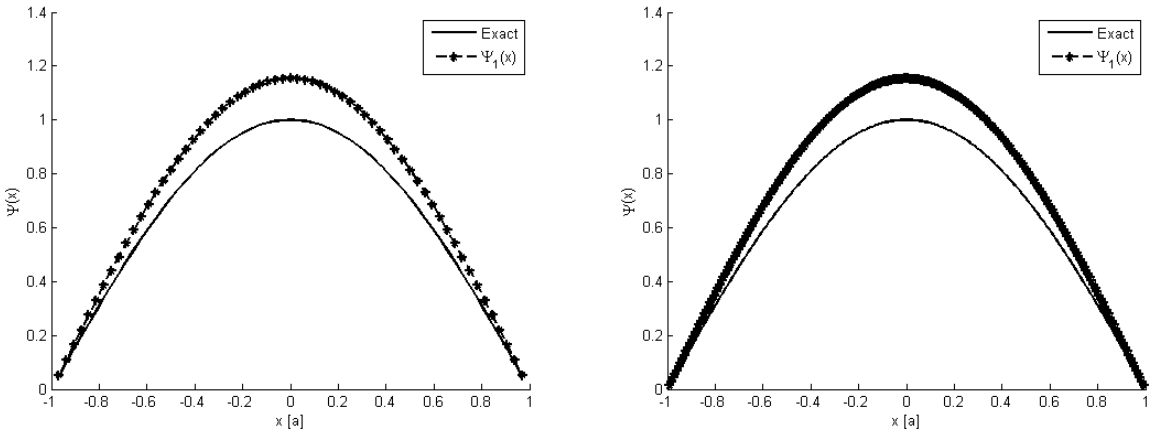
1 Infinite Square Well

The time-independent Schrodinger's equation for a wave function $\psi(x)$ for a single particle of mass m in a infinite square well of width $2a$:

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

with units L = a, E = $\frac{\hbar^2}{ma^2}$.

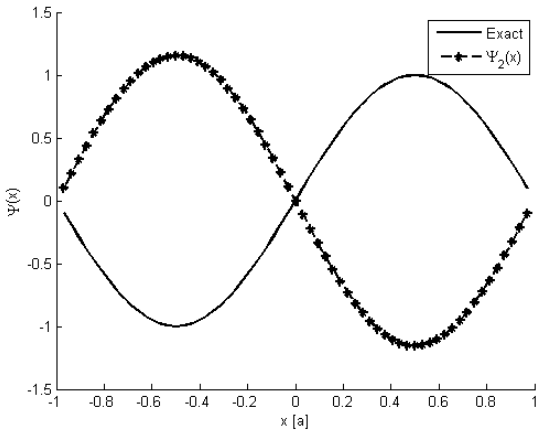
1.1 Non-spurious Modes



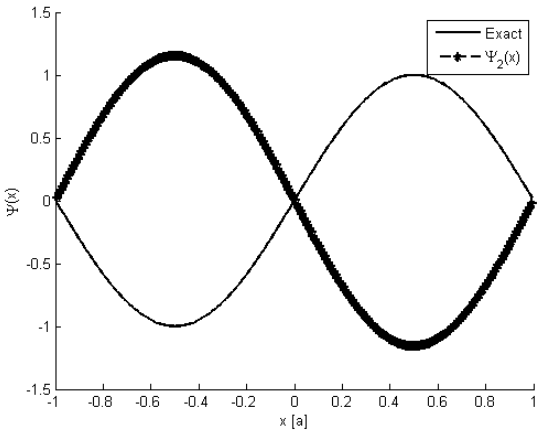
(a) n = 1, N = 64

(b) n = 1, N = 256

Figure 1: The computed eigenvalues for N = 64, 256 are λ = 1.2410, 1.2355, respectively.

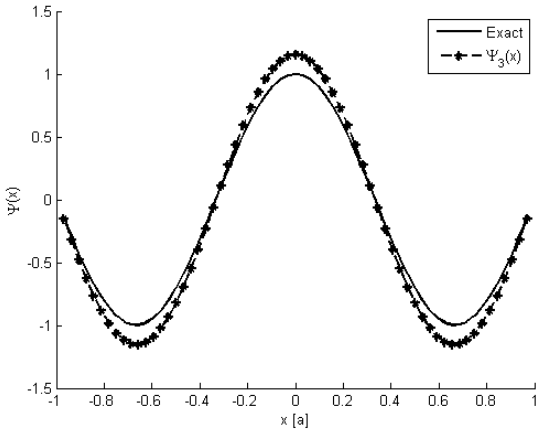


(a) n = 2, N = 64

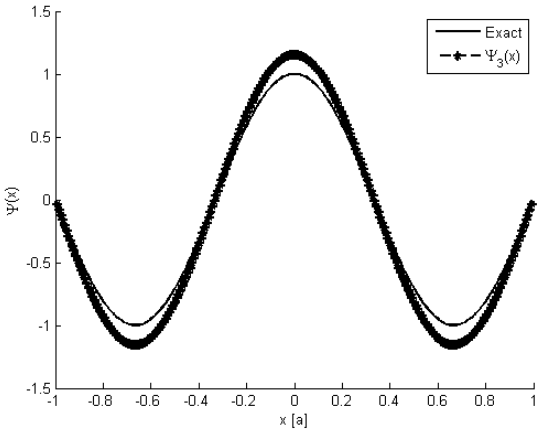


(b) n = 2, N = 256

Figure 2: The computed eigenvalues for N = 64, 256 are $\lambda = 4.9641, 4.9421$, respectively.

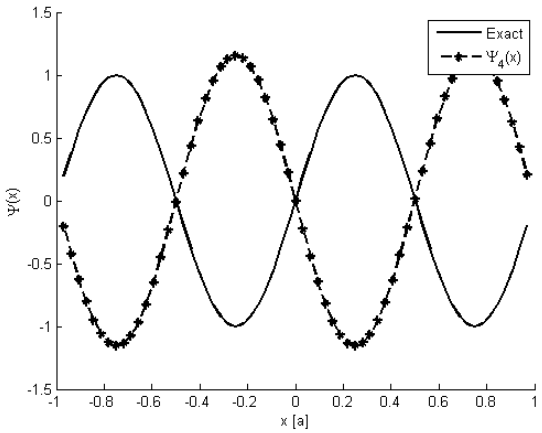


(a) n = 3, N = 64

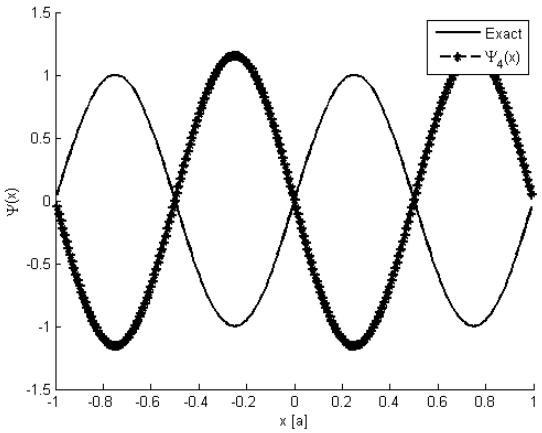


(b) n = 3, N = 256

Figure 3: The computed eigenvalues for N = 64, 256 are $\lambda = 11.1691, 11.1197$, respectively.



(a) n = 4, N = 64



(b) n = 4, N = 256

Figure 4: The computed eigenvalues for N = 64, 256 are λ = 19.8560, 19.7684, respectively.

1.2 Spurious Modes

From the plots it can be inferred that the spurious modes are unphysical. This is due to the fact that the graphs are "aware" of the spacing, h. The wavefunction is not "smooth" like the modes n = 1,2,3,4. The computed eigenvalues have high errors compared to the exact eigenvalues.

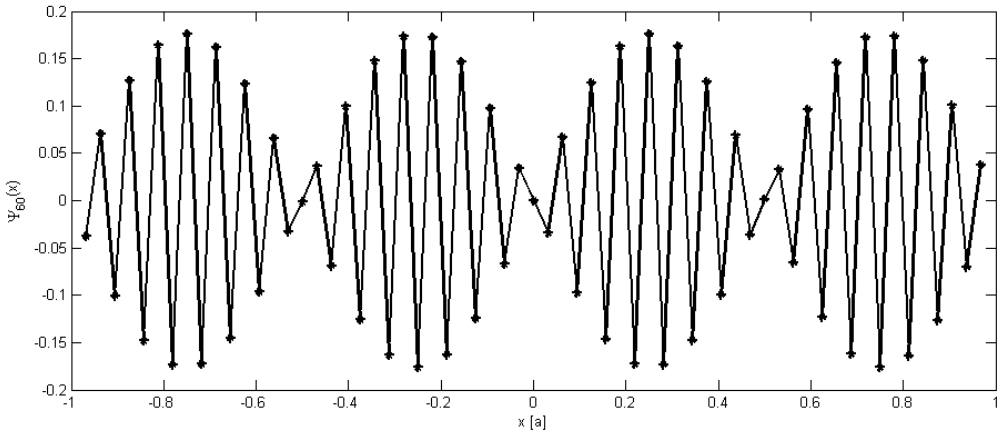


Figure 5: For N = 64 and n = 60, the spurious mode is plotted.

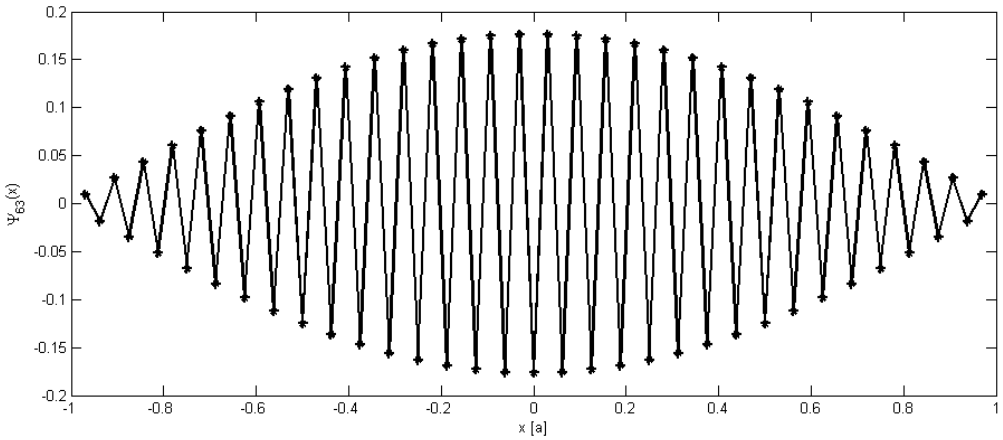


Figure 6: For N = 64 and n = 63, the spurious mode is plotted.

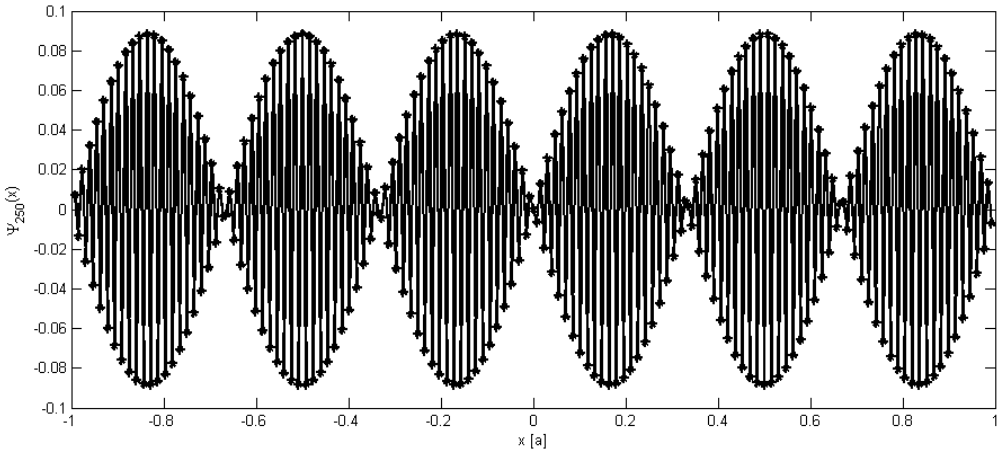


Figure 7: For N = 256 and n = 250, the spurious mode is plotted.

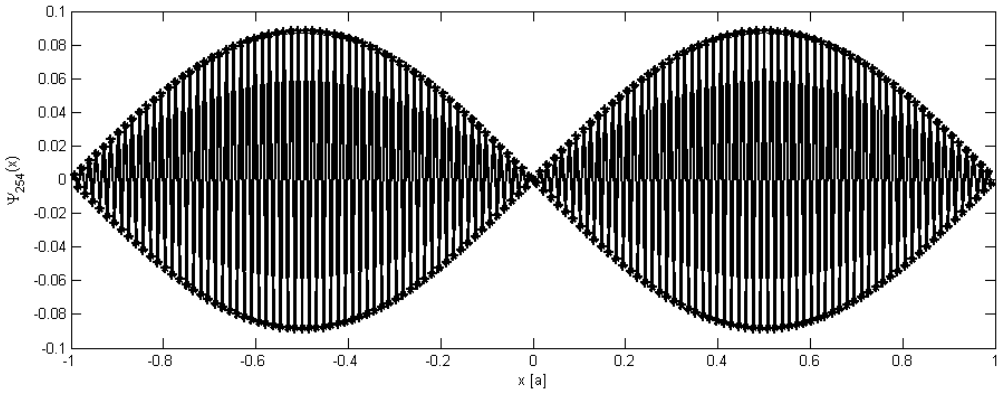
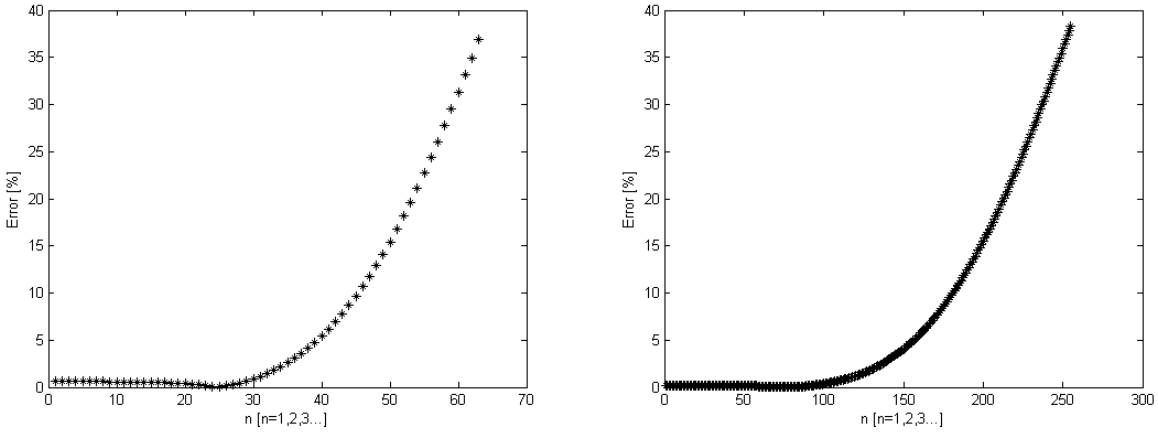


Figure 8: For N = 256 and n = 254, the spurious mode is plotted.

1.3 Error



(a) N = 64

(b) N = 256

Figure 9: The percent error between the exact and computed eigenvalues is plotted for N = 64, 256. For N = 64, the amount of eigenvalues less than 1% is 30. For N = 256, the amount of eigenvalues less than 1% is 116. The large error is most likely due to the spurious modes.

2 Perturbed Infinite Square Well

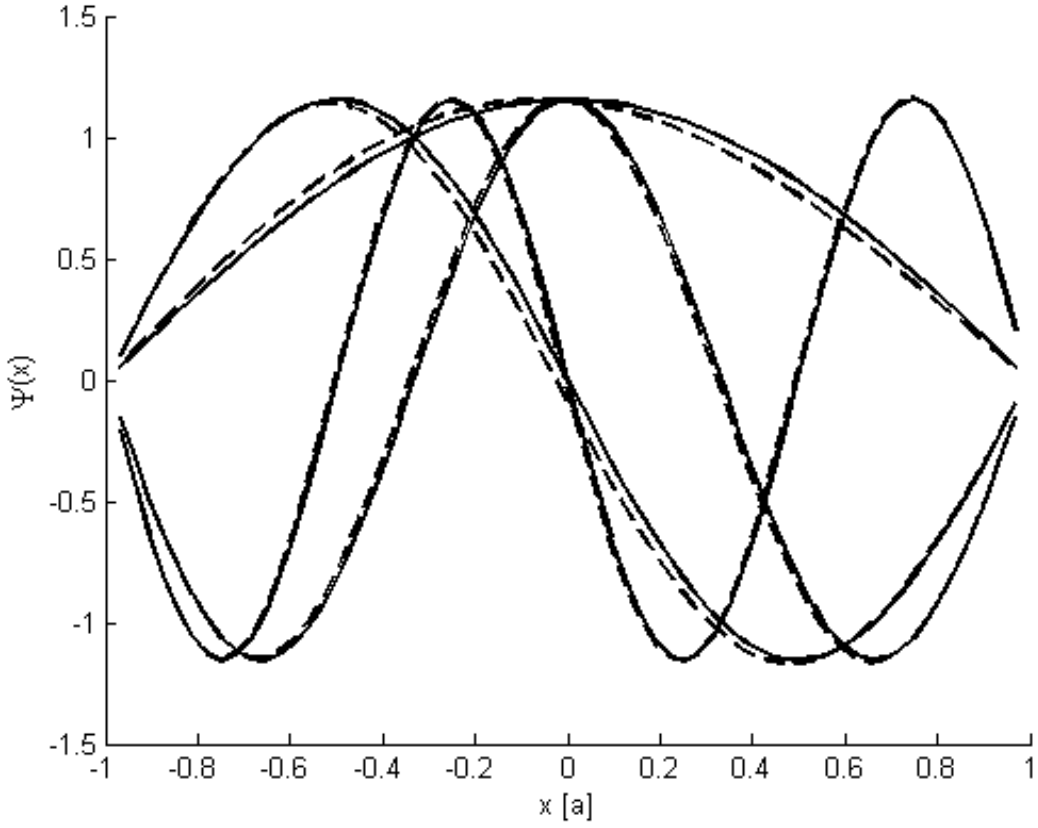


Figure 10: By adding a perturbation of $\frac{x}{2}$ to the potential, the eigenvectors are plotted for n = 1, 2, 3, 4, where the dashed lines are the perturbed square well. The computed eigenvalues for n = 1, 2, 3, 4 are λ = 1.2324, 4.9666, 11.1706, 19.8569, respectively.

3 Quantum Harmonic Oscillator

The time-independent Schrodinger's equation for a wave function $\psi(x)$ for a single particle of mass m in a quantum harmonic oscillator with a $V(x) = \frac{1}{2}m\omega_0^2x^2$:

$$-\frac{1}{2}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

with units L = $\sqrt{\frac{\hbar}{m\omega_0}}$, E = $\hbar\omega_0$.

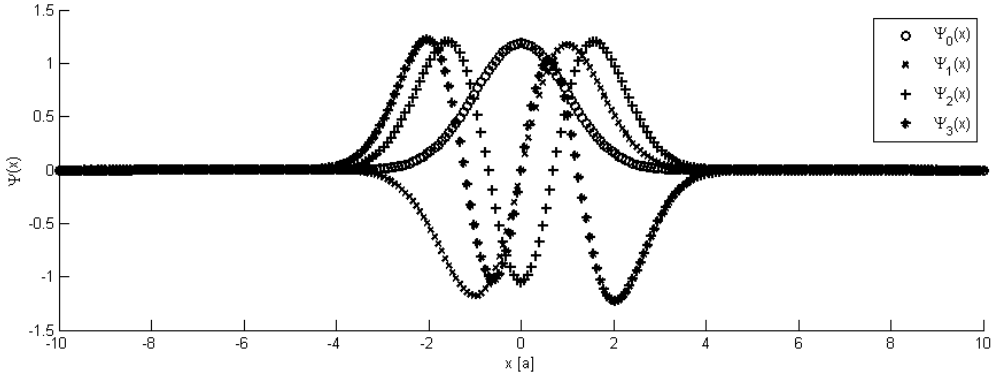
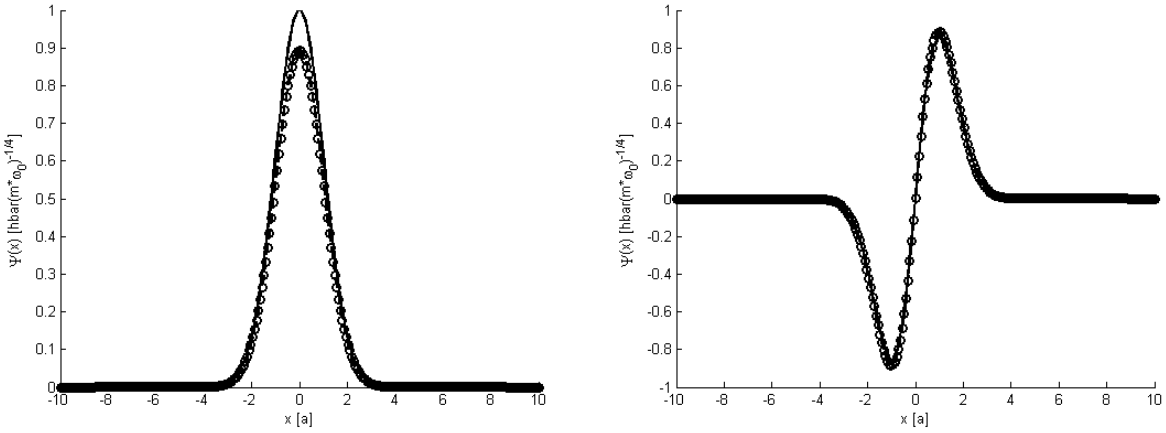


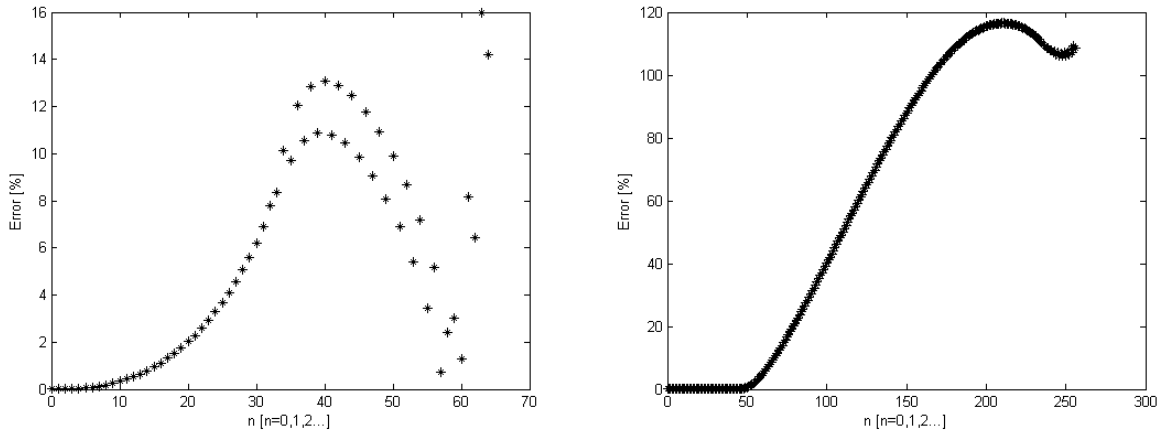
Figure 11: For modes n = 0, 1, 2, 3, the eigenvectors for the quantum harmonic oscialltor are shown. The respective computed eigenvalues are $\lambda = .5, 1.5, 2.5, 3.5$.



(a) n = 0

(b) n = 1

Figure 12: For modes n = 0, 1 and N = 256, the exact and computed wavefunctions are plotted.



(a) N = 64 (b) N = 256

Figure 13: For N = 64, 256, the respective number of eigenvalues less than 1% are 17, 52. The error between the exact and computed eigenvalues are shown The higher error tends to lead to spurious modes of the quantum harmonic oscillator.

4 Perturbed Quantum Harmonic Oscillator

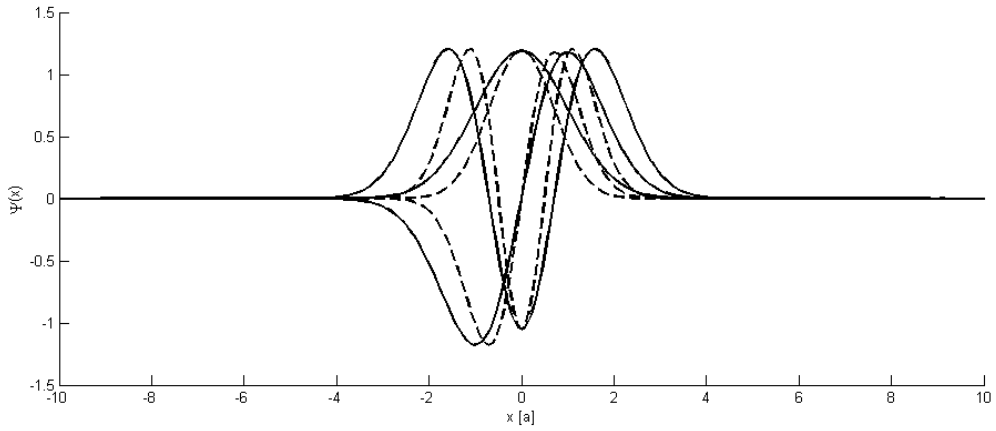


Figure 14: By adding a perturbation of x^2 to the potential, the eigenvectors are plotted for n = 1, 2, 3, where the dashed lines are the perturbed quantum harmonic oscillator. The computed eigenvalues for n = 1, 2, 3 are $\lambda = 1.0$, 3.0, 5.0, respectively.

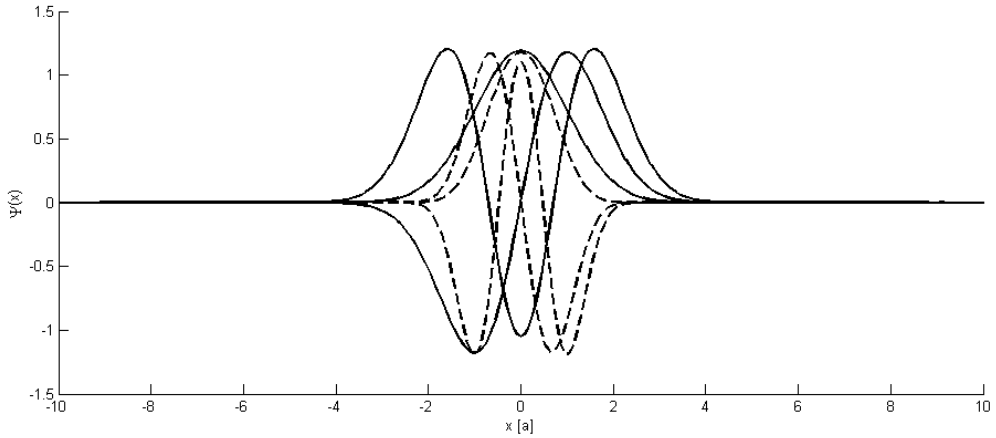


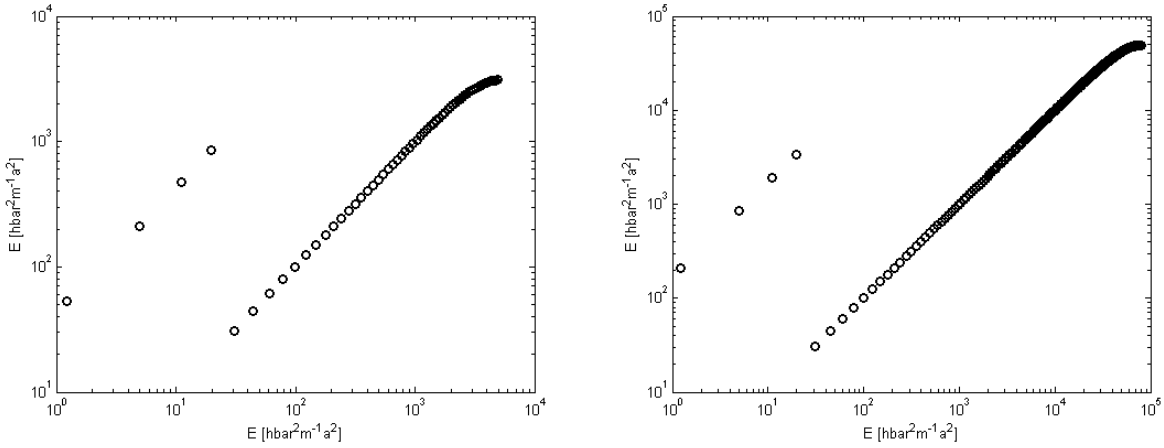
Figure 15: By adding a perturbation of x^4 to the potential, the eigenvectors are plotted for n = 1, 2, 3, where the dashed lines are the perturbed quantum harmonic oscillator. The computed eigenvalues for n = 1, 2, 3 are $\lambda = 0.9263$, 3.0579, 5.6397, respectively.

5 First-order Perturbation Theory

First-order perturbation theory follows:

$$E_n^{(1)} = \langle \psi_n^{(0)} | \, V' \, | \psi_n^{(0)} \rangle$$

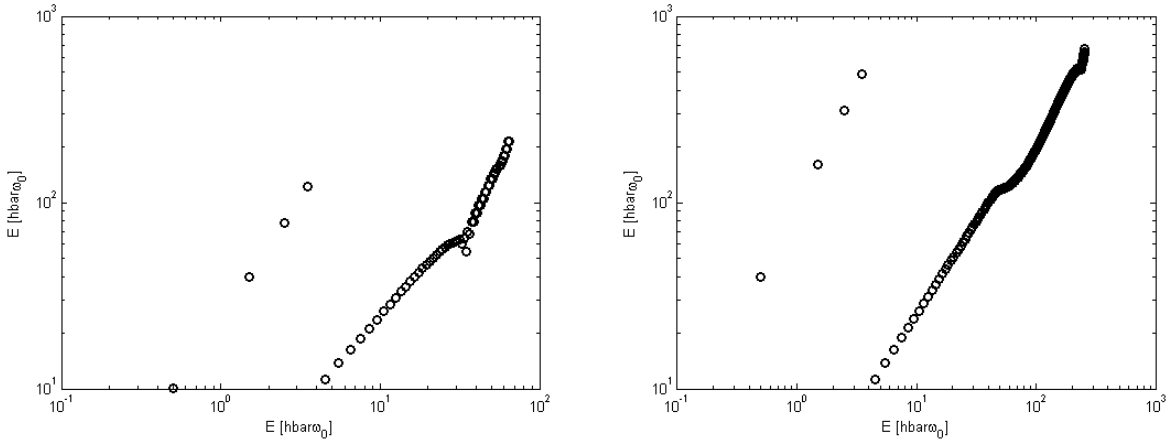
5.1 Infinite Square Well



(a) N = 64 (b) N = 256

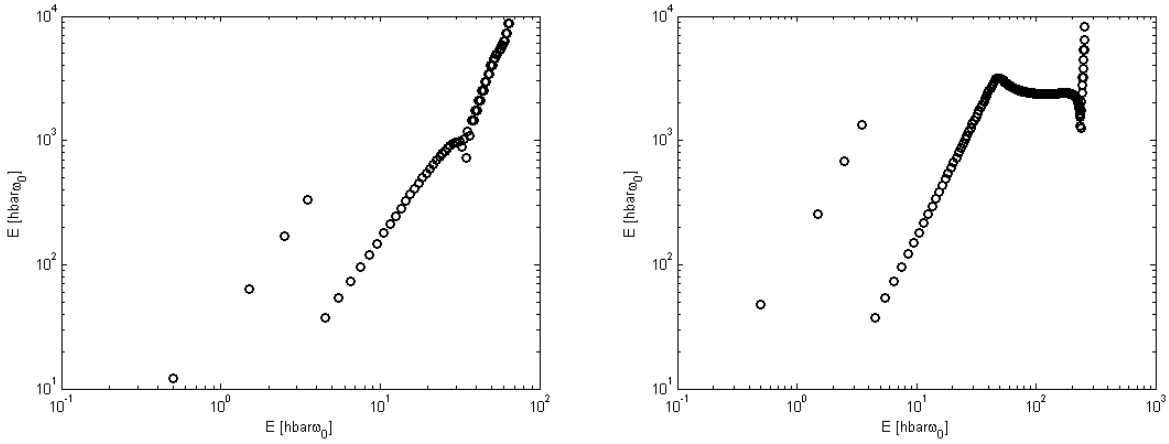
Figure 16: The first-order perturbation theory and computed perturbed eigenmodes are shown. The accuracy is observed for errors less than 1% between the computed and first-order perturbation theory. For N = 64, the eigenmodes have a 93.65% accuracy. For N = 256, the accuracy is 98.82%. The first 4 modes are not within a 1% error to the computed eigenmodes, where the first-order perturbation theory gives higher energy.

5.2 Quantum Harmonic Oscillator



(a) N = 64 (b) N = 256

Figure 17: The first-order perturbation theory and computed perturbed eigenmodes are shown. The accuracy is observed for errors less than 5% between the computed and first-order perturbation theory. For N = 64, the eigenmodes have a 52.31% accuracy. For N = 256, the accuracy is 78.99%. A perturbation proportional to x^2 seems to increase in accuracy for higher N values.



(a) N = 64 (b) N = 256

Figure 18: A anharmonic perturbation proportional to x^4 decreases the accuracy. The accuracy is observed for errors less than 5% between the computed and first-order perturbation theory. For N = 64, the eigenmodes have a 23.08% accuracy. For N = 256, the accuracy is 3.89%. The accuracy is observed to get worse with the increase in perturbation.