1. Consider an infinite square well that runs from 0 to a. As a perturbation, we place a delta-function bump at the center of the well,

$$\hat{H}' = \alpha\delta\left(x - \frac{a}{2}\right),$$

where α is a constant.

   (a) Determine the first-order correction to the allowed energies. Why are the energies for even n unperturbed?

   (b) Determine the first three non-zero terms in the perturbation expansion,

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0,$$

   of the correction to the ground state ψ_1^1.

(a) The first-order correction, E_n^1, is given by Griffiths Equation 7.9 to be

$$E_n^1 = \left\langle \psi_n^0 \middle| \hat{H}' \middle| \psi_n^0 \right\rangle = \int_{-\infty}^{\infty} \psi_n^{0*} \hat{H}' \psi_n^0 \mathrm{d}x.$$

Substituting Griffiths Equation 2.31, the n-th wavefunction for the infinite square well, and our expression for the perturbation hamiltonian yields

$$E_n^1 = \frac{2\alpha}{a} \int_0^a \sin\left(\frac{n\pi}{a}x\right)^2 \delta\left(x - \frac{a}{2}\right) \mathrm{d}x.$$

The δ-function is non-zero at $x = a/2$, which is inside the limits of integration. Thus,

$$E_n^1 = \frac{2\alpha}{a} \sin\left(\frac{n\pi}{2}\right)^2.$$

Notice,

$$E_n^1 = \begin{cases} \frac{2\alpha}{a}, & n \text{ is odd,} \\ 0, & n \text{ is even.} \end{cases}$$

The lack of correction on even energies is a consequence of the wavefunction. We can also think about the shape of the even wavefunctions and how it relates to our perturbation. The even wavefunctions are of probability amplitude 0 at $a/2$. Thus, it makes sense that a perturbation localized only to $a/2$ would not change the wavefunction.

(b) We begin with Griffiths Equation 7.13:

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0.$$

Substituting $n = 1$ yields

$$\psi_1^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle}{E_1^0 - E_m^0} \psi_m^0.$$

We begin with simplifying the denominator:

$$E_1^0 - E_m^0 = \frac{\pi^2 \hbar^2}{2m_p a} - \frac{m^2 \pi^2 \hbar^2}{2m_p a} = (1 - m^2) \frac{\pi^2 \hbar^2}{2m_p a},$$

where m_p refers to the mass of the particle and m is the indexing number. Then,

$$\psi_1^1 = \sum_{m \neq n} \frac{2m_p a^2}{(1 - m^2)\pi^2 \hbar^2} \langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle \psi_m^0.$$

We now focus on the inner-product term; substituting Griffiths Equation 2.37 and the expression for the perturbation hamiltonian yields, after simplification,

$$\langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle = \frac{2\alpha}{a} \int_0^a \sin\left(\frac{m\pi}{a}\right) \sin\left(\frac{\pi}{a} x\right) \delta\left(x - \frac{a}{2}\right) \mathrm{d}x.$$

Here, we could take the simple δ-function interpretation, pulling our sin terms outside the integral and substituting $x = a/2$. However, it is fun to apply the trig identity[1]

$$\sin(\theta)\sin(\phi) = \frac{\cos(\theta - \phi) - \cos(\phi - \theta)}{2},$$

doing so yields

$$\begin{aligned}
\langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle &= \frac{2\alpha}{a} \int_0^a \frac{\cos\left[(m-1)\frac{\pi}{a}x\right] - \cos\left[(1-m)\frac{\pi}{a}x\right]}{2} \delta\left(x - \frac{a}{2}\right) \mathrm{d}x \\
&= \frac{2\alpha}{a} \int_0^a \frac{\cos\left[(m-1)\frac{\pi}{a}x\right] + \cos\left[(m-1)\frac{\pi}{a}x\right]}{2} \delta\left(x - \frac{a}{2}\right) \mathrm{d}x \\
&= \frac{2\alpha}{a} \int_0^a \cos\left[(m-1)\frac{\pi}{a}x\right] \delta\left(x - \frac{a}{2}\right) \mathrm{d}x \\
&= \frac{2\alpha}{a} \cos\left((m-1)\frac{\pi}{a}\frac{a}{2}\right) \\
&= \frac{2\alpha}{a} \cos\left(m\frac{\pi}{a} - \frac{\pi}{2}\right) \\
&= \frac{2\alpha}{a} \sin\left(m\frac{\pi}{a}\right),
\end{aligned}$$

[1] That is, I was not convinced that I could take that interpretation with more complicated functions.

which is what we would have found had we taken the simple δ-function interpretation. Putting all the pieces together yields

$$\psi_1^1 = \sum_{m \neq n} \frac{4m_p a\alpha}{(1-m^2)\pi^2\hbar^2} \sin\left(\frac{m\pi}{2}\right) \psi_m^0.$$

This can be simplified further

$$\psi_1^1 = \frac{4m_p a\alpha}{\pi^2\hbar^2} \sum_{m \neq n} \frac{1}{1-m^2} \sin\left(\frac{m\pi}{2}\right) \psi_m^0.$$

Notice, the m-th term in the summation will be non-zero iff m is odd. Furthermore, the series will alternate positive and negative terms. This makes sense, in part (a) we revealed that there was no first-order correction to even wavefunctions. Then, the third-order (three-term) first-order wavefunction is

$$\psi_1^1 \approx \frac{4m_p a\alpha}{\pi^2\hbar^2} \left(\frac{1}{8}\psi_3^0 - \frac{1}{24}\psi_5^0 + \frac{1}{48}\psi_7^0\right).$$

2. The allowed energies for the harmonic oscillator are

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega,$$

where $\omega = \sqrt{k/m}$ is the classical frequency and the potential energy is

$$V(x) = \frac{1}{2}kx^2.$$

Suppose the spring constant increases lightly, $k \to (1+\epsilon)\,k$.

(a) Determine the exact new energies, then expand the formula as a power series in ϵ up to second order.

(b) Calculate the first-order perturbation to the energy using

$$E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle.$$

To preform this calculation, it will be necessary to determine what $\hat{H}'$ is in this case. Compare this result with the result from part (a).

(a) The exact new energies are given simply by substituting k for $(1+\epsilon)k$. Let

$$\omega' = \sqrt{\frac{(1+\epsilon)k}{m}} = \omega\sqrt{1+\epsilon}.$$

Then,

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega\sqrt{1+\epsilon}.$$

The second-order expansion for E_n is given by

$$E_n \approx \left(n + \frac{1}{2}\right) \hbar\omega \left(1 + \frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2\right).$$

(b) The hamiltonian of a quantum harmonic oscillator can be written as

$$\hat{H} = \frac{1}{2}m\omega^2\hat{x}^2.$$

Then, we let $\omega \to \omega'$. Our hamiltonian becomes

$$\hat{H} = \frac{1}{2}m\omega^2(1+\epsilon)\hat{x}^2 = \frac{1}{2}m\omega^2\hat{x}^2 + \epsilon\frac{1}{2}m\omega^2\hat{x}^2.$$

Here, we see the first term is our zeroth-order hamiltonian, $\hat{H}^0$. Consequently, the second term is our perturbation hamiltonian,

$$\hat{H}' = \epsilon\frac{1}{2}m\omega^2\hat{x}^2 = \epsilon V.$$

This perturbation hamiltonian can be expressed in terms of the raising and lowering operators a_+ and a_-. We recognize that

$$\hat{H}' = \epsilon V = \frac{\epsilon}{2}\hat{H},$$

where the factor of 1/2 comes from the result of Griffiths Example 2.5 where we see that the hamiltonian of a simple harmonic oscillator is divided evenly in potential energy and kinetic energy. Then, as in Griffiths Equation 2.53,

$$\hat{H} = \hbar\omega\left(a_-a_+ - \frac{1}{2}\right).$$

Recognizing that $\hat{H} = \hat{H}'/\epsilon$,

$$\hat{H}' = \frac{1}{2}\epsilon\hbar\omega\left(a_-a_+ - \frac{1}{2}\right).$$

Finally, we may calculate the first-order energy perturbation by Griffiths Equation 7.9:

$$E_n^1 = \langle\psi_n^0|\hat{H}'|\psi_n^0\rangle = \frac{1}{2}\epsilon\hbar\omega\left(\langle\psi_n^0|a_-a_+|\psi_n^0\rangle - \frac{1}{2}\langle\psi_n^0\,|\,\psi_n^0\rangle\right).$$

The raising and lowering operators action on ψ_n is defined in Griffiths Equation 2.66. Then,

$$E_n^1 = \frac{1}{2}\epsilon\hbar\omega\left(\sqrt{n+1}\sqrt{n+1} - \frac{1}{2}\right) = \frac{1}{2}\epsilon\hbar\omega\left(n + \frac{1}{2}\right) = \frac{1}{2}\epsilon E_n^0.$$

This is in direct agreement with the second term (the first-order term) of the expansion in part (a).