Homework No. 6 Using 1st and 2nd Order Perturbation Theory

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I. BACKGROUND

We discussed in class the development of 1st and 2nd order perturbation theory in quantum mechanics. The perturbation H^1 occurs in the hamiltonian as

$$H = H^0 + H'$$

where H^0 is the hamiltonian of a simpler system with known solutions to the Schrodinger equation, $H^0\,\psi_n^0 = E_n^0\,\psi_n^0$. The purpose of this problem is to explore how a small perturbation affects the energy levels and wave functions in a simple quantum mechanics problem, namely the infinitely deep potential well.

The first and second order corrections to the n^{th} energy level are described as follows:

$$E_n^{(1)} = \langle \psi_n^o | H' | \psi_n^o \rangle \tag{1}$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{\left| \left\langle \psi_m^0 | H' | \psi_n^0 \right\rangle \right|^2}{E_n^0 - E_m^0} \tag{2}$$

We also discussed the first order correction to the n^{th} wave function and this described by the following equation:

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\left\langle \psi_m^0 | H' | \psi_n^0 \right\rangle}{E_n^0 - E_m^0}\; \psi_m^0 \tag{3}$$

II. A PERTURBATION IN THE INFINITELY DEEP POTENTIAL WELL

The solutions to the Schrodinger equation for the infinitely deep potential well of width a are well known. The wave functions and energies can be written as follows:

$$\psi_n^0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$E_n^0 = \frac{n^2 \hbar^2 \pi^2}{2ma^2}$$

A. The perturbation

The perturbation for this problem is a small rectangular "bump" that is half the width of the well, and placed symmetrically in the center.

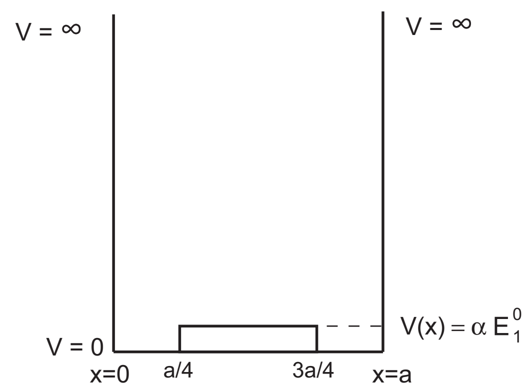

FIG. 1. A perturbation in the potential energy of an infinitely deep well is shown. The perturbation αE_1^0 causes a small shift in the eigenstate energies and changes to the wave functions.

B. Question 1

Find the 1st and 2nd order corrections to the ground state energy. For the 2nd order correction, include the first 10 non-zero terms in your calculation ($m = 3, 5, 7, \ldots, 19, 21$) in order to achieve reasonable accuracy. Write your answer in the form:

$$E_1 = E_1^0 \left(1 + \underline{\hspace{2cm}}\ \alpha\ -\ \underline{\hspace{2cm}}\ \alpha^2\right)$$

Question: If $\alpha = 0.10$, what is the percentage change observed in the ground state energy?

Question: Can you explain from symmetry arguments as to why the even numbered terms in the sum are zero? In other words why are the matrix elements

$$\left\langle \psi_m^0 | H' | \psi_1^0 \right\rangle = 0$$

for all *even* integer values, $m = 2, 4, 6, \ldots$?

Hint: Shift the $x = 0$ axis to the middle of the well and look at the *even* and *odd* nature of the matrix element

$$\left\langle \psi_m^0 | H' | \psi_1^0 \right\rangle \;=\; \langle \text{even} \,|\, \text{even} \,|\, \text{odd} \rangle$$

between symmetric limits of $-a/2$ to $+a/2$.

C. Question 2

Find the 1st order correction to the ground state wave function, once again using the first 10 non-zero terms in the expansion described by Eq. 3. Plot the total ground state wave function by combining the perturbed and unperturbed wave functions. Plot this wave function

$$\psi_{\text{Total}}(x) = \psi_1^0(x) + \psi_1^{(1)}(x) \tag{4}$$

in the region between 0 and a. Assume that $\alpha = 0.50$ in order to see an appreciable change in the wave function.

Note: This new wave function $\psi_{\text{Total}}(x)$ is a "good" approximation to the Schrodinger equation, $H\psi_{\text{Total}}(x) = E_1\, \psi_{\text{Total}}(x)$.

D. Question 3

Is the new wave ground-state wave function in Eq. 4 normalized? Show that it is normalized in the interval $0 \le x \le a$, to at least one part in 1,000. It appears that terminating the series expansion after the first 10 non-zero terms gives a good approximation to the new ground-state wave function ψ_1 that satisfies

$$H\psi_1 = E_1\psi_1$$

where H, ψ_1, and E_1 contain both the zeroth and first order terms:

$$(H^0 + H')(\psi_1^0 + \psi_1^{(1)}) = (E_1^0 + E_1^{(1)})(\psi_1^0 + \psi_1^{(1)}).$$

Note: Feel free to use *Mathematica* or *Matlab* to do your calculations.