Problem 5: Perturbation Theory: (10 Points)

A single particle is in a one dimensional infinite well of length L. The potential $V(x)$ is given by:

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le L \\ \infty, & \text{otherwise} \end{cases}$$

Suppose the potential energy inside the well is changed to

$$V(x) = \epsilon \sin \frac{\pi x}{L}$$

when $0 \le x \le L$.

Note you may use your results from Problem 1 for this problem.

(a) ~~1.~~ Calculate the energy shifts for the perturbed well to first order in ϵ. **(2 Points)**

(b) ~~2.~~ Which energy level is shifted the most to first order in ϵ? **(1 Point)**

(c) ~~3.~~ Calculate the second order (in ϵ) correction to the ground state energy **(2 Points)**

(d) ~~4.~~ Calculate the corrections to the ground state wavefunction to first order in ϵ. **(2 Points)**

(e) 5. Suppose that ϵ is larger than the energy of the first excited state. Carefully sketch the wavefunction versus x for the ground state and for the first excited state. How many nodes, maxima, and minima does the wavefunction have in each state. **(2 Points)**

(f) 6. Suppose the wavefunction is a linear combination of the ground state and the first excited state from part 5. Describe how the maximum of the probability density depends on time. **(1 Point)**

(a)

To first order, we have

$$E^{(1)} = \langle n|V'|n\rangle$$

where

$$|n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right).$$

Then

$$E^{(1)} = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\varepsilon\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)dx$$

$$= \frac{2\varepsilon}{L}\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)dx$$

$$= \frac{2\varepsilon}{L}\int_0^L \frac{1}{2}\left(1-\cos\left(\frac{2n\pi x}{L}\right)\right)\sin\left(\frac{\pi x}{L}\right)dx$$

$$= \frac{\varepsilon}{L}\int_0^L \left(\sin\left(\frac{\pi x}{L}\right) - \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{2n\pi x}{L}\right)\right)dx$$

$$= \frac{\varepsilon}{L}\left[\int_0^L \sin\left(\frac{\pi x}{L}\right)dx - \frac{1}{2}\int_0^L\left(\sin\left(\frac{\pi x}{L} - \frac{2\pi n x}{L}\right) + \sin\left(\frac{2\pi n x}{L} + \frac{\pi x}{L}\right)\right)dx\right]$$

$$= \frac{\varepsilon}{L}\left[\int_0^L \sin\left(\frac{\pi x}{L}\right)dx - \frac{1}{2}\int_0^L \sin\left(x\left(\frac{\pi - 2\pi n}{L}\right)\right)dx - \frac{1}{2}\int_0^L \sin\left(x\left(\frac{2\pi n+\pi}{L}\right)\right)dx\right]$$

$$= \frac{\varepsilon}{L}\left[-\frac{L}{\pi}\cos\left(\frac{\pi x}{L}\right) + \frac{L}{2\pi - 4\pi n}\cos\left(x\left(\frac{\pi - 2\pi n}{L}\right)\right) + \frac{L}{2\pi+4\pi n}\cos\left(x\left(\frac{\pi + 2\pi n}{L}\right)\right)\right]\Bigg|_0^L$$

$$= \frac{\varepsilon}{L}\left[-\frac{L}{\pi}(-1) + \frac{L}{2\pi - 4\pi n}(-1) + \frac{L}{2\pi + 4\pi n}(-1) + \frac{L}{\pi}(1) - \frac{L}{2\pi - 4\pi n}(1) - \frac{L}{2\pi+4\pi n}(1)\right]$$

$$= \frac{\varepsilon}{L}\left[\frac{2L}{\pi} - \frac{2L}{2\pi - 4\pi n} - \frac{2L}{2\pi + 4\pi n}\right]$$

$$\boxed{E^{(1)} = -\frac{8\varepsilon n^2}{\pi(1-2n)(1+2n)}}$$

(b)

The $n=1$ energy level is shifted the most to first order in ε, with the energy shift being

$$E_1^{(1)} = \frac{8\varepsilon}{3\pi}.$$

(c)

The second order correction to the ground state is

$$E^{(2)} = \sum_{m\neq 1} \frac{|\langle m|V'|1\rangle|^2}{E_1^{(0)} - E_m^{(0)}}$$

$$= \sum_{m\neq 1} \frac{1}{E_1^{(0)} - E_m^{(0)}} \left| \int_0^L \frac{2\varepsilon}{L} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{\pi x}{L}\right) dx \right|^2$$

$$= \sum_{m\neq 1} \frac{1}{E_1^{(0)} - E_m^{(0)}} \frac{4\varepsilon^2}{L^2} \left| \int_0^L \sin^2\left(\frac{\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx \right|^2$$

The integral is equal to zero unless $m \in$ odds, with $m \neq 1$. So

$$E^{(2)} = \frac{1}{E_1^{(0)} - E_m^{(0)}} \frac{4\varepsilon^2}{L^2} \left| \frac{2L(\cos(\pi m) - 1)}{\pi m (m^2 - 4)} \right|^2, \quad m = 3, 5, 7, \ldots$$

$$= \frac{1}{E_1^{(0)} - E_m^{(0)}} \frac{4\varepsilon^2}{L^2} \left| \frac{2L(-1) - 1}{m(m^2-4)\pi} \right|^2$$

$$= \frac{1}{E_1^{(0)} - E_m^{(0)}} \frac{4\varepsilon^2}{L^2} \left(\frac{2L + 1}{m(m^2-4)\pi} \right)^2$$

But

$$E_n^{(0)} = \frac{n^2 \pi^2 \hbar^2}{2m' L^2},$$

So

$$E_1^{(0)} = \frac{\pi^2 \hbar^2}{2m' L^2}, \quad E_m^{(0)} = \frac{m^2 \pi^2 \hbar^2}{2m' L^2}$$

(c), cont'd...

$$E^{(2)} = \frac{2m^2L^2}{\pi^2\hbar^2(1-m^2)}\,\frac{4\varepsilon^2}{L^2}\left(\frac{2L+1}{m(m^2-4)\pi}\right)^2$$

$$\boxed{E^{(2)} = \frac{8m^2\varepsilon^2}{\pi^2\hbar^2(1-m^2)}\left(\frac{2L+1}{m(m^2-4)\pi}\right)^2, \quad m = 3,5,7,\ldots}$$

(d)

We know that

$$|n^{(1)}\rangle = \sum_{m\neq 1}\frac{\langle m|V'|1\rangle}{E_1^{(0)}-E_m^{(0)}}\,|m\rangle$$

$$= \sum_{m\neq 1}\frac{1}{E_1^{(0)}-E_m^{(0)}}\int_0^L \frac{2\varepsilon}{L}\sin^2\left(\frac{\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx\,\sqrt{\frac{2}{L}}\sin\left(\frac{m\pi x}{L}\right)$$

$$= -\frac{2m^2L^2}{\pi^2\hbar^2(1-m^2)}\,\frac{2\sqrt{2}\,\varepsilon}{L\sqrt{L}}\left(\frac{2L+1}{m(m^2-4)\pi}\right)\sin\left(\frac{m\pi x}{L}\right)$$

$$|n^{(1)}\rangle = -\frac{4\sqrt{2}\,m^2\varepsilon\sqrt{L}}{\pi^2\hbar^2(1-m^2)}\left(\frac{2L+1}{m(m^2-4)\pi}\right)\sin\left(\frac{m\pi x}{L}\right),$$

So

$$\boxed{|n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) - \frac{4\sqrt{2}\,m^2\varepsilon\sqrt{L}}{\pi^2\hbar^2(1-m^2)}\left(\frac{2L+1}{m(m^2-4)\pi}\right)\sin\left(\frac{m\pi x}{L}\right)}.$$