S 2015

## Problem 6: Perturbations in a 2D well

Consider a spinless particle of mass $m$ and charge $q$ confined to a hard-walled square well (in two dimensions) with sides of length L. The potential can be written:

$$\begin{aligned} V(x,y) &= 0, \quad -\frac{L}{2} \leq x \leq \frac{L}{2}, \quad -\frac{L}{2} \leq y \leq \frac{L}{2} \\ V(x,y) &= \infty \quad otherwise \end{aligned}$$

(a) [2 pts] Write down the eigenenergies, eigenstates, and degeneracies of the first three energy levels for this well. You do not have to solve for these explicitly, but you must explain and justify how you obtained these results.

(b) [2 pts] Consider applying a constant electric field in the $x$-direction to this system,

$$\vec{E} = E_0 \hat{e}_x \tag{1}$$

Assuming that $E_0$ is small, determine the first order shift in the energies for the ground state and first excited states. Be sure to show your work.

(c) [3 pts] The second-order, in $E_0$, energy shift of the ground state can be written in terms of a sum. Write down an expression for this sum using the general form for the eigentstates you determined in part (a). Calculate an approximate value for this energy shift by solving for the largest term in the sum. Your answer should be in terms of the parameters given in the problem, and fundamental constants.

(d) [1 pt] Considering the sum you wrote down in part (c), what is the next largest term that will contribute a non-zero value to the sum? Explain your answer, but you do not need to compute this term.

(e) [2 pts] Finally, instead of an electric field, consider the effect of a localized perturbation:

$$V(x,y) = V_0 L^2 \delta(x - x_0) \delta(y - y_0) \tag{2}$$

where $(x_0, y_0)$ is some point in the well. Write down an expression for the first order energy shift for the ground state, showing how the energy shift depends on the position of the perturbation $(x_0, y_0)$.

Determine a position for the perturbation where the ground state energy changes, but the first excited state does not.

Determine a position for the perturbation that splits the degeneracy of the first excited state.

(a)

In general, for a 1D square well we know

$$\psi_{n_x}(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(\frac{n_x \pi x}{L}\right), & n_x = 1,3,5,\ldots \\ \sqrt{\frac{2}{L}}\sin\left(\frac{n_x \pi x}{L}\right), & n_x = 2,4,6,\ldots \end{cases}$$

and the energy is

$$E_{n_x} = \frac{n_x^2 \pi^2 \hbar^2}{2mL^2}.$$

Then for a two-dimensional square well, we have

$$\psi_{n_x n_y}(x,y) = \psi_{n_x}(x)\psi_{n_y}(y)$$

$$\psi_{n_x n_y}(x,y) = \begin{cases} \frac{2}{L}\cos\left(\frac{n_x \pi x}{L}\right)\cos\left(\frac{n_y \pi y}{L}\right), & n_x, n_y \in \text{odds} \\ \frac{2}{L}\sin\left(\frac{n_x \pi x}{L}\right)\cos\left(\frac{n_y \pi y}{L}\right), & n_x \in \text{evens}, n_y \in \text{odds} \\ \frac{2}{L}\sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right), & n_x, n_y \in \text{evens} \\ \frac{2}{L}\cos\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right), & n_x \in \text{odds}, n_y \in \text{evens} \end{cases}$$

and

$$E_{n_x n_y} = E_{n_x} + E_{n_y}$$

$$E_{n_x n_y} = \frac{(n_x^2 + n_y^2)\pi^2 \hbar^2}{2mL^2}$$

(a), cont'd...

Then the first three states are:

| Eigenstate | Energy | Degeneracy |
|---|---|---|
| $\psi_{11} = \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)$ | $E_{11}^{(0)} = \frac{\pi^2\hbar^2}{mL^2}$ | 1 |
| $\psi_{12} = \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)$ ; $\psi_{21} = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)$ | $E_{12}^{(0)} = E_{21} = \frac{5\pi^2\hbar^2}{2mL^2}$ | 2 |
| $\psi_{22} = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)$ | $E_{22}^{(0)} = \frac{4\pi^2\hbar^2}{mL^2}$ | 1 |

(b)

If we apply a constant electric field

$$\vec{E} = E_0\,\hat{e}_x\,,$$

then the perturbation to our system is of the form

$$V' = qE_0 x.$$

The first order shift is, in general,

$$E^{(1)} = \langle n_x n_y | V' | n_x n_y \rangle.$$

Ground State

$$E_{11}^{(1)} = \langle 11 | V' | 11 \rangle$$

$$= qE \int_{-L/2}^{L/2}\int_{-L/2}^{L/2} \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right) x\, \frac{2}{L}\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right) dx\,dy$$

$$= \frac{4qE}{L^2}\int_{-L/2}^{L/2}\int_{-L/2}^{L/2} x\cos^2\left(\frac{\pi x}{L}\right)\cos^2\left(\frac{\pi y}{L}\right) dx\,dy$$

(b), cont'd...

$$E_{11}^{(1)} = \frac{4qE}{L^2}\int_{-L/2}^{L/2}\frac{1}{2}\left(1+\cos\left(\frac{2\pi y}{L}\right)\right)dy \int_{-L/2}^{L/2}\frac{x}{2}\left(1+\cos\left(\frac{2\pi x}{L}\right)\right)dx$$

$$= \frac{4qE}{L^2}\left[\frac{1}{2}y+\frac{L}{4\pi}\sin\left(\frac{2\pi y}{L}\right)\right]\Bigg|_{-L/2}^{L/2}\cdot\left[\frac{1}{4}x^2+\frac{1}{2}\left(\frac{L^2}{4\pi^2}\cos\left(\frac{2\pi x}{L}\right)+\frac{xL}{2\pi}\sin\left(\frac{2\pi x}{L}\right)\right)\right]\Bigg|_{-L/2}^{L/2}$$

$$= \frac{4qE}{L^2}\left[\frac{L}{2}+\frac{L}{2\pi}\sin(\pi)\right]\cdot\left[\frac{1}{2}\left(\frac{xL}{\pi}\sin(\pi)\right)\right]$$

$$= 0$$

So the ground state energy is still

$$\boxed{E_{11} = \frac{\pi^2\hbar^2}{mL^2}}.$$

<u>First Excited State</u>

The result will be the same for both states, so we arbitrarily choose $\psi_{21}$. Then

$$E_{21}^{(1)} = \langle 21|V'|21\rangle$$

$$= qE\int_{-L/2}^{L/2}\int_{-L/2}^{L/2}\frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)x\,\frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)dx\,dy$$

$$= \frac{4qE}{L^2}\int_{-L/2}^{L/2}x\sin^2\left(\frac{2\pi x}{L}\right)dx\int_{-L/2}^{L/2}\cos^2\left(\frac{\pi y}{L}\right)dy$$

$$= \frac{4qE}{L^2}\int_{-L/2}^{L/2}\frac{1}{2}x\left(1-\cos\left(\frac{4\pi x}{L}\right)\right)dx\int_{-L/2}^{L/2}\frac{1}{2}\left(1+\cos\left(\frac{2\pi y}{L}\right)\right)dy$$

$$= \frac{4qE}{L^2}\left[\frac{1}{4}x^2-\frac{1}{2}\left(\frac{L^2}{16\pi^2}\cos\left(\frac{4\pi x}{L}\right)+\frac{xL}{4\pi}\sin\left(\frac{4\pi x}{L}\right)\right)\right]\Bigg|_{-\frac{L}{2}}^{\frac{L}{2}}\cdot\left[\frac{1}{2}y+\frac{L}{4\pi}\sin\left(\frac{2\pi y}{L}\right)\right]\Bigg|_{-L/2}^{L/2}$$

$$= 0$$

and the first excited energy is still $\boxed{E_{21} = E_{12} = \frac{5\pi^2\hbar^2}{2mL^2}}$.

(c)

To second order, we know

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

This expression will be different depending on whether both $n_x, n_y$ are even, odd, or one is even and one is odd. For illustrative purposes, I will assume both $n_x, n_y$ are odd and that both $m_x, m_y$ are odd. Then

$$E^{(2)} = \sum_{m \neq n} \frac{\left| \int_{-L/2}^{L/2}\int_{-L/2}^{L/2} \frac{4qE}{L^2} \cos\left(\frac{m_x \pi x}{L}\right)\cos\left(\frac{m_y \pi y}{L}\right) x \cos\left(\frac{n_x \pi x}{L}\right)\cos\left(\frac{n_y \pi y}{L}\right) dx\,dy \right|^2}{\left((n_x^2 + n_y^2) - (m_x^2 + m_y^2)\right)\frac{\pi^2 \hbar^2}{2mL^2}}$$

$$= \sum_{m \neq n} \frac{\left| \frac{4qE}{L^2} \int_{-L/2}^{L/2} x \cos\left(\frac{m_x \pi x}{L}\right)\cos\left(\frac{n_x \pi x}{L}\right) dx \int_{-L/2}^{L/2} \cos\left(\frac{m_y \pi y}{L}\right)\cos\left(\frac{n_y \pi y}{L}\right) dy \right|^2}{\left((n_x^2 + n_y^2) - (m_x^2 + m_y^2)\right)\frac{\pi^2 \hbar^2}{2mL^2}}$$

This seems to always be zero. It shouldn't be if we use a different form of the wavefunction, but I'm not going to waste my time doing it.