E6050: Pertrubed particle in a 2D symmetric box

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The problem:

Given a particle with no spin and mass m in a box $x, y \in [-a, a]$.

(1) Write the wave function $\psi(x, y)$ of the ground state.
(2) A potential $V = u\delta(x)\delta(y)$ is added (relates to all questions 3-5 as well). Write three "lowest" (i.e correlating to lowest energies) eigenstates coupled with the ground state by the perturbation.
(3) Write the Hamiltonian $H = H_0 + V$ as a sum of two 4x4 matrices.
(4) Write eigenstates (as column vectors) and eigenenergies up to first order of u.
(5) Calculate ground state energy to second order.

The solution:

(1) In the case of a square box, we can write the hamilotnian of the particle as:

$$\hat{H} = -\frac{\hbar^2}{2m}\left(p_x^2 + p_y^2\right) \tag{1}$$

Boundary conditions are:

$$\psi\left(-a, y\right) = \psi\left(a, y\right) = \psi\left(x, a\right) = \psi(x, -a) = 0 \tag{2}$$

Concluding eigenstates of a particle in a two-dimentional box:

$$\psi(x, y) = \begin{cases} \frac{1}{a}\sin\left(k_{n,x}x\right)\sin(k_{m,y}y) & n, m = even \\ \frac{1}{a}\cos\left(k_{n,x}x\right)\cos(k_{m,y}y) & n, m = odd \\ \frac{1}{a}\sin\left(k_{n,x}x\right)\cos(k_{m,y}y) & n = even, m = odd \\ \frac{1}{a}\cos\left(k_{n,x}x\right)\sin(k_{m,y}y) & n = odd, m = even \end{cases} \tag{3}$$

where

$$k_{n,x} = \frac{\pi}{2a}n \quad ; \quad k_{m,y} = \frac{\pi}{2a}m \tag{4}$$

and the energies are :

$$E_{n,m} = \frac{\hbar^2}{2m}\left(k_{n,x}^2 + k_{m,y}^2\right) = \frac{\hbar^2\pi^2}{8ma^2}\left(n^2 + m^2\right) \tag{5}$$

The unperturbed ground state is achieved by choosing $n, m = 1$, so that the wave function of the ground state is: $\frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos(\frac{\pi}{2a}y)$. The energy is: $E_0 = \frac{\hbar^2\pi^2}{4ma^2}$.

(2) The wave functions which are affected by the aforementioned perturbation are those for which $\psi(0, 0) \neq 0$. We conclude that the 'lowest' three eigenstates are $|n = 1, m = 3\rangle$ $|n = 3, m = 1\rangle$ and $|n = 3, m = 3\rangle$:

$$\begin{aligned} |3, 1\rangle &= |1\rangle = \frac{1}{a}\cos\left(\frac{\pi}{2a}3x\right)\cos(\frac{\pi}{2a}y) \\ |1, 3\rangle &= |2\rangle = \frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos(\frac{\pi}{2a}3y) \\ |3, 3\rangle &= |3\rangle = \frac{1}{a}\cos\left(\frac{\pi}{2a}3x\right)\cos(\frac{\pi}{2a}3y) \end{aligned} \tag{6}$$

and the energies are:

$$E_{1,2} = \frac{10\hbar^2\pi^2}{8ma^2}; \; E_3 = \frac{18\hbar^2\pi^2}{8ma^2} \tag{7}$$

(3) In order to find V we will compute: $\langle n|V|m\rangle = \langle n|u\delta\left(x\right)\delta\left(y\right)|m\rangle$.

$$\langle 0|V|0\rangle = \int_{-a}^{a}\int_{-a}^{a}\frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos\left(\frac{\pi}{2a}y\right)u\delta\left(x\right)\delta\left(y\right)\frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos\left(\frac{\pi}{2a}y\right)dxdy = \frac{u}{a^2} \tag{8}$$

It is obvious that all combinations give the same result, since the δ cooses $\cos(0) = 1$.
The hamiltonian is:

$$H = H_0 + V = E_0\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix} + \frac{u}{a^2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \tag{9}$$

(4) First of all, in order to use perturbation theory we must tackle degeneracies (i.e states $|1\rangle$and $|2\rangle$). Changing basis by using Symmetric and Anti-Symmetric configurations:

$$|A\rangle = \tfrac{1}{\sqrt{2}}\left(|1\rangle + |2\rangle\right) \quad , \; |S\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle - |2\rangle\right) \tag{10}$$

Using the transformation matrix, we derive the new Hamiltonian:

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$P^THP = E_0\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix} + \frac{u}{a^2}\begin{pmatrix} 1 & \sqrt{2} & 0 & 1 \\ \sqrt{2} & 2 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 \\ 1 & \sqrt{2} & 0 & 1 \end{pmatrix} = \tag{11}$$

$$H_{new} = E_0\begin{pmatrix} 1 + \frac{u}{E_0a^2} & 0 & 0 & 0 \\ 0 & 5 + \frac{2u}{E_0a^2} & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 + \frac{u}{E_0a^2} \end{pmatrix} + \frac{u}{a^2}\begin{pmatrix} 0 & \sqrt{2} & 0 & 1 \\ \sqrt{2} & 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 \\ 1 & \sqrt{2} & 0 & 0 \end{pmatrix}$$

In equation (11), one can see the 1^{st} order correction:

$$\epsilon^{[0]} = \epsilon_{n_0} \,;\, \epsilon^{[1]} = V_{n_0,n_0} \rightarrow \epsilon_0 = E_0 + \frac{u}{a^2} \,;\, \epsilon_S = E_1 + \frac{2u}{a^2} \,;\, \epsilon_A = E_1 \,;\, \epsilon_3 = E_3 + \frac{u}{a^2}$$

We will compute the eigenstates to 1^{st} order:

$$\Psi^{[1]} = \frac{V_{n,n_0}}{\epsilon_{n_0} - \epsilon_n}$$

Marking $\frac{u}{a^2} = \lambda$:

$$\Psi_0^{[1]} = \begin{pmatrix} 0 \\ \frac{\sqrt{2}\frac{u}{a^2}}{-4E_0-\frac{u}{a^2}} \\ 0 \\ \frac{u}{-8E_0a^2} \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{\sqrt{2}\lambda}{-4E_0-\lambda} \\ 0 \\ \frac{\lambda}{-8E_0a^2} \end{pmatrix} \rightarrow \Psi_0^{[0]} + \Psi_0^{[1]} = \begin{pmatrix} 1 \\ \frac{\sqrt{2}\lambda}{-4E_0-\lambda} \\ 0 \\ \frac{\lambda}{-8E_0a^2} \end{pmatrix}$$

$$\Psi_s^{[1]} = \begin{pmatrix} \frac{\sqrt{2}\lambda}{4E_0+\lambda} \\ 0 \\ 0 \\ \frac{\sqrt{2}\lambda}{-4E_0+\lambda} \end{pmatrix} \rightarrow \Psi_S^{[0]} + \Psi_S^{[1]} = \begin{pmatrix} \frac{\sqrt{2}\lambda}{4E_0+\lambda} \\ 1 \\ 0 \\ \frac{\sqrt{2}\lambda}{-4E_0+\lambda} \end{pmatrix} \tag{12}$$

$$\Psi_A^{[1]} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \Psi_A^{[0]} + \Psi_A^{[1]} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\Psi_3^{[1]} = \begin{pmatrix} \frac{\lambda}{8E_0} \\ \frac{\sqrt{2}\lambda}{4E_0-2\lambda} \\ 0 \\ 0 \end{pmatrix} \rightarrow \Psi_3^{[0]} + \Psi_3^{[1]} = \begin{pmatrix} \frac{\lambda}{8E_0} \\ \frac{\sqrt{2}\lambda}{4E_0-2\lambda} \\ 0 \\ 1 \end{pmatrix}$$

(5) In order to calculate 2^{nd} order correction of the ground state energy we will use:

$$\epsilon^{[2]} = \sum_m \frac{V_{n_0,m} \cdot V_{m,n_0}}{\epsilon_{n_0} - \epsilon_m} = \{n_0 = 0\} = \frac{V_{0,S} \cdot V_{S,0}}{-4E_0 - \lambda} + \frac{V_{0,A} \cdot V_{A,0}}{-4E_0 + \lambda} + \frac{V_{0,3} \cdot V_{3,0}}{-8E_0} = \tag{13}$$

$$= \frac{2\lambda^2}{-4E_0 - \lambda} + \frac{\lambda^2}{-8E_0}$$