E6050: Pertrubated Particle in a 2D Symmetric Box

Submitted by: Tamir Tapuhy & Omer Koren

The problem:

Given a particle without spin, and mass m in a squared box $x, y \in [-a, a]$. Later we will add the potential $V = u\delta(x)\delta(y)$.

(1) Write the wave function $\psi(x, y)$ of the unperturbated ground state.
(2) Write the lowest 3 eigenstates which are coupled to the ground state by the perturbation.
(3) Write the Hemiltonian $H = H_0 + V$, as a sum of two 4x4 matrices.
(4) Write the eigenstates (as column vectors) and the first order eigen energies of u.
(5) Calculate the correction of the second order to the ground state energy.

The solution:

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

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

The particle is limited to be in the box so the boundary conditions of the wave functions are:

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

We can deal with the hemiltonian by separation of the variables x and y, and finding a solution of the form:

$$\psi(x, y) = X(x) \cdot Y(y) \tag{3}$$

The solution for each axis is of the form of an infinite well: $A_{n,m} \sin(k_x x) \sin(k_y y)$,
while $k_x = \frac{\pi}{2a} n; k_y = \frac{\pi}{2a} m$, n, m - integers. Let us compute the normalization factor:

$$A_{n,m}^2 \int_{-a}^{a} \int_{-a}^{a} \sin^2(k_x x) \cos^2(k_y y)\, dx dy = 1 \tag{4}$$

$$A_{n,m}^2 \int_{-a}^{a} \left(\frac{1 - \cos\left(\frac{2\pi}{2a} n \cdot x\right)}{2}\right) dx \int_{-a}^{a} \left(\frac{1 + \cos\left(\frac{2\pi}{2a} m \cdot y\right)}{2}\right) dy = 1 \tag{5}$$

$$A_{n,m}^2 = \frac{1}{a^2} \rightarrow A_{n,m} = \frac{1}{a} \tag{6}$$

We can now write the eigenfunction of the hamiltonian:

$$\psi(x, y) = \begin{cases} \frac{1}{a} \sin(k_x x) \sin(k_y y) & n, m = even \\ \frac{1}{a} \cos(k_x x) \cos(k_y y) & n, m = odd \\ \frac{1}{a} \sin(k_x x) \cos(k_y y) & n = even, m = odd \\ \frac{1}{a} \cos(k_x x) \sin(k_y y) & n = odd, m = even \end{cases} \tag{7}$$

and the energies :

$$E_{n,m} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right) = \frac{\hbar^2 \pi^2}{8ma^2}\left(n^2 + m^2\right) \tag{8}$$

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

(2) The wave functions which are affected by the perturbation mentioned earlier are those that are not equal to zero at $x, y = 0$ (the place of the perturbation). We can conclude that the lowest three eigenstate achieved by choosing $n = 1, m = 3,\ n = 3, m = 1$ and $n, m = 3$. So the three talked-about eigenstates are:

$$\begin{array}{l} |1\rangle = \frac{1}{a}\cos\left(\frac{\pi}{2a}3x\right)\cos(\frac{\pi}{2a}y) \\ |2\rangle = \frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos(\frac{\pi}{2a}3y) \\ |3\rangle = \frac{1}{a}\cos\left(\frac{\pi}{2a}3x\right)\cos(\frac{\pi}{2a}3y) \end{array} \tag{9}$$

and the energies:

$$E_1 = \frac{10\hbar^2\pi^2}{8ma^2} = E_2;\ E_3 = \frac{18\hbar^2\pi^2}{8ma^2} \tag{10}$$

(3) It can be immidiately seen that H_0 is a diagonal matrix of the eigenvalues of the unperturbated hamiltonian. In order to find the matrix V we will compute: $\langle n|V|m\rangle = \langle n|u\delta(x)\delta(y)|m\rangle$.

$$\langle 0|V|0\rangle = \int_{-a}^{a}\int_{-a}^{a}\frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos\left(\frac{\pi}{2a}y\right)u\delta(x)\delta(y)\frac{1}{a}\cos\left(\frac{\pi}{2a}x\right)\cos\left(\frac{\pi}{2a}y\right)dxdy = \frac{u}{a^2} \tag{11}$$

It is obvious that all the combination will give the same result, because of the integral with the Delta function.
The wanted hamiltonian is:

$$H = H_0 + V = E_0\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix} + \frac{u}{a^2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \tag{12}$$

(4) First of all, in order to use perturbation theory we must deal with the degeneracy between the states $|1\rangle$and $|2\rangle$. We will chage the base by using the Symmetric and Anti-Symmetric configurations:

$$|A\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \quad , |S\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \tag{13}$$

By using the transformation matrix, built of the eigenstaes $|0\rangle, |S\rangle, |A\rangle and\, |4\rangle$we get the new Hamiltonian:

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

$$P^T H P = E_0\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix} + \frac{u}{a^2}\begin{pmatrix} 1 & \sqrt{2} & 0 & 1 \\ \sqrt{2} & 2 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 \\ 1 & \sqrt{2} & 0 & 1 \end{pmatrix} = \tag{14}$$

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

In equation number 14 above, one can see the energy with the first order correction.

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

Now, as asked we will compute the eigenstates of the first order and present it as column vectors.

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

We will mark $\frac{u}{a^2} = \lambda$ as accepted.

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

$$\Psi_s^{[1]} = \begin{pmatrix} \frac{\sqrt{2}\lambda}{4E_0 + \lambda} \\ 0 \\ 0 \\ \frac{\sqrt{2}\lambda}{-4E_0 + \lambda} \end{pmatrix} \rightarrow \Psi_S^{[0]} + \Psi_S^{[1]} = \begin{pmatrix} \frac{\sqrt{2}\lambda}{4E_0 + \lambda} \\ 1 \\ 0 \\ \frac{\sqrt{2}\lambda}{-4E_0 + \lambda} \end{pmatrix} \tag{15}$$

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

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

(5) In order to Calculate the correction of the second order to the ground state energy we will use the expression:

$$\epsilon^{[2]} = \sum_m \frac{V_{n_0,m} \cdot V_{m,n_0}}{\epsilon_{n_0} - \epsilon_m} = \{n_0 = 0\} = \frac{V_{0,S} \cdot V_{S,0}}{-4E_0 - \lambda} + \frac{V_{0,A} \cdot V_{A,0}}{-4E_0 + \lambda} + \frac{V_{0,3} \cdot V_{3,0}}{-8E_0} = \tag{16}$$

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

As we know, the second order correction, for the ground state, will allways be negative, and one can see it in the result that we got.