6050: Perturbed particle in a square box

Submitted by: Elperin Ariel

The problem:

A particle with no spin, of mass m, in placed in a square box x,y$\in [-a, a]$. Later the particle is presented with the perturbation V=u$\delta(x)\delta(y)$.

(1) Write the wavefunction $\psi(x, y)$ of the unperturbed ground state.
(2) Write the wavefunction of the 3 lowest states which are coupled by the perturbation to the ground state.
(3) Write the hamiltonian $H = H_0 + V$ as a sum of two 4x4 matrices.
(4) Write the eigenstates and the first order eigenenergies in u.
(5) Calculate the second order energy shift for the ground state energy.

The solution:

(1)
we have a particle in the potential:

$$V(x.y) = \begin{cases} 0 & x, y \in [-a, a] \\ \infty & x, y \notin [-a, a] \end{cases}$$

In order to find the eigenstates, we need to solve:

$$H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

After losing the time dependence, since $\psi = \psi(x, y)e^{-i\frac{E}{\hbar}t}$, and using separation of variables $\psi(x, y) = X(x)Y(y)$ we get an infinite well in each axis. After adding the boundary conditions: $\psi(x, -a) = \psi(x, a) = \psi(y, -a) = \psi(y, a) = 0$ we have:

$$X(x) = \begin{cases} A_n \sin(\frac{\pi n}{2a}x) & \text{n is even} \\ A_n \cos(\frac{\pi n}{2a}x) & \text{n is odd} \end{cases}$$

Since we have the same solution for Y(y), after normalizing we get:

$$\psi(x, y) = \begin{cases} \frac{1}{a}\sin(\frac{\pi n}{2a}x)\sin(\frac{\pi m}{2a}y) & \text{n,m=even} \\ \frac{1}{a}\sin(\frac{\pi n}{2a}x)\cos(\frac{\pi m}{2a}y) & \text{n=even , m=odd} \\ \frac{1}{a}\cos(\frac{\pi n}{2a}x)\sin(\frac{\pi m}{2a}y) & \text{n=odd, m=even} \\ \frac{1}{a}\cos(\frac{\pi n}{2a}x)\cos(\frac{\pi m}{2a}y) & \text{n,m=odd} \end{cases}$$

with the corresponding eigenenergies:

$$E_{n,m} = \frac{\hbar^2\pi^2}{8a^2}(n^2 + m^2)$$

The ground state is $n = m = 1$, and has the wavefunction:

$$\psi(x, y) = \frac{1}{a}\cos(\frac{\pi x}{2a})\cos(\frac{\pi y}{2a})$$

And energy:

$$E_0 = \frac{\hbar^2\pi^2}{4a^2}$$

(2)
The perturbation $V(x) = u\delta(x)\delta(y)$ only affects states with a wavefunction $\psi(x,y)$ such that $\psi(0,0) \neq 0$, otherwise the particle already cannot be found in (0,0) and the perturbation has no effect. This happens only for states ψ_{nm} in which n,m are odd.

Therefore, the lowest states which are coupled by the perturbation to the ground state are ψ_{13}, ψ_{31}, ψ_{33}.

$$|1,3\rangle \equiv |1\rangle = \frac{1}{a}\cos(\frac{\pi}{2a}x)\cos(\frac{3\pi}{2a}y)$$
$$|3,1\rangle \equiv |2\rangle = \frac{1}{a}\cos(\frac{3\pi}{2a}x)\cos(\frac{\pi}{2a}y)$$
$$|3,3\rangle \equiv |3\rangle = \frac{1}{a}\cos(\frac{3\pi}{2a}x)\cos(\frac{3\pi}{2a}y)$$

(3) We shall now find the perturbation matrix V_{ij} in the basis $|0\rangle, |1\rangle, |2\rangle, |3\rangle$ when $|0\rangle = \psi_{11}$

$$V_{00} = \langle 0|V|0\rangle = \frac{1}{a^2}\int_{-a}^{a}\int_{-a}^{a}\cos(\frac{\pi}{2a}x)\cos(\frac{\pi}{2a}y)u\delta(x)\delta(y)\cos(\frac{\pi}{2a}x)\cos(\frac{\pi}{2a}y)\,dx\,dy = \frac{u}{a^2}$$

It is obvious that $\forall i,j\ \ \langle i|V|j\rangle = \langle 0|V|0\rangle$, Therefore the representation of V in our basis is as follows:

$$V = \frac{u}{a^2}\begin{pmatrix}1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\end{pmatrix}$$

The unperturbed hamiltonian is diagonal, with the eigenenergies:

$$H_0|0\rangle = E_0|0\rangle, H_0|1\rangle = 5E_0|1\rangle, H_0|2\rangle = 5E_0|2\rangle, H_0|3\rangle = 9E_0|3\rangle$$

where $E_0 = \frac{\hbar^2\pi^2}{16a^2}$.

Hence, the perturbed hamiltonian is:

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

(4) We notice that there is degeneracy in the eigenenergy $E = 5E_0$ which corresponds to the two different eigenstates : $|1\rangle, |2\rangle$. In order to use the perturbation theory, we must first get rid of this degeneracy. We shall do this by the following transformation of basis:

$$|0\rangle \to |0\rangle\ \ |1\rangle \to |S\rangle\ \ |2\rangle \to |A\rangle\ \ |3\rangle \to |3\rangle$$

where

$$|S\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)\ \ and\ \ |A\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle).$$

The transformation matrix is:

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

The unperturbed hamiltonian H_0 has the same representation in the new basis, hence, in the new basis we have:

$$H_{new} = H_0 + T^{-1}VT = E_0 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix} + \frac{u}{a^2} \begin{pmatrix} 1 & \sqrt{2} & 0 & 1 \\ \sqrt{2} & 2 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 \\ 1 & \sqrt{2} & 0 & 1 \end{pmatrix}$$

We notice that the perturbation V does not couple eigenstates with the same eigenenergey anymore, therefore we can now use the approximation:

$$E_n = E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum_{k \neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$|n\rangle = |n^{(0)}\rangle + \lambda \sum_{k \neq n} \frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$$

where

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$$

Using the approximation, we have the first order correction in $\frac{u}{a^2}$ to the eigenenergies:

$$E_0 = E_0^{(0)} + \frac{u}{a^2}, \quad E_S = E_S^{(0)} + \frac{2u}{a^2}, \quad E_A = E_A^{(0)}, \quad E_3 = E_3^{(0)} + \frac{u}{a^2}$$

And the first order correction to the eigenstates:

$$|0\rangle = |0^{(0)}\rangle + \frac{u}{a^2} \left(\frac{\sqrt{2}}{-4E_0} |S^{(0)}\rangle + \frac{1}{-8E_0} |3^{(0)}\rangle \right) = \begin{pmatrix} 1 \\ -\frac{1}{2\sqrt{2}E_0} \frac{u}{a^2} \\ 0 \\ -\frac{1}{8E_0} \frac{u}{a^2} \end{pmatrix}$$

$$|S\rangle = |S^{(0)}\rangle + \frac{u}{a^2} \left(\frac{\sqrt{2}}{4E_0} |0^{(0)}\rangle + \frac{\sqrt{2}}{-4E_0} |3^{(0)}\rangle \right) = \begin{pmatrix} \frac{1}{2\sqrt{2}E_0} \frac{u}{a^2} \\ 1 \\ 0 \\ -\frac{1}{2\sqrt{2}E_0} \frac{u}{a^2} \end{pmatrix}$$

$$|A\rangle = |A^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|3\rangle = |3^{(0)}\rangle + \frac{u}{a^2} \left(\frac{1}{8E_0} |0^{(0)}\rangle + \frac{\sqrt{2}}{4E_0} |S^{(0)}\rangle \right) = \begin{pmatrix} \frac{1}{8E_0} \frac{u}{a^2} \\ \frac{1}{2\sqrt{2}E_0} \frac{u}{a^2} \\ 0 \\ 1 \end{pmatrix}$$

(5) The correction of the ground state energy up to the second order is:

$$E_0 = E_0^{(0)} + \frac{u}{a^2} + \frac{u^2}{a^4} \left(\frac{2}{-4E_0} + \frac{1}{-8E_0} \right)$$