E6050: Pertrubation in a symmetric square box

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The problem:

A particle without spin, with mass m, is placed in a square box $x, y \in [-a, a]$. We then add a pertrubation of the form $V = u\delta(x)\delta(y)$

(1) Write the Wavefunctions for the unpertrubed particle's ground state.
(2) Also write the first three eigenstates that are coupled to the ground state.
(3) Write the Hamiltonian as a sum of two 4×4 matrices: $H = H_0 + V$
(4) Write the eigenstates (as column vectors) and the eigen energies in the first order of u.
(5) Calculate the second order correction to the energy of the ground state.

The solution:

The Hamiltonian without the pertrubation is:

$$i\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi \rightarrow V = \begin{cases} 0 & x, y \in [-a, a] \\ \infty & otherwise \end{cases}$$

As usual the solution is time dependante according to $\Psi(x, y, t) = \psi(x, y)e^{i\frac{E}{\hbar}t}$ and we must now solve the eigenvector problem in the space coordinates only. We can also assume an independant solution for $x, y \rightarrow \psi(x, y) = \chi(x)\eta(y)$ when the obvious solutions are sin and cos functions.

So now we can calculate the solutions, taking into account the boundry conditions of the box:

$$\chi(x) = N_x \sin(k_x x)\mid_{x=\pm a} = 0 \qquad \int_{-a}^{a} N_x \sin^2(k_x x)dx = 1 \rightarrow N_x = \sqrt{\frac{1}{a}}$$

The same goes for cosine solutions. The results for y are the same as for x (for obvious reasons). We now have a full discription of all the eigenfuntions of this Hamiltonian:

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

with the energy given by substitution into the Hamiltonian:

$$E_{n,m}\psi(x, y) = -\frac{\hbar^2}{2m}\nabla^2\psi(x, y) = \frac{\hbar^2\pi^2}{8ma^2}(n^2 + m^2)$$

(1) The ground state wavefunction is then $\frac{1}{a}\cos(\frac{\pi}{2a}x)\cos(\frac{\pi}{2a}y)$ for $n = m = 1$ and the energy $E_{1,1} = \frac{\hbar^2\pi^2}{4ma^2} \equiv E_0$

(2) The only wavefunctions that are in any way affected by the $\delta(x)\delta(y)$ scatterer are those that are not zero at $x, y = 0$, which means only the cosine functions. so we get $n = 1, 3$ and $m = 1, 3$ with all combinations allowed (notice that $n = m = 1$ is the ground state). we can define:

$$|1>= \frac{1}{a}\cos(\frac{\pi}{2a}x)cos(\frac{\pi}{2a}y)$$

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

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

$$|4>= \frac{1}{a}cos(\frac{3\pi}{2a}x)cos(\frac{3\pi}{2a}y)$$

The energies involved are $E_1 = \frac{\hbar^2\pi^2}{4ma^2}$, $E_2 = E_3 = \frac{\hbar^2\pi^2}{8ma^2}10$, $E_4 = \frac{\hbar^2\pi^2}{8ma^2}18$
(3) In the given basis we get the unpertrubed Hamiltonian to be:

$$H_0 = \frac{\hbar^2\pi^2}{8ma^2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 10 & 0 & 0 \\ 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 18 \end{pmatrix}$$

Now we must find the pertrubing potential matrix by sandwiching the different wavefunctions of our base, according to the Hamiltonian with the $\delta(x)\delta(y)$ function:

$$E_{n,m} =< n|E|m >=< n|H|M >= \int_{-a}^{a}\int_{-a}^{a}\frac{1}{a^2}\cos(\frac{\pi n}{2a}x)\cos(\frac{\pi n}{2a}y)(\frac{\partial^2}{\partial x^2}\cos(\frac{\pi m}{2a}x)\cos(\frac{\pi m}{2a}y)dxdy+$$

$$\int_{-a}^{a}\int_{-a}^{a}\frac{1}{a^2}\cos(\frac{\pi n}{2a}x)\cos(\frac{\pi n}{2a}y)\,[u\delta(x,y)]\cos(\frac{\pi m}{2a}x)\cos(\frac{\pi m}{2a}y)dxdy$$

The first integral gives the energies of the unpertrubed Hamiltonian, which is the diagonal matrix H_0. The second integral simply gives $< n|V|m >= \frac{u}{a^2}$ for any n,m.

$$H = H_0 + V = \frac{\hbar^2\pi^2}{8ma^2}\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 10 & 0 & 0 \\ 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 18 \end{pmatrix} + \frac{u}{a^2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

we can also define the following constants to shorten writing: $E_0 = \frac{\hbar^2\pi^2}{4ma^2}$ $\lambda = \frac{u}{a^2}$, giving the following matrix:

$$H = H_0 + V = E_0\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 9 \end{pmatrix} + \lambda\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

Notice that we have a degeneracy in the energies E_2, E_3. we will use the symmetric and anti symmetric solutions to avoid this problem.

$$|S>= \frac{1}{\sqrt{2}}(|2>+|3>) \quad , \quad |A>= \frac{1}{\sqrt{2}}(|2>-|3>)$$

We may find the matrix V in the new basis by operating the old V on the $|A>$ and $|S>$ states in the standard base. We also add the diagonal elements of V to the already diagonal matrix H_0.We end up with the following states: $|1>, |A>, |S>, |4>$.
In the new base our matrices take the following form:

$$H = H_0 + V = E_0 \begin{pmatrix} 1+\frac{\lambda}{E_0} & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5+2\frac{\lambda}{E_0} & 2 \\ 0 & 0 & 0 & 9+\frac{\lambda}{E_0} \end{pmatrix} + \lambda \begin{pmatrix} 0 & 0 & \sqrt{2} & 1 \\ 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & \sqrt{2} \\ 1 & 0 & \sqrt{2} & 0 \end{pmatrix}$$

So we can now easily find the eigenstates and energies of the first order in λ:

$$\Psi_n^{[0,1]} = \Psi_n^{[0]} + \Psi_n^{[1]} = \Psi_n^{[0]} + \frac{V_{n,n_0}}{E_{n_0}^{[0]} - E_n^{[0]}}$$

With the (first order) energy corrections given directly from the addition of the diagonal elements of V into H_0 i.e:

$$E_1^{[0,1]} = E_0 + \lambda \quad , \quad E_A^{[0,1]} = 5E_0 \quad , \quad E_S^{[0,1]} = 5E_0 + 2\lambda \quad , \quad E_4^{[0,1]} = 9E_0 + \lambda$$

The eigenstates given in coloumn form in the previous base $(|1>, |A>, |S>, |4>)$:

$$|\Psi_1^{[0,1]}>= \begin{pmatrix} 1 \\ -\frac{\sqrt{2}\lambda}{4E_0-\lambda} \\ 0 \\ -\frac{\lambda}{8E_0} \end{pmatrix} \quad , \quad |\Psi_A^{[0,1]}>= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|\Psi_S^{[0,1]}>= \begin{pmatrix} \frac{\sqrt{2}\lambda}{4E_0+\lambda} \\ 0 \\ 1 \\ -\frac{\sqrt{2}\lambda}{4E_0+\lambda} \end{pmatrix} \quad , \quad |\Psi_4^{[0,1]}>= \begin{pmatrix} \frac{\lambda}{8E_0} \\ \frac{\sqrt{2}\lambda}{4E_0+\lambda} \\ 0 \\ 1 \end{pmatrix}$$

We can see the Anti Symmetric solution is unaffected by the pertrubation. That is because the wavefunction $\frac{1}{\sqrt{2}a}(\cos(\frac{3\pi}{2a}x)\cos(\frac{\pi}{2a}y) - \cos(\frac{\pi}{2a}x)\cos(\frac{3\pi}{2a}y))$ is zero at $(0,0)$ and so does not feel the pertrubation.
(5) We can calculate the second order correction to the energy using: $\sum_{m(=n_0)} \frac{|Vn_0, m|^2}{E_{n_0}^{[0]} - E_n^{[0]}}$

$$E_1^{[2]} = \frac{V_{1,A}^2}{E_1^{[0]} - E_A^{[0]}} + \frac{V_{1,S}^2}{E_1^{[0]} - E_S^{[0]}} + \frac{V_{1,4}^2}{E_1^{[0]} - E_4^{[0]}} = -\frac{2\lambda^2}{4E_0+\lambda} - \frac{\lambda^2}{8E_0}$$

The first term is zero (anti symmetric solution). We can see both states $|S>$ and $|4>$ 'push' down the ground state energy (the term is always negative for ground state energies).