Ex6051: Particle in a square box with perturbations

Submitted by: Osher Shoval and Bar Zohar

The problem:

A spinless particle of mass M is placed in a square box $x, y \in [-a, a]$. A perturbation is added $u\delta(x)\delta(y)$ represented by the matrix V and a potential $c(x^2 + y^2)$ represented by the matrix W.

(1) Write the wave function $\psi(x, y)$ of the unperturbed ground state and the wave functions of the 3 lowest excited states coupled by the perturbation V to the ground state.
(2) Write an expression for the unperturbed ground state energy E_0. Express the rest of the unperturbed energies as a multiples of E_0.
(3) Write 4×4 matrix representation of V in the above basis.
(4) Write 4×4 matrix representation of W in the above basis.
(5) Calculate the corrections for the ground state energy to the second order in perturbation theory.
(6) Find frequency of small oscillations for a particle prepared in the middle eigenstate.

Guidance:

Express your answer in terms of ground state energy E_0 (so that the mass does not appear).
The answer in section 4 will include the numerical coefficients:
$\alpha_{nm} = \int_{-1}^{1} x^2 \cos\left(\frac{n\pi x}{2}\right) \cos\left(\frac{m\pi x}{2}\right) dx$
In section 5 ignore the error due to omitting the energy states in section 1.
In section 6 approximation of 2 states is sufficient.

The solution:

(1) $$\Psi_{nm}(x,y) = |n,m> = \begin{cases} \frac{1}{a}\cos(k_x x)\cos(k_y y)\ , & \text{for n odd \& m odd} \\ \frac{1}{a}\cos(k_x x)\sin(k_y y)\ , & \text{for n odd \& m even} \\ \frac{1}{a}\sin(k_x x)\cos(k_y y)\ , & \text{for n even \& m odd} \\ \frac{1}{a}\sin(k_x x)\sin(k_y y)\ , & \text{for n even \& m even} \end{cases}$$

$k_x = \frac{\pi}{2a}n\ ,\ k_y = \frac{\pi}{2a}m$

$$\Psi_{11}(x,y) = \frac{1}{a}\cos\left(\frac{\pi x}{2a}\right)\cos\left(\frac{\pi y}{2a}\right)$$

$$< \Psi_{nm}|V|\Psi_{n'm'} > = \int_{-a}^{a}\int_{-a}^{a} \Psi_{nm}(x,y) u\delta(x)\delta(y)\Psi_{n'm'} dxdy$$

It is easy to see that the integral will take on non-zero values only for purely even states (n,m odd). Therefore the 3 lowest excited states are:

$$\Psi_{31}(x,y) = \frac{1}{a}\cos\left(\frac{3\pi x}{2a}\right)\cos\left(\frac{\pi y}{2a}\right)$$
$$\Psi_{13}(x,y) = \frac{1}{a}\cos\left(\frac{\pi x}{2a}\right)\cos\left(\frac{3\pi y}{2a}\right)$$
$$\Psi_{33}(x,y) = \frac{1}{a}\cos\left(\frac{3\pi x}{2a}\right)\cos\left(\frac{3\pi y}{2a}\right)$$

(2) $$E_{nm} = \frac{\pi^2}{2M(2a)^2}(n^2 + m^2)$$

$E_0 = E_{11} = \dfrac{\pi^2}{4Ma^2}$, $E_{31} = E_{13} = \dfrac{5\pi^2}{4Ma^2} = 5E_0$, $E_{33} = \dfrac{9\pi^2}{4Ma^2} = 9E_0$

(3) $V_{nm,n'm'} = \dfrac{u}{a^2}\displaystyle\int_{-a}^{a}\int_{-a}^{a} \cos\left(\frac{n\pi x}{2a}\right)\cos\left(\frac{m\pi y}{2a}\right)\delta(x)\delta(y)\cos\left(\frac{n'\pi x}{2a}\right)\cos\left(\frac{m'\pi y}{2a}\right)dxdy$

In the basis $|11>, |13>, |31>, |33>$:

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

(4) $W_{nm,n'm'} = \dfrac{c}{a^2}\displaystyle\int_{-a}^{a}\int_{-a}^{a} \cos\left(\frac{n\pi x}{2a}\right)\cos\left(\frac{m\pi y}{2a}\right)(x^2+y^2)\cos\left(\frac{n'\pi x}{2a}\right)\cos\left(\frac{m'\pi y}{2a}\right)dxdy$

$\{x' = \dfrac{x}{a}$, $y' = \dfrac{y}{a}\}$

$= ca^2\displaystyle\int_{-a}^{a}\int_{-a}^{a} \cos\left(\frac{n\pi x'}{2}\right)\cos\left(\frac{m\pi y'}{2}\right)(x'^2+y'^2)\cos\left(\frac{n'\pi x'}{2}\right)\cos\left(\frac{m'\pi y'}{2}\right)dx'dy'$

Using the given α define: $\alpha_{31} = \eta$, $\alpha_{11} - \alpha_{33} = \zeta$. In the same basis:

$$W = ca^2\begin{pmatrix} 0 & -\eta & \eta & 0 \\ -\eta & \zeta & 0 & \eta \\ \eta & 0 & -\zeta & -\eta \\ 0 & \eta & -\eta & 0 \end{pmatrix}$$

(5) $E_{_0}^{(1)} =< \Psi_{11}|V|\Psi_{11} >= \dfrac{u}{a^2}$

$$E_{_0}^{(2)} = \sum_{nm\neq 11}\frac{|<\Psi_{nm}|V|\Psi_{11}>|^2}{E_0 - E_{nm}} = \frac{(\frac{u}{a^2} - ca^2\eta)^2}{-4E_0} + \frac{(\frac{u}{a^2} + ca^2\eta)^2}{-4E_0} + \frac{\frac{u}{a^2}}{-8E_0} = -\frac{5u^2}{8a^4E_0} - \frac{c^2a^4\alpha_{13}^2}{2E_0}$$

$$\tilde{E_0} = E_0 + \frac{u}{a^2} - \frac{5u^2}{8a^4E_0} - \frac{c^2a^4\alpha_{13}^2}{2E_0}$$

(6) Using the basis for the middle eigenstates: $|13>$, $|31>$:

$$\text{H} = E_0\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} + \tfrac{u}{a^2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + ca^2\begin{pmatrix} \zeta & 0 \\ 0 & -\zeta \end{pmatrix} \qquad \Omega = \sqrt{(2ca^2(\alpha_{11} - \alpha_{33}))^2 + (2\frac{u}{a^2})^2}$$