E6040: First order perturbation theory for two dimensional box with a displaced wall

Submitted by: Maxim Sokol & Dekel Shapira

The problem:

A particle of mass M is placed in two dimensional box having side-length a, $x, y \in [0, a]$. The displacement of the left wall is given by $x = \epsilon(y)$. If it were a one dimensional box, the addition to the perturbed Hamiltonian would be: $\langle\psi|V|\phi\rangle = \left(\frac{\epsilon}{2M}\right)\left[\frac{\partial\psi}{\partial x}\right]\left[\frac{\partial\phi}{\partial x}\right]$
where ϵ is small and the derivatives are being calculated at $x = 0$.

(1) Write the two dimensional generalization of the above formula. you may assume the wall is inclined in a small angle and $\epsilon(0) = -\epsilon_0/2$, $\epsilon(a) = +\epsilon_0/2$
(2) Write the Hamiltonian for the three lowest states (in the unperturbed base)
(3) Write the leading order of the ground state energy
(4) Write the leading order of the excited states energy

The solution:

(1) The two dimensional generalization of the above formula:

$$\langle\psi|V|\phi\rangle = \int_0^a \left(\frac{\epsilon(y)}{2M}\right)\left[\frac{\partial\psi}{\partial x}\right]\left[\frac{\partial\phi}{\partial x}\right] dy$$

(2) The Hamiltonian of the unperturbed system:

$$\mathcal{H} = \frac{p^2}{2M}$$

And the eigenenergies and eigenstates according to the boundary conditions:

$$\langle\psi|n, m\rangle = \frac{2}{a}\sin(\frac{\pi m y}{a})\sin(\frac{\pi n x}{a})$$

The Hamiltonian in the unperturbed base:

$$\mathcal{H} = \mathcal{H}_0 + V = \frac{\pi^2}{2Ma^2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix} - \frac{1}{M}\cdot\frac{16\epsilon}{9a^3}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$$

(3)

$$E_0^{[0]} = \frac{\pi^2}{2Ma^2}$$

$$E_0^{[1]} = V_{n0,n0}$$

$$E_0^{[2]} = \sum \frac{V_{n0,m}V_{m,n0}}{\epsilon_0 - \epsilon_m}$$

$$E_0 = E_0^{[0]} + E_0^{[1]} + E_0^{[2]} = \frac{\pi^2}{2Ma^2} + 0 - \frac{512\epsilon^2}{243Ma^4\pi^2} = \frac{\pi^2}{2Ma^2} - \frac{512\epsilon^2}{243Ma^4\pi^2}$$

(4) Before using Perturbation theory, degeneracy must be removed:

$$\mathcal{H}^{excited} = \frac{\pi^2}{2Ma^2}\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} - \frac{1}{M} \cdot \frac{16\epsilon}{9a^3}\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}$$

After diagonalizing (using the symmetric and anti-symmetric base):

$$\mathcal{H}^{excited}_{|s\rangle,|a\rangle} = \frac{\pi^2}{2Ma^2}\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} - \frac{1}{M} \cdot \frac{16\epsilon}{9a^3}\begin{pmatrix} -2 & 0 \\ 0 & 2 \end{pmatrix}$$

$$E^{[1]}_{|s\rangle} = 5\frac{\pi^2}{2Ma^2} - 2\frac{1}{M} \cdot \frac{16\epsilon}{9a^3}$$

$$E^{[1]}_{|a\rangle} = 5\frac{\pi^2}{2Ma^2} + 2\frac{1}{M} \cdot \frac{16\epsilon}{9a^3}$$