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

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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.

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 inside the box:

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

And the eigenstates according to the boundary conditions:

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

Therefore, the Values of $\mathcal{H}\prime$ in the unperturbed basis:

$$\langle n', m'|\mathcal{H}\prime|n, m\rangle = \frac{\pi^2}{2Ma^2}\left(n^2 + m^2\right)\delta_{n,n'}\delta_{m,m'}$$

The derivative of the state $|n, m\rangle$ with respect to x, at x=0:

$$\frac{\partial\psi_{n,m}}{\partial x}|_{x=0} = \frac{2\pi n}{a^2}\sin\left(\frac{\pi m y}{a}\right)$$

V in the unperturbed basis:

$$\epsilon(y) = \frac{\epsilon_0}{a}\left(y - \frac{a}{2}\right)$$

$$\langle n, m|V|n', m'\rangle = \frac{2\pi n' n\epsilon_0}{Ma^4}\int_0^a \frac{\pi}{a}\left(y - \frac{a}{2}\right)\sin\left(\frac{\pi m y}{a}\right)\sin\left(\frac{\pi m' y}{a}\right)dy$$

The Hamiltonian in the unperturbed basis for the three lowest states:

$$\mathcal{H} = \mathcal{H}_0 + V = \frac{\pi^2}{2Ma^2}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix} - \frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$$

(3) The state $|1,1\rangle$ is coupled only with the state $|1,2\rangle$,:

$$\mathcal{H}'_0 + V' = \frac{\pi^2}{2Ma^2}\begin{pmatrix} 2 & 0 \\ 0 & 5 \end{pmatrix} - \frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

$$E_0^{[1]} = V_{n0,n0} = 0$$

$$E_0^{[2]} = \sum \frac{V_{n0,m}V_{m,n0}}{\epsilon_0 - \epsilon_m} = -\frac{1}{3} \cdot \frac{2Ma^2}{\pi^2} \cdot \left(\frac{16\epsilon_0}{9Ma^3}\right)^2$$

$$E_0 = E_0^{[0]} + E_0^{[1]} + E_0^{[2]} = \frac{\pi^2}{Ma^2} + 0 - \frac{512\epsilon_0^2}{243Ma^4\pi^2} = \frac{\pi^2}{Ma^2} - \frac{512\epsilon_0^2}{243Ma^4\pi^2}$$

(4) Removing degeneracy first:

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

In symmetric and anti-symmetric basis:

$$\mathcal{H}^{excited}_{|s\rangle,|a\rangle} = \frac{\pi^2}{2Ma^2}\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} - \frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}\begin{pmatrix} -2 & 0 \\ 0 & 2 \end{pmatrix}$$

For convenience reasons we shall define:

$$b := \frac{\pi^2}{2Ma^2}$$

$$\delta := \frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}$$

$$\mathcal{H}^{excited}_{|s\rangle,|a\rangle} = b\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} - \delta\begin{pmatrix} -2 & 0 \\ 0 & 2 \end{pmatrix}$$

The leading order is $E^{[0]}$ of the diagonalized hamiltonian:

$$\mathcal{H}^{excited}_{|s\rangle,|a\rangle} = \begin{pmatrix} 5b + 2\delta & 0 \\ 0 & 5b - 2\delta \end{pmatrix}$$

$$E_{|a\rangle}^{[0]} = 5\frac{\pi^2}{2Ma^2} + 2\frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}$$

$$E_{|s\rangle}^{[0]} = 5\frac{\pi^2}{2Ma^2} - 2\frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}$$

(3)+(4) Step by Step approach
Degeneracy shall be removed using the new basis [$|1,1\rangle$, $|a\rangle$, $|s\rangle$]:
$|a\rangle = \frac{1}{\sqrt{2}}(|1,2\rangle - |2,1\rangle)$
$|b\rangle = \frac{1}{\sqrt{2}}(|1,2\rangle + |2,1\rangle)$

with b and δ as in (3)
The new hamiltonian:

$$\mathcal{H}_0^{new} + V^{new} = \begin{pmatrix} 2b & 0 & 0 \\ 0 & 5b+2\delta & 0 \\ 0 & 0 & 5b-2\delta \end{pmatrix} - \frac{\delta}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

For each one of the obtained eigenstates (Energy values):

$$E = E^{[0]} + E^{[1]} + E^{[2]} + ...$$

3) Leading order of the ground state energy:

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

$$E_0^{[1]} = V_{n_0,n_0}^{new} = 0$$

$$E_0^{[2]} = \sum \frac{V_{n_0,m}^{new} V_{m,n_0}^{new}}{\epsilon_0^{new} - \epsilon_m^{new}} = \frac{1}{-3b-2\delta} \cdot \frac{\delta^2}{2} + \frac{1}{-3b+2\delta} \cdot \frac{\delta^2}{2}$$

Leading order expansion:

$$E_0^{[2]} = -\frac{\delta^2}{3b} = -\frac{1}{3} \cdot \frac{2Ma^2}{\pi^2} \cdot \left(\frac{16\epsilon_0}{9Ma^3}\right)^2$$

4) Leading order of the excited states energy:
Using the same method as in 3) we obtain:

$$E_{|a\rangle,|s\rangle} = 5b \pm 2\delta + \frac{1}{5b \pm 2\delta - 2b} \cdot \frac{\delta^2}{2}$$

Leading order expansion:

$$E_{|a\rangle,|s\rangle} = 5b \pm 2\delta = 5\frac{\pi^2}{2Ma^2} \pm 2\frac{1}{M} \cdot \frac{16\epsilon_0}{9a^3}$$

We obtain the same results as before