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PHY F311 QM-2

COMPRE PART-A

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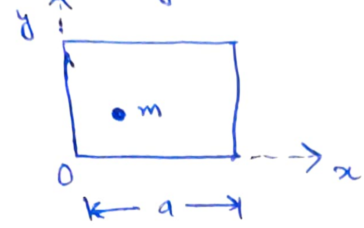
- System : A quantum particle of mass m confined to a 2-d square box of length a.



1.

Let's consider the Schrodinger equation for the given particle, confined in the box : $[0<x<a \ , \ 0<y<a]$.

$\therefore$ Schrodinger eqn for this system can be written as:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)+V(x,y)\,\psi(x,y)=E\,\psi(x,y)$$

For this system, given that the box has finite rigidity, we can say that

$$\begin{cases} V(x,y)=0 & \text{inside the box} \\ V(x,y)=\infty & \text{outside the box} \end{cases}$$

$\therefore$ Schrodinger's eqn becomes:

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)=E\psi\right] \quad \text{—— (1)}$$

Now, the Hamiltonian in eq (1) (LHS) is a sum of two independent terms. $\therefore$ we can assume a solution for $\psi(x,y)$ by separation of variables as:

$$\psi(x,y)=X(x)\,Y(y) \quad \text{—— (2)}$$

$\therefore$ Eq ① can be expressed in terms of $X(x)$ and $Y(y)$:

(terms)

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2 X(x)}{\partial x^2}\right) = \mathcal{E}_x X(x) \quad \text{— ③}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2 Y(y)}{\partial y^2}\right) = \mathcal{E}_y Y(y) \quad \text{— ④}$$

& total energy E is:

$$E = \mathcal{E}_x + \mathcal{E}_y$$

Solving eq ③ & ④, we get the foll solutions:

$$X(x) = A_x \sin(k_x x) + B_x \cos(k_x x) \quad \text{— ⑤}$$

$$Y(y) = A_y \sin(k_y y) + B_y \cos(k_y y) \quad \text{— ⑥}$$

Apply boundary conditions:

(i) $\psi(0, y) = 0 \Rightarrow B_x = 0$

(ii) $\psi(x, 0) = 0 \Rightarrow B_y = 0$

$\therefore$ Subst. eq ⑤ & ⑥ in eq ②, we get:

$$\psi(x,y) = \underbrace{A_x A_y}_{\substack{N \\ (\text{say})}} \sin(k_x x)\sin(k_y y)$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Rightarrow \left[\psi(x,y) = N \sin\left(\sqrt{\frac{2m\mathcal{E}_x}{\hbar^2}}\, x\right)\sin\left(\sqrt{\frac{2m\mathcal{E}_y}{\hbar^2}}\, y\right)\right] \quad \text{— ⑦}$$

Apply boundary conditions:

(iii) $\psi(a, y) = 0$

$$\Rightarrow N \sin\left(\sqrt{\frac{2m\mathcal{E}_x}{\hbar^2}}\, a\right) \sin\left(\sqrt{\frac{2m\mathcal{E}_y}{\hbar^2}}\, y\right) = 0$$

(iv) $\psi(x, a) = 0$

$$\Rightarrow N \sin\left(\sqrt{\frac{2m\mathcal{E}_x}{\hbar^2}}\, x\right) \sin\left(\sqrt{\frac{2m\mathcal{E}_y}{\hbar^2}}\, a\right) = 0$$

Both these conditions (iii) and (iv) will be satisfied if:

$$\sin\left(\sqrt{\frac{2m\mathcal{E}_x}{\hbar^2}}\, a\right) = 0 \qquad \text{— (8)}$$

and

$$\sin\left(\sqrt{\frac{2m\mathcal{E}_y}{\hbar^2}}\, a\right) = 0 \qquad \text{— (9)}$$

$$\therefore \sqrt{\frac{2m\mathcal{E}_x}{\hbar^2}}\, a = n_x \pi \quad \& \quad \sqrt{\frac{2m\mathcal{E}_y}{\hbar^2}}\, a = n_y \pi$$

$$\Rightarrow \left[\mathcal{E}_{nx} = \frac{\pi^2 \hbar^2}{2ma^2} n_x^2\right] \quad \Rightarrow \left[\mathcal{E}_{ny} = \frac{\pi^2 \hbar^2}{2ma^2} n_y^2\right]$$

Since $\mathcal{E}_{nx}$ and $\mathcal{E}_{ny}$ are independent terms, total energy can be written as:

$$E = \mathcal{E}_{nx} + \mathcal{E}_{ny} \qquad \text{— (10)}$$

$$\therefore \boxed{E_{n_x, n_y} = \frac{\pi^2 \hbar^2}{2ma^2}\left(n_x^2 + n_y^2\right)}$$ — Energy eigenvalues

$(n_x, n_y = 1, 2, 3, \ldots)$

Now, substituting the values of E_{nx}, E_{ny} in eq (7) we get:

$$\psi(x,y) = N \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right)$$

where N is the normalization constant.

To determine N :

$$\int_0^a \int_0^a |\psi(x,y)|^2 \, dx\, dy = 1$$

$$N^2 \int_0^a \sin^2\left(\frac{n_x \pi x}{a}\right) dx \int_0^a \sin^2\left(\frac{n_y \pi y}{a}\right) dy = 1$$

$$N^2 \cdot \left(\frac{1}{2}x - \frac{1}{2} \sin \frac{2n_x\pi x}{a} \cdot \frac{a}{2n_x\pi}\right)\Bigg|_0^a \cdot \left(\frac{1}{2}y - \frac{1}{2} \sin \frac{2n_y\pi y}{a} \cdot \frac{a}{2n_y\pi}\right)\Bigg|_0^a = 1$$

$$N^2 \cdot \left(\frac{a}{2}\right) \cdot \left(\frac{a}{2}\right) = 1$$

$$N = \frac{2}{a}$$

$\therefore$ Normalised wavefunction is :

$$\boxed{\psi(x,y) = \frac{2}{a} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right)}$$

Degeneracy

In the first three wavefunctions, there is one degeneracy for the second wavefunction (1st excited state), for $(n_x, n_y) = (1,2)$ and $(2,1)$.

The energies of this first excited state are:

Using eq (10)

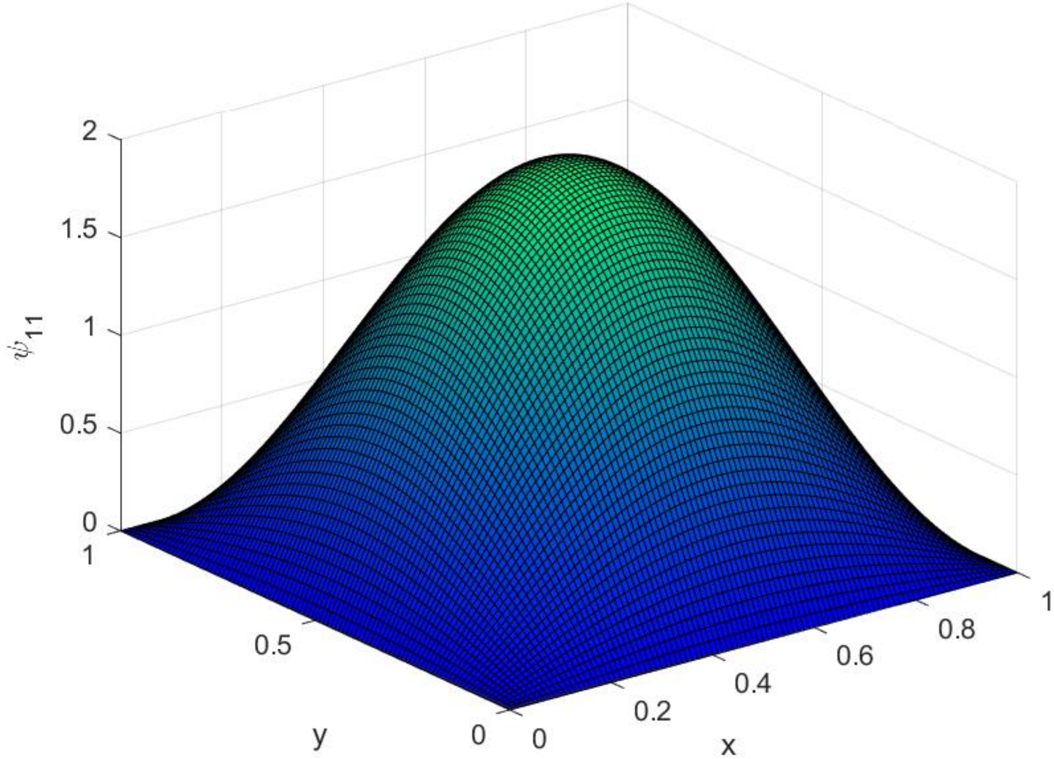
$$E_{1,2} = E_{2,1} = \frac{\pi^2 \hbar^2}{2ma^2}(1^2 + 2^2) = \frac{5\pi^2\hbar^2}{2ma^2}$$

The two wavefunctions / states with this energy are

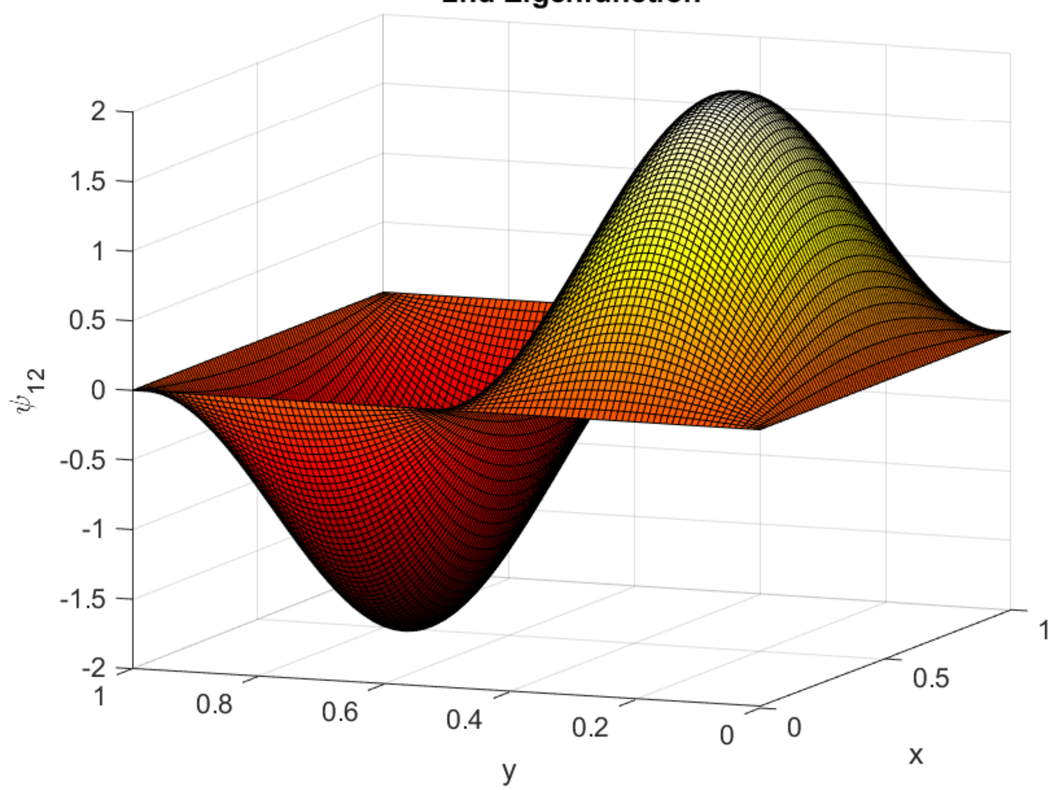
$$\psi_{1,2} = \frac{2}{a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)$$

$$\psi_{2,1} = \frac{2}{a}\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right).$$

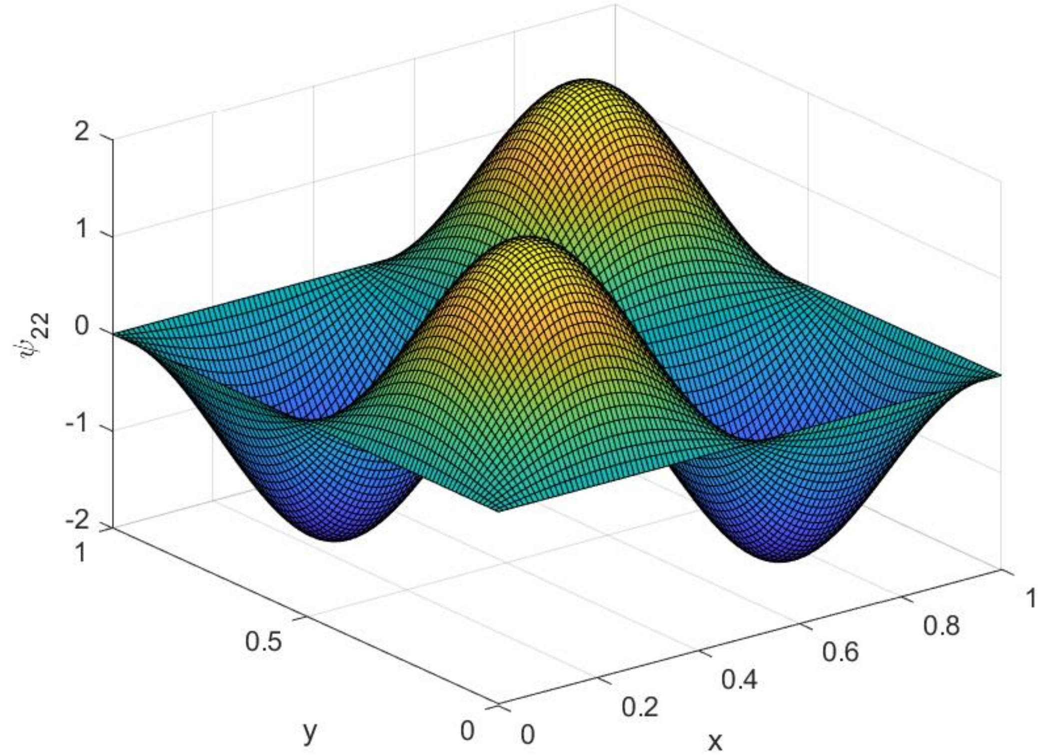
1st Eigenfunction



2nd Eigenfunction



3rd Eigenfunction



MATLAB CODE FOR PART 1

```
%parameters
a = 1.0; % length of the box

[x,y] = meshgrid(0:0.01:1,0:0.01:1);

psi_11 = (2/a).*(sin(1.*pi.*x/a)).*(sin(1.*pi.*y/a));
%first eigenfunction
psi_12 = (2/a).*(sin(1.*pi.*x/a)).*(sin(2.*pi.*y/a));
%second eigenfunction
psi_22 = (2/a).*(sin(2.*pi.*x/a)).*(sin(2.*pi.*y/a));
%third eigenfunction

figure
z1 = surf(x,y,psi_11);
colormap(winter);
title("1st Eigenfunction");
xlabel("x"),ylabel("y"),zlabel("\psi_1_1");

figure
z2 = surf(x,y,psi_12);
colormap(hot);
title("2nd Eigenfunction");
xlabel("x"),ylabel("y"),zlabel("\psi_1_2");

figure
z3 = surf(x,y,psi_22);
colormap(parula);
title("3rd Eigenfunction");
xlabel("x"),ylabel("y"),zlabel("\psi_2_2");
```

2.

Perturbation : weak potential $V = V_0 xy$.

Unperturbed wave func :

$$\psi^{(0)}(x,y) = \frac{2}{a} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right)$$

For ground state, $n_x = 1$ & $n_y = 1$.

$$\therefore \quad \psi_0^{(0)}(x,y) = \frac{2}{a} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a}$$

The ground state is non-degenerate.

Energy is:

$$E_0^0 = \frac{\pi^2 \hbar^2}{ma^2}$$

The first order energy shift for ground state is

$$E_0^{(1)} = \langle \psi_0^0 | V | \psi_0^0 \rangle$$

$$= \langle \psi_0^0 | V_0 xy | \psi_0^0 \rangle$$

$$= \int_0^a \int_0^a \frac{2}{a} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \cdot V_0 xy \cdot \frac{2}{a} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \cdot dx dy$$

$$= \frac{4V_0}{a^2} \int_0^a x \sin^2\frac{\pi x}{a}\, dx \int_0^a y \sin^2\frac{\pi y}{a}\, dy$$

(independent functions)

$$= \frac{4V_0}{a^2} \cdot \frac{a^2}{4} \cdot \frac{a^2}{4}$$

$$\boxed{E_0^{(1)} = \frac{V_0 a^2}{4}}$$

First excited state

The first excited state is doubly degenerate, with the following eigenfunctions:

$$\psi_{12}^{(0)}(x,y) = \frac{2}{a}\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a} = \psi_a \quad \text{(say)}$$

and $$\psi_{21}^{(0)}(x,y) = \frac{2}{a}\sin\frac{2\pi x}{a}\sin\frac{\pi y}{a} = \psi_b \quad \text{(say)}$$

and has energy:

$$E_1^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+2^2) = \frac{5\pi^2\hbar^2}{2ma^2}$$

Now, we need to construct a 2x2 $\tilde{V}$ matrix, and then diagonalize it in the degenerate subspace of the perturbed Hilbert space.

For the complete Hamiltonian (H) after perturbation, we want the system to have $|n\rangle$ eigenstates with E_n energy eigenvalues, and out of the $|n\rangle$ states, the two degenerate states linearly combine to form the ~~perturbed~~ energy eigenfunction.

Here $(V = V_0 xy)$

$$H = H_0 + V \longrightarrow \{|n\rangle, E_n\}$$

and say $$\psi^0 = c_1\psi_a^0 + c_2\psi_b^0 \qquad (1)$$

Applying normal perturbation theory to $H_0\psi^0 = E^0\psi^0$, we get the foll eqn for 1st order:

$$H_0\psi^{(1)} + V\psi^{(0)} = E^{(1)}\psi^{(0)} + E^{(0)}\psi^{(1)} \qquad (2)$$

Now, take inner product of eq (2) first with ψ_a and then with ψ_b.

We get the foll. two equations:

$$c_1 V_{aa} + c_2 V_{ab} = c_1 E^{(1)} \quad \text{— ③}$$

&

$$c_1 V_{ba} + c_2 V_{bb} = c_2 E^{(1)} \quad \text{— ④}$$

where $V_{ij} = \langle \psi_i | V | \psi_j \rangle$

$i, j = a, b$

Writing these in matrix form:

$$\begin{pmatrix} V_{aa} & V_{ab} \\ V_{ba} & V_{bb} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E^{(1)} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

It is clearly visible that $E^{(1)}$ are the energy eigenvalues for the matrix $\tilde{V}$, and the linear combination of the unperturbed states are the eigenvectors of $\tilde{V}$.

Now, the diagonal elements of V are:

$$V_{aa} = \int \psi_a^{(0)} V \psi_a^{(0)} d\tau$$

$$= \frac{4V_0}{a^2} \int_0^a \int_0^a \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \cdot xy \cdot \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \, dx\,dy$$

$$= \frac{4V_0}{a^2} \int_0^a x \sin^2\frac{\pi x}{a} \, dx \int_0^a y \sin^2\frac{\pi y}{a} \, dy$$

$$= \frac{V_0 a^2}{4}$$

$$\therefore \left[V_{aa} = \frac{V_0 a^2}{4} = V_{bb} \right]$$

Off-diagonal elements:

$$V_{ab} = \int \psi_a V \psi_b \, d\tau = \int_0^a \int_0^a \frac{4V_0}{a^2} x \sin\frac{\pi x}{a} \sin\frac{2\pi x}{a} \cdot y \sin\frac{\pi y}{a} \sin\frac{2\pi y}{a} \, dx\,dy$$

$$= \frac{4V_0}{a^2}\int_0^a x \sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\,dx \int_0^a y \sin\frac{\pi y}{a}\sin\frac{2\pi y}{a}\,dy$$

$$= \frac{4V_0}{a^2}\cdot + \frac{8a^2}{9\pi^2}\cdot + \frac{8a^2}{9\pi^2}$$

$$= \frac{256\, V_0 a^2}{81\pi^4}$$

$$\therefore \quad V_{ab} = \frac{256\, V_0 a^2}{81\pi^4} = V_{ba}$$

Thus, the matrix is :

$$V = \begin{pmatrix} \frac{V_0 a^2}{4} & \frac{256\, V_0 a^2}{81\pi^4} \\ \frac{256\, V_0 a^2}{81\pi^4} & \frac{V_0 a^2}{4} \end{pmatrix}$$

The 1st order energy shifts are the eigenvalues $E_1^{(1)}$ of this matrix V.

The characteristic eqn for V is :

$$\left(\frac{V_0 a^2}{4} - E_1^{(1)}\right)^2 - \left(\frac{256 V_0 a^2}{81\pi^4}\right)^2 = 0$$

$$\Rightarrow \quad E_1^{(1)} = \frac{V_0 a^2}{4} \pm \frac{256 V_0 a^2}{81\pi^4}$$

$$= V_0 a^2\left(\frac{1}{4} \pm \frac{256}{81\pi^4}\right)$$

$\therefore$ Eigenvalues are :

$$e_1 = V_0 a^2\left(\frac{1}{4} + \frac{256}{81\pi^4}\right) \approx V_0 a^2 (0.282)$$

$$e_2 = V_0 a^2\left(\frac{1}{4} - \frac{256}{81\pi^4}\right) \approx V_0 a^2 (0.218)$$

1st order
$\therefore$ The splitting of energy of the first excited state is

$$E_1(\lambda) = \begin{cases} E_1^{(0)} + \lambda V_0 a^2 (0.282) \\ E_1^{(0)} + \lambda V_0 a^2 (0.218) \end{cases}$$

where $E_1^{(0)}$ is the unperturbed energy.

3. Perturbed energy eigenfunction.

$$\psi^0 = c_1 \psi_a^0 + c_2 \psi_b^0$$

where (c_1, c_2) form the eigenvectors of matrix V:

$$V_0 a^2 \begin{pmatrix} \frac{1}{4} & \left(\frac{4}{3\pi}\right)^4 \\ \left(\frac{4}{3\pi}\right)^4 & \frac{1}{4} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E_1^{(1)} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Let $\left(\frac{4}{3\pi}\right)^4 = l$.

Then for eigenvalues: $E_1^{(1)} = V_0 a^2 \left(\frac{1}{4} \pm l\right)$

$$V_0 a^2 \left[\frac{1}{4} c_1 + l c_2\right] = V_0 a^2 \left(\frac{1}{4} \pm l\right) c_1$$

& $$V_0 a^2 \left[l c_1 + \frac{1}{4} c_2\right] = V_0 a^2 \left(\frac{1}{4} \pm l\right) c_2$$

$\therefore$ The corresponding eigenvalues are $c_1 = \pm c_2 = 1$

$\therefore$ $v_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $v_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$$\therefore \quad \psi_\alpha^0 = \psi_a^0 \pm \psi_b^0$$

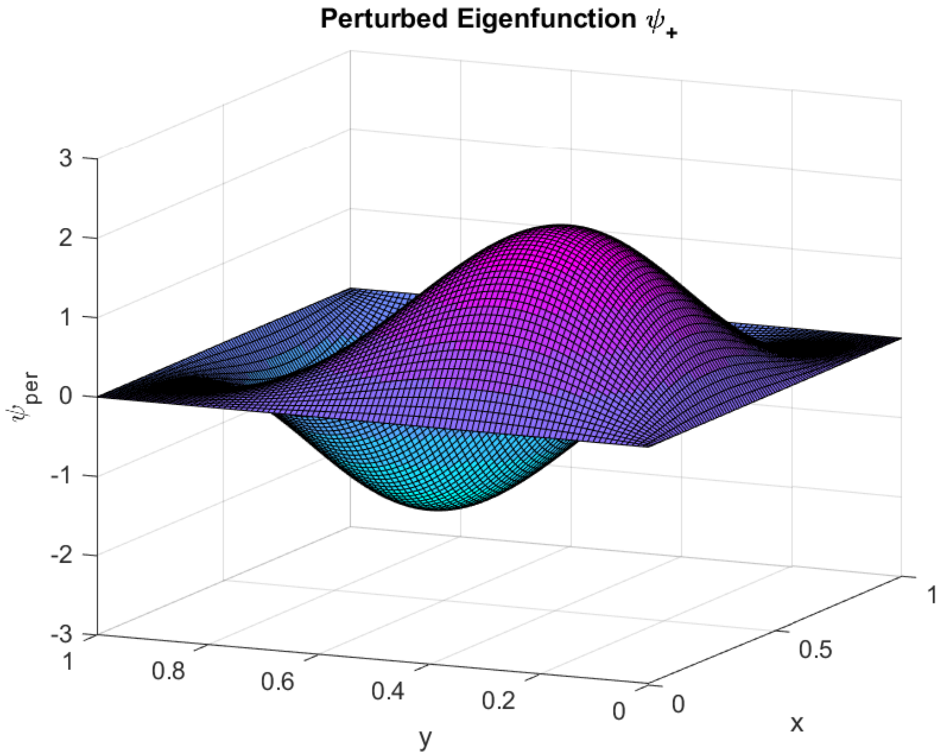
After normalization,

$$\psi_\alpha^0 = \frac{1}{\sqrt{2}} \left(\psi_a^0 \pm \psi_b^0 \right)$$

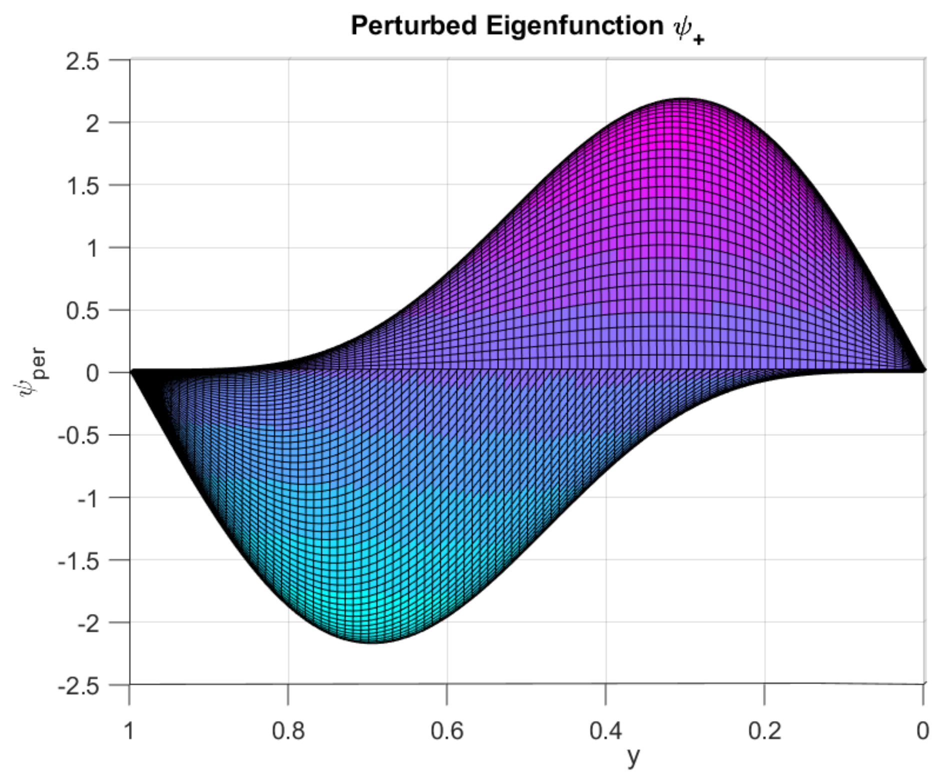
(normalized)

$$\boxed{\psi^0 = \frac{1}{\sqrt{2}} \left(\psi_{12}^0 \pm \psi_{21}^0 \right)}$$

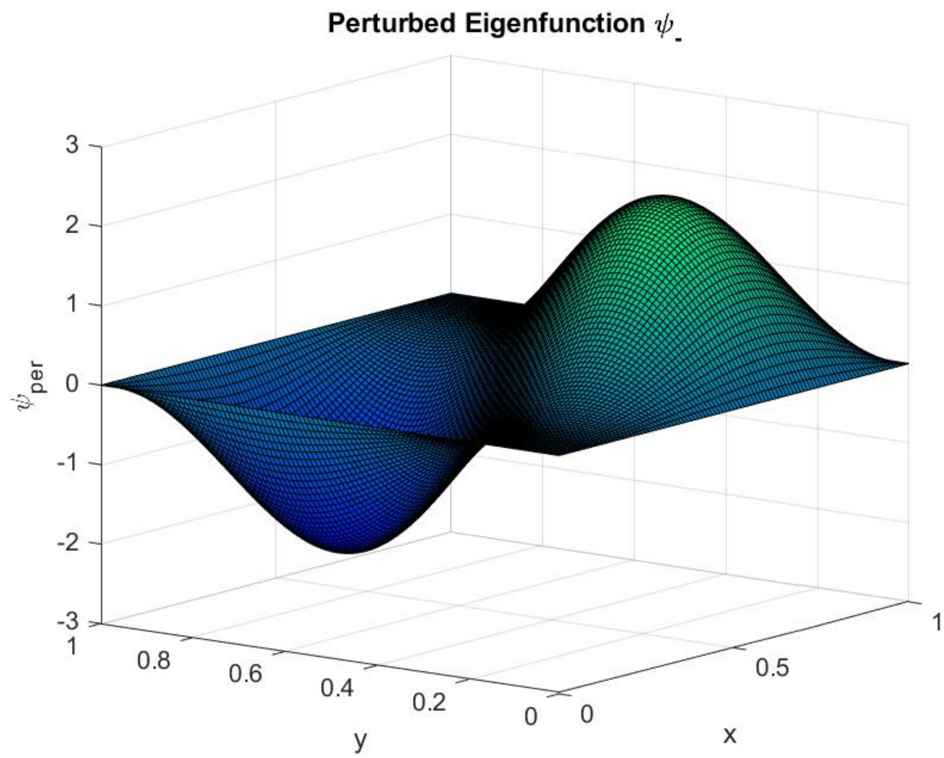
$$\therefore \quad \psi^0 = \begin{cases} \frac{1}{\sqrt{2}} \left(\psi_{12}^0 + \psi_{21}^0 \right) = \psi_+ \\ \frac{1}{\sqrt{2}} \left(\psi_{12}^0 - \psi_{21}^0 \right) = \psi_- \end{cases}$$



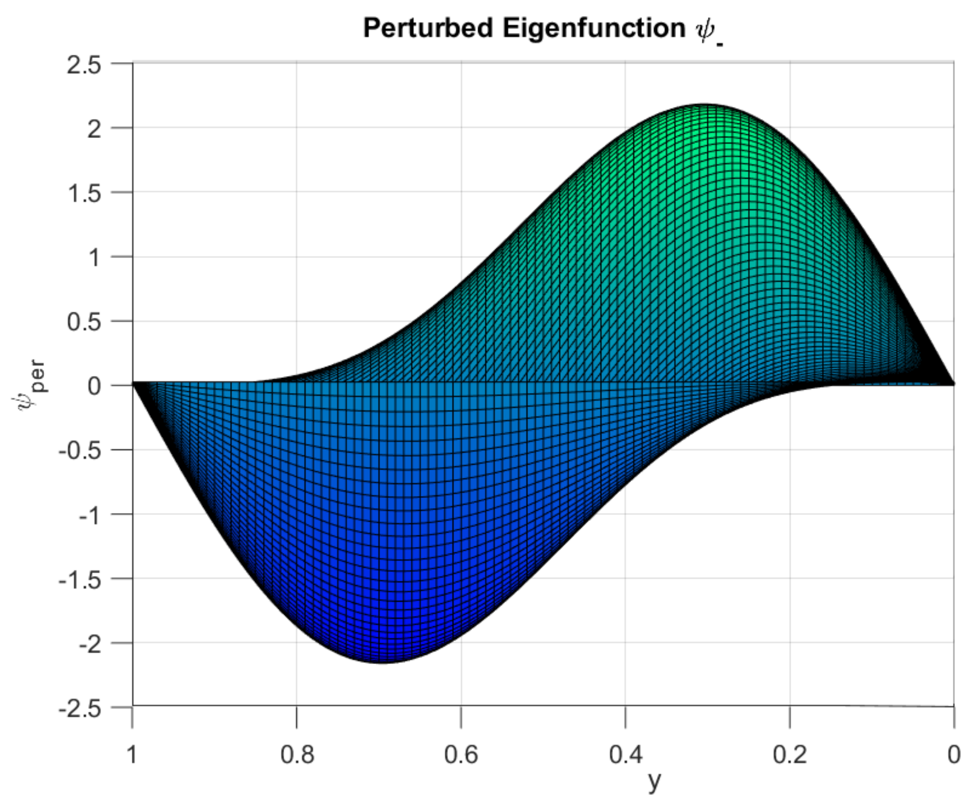
3-d view



2-d view



3-d view



2-d view

MATLAB CODE FOR PART 3

```
%parameters
a = 1.0; % length in metres

[x,y] = meshgrid(0:0.01:1,0:0.01:1);

psi_12 = (2/a).*(sin(1.*pi.*x/a)).*(sin(2.*pi.*y/a));
%second eigenfunction
psi_21 = (2/a).*(sin(2.*pi.*x/a)).*(sin(1.*pi.*y/a));
%second eigenfunction
zper1 = 1/sqrt(2)*(psi_12+psi_21);
zper2 = 1/sqrt(2)*(psi_12-psi_21);

figure
z1 = surf(x,y,zper1);
colormap(cool(10));
title("Perturbed Eigenfunction \psi_+");
xlabel("x"),ylabel("y"),zlabel("\psi_p_e_r");

figure
z2 = surf(x,y,zper2);
colormap(winter);
title("Perturbed Eigenfunction \psi_-");
xlabel("x"),ylabel("y"),zlabel("\psi_p_e_r");
```

References

- Modern Quantum Mechanics. Second Edition. JJ Sakurai, Jim Napolitano
- Introduction to Quantum Mechanics. Second Edition. David J. Griffiths
- https://in.mathworks.com/help/matlab/
- Lecture notes

4. Energy Spectrum :