PHY 362K Homework 2

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We know that $E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$

For a particle in an infinite square well, we get $\psi_n^{(0)} = \sqrt{\frac{2}{a}} \sin(\frac{n\pi}{a} x)$

$\therefore E_n^{(1)} = \int_0^a |\psi_n^0|^2 H'(x) dx = \frac{2\alpha}{a} \int_0^a \sin^2(\frac{n\pi}{a} x) \delta(x - \frac{a}{2}) dx = \boxed{\dfrac{2\alpha}{a} \sin^2(2n\pi)}$

From the equation above we can know that $E_n^{(1)} = 0$ when n is even. This is because when n is even, the wave function has a node at location $\frac{a}{2}$. Therefore H' does not affect the wave function there. This means the first order energies are not perturbed to the first order for even n.

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From the question we can know that $E_0 \approx E_0^{(0)} + E_0^{(1)} + E_0^{(2)}$

$E_0^{(0)} = \frac{1}{2} \hbar \omega$

$E_0^{(1)} = \langle \psi_0^{(0)} | H' | \psi_0^{(0)} \rangle = \int_{-\infty}^{\infty} |\psi_0^{(0)}|^2 H' dx = \alpha \sqrt{\frac{m\omega}{\hbar}} \int_{-\infty}^{\infty} x^3 e^{-\frac{m\omega}{\hbar} x^2} dx = 0$

$E_0^{(2)} = \sum_{m \neq 0} \frac{|\langle \psi_m^{(0)} | H' | \psi_0^{(0)} \rangle|^2}{E_0^{(0)} - E_m^{(0)}}$

We know that $E_0^{(0)} - E_m^{(0)} = (\frac{1}{2} - m + \frac{1}{2}) \hbar \omega = -m \hbar \omega$

$\langle\psi_m^{(0)}|H'|\psi_0^{(0)}\rangle = \alpha\int_{-\infty}^{\infty}\psi_m^{(0)*}\psi_0^{(0)}x^3dx$

$x^3\psi_0^{(0)} = x^3\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}} = \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}\xi^3\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{\xi^2}{2}} = \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}\xi^3\psi_0^{(0)}$ where $\xi = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}x$

$\because \psi_n^{(0)}(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\frac{\xi^2}{2}} = \frac{1}{\sqrt{2^n n!}}H_n(\xi)\psi_0^{(0)}$

$\therefore x^3\psi_0^{(0)} = \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}(c_1\psi_1^{(0)} + c_3\psi_3^{(0)}) = \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}(c_1\frac{2}{\sqrt{2}}\xi\psi_0^{(0)} + c_2\frac{2}{\sqrt{3}}\xi^3\psi_0^{(0)} - c_2\frac{3}{\sqrt{3}}\xi\psi_0^{(0)})$

From the above equations we can get $c_1 = \frac{3\sqrt{2}}{4}$ and $c_2 = \frac{\sqrt{3}}{2}$

$\langle\psi_m^{(0)}|\alpha x^3|\psi_0^{(0)}\rangle = \alpha\left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}\left(\frac{3\sqrt{2}}{4}\int_{-\infty}^{\infty}\psi_m^{(0)*}\psi_1^{(0)}dx + \frac{\sqrt{3}}{2}\int_{-\infty}^{\infty}\psi_m^{(0)*}\psi_3^{(0)}dx\right)$

Since $\psi_m^{(0)*}\psi_n^{(0)} = \delta_{mn}$, the only two non-degenerate terms are $m = 1$ and $m = 3$

$\langle\psi_1^{(0)}|\alpha x^3|\psi_0^{(0)}\rangle = \alpha\left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}\frac{3\sqrt{2}}{4}$

$\langle\psi_3^{(0)}|\alpha x^3|\psi_0^{(0)}\rangle = \alpha\left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}\frac{\sqrt{3}}{2}$

$\therefore E_0^{(2)} = \frac{|\langle\psi_1^{(0)}|\alpha x^3|\psi_0^{(0)}\rangle|^2}{E_0^{(0)} - E_1^{(0)}} + \frac{|\langle\psi_3^{(0)}|\alpha x^3|\psi_0^{(0)}\rangle|^2}{E_0^{(0)} - E_m^{(0)}} = -\frac{11}{8}\alpha^2\left(\frac{\hbar}{m\omega}\right)^3\frac{1}{\hbar\omega}$

$$\therefore \boxed{E_0 = \frac{1}{2}\hbar\omega - \frac{11}{8}\alpha^2\left(\frac{\hbar}{m\omega}\right)^3\frac{1}{\hbar\omega}}$$

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(a)

For a particle in an infinite square well, we get $\psi_n^{(0)} = \sqrt{\frac{2}{a}}\sin(\frac{n\pi}{a}x)$

$$H'(x) = \begin{cases} V_0, & \frac{3a}{8} \leq x \leq \frac{5a}{8} \quad (1) \\ \\ 0, & \text{otherwise} \quad (2) \end{cases}$$

$E_1^{(1)} = \langle\psi_1^{(0)}|H'|\psi_1^{(0)}\rangle = \frac{2}{a}V_0\int_{\frac{3a}{8}}^{\frac{5a}{8}}\sin^2(\frac{\pi}{a}x)dx = \boxed{(\frac{1}{4} + \frac{1}{\sqrt{2}\pi})V_0}$

$E_2^{(1)} = \langle\psi_2^{(0)}|H'|\psi_2^{(0)}\rangle = \frac{2}{a}V_0\int_{\frac{3a}{8}}^{\frac{5a}{8}}\sin^2(\frac{2\pi}{a}x)dx = \boxed{(\frac{\pi-2}{4\pi})V_0}$

$E_3^{(1)} = \langle\psi_3^{(0)}|H'|\psi_3^{(0)}\rangle = \frac{2}{a}V_0\int_{\frac{3a}{8}}^{\frac{5a}{8}}\sin^2(\frac{3\pi}{a}x)dx = \boxed{\frac{1}{12}\left(3+\frac{2\sqrt{2}}{\pi}\right)V_0}$

$E_4^{(1)} = \langle\psi_4^{(0)}|H'|\psi_4^{(0)}\rangle = \frac{2}{a}V_0\int_{\frac{3a}{8}}^{\frac{5a}{8}}\sin^2(\frac{4\pi}{a}x)dx = \boxed{\frac{1}{4}V_0}$

$E_5^{(1)} = \langle\psi_5^{(0)}|H'|\psi_5^{(0)}\rangle = \frac{2}{a}V_0\int_{\frac{3a}{8}}^{\frac{5a}{8}}\sin^2(\frac{5\pi}{a}x)dx = \boxed{(\frac{1}{4}-\frac{1}{5\sqrt{2}\pi})V_0}$

(b)

We know that $|\psi_1^{(1)} = \sum_{n\neq 1}\frac{\langle\psi_n^{(0)}|V_0|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_n^{(0)}}|\psi_n^{(0)}\rangle = \sum_{n\neq 1}c_n|\psi_n^{(0)}\rangle$

$E_1^{(0)} - E_n^(0) = \frac{\pi^2\left(1-n^2\right)\hbar^2}{2a^2m}$

We plug in the values above and get:

$c_3 = \frac{\langle\psi_3^{(0)}|V_0|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_3^{(0)}} = \boxed{\frac{\left(1+\sqrt{2}\right)a^2mV_0}{8\pi^3\hbar^2}}$

$c_5 = \frac{\langle\psi_5^{(0)}|V_0|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_5^{(0)}} = \boxed{-\frac{\left(3+\sqrt{2}\right)a^2mV_0}{72\pi^3\hbar^2}}$

$c_7 = \frac{\langle\psi_7^{(0)}|V_0|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_7^{(0)}} = \boxed{\frac{a^2mV_0}{72\sqrt{2}\pi^3\hbar^2}}$

$c_9 = \frac{\langle\psi_9^{(0)}|V_0|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_9^{(0)}} = \boxed{\frac{a^2mV_0}{200\sqrt{2}\pi^3\hbar^2}}$

$c_{11} = \frac{\langle\psi_{11}^{(0)}|V_0|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_{11}^{(0)}} = \boxed{-\frac{\left(5+3\sqrt{2}\right)a^2mV_0}{1800\pi^3\hbar^2}}$

(c)

For the case $V_0 = \frac{3\pi^2\hbar^2}{ma^2}$, the plot of $\psi_1^{(1)}$ is shown in Figure 1

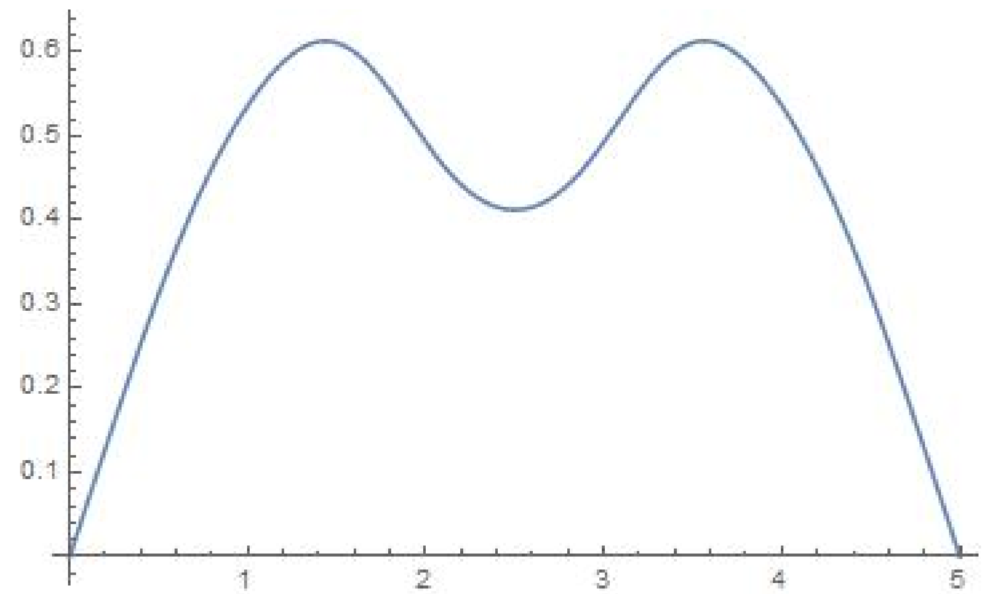

Figure 1: The plot of $\psi_1^{(1)}$

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(a)

When $\epsilon = 0$, the Hamiltonian matrix becomes:

$$\mathbf{H} = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Suppose the eigenvalue is E and the eigenvector is $|\psi^0\rangle$

Therefore, $\begin{pmatrix} V_0 & 0 & 0 \\ 0 & V_0 & 0 \\ 0 & 0 & 2V_0 \end{pmatrix} |\psi^0\rangle = E|\psi^0\rangle$

$$\therefore \begin{vmatrix} V_0 - E & 0 & 0 \\ 0 & V_0 - E & 0 \\ 0 & 0 & 2V_0 - E \end{vmatrix} = 0$$

$$-E^3 + 4VE^2 + 5V^2E + 2V^3 = 0$$

$\therefore E = V_0 or 2V_0$

We let $|\psi^0\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$

When $E = V_0$,

$$\begin{pmatrix} V_0 & 0 & 0 \\ 0 & V_0 & 0 \\ 0 & 0 & 2V_0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} V_0 a \\ V_0 b \\ V_0 c \end{pmatrix}$$

In this case, we can have two orthonormal eigenstates $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

When $E = 2V_0$,

$$\begin{pmatrix} V_0 & 0 & 0 \\ 0 & V_0 & 0 \\ 0 & 0 & 2V_0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 2V_0 a \\ 2V_0 b \\ 2V_0 c \end{pmatrix}$$

In this case, we can have eigenstate $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

(b)

When the system is perturbed, we have

$$\mathbf{H} = V_0 \begin{pmatrix} (1-\epsilon) & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}$$

Let the eigenvalue to be E and the eigenvector to be $|\psi^1\rangle$

Then the eigenvalues are $E = (1-\epsilon)V_0,\ \frac{V_0}{2}(3-\sqrt{1+4\epsilon^2}),\ \frac{V_0}{2}(3+\sqrt{1+4\epsilon^2})$

Using power expansion, we can get $E = (1-\epsilon)V_0,\ \frac{V_0}{2}(3-1-2\epsilon^2) = V_0(1-\epsilon^2),\ \frac{V_0}{2}(3+1+2\epsilon^2) = V_0(2+\epsilon^2)$

(c)

From the question we can know that $H' = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

We let $|\psi_1^0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\psi_2^0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $|\psi_3^0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$$\therefore E_1^1 = \langle\psi_1^0|H'|\psi_1^0\rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = -\epsilon V_0$$

$$E_2^1 = \langle\psi_2^0|H'|\psi_2^0\rangle = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$E_3^1 = \langle\psi_3^0|H'|\psi_3^0\rangle = \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

The equation for calculating the second order eigenvalues is $E_n^2 = \sum_{m\neq n} \frac{|\langle\psi_m^0|H'|\psi_n^0\rangle|^2}{E_n^0 - E_m^0}$

Since $|\psi_1^0\rangle$ and $|\psi_2^0\rangle$ share the same eigenvalues V_0, the non-degenerate method only applies to $|\psi_3^0\rangle$

Therefore, $E_3^2 = \frac{|\langle\psi_1^0|H'|\psi_3^0\rangle|^2}{E_3^0 - E_1^0} + \frac{|\langle\psi_2^0|H'|\psi_3^0\rangle|^2}{E_3^0 - E_2^0} = \frac{|\langle\psi_1^0|H'|\psi_3^0\rangle|^2 + |\langle\psi_2^0|H'|\psi_3^0\rangle|^2}{V_0} = \epsilon^2 V_0$

$E_3 = E_3^0 + E_3^1 + E_3^2 = 2V_0 + \epsilon^2 V_0 = V_0(2 + \epsilon^2)$

This matches the answer in part (b)

(d)

We let $\mathbf{W} = \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix}$, where $W_{ij} = \langle\psi_i^0|H'|\psi_j^0\rangle$

$\therefore W = \epsilon V_0 \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}$

The eigenvalues therefore are $E_1^1 = -\epsilon V_0$ and $E_2^1 = 0$

$E_1 = V_0 - \epsilon V_0$ and $E_2 = V_0$

This matches the results in (b) up to the first order of ϵ

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(a)

From the question we know that the perturbation matrix $H' = \begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix}$, where $H'_{ij} = \langle \widetilde{\psi}^{(0)}_{2i} | H' | \widetilde{\psi}^{(0)}_{2j} \rangle$

We let $\widetilde{\psi}^{(0)}_{21} = \psi^{(0)}_{21}$ and $\widetilde{\psi}^{(0)}_{22} = \psi^{(0)}_{12}$

Plug in the values given in the question, we get

$H'_{11} = \int_{x=\frac{a}{2}}^{a} \int_{y=0}^{\frac{a}{2}} \widetilde{\psi}^{(0)}_{21} * \widetilde{\psi}^{(0)}_{21} * H' \; dy \; dx = \frac{\hbar^2}{3a^2m}$

$H'_{12} = \int_{x=\frac{a}{2}}^{a} \int_{y=0}^{\frac{a}{2}} \widetilde{\psi}^{(0)}_{21} * \widetilde{\psi}^{(0)}_{22} * H' \; dy \; dx = -\frac{64\hbar^2}{225a^2m}$

$H'_{21} = \int_{x=\frac{a}{2}}^{a} \int_{y=0}^{\frac{a}{2}} \widetilde{\psi}^{(0)}_{22} * \widetilde{\psi}^{(0)}_{21} * H' \; dy \; dx = -\frac{64\hbar^2}{225a^2m}$

$H'_{22} = \int_{x=\frac{a}{2}}^{a} \int_{y=0}^{\frac{a}{2}} \widetilde{\psi}^{(0)}_{22} * \widetilde{\psi}^{(0)}_{22} * H' \; dy \; dx = \frac{\hbar^2}{3a^2m}$

$$\therefore \boxed{H' = \begin{pmatrix} \frac{\hbar^2}{3a^2m} & -\frac{64\hbar^2}{225a^2m} \\ -\frac{64\hbar^2}{225a^2m} & \frac{\hbar^2}{3a^2m} \end{pmatrix}}$$

(b)

Suppose $\begin{pmatrix} \frac{\hbar^2}{3a^2m} & -\frac{64\hbar^2}{225a^2m} \\ -\frac{64\hbar^2}{225a^2m} & \frac{\hbar^2}{3a^2m} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E^{(1)}_2 \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$, where $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ is the eigenstate and $E^{(1)}_2$ is the eigenvalue

We get that $E^{(1)}_2 = \boxed{\dfrac{139\hbar^2}{225a^2m}}$ or $\boxed{\dfrac{11\hbar^2}{225a^2m}}$

The corresponding eigenstates are $\begin{pmatrix} c_{11} \\ c_{12} \end{pmatrix} = \boxed{\begin{pmatrix} -1 \\ 1 \end{pmatrix}}$ and $\begin{pmatrix} c_{21} \\ c_{22} \end{pmatrix} = \boxed{\begin{pmatrix} 1 \\ 1 \end{pmatrix}}$

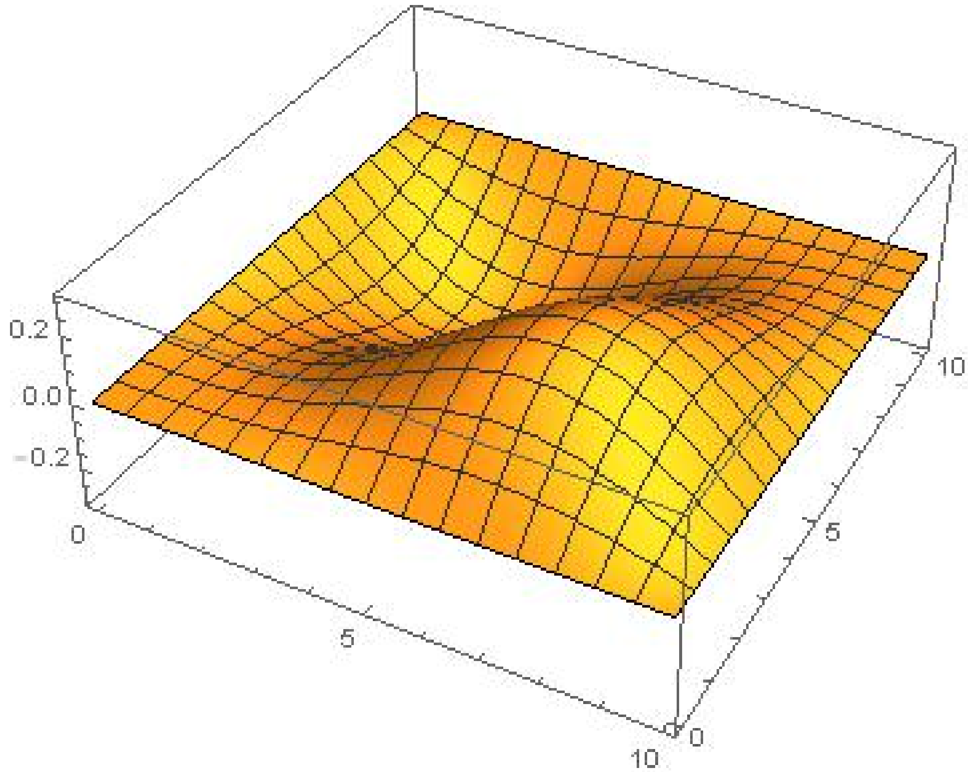

Figure 2: The plot of $|\phi_{21}^{(0)}\rangle$

(c)

According to part (b), when $E_2^{(1)} = \frac{139\hbar^2}{225a^2m}$

$|\phi_{21}^{(0)}\rangle = c_{11}|\widetilde{\psi}_{21}^{(0)}\rangle + c_{12}|\widetilde{\psi}_{22}^{(0)}\rangle = -\frac{2}{a}\sin(\frac{2\pi x}{a})\sin(\frac{\pi y}{a}) + \frac{2}{a}\sin(\frac{\pi x}{a})\sin(\frac{2\pi y}{a})$

The Plot of $|\phi_{21}^{(0)}\rangle$ is shown in Figure 2

when $E_2^{(1)} = \frac{11\hbar^2}{225a^2m}$

$|\phi_{22}^{(0)}\rangle = c_{21}|\widetilde{\psi}_{21}^{(0)}\rangle + c_{22}|\widetilde{\psi}_{22}^{(0)}\rangle = \frac{2}{a}\sin(\frac{2\pi x}{a})\sin(\frac{\pi y}{a}) + \frac{2}{a}\sin(\frac{\pi x}{a})\sin(\frac{2\pi y}{a})$

The Plot of $|\phi_{22}^{(0)}\rangle$ is shown in Figure 3

According to Figure 2 and Figure 3, we can see that $|\phi_{21}^{(0)}\rangle$ has higher amplitude than $|\phi_{22}^{(0)}\rangle$ in the perturbation area. Therefore the energy with eigenstate $|\phi_{21}^{(0)}\rangle$ is higher

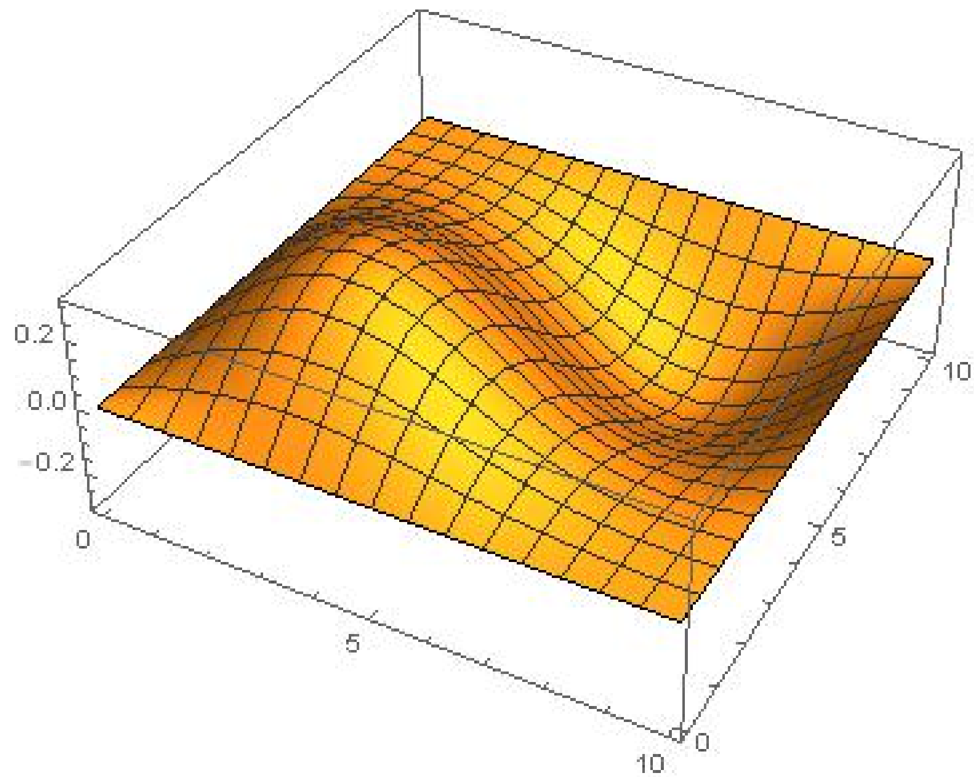

Figure 3: The plot of $|\phi_{22}^{(0)}\rangle$