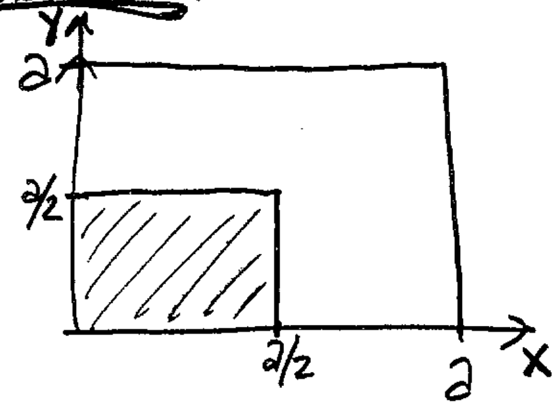
Problem Set II Key (continued):

Problem 2.



Unperturbed states are:

$$\psi^{(0)}_{(x,y)} = A \sin\left(\frac{\ell\pi x}{a}\right)\sin\left(\frac{n\pi y}{a}\right)$$

where $\ell = 1, 2, \ldots$ and $n = 1, 2, \ldots$

Since $0 = \psi^{(0)}_{(x,0)} = \psi^{(0)}_{(x,a)} = \psi^{(0)}_{(0,y)} = \psi^{(0)}_{(a,y)}$

Find normalization factor: $1 = \int_0^a\int_0^a |\psi|^2 dx\,dy = |A|^2 \int_0^a dx \sin^2\frac{\ell\pi x}{a} \int_0^a dy \sin^2\frac{n\pi y}{a}$

$$\left[\begin{array}{l} \cos 2\theta = \cos^2\theta - \sin^2\theta = 1 - 2\sin^2\theta \\ \text{so } \sin^2\theta = \frac{1}{2}(1 - \cos 2\theta) \\ \int_0^P \sin^2\frac{\ell\pi x}{a}\,dx = \frac{a}{2\ell\pi}\int_0^{\frac{\ell\pi P}{a}} (1 - \cos 2\theta)\,d\theta = \frac{P}{2} - \frac{a}{4\ell\pi}\sin\left(\frac{2\ell\pi P}{a}\right) \end{array}\right]$$

So $1 = |A|^2 \, \frac{a}{2}\cdot\frac{a}{2}$, $A = \frac{2}{a}$

Normalized unperturbed states are: $\psi_{\ell n}(x,y) = \frac{2}{a}\sin\left(\frac{\ell\pi x}{a}\right)\sin\left(\frac{n\pi y}{a}\right)$

with energy $\mathcal{H}_0 \psi^{(0)}_{\ell n} = -\frac{\hbar^2}{2m}\left[\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right]\frac{2}{a}\sin\left(\frac{\ell\pi x}{a}\right)\sin\left(\frac{n\pi y}{a}\right)$

$$= -\frac{\hbar^2}{2m}\frac{2}{a}\left[-\left(\frac{\ell\pi}{a}\right)^2 - \left(\frac{n\pi}{a}\right)^2\right]\sin\left(\frac{\ell\pi x}{a}\right)\sin\left(\frac{n\pi y}{a}\right)$$

$$= \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2(\ell^2 + n^2)\,\psi_{\ell n}(x,y)$$

$$\underline{E^{(0)}_{\ell n} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2(\ell^2 + n^2)}$$

a. Ground state: Unperturbed $\psi_{11}^{(0)}(x,y) = \frac{2}{a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)$

energy $\mathcal{E}_{11}^{(0)} = \frac{1}{m}\left(\frac{\hbar\pi}{a}\right)^2$

First order correction to energy:

$$Q_1 = \langle \psi_{11} | \mathcal{H}' | \psi_{11} \rangle$$

$$= \left(\frac{2}{a}\right)^2 W_0 \underbrace{\int_0^{a/2} \sin^2\frac{\pi x}{a}\, dx}_{\frac{a}{4}} \underbrace{\int_0^{a/2} \sin^2\frac{\pi y}{a}\, dy}_{\frac{a}{4}}$$

$$= \frac{4\ W_0}{a^2}\ \frac{\cancel{a^2}}{4^2} = \frac{W_0}{4}$$

So to first order in W_0 the ground state energy is $\underline{\underline{\frac{1}{m}\left(\frac{\hbar\pi}{a}\right)^2 + \frac{W_0}{4}}}$

b. First excited state:

This energy level is degenerate $\mathcal{E}_{21}^{(0)} = \mathcal{E}_{12}^{(0)} = \frac{5}{2m}\left(\frac{\hbar\pi}{a}\right)^2$

The zeroth order wavefunction can be any linear combination of the two states

$$\psi^{(0)} = \alpha\,\psi_{21} + \beta\,\psi_{12}$$

$$= \frac{2}{a}\left(\alpha \sin\frac{2\pi x}{a}\sin\frac{\pi y}{a} + \beta\sin\frac{\pi x}{a}\sin\frac{2\pi y}{a}\right)$$

Need the matrix elements:

$W_{AB} = \langle \psi_{ln} | W | \psi_{l'n'} \rangle$ where ln is either 12 or 21 and $l'n'$ is either 12 or 21.

First find $W_{21,12} = W_{12,21} = W_0\left(\frac{2}{a}\right)^2 \underbrace{\int_0^{a/2} dx \sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}}\int_0^{a/2} dy \sin\frac{\pi y}{a}\sin\frac{2\pi y}{a}$

$\sin 2x = 2\sin x\cos x$

$$\to 2\int_0^{a/2} dx \sin^2\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right)$$

Let $\theta = \cos\frac{\pi x}{a}$

$d\theta = -\sin\left(\frac{\pi x}{a}\right)\frac{\pi}{a}$

$$= \frac{2a}{\pi}\int_0^1 \theta^2 d\theta = \underline{\frac{2a}{3\pi}}$$

So $W_{21,12} = W_{12,21} = W_0\left(\frac{2}{a}\right)^2\left(\frac{2a}{3\pi}\right)^2 = \underline{W_0\left(\frac{4}{3\pi}\right)^2}$

Then find $W_{12,12} = W_{21,21} = W_0\left(\frac{2}{a}\right)^2\int_0^{a/2} dx \sin^2\left(\frac{2\pi x}{a}\right)\int_0^{a/2} dy \sin^2\left(\frac{\pi y}{a}\right)$

$$= W_0\left(\frac{2}{a}\right)^2\left(\frac{a}{4}\cdot\frac{a}{4}\right) = \underline{W_0/4}$$

Diagonalize:

$$\begin{pmatrix} W_{12,12} - Q_1 & W_{12,21} \\ W_{21,12} & W_{21,21} - Q_1 \end{pmatrix}\begin{pmatrix}\alpha \\ \beta\end{pmatrix} = 0$$

determinant has to vanish:

$$\left(W_{12,12} - Q_1\right)\left(W_{21,21} - Q_1\right) - W_{12,21}W_{21,12} = 0$$

Substitute: $\left(\frac{W_0}{4} - Q_1\right)^2 - W_0^2\left(\frac{4}{3\pi}\right)^4 = 0$

$$\frac{W_0}{4} - Q_1 = \pm W_0 \left(\frac{4}{3\pi}\right)^2$$

$$Q_1 = \frac{W_0}{4} \pm W_0 \left(\frac{4}{3\pi}\right)^2$$

$$= W_0 \left(\frac{1}{4} \pm \frac{16}{9\pi^2}\right)$$

To first order the energy is:

$$E_+ = \frac{5}{2m}\left(\frac{\hbar\pi}{a}\right)^2 + W_0\left(\frac{1}{4} + \frac{16}{9\pi^2}\right)$$

and $$E_- = \frac{5}{2m}\left(\frac{\hbar\pi}{a}\right)^2 + W_0\left(\frac{1}{4} - \frac{16}{9\pi^2}\right)$$

The wave function to zeroth order is $\psi^{(0)} = \alpha \psi_{21} + \beta \psi_{12}$

find α and β:

$\boxed{\psi_+^{(0)}:}$ Substitute $Q_1 = \left(\frac{1}{4} + \frac{16}{9\pi^2}\right) W_0$ into the matrix eqn.

$$\left(\cancel{\frac{W_0}{4}} - \cancel{\frac{W_0}{4}} - \frac{16 W_0}{9\pi^2}\right)\alpha + \frac{16 W_0}{9\pi^2}\beta = 0$$

i.e. $\alpha = \beta$

Normalization gives $\alpha = \beta = \frac{1}{\sqrt{2}}$

$\boxed{\psi_-^{(0)}:}$ Substitute $Q_1 = \left(\frac{1}{4} - \frac{16}{9\pi^2}\right) W_0$ into matrix eqn.

get $\alpha = -\beta$

So: $\psi_+^{(0)} = \frac{1}{\sqrt{2}}\left(\psi_{12} + \psi_{21}\right)$ and $\psi_-^{(0)} = \frac{1}{\sqrt{2}}\left(\psi_{12} - \psi_{21}\right)$