5.3 We have an infinite 2-D square well ($V_0 = 0$ for $0 \le x, y \le L$, ∞ elsewhere). I know that we should all just "know" the energy eigenfunctions, but I'll rederive them here for practice.

Assume a seperable form $\psi(x,y) = f(x)\,g(y)$

Schrödinger's Equation then gives us $\frac{-\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + V(x,y)\psi = E\psi$.

The wavefunction vanishes outside the well, so from now on we'll only focus on $0 \le x, y \le L$. Inside the well, $V(x,y) = 0$.

$$-\frac{\hbar^2}{2m}(gf'' + fg'') = Efg \Rightarrow -\frac{2mE}{\hbar^2} = \frac{1}{f}\frac{\partial^2 f}{\partial x^2} + \frac{1}{g}\frac{\partial^2 g}{\partial y^2}$$

$$\Rightarrow -\frac{1}{g}\frac{\partial^2 g}{\partial y^2} = \frac{2mE}{\hbar^2} + \frac{1}{f}\frac{\partial^2 f}{\partial x^2}$$

Since we have seperated this, the two sides of the equation must always be true, and thus equal to the same constat. Call that constant k_y^2.

$$\rightarrow -\frac{1}{g}\frac{\partial^2 g}{\partial y^2} = -k_y^2 \Longrightarrow g'' = g k_y^2$$

when $k_y^2 < 0$, $g(y) = C_1 \sinh(y k_y) + C_2 \cosh(y k_y)$

Applying Boundary Conditions: $g(0) = 0 \Rightarrow C_2 = 0$, so $g(y) = C_1 \sinh(y k_y)$.

also $g(L) = 0 \Rightarrow k_y = 0$, or $C_1 = 0$. Thus $k_y^2 < 0$ yields no solutions.

when $k_y^2 > 0$, $g(y) = C_1 \sin(y k_y) + C_2 \cos(y k_y)$

Applying Boundary Conditions: $g(0) = 0 \Rightarrow C_2 = 0$, so $g(y) = C_1 \sinh(y k_y)$.

also $g(L) = 0 \Rightarrow k_y = \frac{n_y \pi}{L}$

1 $\Rightarrow g(y) = C_1 \sin(k_y y)$, $k_y = \frac{n_y \pi}{L}$

$$\rightarrow \frac{2mE}{\hbar^2} + \frac{1}{f}\frac{\partial^2 f}{\partial x^2} = k_y^2$$, let $-k_x^2 = \frac{2mE}{\hbar^2} - k_y^2$, then

$$-\frac{1}{f}\frac{\partial^2 f}{\partial x^2} = -k_x^2 \Longrightarrow f'' = f k_x^2$$

Following the same logic as above,

2 $\Rightarrow f(x) = D_1 \sin(k_x x)$, $k_x = \frac{n_x \pi}{L}$

Combing 1 and 2, and redefing $A = C_1 D_1$, we get

$$\psi(x,y) = A \sin(k_y y) \sin(k_x x)$$

Normalize to get A.

$$1 = A^2 \int_0^L \int_0^L |\psi(x,y)|^2 \, dx\,dy = A^2 \int_0^L \int_0^L \sin^2\left(\frac{n_x \pi x}{L}\right) \sin^2\left(\frac{n_y \pi y}{L}\right) dx\,dy = \frac{A^2 L^2}{4} \Rightarrow A = \frac{2}{L}$$

3 $\psi(x,y) = \frac{2}{L} \sin(k_y y) \sin(k_x x)$

For kicks, we also get

$$k_x = \frac{n_x \pi}{L} = \sqrt{\frac{2mE}{\hbar^2} - k_y^2} \Rightarrow \frac{n_x^2 \pi^2}{L^2} + \frac{n_y^2 \pi}{L^2} = \frac{2mE}{\hbar^2} \rightarrow E = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2)$$

5.3, cont.

Thus, from ③

$$\boxed{\begin{array}{ll} \text{Ground State } (n=1), & \psi_1(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) \\ \text{First Excited State } (n=2), & \psi_{2a}(x,y) = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) \\ & \text{or } \psi_{2b}(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right) \end{array}}$$

2-fold degenerscy.

Ground State $(n=1)$

→ Zeroth-order energy eigenfuction: $\boxed{\psi_1^{(0)}(x,y) = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)}$

→ 1^{st}-order energy shift

we have the perturbation $V_1 = \lambda xy$

In general, $\Delta_n^{(1)} = \langle n^{(0)}|V_1|n^{(0)}\rangle$ where $|n^{(0)}\rangle$ is the zeroth order energy eigenket of the n^{th} excited state.

Here we have $\Delta_1^{(1)} = \langle 1^{(0)}|xy|1^{(0)}\rangle\lambda = \lambda\int_0^L\int_0^L |\psi_1^0(x,y)|^2 xy\,dx\,dy$

$$= \frac{4\lambda}{L^2}\int_0^L\int_0^L xy\sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right)dx\,dy = \frac{1}{4}\lambda L^2 \quad \Rightarrow \boxed{\Delta_1^{(1)} = \frac{\lambda L^2}{4}}$$

1^{st} Excited state $(n=2)$

→ 1^{st}-order energy shift: $\Delta_2^{(1)} = \langle 2^{(0)}|V_1|2^{(0)}\rangle = \lambda\langle 2^{(0)}|xy|2^{(0)}\rangle$

This becomes a 2x2 matrix because of the 2-fold degenracy

$$\Delta_2^{(1)} = \lambda\begin{bmatrix}\langle\psi_{2a}|xy|\psi_{2a}\rangle & \langle\psi_{2a}|xy|\psi_{2b}\rangle \\ \langle\psi_{2b}|xy|\psi_{2a}\rangle & \langle\psi_{2b}|xy|\psi_{2b}\rangle\end{bmatrix}$$

calculate the matrix elemts.

$$\langle\psi_{2a}|xy|\psi_{2a}\rangle = \frac{4}{L^2}\int_0^L\int_0^L \sin^2\left(\frac{2\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right)xy\,dx\,dy = \frac{L^2}{4}$$

also $\langle\psi_{2a}|xy|\psi_{2a}\rangle = \langle\psi_{2b}|xy|\psi_{2b}\rangle$ b/c symmetric in x vs. y.

$$\langle\psi_{2a}|xy|\psi_{2b}\rangle = \frac{4}{L^2}\int_0^L\int_0^L \sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)\sin\left(\frac{\pi y}{L}\right)xy\,dx\,dy = \frac{256\,L^2}{\pi^4\,81}$$

also $\langle\psi_{2a}|xy|\psi_{2b}\rangle = \langle\psi_{2b}|xy|\psi_{2a}\rangle$ b/c the wavefuctions are real.

$$\Rightarrow \Delta_2^{(1)} = \lambda L^2\begin{bmatrix}\frac{1}{4} & \frac{256}{81\pi^4} \\ \frac{256}{81\pi^4} & 1/4\end{bmatrix}$$

Now diagonalize this. $|\Delta_2^{(1)} - \xi I| = 0 \Rightarrow \lambda L^2\begin{vmatrix}1/4-\xi & \frac{256}{81\pi^4} \\ \frac{256}{81\pi^4} & 1/4-\xi\end{vmatrix} = 0$

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$$\Rightarrow \xi_\pm = \frac{81\pi^4 \pm 1024}{324\pi^4}\lambda L^2$$

Crunching the numbers, we get the energy shifts: $\boxed{\begin{array}{l}\Delta_{2a}^{(1)} = 0.28\lambda L^2 \\ \Delta_{2b}^{(1)} = 0.22\lambda L^2\end{array}}$

→ Zeroth-order energy eigenfuctions.

$$\Delta_2^{(1)} - \xi_a I = \frac{256L^2}{81\pi^4}\begin{bmatrix}-1 & 1 \\ 1 & -1\end{bmatrix} \Rightarrow \boxed{\psi_{2a}^{(0)} = \frac{1}{\sqrt2}\begin{bmatrix}1\\1\end{bmatrix} = \frac{\sqrt2}{L}\left(\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) + \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)\right)}$$

$$\Delta_2^{(1)} - \xi_b I = \frac{256L^2}{81\pi^4}\begin{bmatrix}1 & 1 \\ 1 & 1\end{bmatrix} \Rightarrow \boxed{\psi_{2b}^{(0)} = \frac{1}{\sqrt2}\begin{bmatrix}1\\-1\end{bmatrix} = \frac{\sqrt2}{L}\left(\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) - \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)\right)}$$