4) A particle of mass m is stuck in a 2-D rectangular box of length a and width b. Derive the normalized wavefunctions and allowed energies for the ground and first excited states using the Schrodinger equation.

The potential is given by:

$$V(x,y) = \begin{cases} 0 & 0 \le x \le a \\ & 0 \le y \le b \\ \infty & \text{otherwise} \end{cases}$$

Use Schrodinger's equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(x,y) = E\psi(x,y) \qquad (1)$$

Try separation of variables; $\psi(x,y) = X(x)\,Y(y)$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right] X(x)\,Y(y) = E\,X(x)\,Y(y)$$

$$-\frac{\hbar^2}{2m}\left[\frac{d^2 X(x)}{dx^2} Y(y) + X(x)\frac{d^2 Y(y)}{dy^2}\right] = E\,X(x)\,Y(y)$$

Divide by $X(x)\,Y(y)$ and multiply by $-\frac{2m}{\hbar^2}$

$$\underbrace{\frac{1}{X(x)}\frac{d^2X(x)}{dx^2}}_{\text{const}} + \underbrace{\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2}}_{\text{const}} = -\frac{2mE}{\hbar^2} \qquad (2)$$

By the usual arguments of seperation of variables the two highlighted portions must be constant.

<u>$X(x)$</u>

$$\frac{1}{X(x)}\frac{d^2X(x)}{dx^2} = \lambda_x \qquad (3)$$

From the boundary conditions we need:

$$X(0) = 0 \qquad \text{BC1 a}$$
$$X(a) = 0 \qquad \text{BC1 b}$$

If $\lambda_x = 0$ then $X(x)$ is linear. From BC 1a and 1b it must be $X(x) = 0$. This state is <u>not</u> normalizable, hence not a solution.

If $\lambda_x > 0$

$$X(x) = d_1 \cosh(\sqrt{\lambda_x}\, x) + d_2 \sinh(\sqrt{\lambda_x}\, x)$$

From $X(0) = 0$

$$0 = d_1 (1) + d_2 (0)$$

$$\Rightarrow d_1 = 0$$

From, $X(a) = 0$

$$0 = d_2 \sinh(\sqrt{\lambda_x}\, a)$$

$$0 = \sinh(\sqrt{\lambda_x}\, a)$$

$$0 = \frac{1}{2}\left(e^{\sqrt{\lambda_x}a} - e^{-\sqrt{\lambda_x}a}\right)$$

$$e^{-\sqrt{\lambda_x}a} = e^{\sqrt{\lambda_x}a}$$ ln both sides

$$-\sqrt{\lambda_x}\,a = \sqrt{\lambda_x}\,a \qquad (4)$$

Since $a \neq 0$ and $\lambda_x \neq 0$

Eq. (4) not possible.

Therefore λ_x must be negative.

For convenience, let

$$\lambda_x = -k_x^2$$

Then the solution to Eq. (3) is:

$$X(x) = c_1 \cos(k_x x) + c_2 \sin(k_x x)$$

from $X(0)=0$,

$$0 = c_1(1) + c_2(0)$$
$$\Rightarrow c_1 = 0$$

From $X(a)=0$

$$0 = c_2 \sin(k_x a)$$

Cannot have $c_2 = 0$ since otherwise we have non-normalizable zero solution. Therefore,

$$\boxed{k_x a = m\pi}$$

m is an integer

And,

$$\boxed{X(x) = c_2 \sin\left(\frac{m\pi x}{a}\right)}$$

The logic for $Y(y)$ is the same.

$$\boxed{k_y a = n\pi}$$ n integer

$$\boxed{Y(y) = b_2 \sin\left(\frac{n\pi}{b} y\right)}$$

Thus, an eigenfunction is

$$\psi_{mn}(x,y) = C_{mn} \sin\left(\frac{m\pi}{a}x\right) \sin\left(\frac{n\pi}{b}y\right)$$

The normalization condition implies,

$$\int_0^b dy \int_0^a dx \, |\psi_{mn}(x,y)|^2 = 1$$

$$|C_{mn}|^2 \int_0^b dy \, \sin^2\left(\frac{n\pi}{b}x\right) \int_0^a \sin^2\left(\frac{m\pi x}{a}\right) = 1$$

$$|C_{mn}|^2 \, \frac{b}{2} \, \frac{a}{2} = 1$$

$$\Rightarrow \quad c_{mn} = \frac{2}{\sqrt{ab}}$$

Therefore,

$$\boxed{\psi_{mn}(x,y) = \frac{2}{\sqrt{ab}} \sin\left(\frac{m\pi}{a}x\right) \sin\left(\frac{n\pi}{a}y\right)}$$

Note: neither m or n can be zero to be normalizable.

Energy levels

From (2)

$$-k_x^2 - k_y^2 = -\frac{2mE}{\hbar^2}$$

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$

$$E = \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2\right]$$

$$\boxed{E_{m,n} = \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{m}{a}\right)^2 + \left(\frac{n}{b}\right)^2\right]}$$

The ground state is:

- $$E_{ground} = E_{1,1} = \frac{\hbar^2\pi^2}{2m}\left[\frac{1}{a^2} + \frac{1}{b^2}\right]$$

The next two states are

- $$E_{1,2} = \frac{\hbar^2\pi^2}{2m}\left[\frac{1}{a^2} + \frac{4}{b^2}\right]$$
- $$E_{2,1} = \frac{\hbar^2\pi^2}{2m}\left[\frac{4}{a^2} + \frac{1}{b^2}\right]$$