Particle in a 2-D Box: Problem TZDII¹ 8.12 Class Work, Wednesday, 1/24/24

Consider a particle in a 2-D box with sides of length a.

The wave function is

$$\psi(x,y) = A \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{a}\right) \quad TZDII (8.23)$$

Write down probability density $|\psi|^2$ and determine where the particle is most likely to be found. How many such points are there? Sketch a contour map similar to those in Fig. 8.4. For

- a) $n_x = 1$, $n_y = 2$
- b) $n_x = 2$, $n_y = 2$
- c) $n_x = 4$, $n_y = 3$

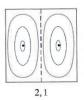






FIGURE 8.4

Contour maps of $|\psi|^2$ for three excited states of the square box. The two numbers under each picture are n_x and n_y . The dashed lines are nodal lines, where $|\psi|^2$ vanishes; these occur where ψ passes through zero as it oscillates from positive to negative values.

a) For
$$n_x = 1$$
 and $n_y = 2$, the probability density $\left| \psi(x,y) \right|^2$ is $\left| \psi(x,y) \right|^2 = A^2 \sin^2 \left(\frac{\pi x}{a} \right) \sin^2 \left(\frac{2\pi y}{a} \right)$

Find A by normalization

$$\int_{0}^{a} \int_{0}^{a} \left| \psi(\mathbf{x}, \mathbf{y}) \right|^{2} d\mathbf{x} d\mathbf{y} = \mathbf{A}^{2} \int_{0}^{a} \int_{0}^{a} \sin^{2} \left(\frac{\pi \mathbf{x}}{a} \right) \sin^{2} \left(\frac{2\pi \mathbf{y}}{a} \right) d\mathbf{x} d\mathbf{y} = 1$$

Integral #176 in the CRC gives

$$\int \sin^2(\alpha x) dx = \frac{1}{2}x - \frac{1}{4\alpha}\sin(2\alpha x)$$

Thus, in general

$$\int_{0}^{a} \int_{0}^{a} \left| \psi(\mathbf{x}, \mathbf{y}) \right|^{2} d\mathbf{x} d\mathbf{y} = \mathbf{A}^{2} \left[\frac{\mathbf{x}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{x}\pi} \sin\left(\frac{4\mathbf{n}_{x}\pi\mathbf{x}}{\mathbf{a}}\right)_{0}^{a} \right] \left[\frac{\mathbf{y}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{y}\pi} \sin\left(\frac{4\mathbf{n}_{x}\pi\mathbf{y}}{\mathbf{a}}\right)_{0}^{a} \right] = 1$$

For $n_x = 1$ and $n_y = 2$, this becomes

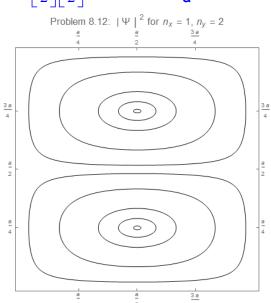
$$\mathbf{A}^{2} \left[\frac{\mathbf{x}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{x}\pi} \sin \left(\frac{4\pi \mathbf{x}}{\mathbf{a}} \right)_{0}^{\mathbf{a}} \right] \left[\frac{\mathbf{y}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{y}\pi} \sin \left(\frac{8\pi \mathbf{y}}{\mathbf{a}} \right)_{0}^{\mathbf{a}} \right] = \mathbf{A}^{2} \left[\frac{\mathbf{a}}{2} \right] \left[\frac{\mathbf{a}}{2} \right] = 1 \quad \Rightarrow \quad \mathbf{A} = \frac{2}{\mathbf{a}}$$

And the probability density is

$$\left|\psi(\mathbf{x},\mathbf{y})\right|^2 = \frac{4}{a^2} \sin^2\left(\frac{\pi \mathbf{x}}{a}\right) \sin^2\left(\frac{2\pi \mathbf{y}}{a}\right)$$

Making a contour plot of this in Mathematica (see T:\O'Donoghue\Modern\TZDIIPr08_12) gives the image to the right. This has one maximum in x at x = 0.5a and two in y at y = 0.25a & y = 0.75a.

¹ Modern Physics for Scientists and Engineers, 2nd Ed., John R. Taylor, Chris D. Zafiratos, & Michael A. Dubson (Prentice Hall, 2002



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

b) For $n_x = 2$ and $n_y = 2$, the probability density $|\psi(x,y)|^2$, for $n_x = 1$ and $n_y = 2$ is

$$\left|\psi(x,y)\right|^2 = A^2 \sin^2\left(\frac{2\pi x}{a}\right) \sin^2\left(\frac{2\pi y}{a}\right)$$

Find A by normalization

$$\int_{0}^{a} \int_{0}^{a} \left| \psi(\mathbf{x}, \mathbf{y}) \right|^{2} d\mathbf{x} d\mathbf{y} = \mathbf{A}^{2} \int_{0}^{a} \int_{0}^{a} \sin^{2} \left(\frac{\pi \mathbf{x}}{a} \right) \sin^{2} \left(\frac{2\pi \mathbf{y}}{a} \right) d\mathbf{x} d\mathbf{y} = 1$$

Integral #176 in the CRC gives

$$\int \sin^2(ax) dx = \frac{1}{2}x - \frac{1}{4a}\sin(2ax)$$

Thus, in general

$$\int_{0}^{a} \int_{0}^{a} \left| \psi(\mathbf{x}, \mathbf{y}) \right|^{2} d\mathbf{x} d\mathbf{y} = \mathbf{A}^{2} \left[\frac{\mathbf{x}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{x}\pi} \sin\left(\frac{4\mathbf{n}_{x}\pi\mathbf{x}}{\mathbf{a}}\right)_{0}^{a} \right] \left[\frac{\mathbf{y}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{y}\pi} \sin\left(\frac{4\mathbf{n}_{x}\pi\mathbf{y}}{\mathbf{a}}\right)_{0}^{a} \right] = 1$$

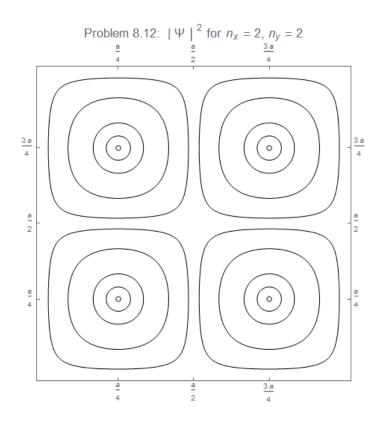
For $n_x = 1$ and $n_y = 2$, this becomes

$$\mathbf{A}^{2} \left[\frac{\mathbf{x}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{x}\pi} \sin \left(\frac{8\pi \mathbf{x}}{\mathbf{a}} \right)_{0}^{\mathbf{a}} \right] \left[\frac{\mathbf{y}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{y}\pi} \sin \left(\frac{8\pi \mathbf{y}}{\mathbf{a}} \right)_{0}^{\mathbf{a}} \right] = \mathbf{A}^{2} \left[\frac{\mathbf{a}}{2} \right] \left[\frac{\mathbf{a}}{2} \right] = 1 \quad \Rightarrow \quad \mathbf{A} = \frac{2}{\mathbf{a}}$$

And the probability density is

$$\left|\psi(x,y)\right|^2 = \frac{4}{a^2} \sin^2\left(\frac{2\pi x}{a}\right) \sin^2\left(\frac{2\pi y}{a}\right)$$

Making a contour plot of this in Mathematica (see T:\O'Donoghue\Modern\TZDIIPr08_12) gives the image to the right. This has two maxima in each direction at x = 0.25a & x = 0.75a and y = 0.25a & y = 0.75a.



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

c) For n_x = 4 and n_y = 3, the probability density $\left|\psi(x,y)\right|^2$ is

$$\left|\psi(x,y)\right|^2 = A^2 \sin^2\left(\frac{4\pi x}{a}\right) \sin^2\left(\frac{3\pi y}{a}\right)$$

Find A by normalization

$$\int_{0}^{a} \int_{0}^{a} \left| \psi(\mathbf{x}, \mathbf{y}) \right|^{2} d\mathbf{x} d\mathbf{y} = \mathbf{A}^{2} \int_{0}^{a} \int_{0}^{a} \sin^{2} \left(\frac{4\pi \mathbf{x}}{a} \right) \sin^{2} \left(\frac{3\pi \mathbf{y}}{a} \right) d\mathbf{x} d\mathbf{y} = 1$$

Integral #176 in the CRC gives

$$\int \sin^2(ax) dx = \frac{1}{2}x - \frac{1}{4a}\sin(2ax)$$

Thus, in general

$$\int_{0}^{a} \int_{0}^{a} \left| \psi(\mathbf{x}, \mathbf{y}) \right|^{2} d\mathbf{x} d\mathbf{y} = \mathbf{A}^{2} \left[\frac{\mathbf{x}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{x}\pi} \sin\left(\frac{4\mathbf{n}_{x}\pi\mathbf{x}}{\mathbf{a}}\right)_{0}^{a} \right] \left[\frac{\mathbf{y}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{y}\pi} \sin\left(\frac{4\mathbf{n}_{x}\pi\mathbf{y}}{\mathbf{a}}\right)_{0}^{a} \right] = 1$$

For $n_x = 1$ and $n_y = 2$, this becomes

$$\mathbf{A}^{2} \left[\frac{\mathbf{x}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{x}\pi} \sin \left(\frac{8\pi \mathbf{x}}{\mathbf{a}} \right)_{0}^{\mathbf{a}} \right] \left[\frac{\mathbf{y}}{2} - \frac{\mathbf{a}}{4\mathbf{n}_{y}\pi} \sin \left(\frac{6\pi \mathbf{y}}{\mathbf{a}} \right)_{0}^{\mathbf{a}} \right] = \mathbf{A}^{2} \left[\frac{\mathbf{a}}{2} \right] \left[\frac{\mathbf{a}}{2} \right] = 1 \quad \Rightarrow \quad \mathbf{A} = \frac{2}{\mathbf{a}}$$

And the probability density is

$$\left|\psi(x,y)\right|^2 = \frac{4}{a^2} \sin^2\left(\frac{4\pi x}{a}\right) \sin^2\left(\frac{3\pi y}{a}\right)$$

Making a contour plot of this in Mathematica (see T:\O'Donoghue\Modern\TZDIIPr08_12) gives the image to the right. This has four maxima in x at x = a/8, 3a/8, 5a/8, & 7a/8 and three maxima in y at y = a/6, 3a/6, & 5a/6.

