Particle in a Box (2 Dimensions)

The time independent Schrödinger equation for a particle equation moving in more than one dimension:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathrm{x},\mathrm{y}) + V(x,y)\Psi(\mathrm{x},\mathrm{y}) = E\Psi(\mathrm{x},\mathrm{y})$$

Where:

$\hbar$	$\frac{h}{2\pi}$ (reduced Plank's constant)
h	Plank's constant (describes size of quanta in quantum mechanics)
m	mass of particle
∇^2	Laplacian operator ($= \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2}$ in 2D rectangular coordinates)
Ψ	wave function (replaces the concept of trajectory in classical mechanics)
$V(x,y)$	potential energy of particle
E	total energy of particle

We expand the Laplacian and rewrite the equation as:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right) + V(x,y)\Psi = E\Psi$$

For a particle in a two-dimensional box of length L and height H, the potential energy function is

$$V(x,y) = \begin{cases} 0 & 0 < x < L \; and \; 0 < y < H \\ \infty & \text{elsewhere} \end{cases}.$$

This implies that the particle can only exist inside the box where $V(x,y) = 0$. Using this fact and letting $k^2 = \frac{2mE}{\hbar^2}$ allows us to rewrite the equation:

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} = -k^2\Psi$$

The result is a homogeneous 2nd order partial differential equation (PDE) with constant coefficients. We use the separation of variables method to solve the above equation. Assume that the wave function $\Psi(\mathrm{x},\mathrm{y})$ is separable into two functions $X(x)$ and $Y(y)$, i.e. $\Psi(\mathrm{x},\mathrm{y}) = \mathrm{X}(\mathrm{x})\mathrm{Y}(\mathrm{y})$ or, for brevity, $\Psi = \mathrm{XY}$.

Therefore $\frac{\partial^2\Psi}{\partial x^2} = X''Y$ and $\frac{\partial^2\Psi}{\partial y^2} = XY''$. This allows us to rewrite the PDE as:

$$X''Y + XY'' = -k^2XY$$

Dividing both sides by XY yields

$$\frac{X''}{X} + \frac{Y''}{Y} = -k^2$$

The variables are separated by shifting the Y term to the right-hand side of the equation:

$$\frac{X''}{X} = -\frac{Y''}{Y} - k^2 = -\lambda^2$$

Since the variables have been fully separated, we can set both equations equal to the constant $-\lambda^2$. (Note: I use $-\lambda^2$ vice $-\lambda$ for convenience.)

We first solve for X, i.e. :

$$\frac{X''}{X} = -\lambda^2 \xrightarrow{yields} X'' + \lambda^2 X = 0$$

We know that the only non-trivial solution has the form:

$$X = \mathrm{c}_1 \sin(\lambda \mathrm{x}) + \mathrm{c}_2 \cos(\lambda \mathrm{x})$$

Since the particle cannot be outside the box:

$$\mathrm{X}(0) = \mathrm{c}_1 \sin(0) + \mathrm{c}_2 \cos(0) = 0 \xrightarrow{\text{yields}} \mathrm{c}_2 = 0 \xrightarrow{\text{yields}} \mathrm{X}(\mathrm{x}) = \mathrm{c}_1 \sin(\lambda \mathrm{x}),$$

and:

$$\mathrm{X}(\mathrm{L}) = \mathrm{c}_1 \sin(\lambda L) = 0 \xrightarrow{\text{yields}} \lambda L = n\pi \xrightarrow{yields} \lambda_n = \frac{n\pi}{L},$$

where n is a positive integer. Therefore:

$$\mathrm{X}_\mathrm{n}(\mathrm{x}) = \mathrm{c}_\mathrm{n} \sin\left(\frac{\mathrm{n}\pi\mathrm{x}}{\mathrm{L}}\right).$$

We now turn our attention to Y and solve:

$$-\frac{Y''}{Y} - k^2 = -\lambda^2 \xrightarrow{yields} Y'' + (k^2 - \lambda^2)\, Y = 0.$$

Again, the only non-trivial solution is:

$$Y = \mathrm{c}_3 \sin\left(\sqrt{k^2 - \lambda^2}\mathrm{y}\right) + \mathrm{c}_4 \cos\left(\sqrt{k^2 - \lambda^2}\mathrm{y}\right).$$

As before, the particle cannot be outside the box:

$$Y(0) = \mathrm{c}_3 \sin(0) + \mathrm{c}_4 \cos(0) \xrightarrow{yields} \mathrm{c}_4 = 0 \xrightarrow{\text{yields}} \mathrm{Y}(\mathrm{y}) = \mathrm{c}_3 \sin\left(\sqrt{k^2 - \lambda^2}\mathrm{y}\right),$$

and:

$$\mathrm{Y(H)} = \mathrm{c}_3 \sin\left(\sqrt{k^2-\lambda^2}\mathrm{H}\right) = 0 \xrightarrow{\text{yields}} \sqrt{k^2-\lambda^2}\mathrm{H} = \mathrm{p}\pi \xrightarrow{\text{yields}} \sqrt{k^2-\lambda^2} = \frac{\mathrm{p}\pi}{\mathrm{H}},$$

where p is a positive integer. Therefore:

$$\mathrm{Y_p(y)} = \mathrm{c_p} \sin\left(\frac{\mathrm{p}\pi\mathrm{y}}{\mathrm{H}}\right).$$

Since $\Psi = \mathrm{XY}$ we have:

$$\Psi_{\mathrm{np}} = \mathrm{c_{np}} \sin\left(\frac{\mathrm{n}\pi\mathrm{x}}{\mathrm{L}}\right) \sin\left(\frac{\mathrm{p}\pi\mathrm{y}}{\mathrm{H}}\right).$$

Note that $\mathrm{c_{np}} = \mathrm{c_n c_p}$. Here the wave function Ψ_{np} varies with integer values of n and p.

Since $\left|\Psi_{\mathrm{np}}(\mathrm{x,y})\right|^2$ is the probability distribution function and since we know that the particle will be somewhere in the box, we know that $\left|\Psi_{\mathrm{np}}(\mathrm{x})\right|^2$=1 for $0 < x < L$ and $0 < y < H$, i.e. there is a 100% probability that the particle is somewhere inside the box. Therefore:

$$c_{np}^2 \int_0^H \int_0^L \sin^2\left(\frac{\mathrm{n}\pi\mathrm{x}}{\mathrm{L}}\right) \sin^2\left(\frac{\mathrm{p}\pi\mathrm{y}}{\mathrm{H}}\right) dxdy = 1.$$

We can separate the integrals as follows (this is possible because the x and y variables are independent):

$$c_{np}^2 \left(\int_0^L \sin^2\left(\frac{\mathrm{n}\pi\mathrm{x}}{\mathrm{L}}\right) dx\right)\left(\int_0^H \sin^2\left(\frac{\mathrm{p}\pi\mathrm{y}}{\mathrm{H}}\right) dy\right) = 1,$$

which yields,

$$c_{np}^2 \left(\frac{L}{2}\right)\left(\frac{H}{2}\right) dy = 1 \xrightarrow{yields} c_{\ np} = \frac{2}{\sqrt{LH}}.$$

Therefore:

$$\boxed{\Psi_{\mathrm{np}} = \frac{2}{\sqrt{LH}} \sin\left(\frac{\mathrm{n}\pi\mathrm{x}}{\mathrm{L}}\right) \sin\left(\frac{\mathrm{p}\pi\mathrm{y}}{\mathrm{H}}\right).}$$

This is the solution to the wave equation for the particle in a two dimensional box.

We now turn our attention to the total energy. Recall:

$$k^2 = \frac{2mE}{\hbar^2} \text{ and } \hbar = \frac{h}{2\pi}.$$

Since:

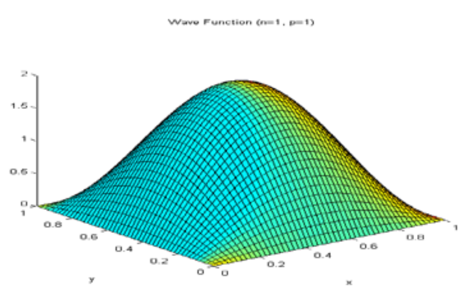
$$\sqrt{k^2 - \lambda^2} = \frac{p\pi}{H} \text{ and } \lambda = \frac{n\pi}{L} \xrightarrow{yields} k^2 = \left(\frac{n\pi}{L}\right)^2 + \left(\frac{p\pi}{H}\right)^2,$$

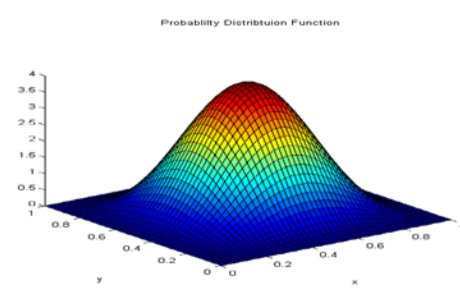
we get:

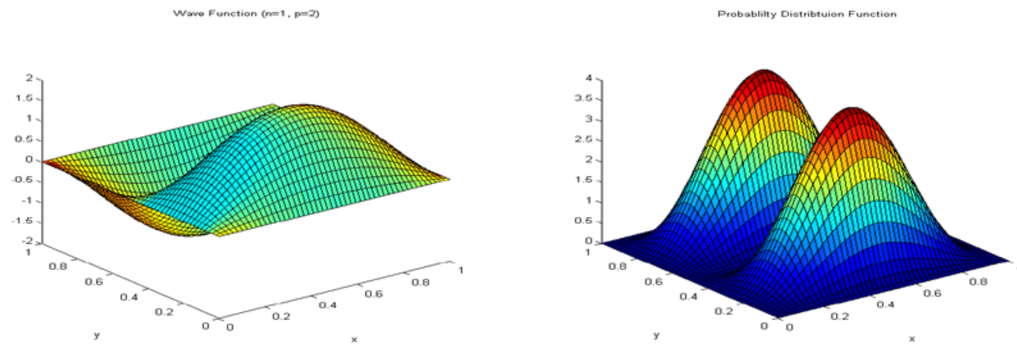
$$E = \left(\left(\frac{n\pi}{L}\right)^2 + \left(\frac{p\pi}{H}\right)^2\right)\left(\frac{h^2}{4\pi^2}\right)\left(\frac{1}{2m}\right) \xrightarrow{yields} \boxed{E = \frac{h^2}{8m}\left(\frac{n^2}{L^2} + \frac{p^2}{H^2}\right)}.$$

Note that this implies that the total energy for a particle is quantized.

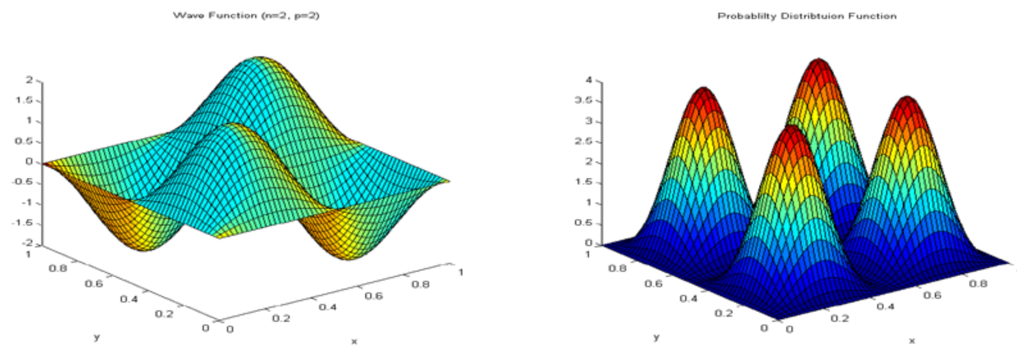
The figures below depict wave functions and probability distribution functions for various values of n and p. In each diagram L=1 and H=1.






Wave Function (n=1, p=2)
Probablilty Distribtuion Function
x
y

n=1, p=2


Wave Function (n=2, p=2)
Probablilty Distribtuion Function
x
y

n=2, p=2

Homework Questions:

1. (5 pts) Let L=1 and H=1. What is the wave equation for Ψ_{23}? What is the total energy of the particle with mass *m* that exists in the state Ψ_{23}?

2. (10 pts) Recall that $\left|\Psi_{\mathrm{np}}\right|^2$ is a probability distribution function where:
Pr($a \leq x \leq b, c \leq y \leq d) = \int_c^d \int_a^b \left|\Psi_{\mathrm{np}}\right|^2 dxdy$. If L=3 and H=2, find
Pr(1≤ $x \leq$ 2, 1/2≤ $y \leq 3/2$) for Ψ_{14}.

3. (5 pts) Find an expression for the total energy of a particle in the state Ψ_{np} if

$$V(x,y) = \begin{cases} a & 0 < x < 1 \text{ and } 0 < y < 1 \\ \infty & \text{elsewhere} \end{cases}$$