Particle in a Box (2 Dimensions)

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

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

Where:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hbar$</td>
<td>reduced Plank’s constant</td>
</tr>
<tr>
<td>$\hbar$</td>
<td>Plank’s constant (describes size of quanta in quantum mechanics)</td>
</tr>
<tr>
<td>$m$</td>
<td>mass of particle</td>
</tr>
<tr>
<td>$\nabla^2$</td>
<td>Laplacian operator ($= \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2}$ in 2D rectangular coordinates)</td>
</tr>
<tr>
<td>$\Psi$</td>
<td>wave function (replaces the concept of trajectory in classical mechanics)</td>
</tr>
<tr>
<td>$V(x,y)$</td>
<td>potential energy of particle</td>
</tr>
<tr>
<td>$E$</td>
<td>total energy of particle</td>
</tr>
</tbody>
</table>

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

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

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 $\Psi(x,y)$ is separable into two functions $X(x)$ and $Y(y)$, i.e. $\Psi(x,y) = X(x)Y(y)$ or, for brevity, $\Psi = XY$.

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

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

Dividing both sides by $XY$ yields
The variables are separated by shifting the Y term to the right-hand side of the equation:

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

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.:

\[ \frac{X''}{X} = -\lambda^2 \quad \Rightarrow \quad X'' + \lambda^2 X = 0 \]

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

\[ X = c_1 \sin(\lambda x) + c_2 \cos(\lambda x) \]

Since the particle cannot be outside the box:

\[ X(0) = c_1 \sin(0) + c_2 \cos(0) = 0 \quad \Rightarrow \quad c_2 = 0 \quad \Rightarrow \quad X(x) = c_1 \sin(\lambda x), \]

and:

\[ X(L) = c_1 \sin(\lambda L) = 0 \quad \Rightarrow \quad \lambda L = n\pi \quad \Rightarrow \quad \lambda_n = \frac{n\pi}{L}, \]

where \(n\) is a positive integer. Therefore:

\[ X_n(x) = c_n \sin\left(\frac{n\pi x}{L}\right). \]

We now turn our attention to \(Y\) and solve:

\[ -\frac{Y''}{Y} - k^2 = -\lambda^2 \quad \Rightarrow \quad Y'' + (k^2 - \lambda^2)Y = 0. \]

Again, the only non-trivial solution is:

\[ Y = c_3 \sin(\sqrt{k^2 - \lambda^2}y) + c_4 \cos(\sqrt{k^2 - \lambda^2}y). \]

As before, the particle cannot be outside the box:

\[ Y(0) = c_3 \sin(0) + c_4 \cos(0) \quad \Rightarrow \quad c_4 = 0 \quad \Rightarrow \quad Y(y) = c_3 \sin(\sqrt{k^2 - \lambda^2}y), \]
and:

\[ Y(H) = c_3 \sin \left( \sqrt{k^2 - \lambda^2} H \right) = 0 \quad \text{yields} \quad \sqrt{k^2 - \lambda^2} H = p\pi \quad \text{yields} \quad \sqrt{k^2 - \lambda^2} = \frac{p\pi}{H}, \]

where \( p \) is a positive integer. Therefore:

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

Since \( \Psi = XY \) we have:

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

Note that \( c_{np} = c_n c_p \). Here the wave function \( \Psi_{np} \) varies with integer values of \( n \) and \( p \).

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

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

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

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

which yields,

\[ c_{np}^2 \left( \frac{L}{2} \right) \left( \frac{H}{2} \right) dy = 1 \quad \text{yields} \quad c_{np} = \frac{2}{\sqrt{LH}}. \]

Therefore:

\[ \Psi_{np} = \frac{2}{\sqrt{LH}} \sin \left( \frac{n\pi x}{L} \right) \sin \left( \frac{p\pi y}{H} \right). \]
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:

\[ k^2 = \frac{2mE}{\hbar^2} \text{ and } \hbar = \frac{\hbar}{2\pi}. \]

Since:

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

we get:

\[ E = \left(\frac{n\pi}{L}\right)^2 + \left(\frac{p\pi}{H}\right)^2 \left(\frac{h^2}{4\pi^2}\right) \left(\frac{1}{2m}\right) \implies E = \frac{h^2}{8m} \left(\frac{n^2}{L^2} + \frac{p^2}{H^2}\right). \]

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 \( H=1 \).
Particle in a Box (2D)

$n=1, \ p=2$

$n=2, \ p=2$
Homework Questions:

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

2. (10 pts) Recall that \( |\Psi_{np}|^2 \) is a probability distribution function where:
   \[
   \Pr(a \leq x \leq b, c \leq y \leq d) = \int_c^d \int_a^b |\Psi_{np}|^2 \, dx \, dy.
   \]
   If \( L=3 \) and \( H=2 \), find \( \Pr(1 \leq x \leq 2, 1/2 \leq y \leq 3/2) \) for \( \Psi_{41} \).

3. (5 pts) Find an expression for the total energy of a particle in the state \( \Psi_{np} \) if
   \[
   V(x, y) = \begin{cases} 
   a & 0 < x < 1 \text{ and } 0 < y < 1 \\
   \infty & \text{elsewhere}
   \end{cases}
   \]