1 Solution by Separation of Variables: Two Dimensional Square Well

Suppose we have a two dimensional potential energy. Inside a region bounded by $0 < x < L$ and $0 < y < L$ the potential energy is zero, outside that region the potential is infinite. Outside the well the wavefunction must be identically zero.\(^1\)

Inside the well we will look for a solution that is separable, that is a solution that can be written as

$$\psi(x, y) = f(x)g(y)$$ (1)

Schroedinger’s Equation in 2D will just be an extension of the 1D equation.

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

and using the expression for $\psi$ from Equation (1), Equation (2) becomes

$$\frac{-\hbar^2}{2m} \left( g \frac{d^2 f}{dx^2} + f \frac{d^2 g}{dy^2} \right) + U(x, y)fg = Ef g$$ (3)

Now consider the potential energy for the square well. It is zero inside the well. So inside the well we can divide by the wavefunction $fg$ and rearrange to get

$$\frac{1}{f} \frac{d^2 f}{dx^2} + \left( \frac{2mE}{\hbar^2} \right) = -\frac{1}{g} \frac{d^2 g}{dy^2}$$ (4)

The left side of Equation (4) depends only on the variable $x$ while the right side only depends on $y$. And this must be true for all possible values of $x$ and $y$. Hence both sides must equal a constant.

$$\frac{1}{f} \frac{d^2 f}{dx^2} + \left( \frac{2mE}{\hbar^2} \right) = -\frac{1}{g} \frac{d^2 g}{dy^2} = Constant$$ (5)

What happens if the constant is negative, $Constant = -\kappa_y^2$? The solution of

$$-\frac{1}{g} \frac{d^2 g}{dy^2} = -\kappa_y^2$$ (6)

is

$$g(y) = A \exp -\kappa_y y + B \exp \kappa_y y$$ (7)

\(^1\)I love the phrase identically zero, I recall it from when I took calculus, and will not pretend to be able to explain exactly what it means.
Applying the boundary condition that \( g \) is continuous at \( x = 0 \), tells us that \( A + B = 0 \). Trying to apply the boundary condition at \( x = L \) fails. This means that solutions of Equation (5) do not exist if the constant is negative.

Do they exist if the constant is positive, \( \text{Constant} = +k_y^2 \)?

\[
-\frac{1}{g} \frac{d^2g}{dy^2} = k_y^2
\]  

(8)

has a solution

\[
g(y) = A \sin(k_y y) + B \cos(k_y y)
\]  

(9)

At \( x = 0 \) we get \( B = 0 \), and at \( x = L \) we get a solution providing that

\[
k_y = \frac{n_y \pi}{L} \quad \text{for } n_y = 1, 2, \cdots
\]  

(10)

Now we must solve for \( f(x) \). We had

\[
\frac{1}{f} \frac{d^2f}{dx^2} + \left( \frac{2mE}{\hbar^2} \right) = \text{Constant} = k_y^2
\]  

(11)

or

\[
\frac{1}{f} \frac{d^2f}{dx^2} = \left( \frac{2mE}{\hbar^2} \right) - k_y^2
\]  

(12)

For this have a solution that can have boundary conditions on \( x \) applied successfully, the constant on the right hand side must be positive,

\[
\left( \frac{2mE}{\hbar^2} \right) - k_y^2 = k_x^2
\]  

(13)

The general solution is

\[
f(x) = C \sin(k_x x) + D \cos(k_x x)
\]  

(14)

and when the boundary conditions are applied, \( D = 0 \) and

\[
k_x = \frac{n_x \pi}{L} \quad \text{for } n_x = 1, 2, \cdots
\]  

(15)

In summary, the acceptable solution, using the definitions in Equations (10) and (15) is

\[
\psi = AC \sin(k_x x) \sin(k_y y) \quad \text{inside}
\]

\[
= 0 \quad \text{outside}
\]  

(16)

with

\[
E = \frac{\hbar^2 \pi^2}{2m} \left( n_x^2 + n_y^2 \right) = \left( n_x^2 + n_y^2 \right) E_0
\]  

(17)