

Numerical Solver of 2D Infinite Well

This script is a numerical Solver for the 2D infinite well scenario utilising finite differences of the second order derivative.

Preparing Values

m is mass, where here it is set to that of the electron rest mass in $\text{eV} \cdot \text{s}^2 \cdot \text{m}^{-2}$.

A is the width of the infinite well in m^2 .

a is the width of the segments of the infinite well for the finite differences approximation, in the same units.

```
In[2]:= m = 0.511 * 10^6 / (9 * 10^16);  
Ax = 0.53 * 10^-10;  
Ay = 0.73 * 10^-10;
```

n_x is the number of points segmenting the domain of the infinite well in the x direction, and n_y in the y direction.

ie. $n = \text{sidelength} - 2$

```
In[5]:= nx = 4;  
ny = 10;
```

```
In[7]:= ax = Ax / (nx + 1);  
ay = Ay / (ny + 1);
```

$node$ is the n th harmonic to be displayed by the graphing solution below.

```
In[9]:= node = 5;
```

Preparing Eigensystem

```
In[10]:= ij = Flatten[Table[{i, j}, {j, ny}, {i, nx}], 1];
```

```
In[11]:= getMatrixElement[k1_, k2_, nx_, ny_] :=  
If[k1 == k2, 4,  
If[k1 == k2 - 1 || k1 == k2 + 1 || k1 == k2 + nx || k1 == k2 - nx, -1, 0]]
```

Here we construct the matrix resulting from applying the finite differences approximation to the TISE.

```
In[12]:= finiteDifferencesMatrix = Table[  
Table [  
getMatrixElement[j, i, nx, ny]  
, {j, nx * ny}]  
, {i, nx * ny}];
```

Solving Eigenproblem and Plotting Results

Solve the eigenproblem and obtain the resulting eigensystem.

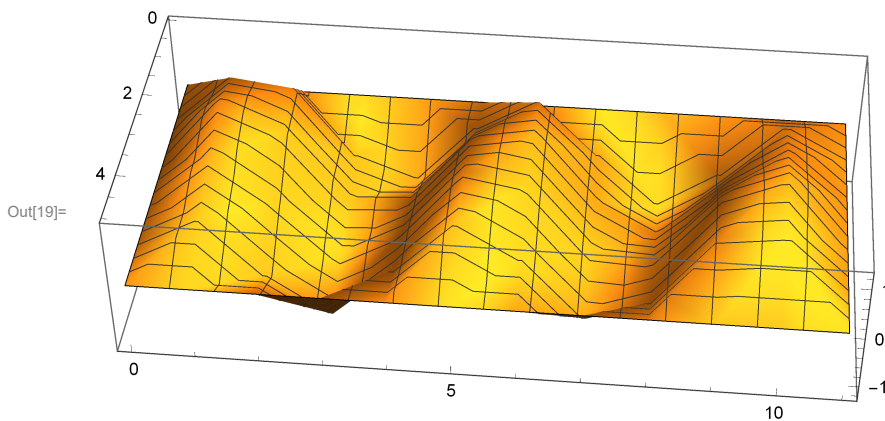
```
In[13]:= eigensystem = Eigensystem[finiteDifferencesMatrix];
```

This shows the first harmonic of the wave function for a particle in the constructed infinite well, and its respective energy.

```
In[14]:= plot = Table[Join[ij[[k]], {eigensystem[[2, -node, k]]}], {k, nx * ny}];
For[x = 0, x < (nx + 2), x++, AppendTo[plot, {x, 0, 0}]];
For[x = 0, x < (nx + 2), x++, AppendTo[plot, {x, ny + 1, 0}]];
For[y = 1, y < (ny + 1), y++, AppendTo[plot, {0, y, 0}]];
For[y = 1, y < (ny + 1), y++, AppendTo[plot, {nx + 1, y, 0}]];
```

Plot results!

```
In[19]:= ListPlot3D[plot, BoxRatios -> Automatic]
```



Plot of the square of the wavefunction:

```

In[20]:= plot2 = Table[Join[ij[[k]], {eigensystem[[2, -node, k]]^2}], {k, nx * ny}];
For[x = 0, x < (nx + 2), x++, AppendTo[plot2, {x, 0, 0}]];
For[x = 0, x < (nx + 2), x++, AppendTo[plot2, {x, ny + 1, 0}]];
For[y = 1, y < (ny + 1), y++, AppendTo[plot2, {0, y, 0}]];
For[y = 1, y < (ny + 1), y++, AppendTo[plot2, {nx + 1, y, 0}]];

ListPlot3D[plot2, BoxRatios -> Automatic]

```

