

Numerical Solver of 1D Infinite Well

This script is a numerical Solver for the 1D 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.

```
m = 0.511 * 10^6 / (9 * 10^16);
```

```
A = 0.53 * 10^-10;
```

```
a = A / 101;
```

n is the number of steps segmenting the domain of the infinite well.

```
n = 100;
```

This function determines what the matrix element's value should be at the given coordinates.

Preparing Eigensystem

```
getMatrixElement[x_, y_] :=  
  If[x == y, 2,  
    If[x == y - 1, -1,  
      If[x == y + 1, -1, 0]]];
```

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

```
finiteDifferencesMatrix = Table [  
  Table [  
    getMatrixElement[j, i]  
    , {j, 1, n}]  
  , {i, 1, n}];
```

Solving Eigenproblem and Plotting Results

Solve the eigenproblem and obtain the resulting eigensystem.

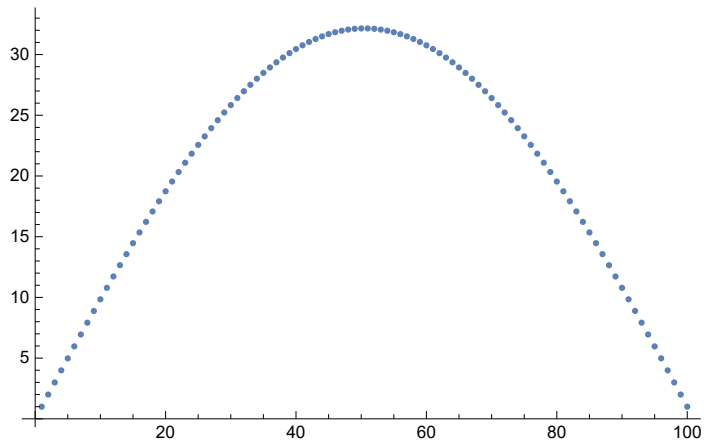
```
eigensystem = Eigensystem[finiteDifferencesMatrix];
```

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

```
(N[eigensystem[[1, -1]]] * ((6.582 * 10^-16)^2)) / (2 * m * (a^2)))
```

134.036

```
ListPlot[eigensystem[[2, -1]]]
```

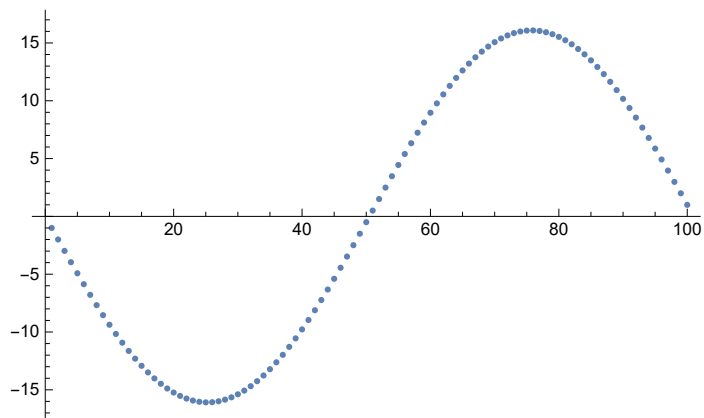


This shows the second harmonic of the wave function for a particle in the constructed infinite well, and its respective energy.

```
(N[eigensystem[[1, -2]]] * ((6.582 * 10^-16)^2)) / (2 * m * (a^2)))
```

536.013

```
ListPlot[eigensystem[[2, -2]]]
```

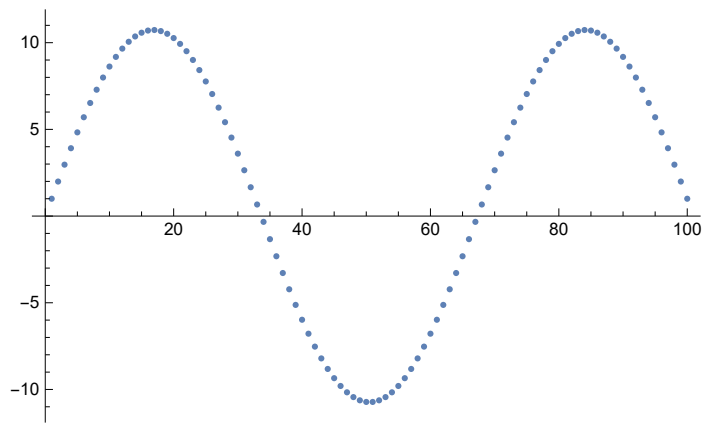


This shows the third harmonic of the wave function for a particle in the constructed infinite well, and its respective energy.

```
(N[eigensystem[[1, -3]]] * ((6.582 * 10^-16)^2)) / (2 * m * (a^2)))
```

1205.54

```
ListPlot[eigensystem[[2, -3]]]
```



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

```
((N[eigensystem[[1, -4]]] * ((6.582 * 10^-16)^2)) / (2 * m * (a^2)))
```

```
2141.98
```

```
ListPlot[eigensystem[[2, -4]]]
```

