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 $\mathrm{eV} \cdot s^2 \cdot m^{-2}$.
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;
```

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.

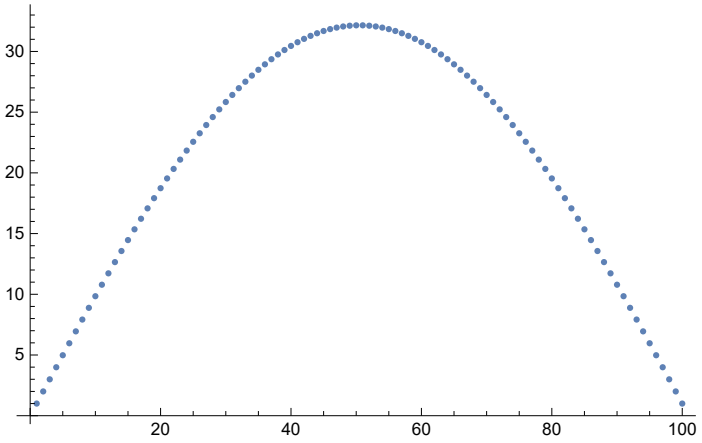
```
eigensystem = Eigensystem[finiteDifferencesMatrix];
```

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]]]
```

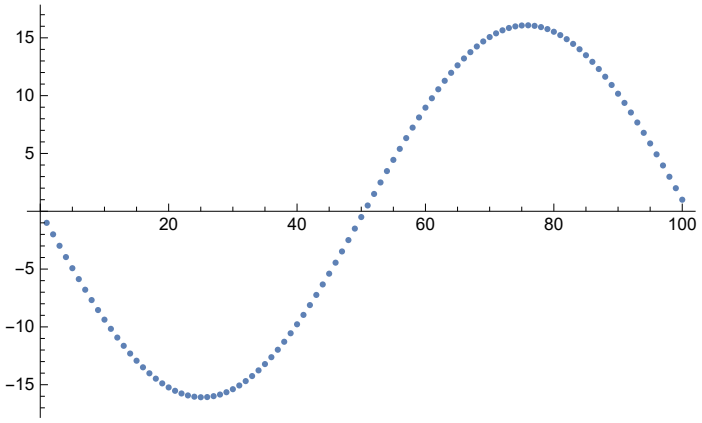


This shows the second harmonic of the wave function for a particle in the constructed infinite well, and its respective energy.

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

```
536.013
```

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

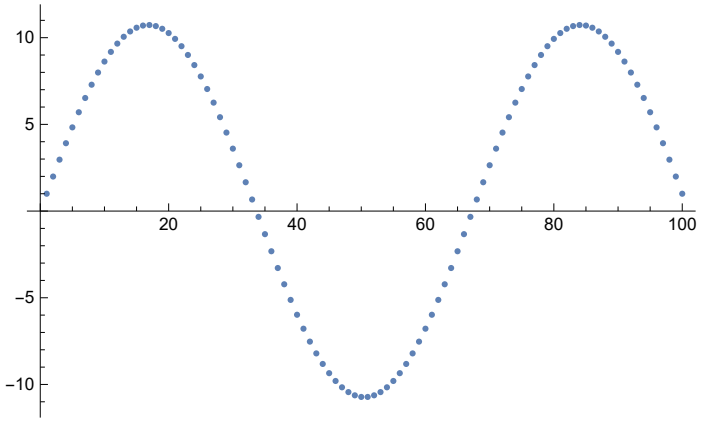


This shows the third harmonic of the wave function for a particle in the constructed infinite well, and its respective energy.

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

```
1205.54
```

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

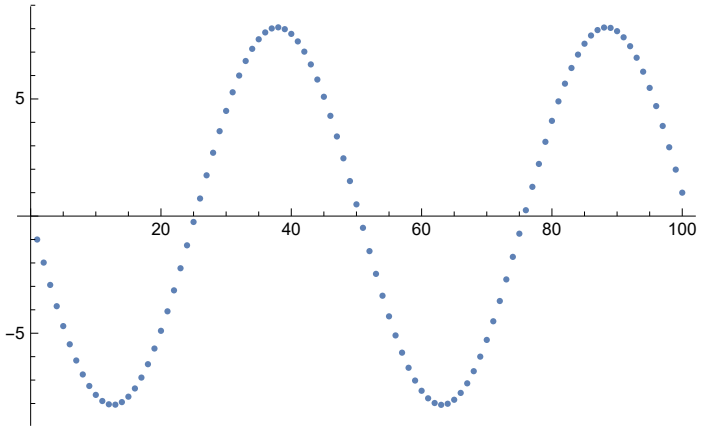


This shows the fourth harmonic of the wave function for a particle in the constructed infinite well, and its respective energy.

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

```
2141.98
```

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



Exploring Progression of Error

Here we plot the actual eigenvalues (orange) against the eigenvalues obtained via the approximation (blue) to show how accuracy is lost towards the halfway-eigenvalue after which the approximation begins to deviate from the actual value rapidly, converging on

```
ListPlot[{Reverse[Eigenvalues[finiteDifferencesMatrix]],
  Flatten[Table[a^2 * x^2 * Pi^2/A^2, {x, 100}]]}, PlotRange → {0, 4}]
```