

Python code and analysis

```
1 import numpy as np
2 import matplotlib.pyplot as plt
3
4 a = 3.0          # the half width of the well in angstroms
5 m = 1.0          # mass of electron in 1 me units
6 V0 = 10.0        # height/depth of well in eV
7 hbar = 1.0       # hbar
8 delta = np.sqrt(2.0*m*V0*(a**2.0)/(hbar**2.0)) # Defined in the hand written solution
9 eta = np.arange(0.001,2*np.pi,0.01) # Defined in the hand written solution
10
11 def f(f,eta):
12     """
13     This is the lhs in the transcendental equations.
14     """
15     return np.sqrt(((delta/eta)**2.0)-1.0)
16
17 def f1(eta):
18     """
19     The equation whose zeros are to be found to obtain the even solution.
20     """
21     return f(eta) - np.tan(eta)
22
23 def f2(eta):
24     """
25     The equation whose zeros are to be found to obtain the odd solution.
26     """
27     return f(eta) + (1.0/np.tan(eta))
28
29 def firstDerivative_O4(function ,x0,stepsize):
30     """
31     Returns first derivative of the function "function" at the point x0 by considering points , one and two
32     steps on either side of x0.
33     The Accuracy is of order (stepsize)^4.
34     """
35     return (function(x0 - 2.0*stepsize) - 8.0*function(x0 - stepsize) + 8.0*function(x0 + stepsize) -
36             function(x0 + 2.0*stepsize))/(12.0*stepsize)
37
38 def Newton_Raphson(f,x0,stepsize):
39     """
40     Returns the zero of f. x0 is the guess. stepsize will be used for determining the first derivative of
41     f.
42     """
43     fprime = firstDerivative_O4(f,x0,stepsize)
44     x1 = x0 - (f(x0)/fprime)
45     while((x0 - x1) >= stepsize**(8.0)):
46         x0 = x1
47         fprime = firstDerivative_O4(f,x0,stepsize)
48         x1 = x0 - f(x0)/fprime
49     return x1
50
51 def get_energy(eta):
52     """
53     Gets energy value for given eta value.
54     """
55     return (eta**2.0)*(hbar**2.0)/(2.0*m*(a**2.0))
56
57 ##### Main portion begins #####
58
59 even_guess = np.pi/4.0 # Guess for even solution
60 odd_guess = 0.999*np.pi # Guess for odd solution
61 even_sol = Newton_Raphson(f1 ,even_guess ,10**(-3)) # Obtaining the solution using the Newton Raphson method
62 odd_sol = Newton_Raphson(f2 ,odd_guess ,10**(-3)) # Obtaining the solution using the Newton Raphson method
63
64 #### Printing the solutions
65 print("eta for even sol : {etev:0.6f}".format(etev=even_sol))
66 print("eta for odd sol : {etod:0.6f}".format(etod=odd_sol))
67 print("Energy for even state is : {e2:0.6f}".format(e2=get_energy(even_sol)))
68 print("Energy for odd state is : {e1:0.6f}".format(e1=get_energy(odd_sol)))
```

The outputs are shown below :

Even solution (η)	Odd solution (η)	Even energy (eV)	Odd energy (eV)
1.460	2.922	0.118	0.474

C++ code and analysis

```

1 #include <iostream>
2 #include <math.h>
3 using namespace std;
4
5 double lhs(double delta, double eta){
6     return sqrt(pow((delta/eta),2.0)-1.0);
7 }
8 double f1(double delta, double eta){
9     return lhs(delta, eta) - tan(eta);
10 }
11 double f2(double delta, double eta){
12     return lhs(delta, eta) + 1.0/tan(eta);
13 }
14 double df1(double delta, double x0, double stepsize){
15     return (f1(delta, x0 - 2*stepsize) - 8*f1(delta, x0 - stepsize) + 8*f1(delta, x0 + stepsize) - f1(
delta, x0 + 2*stepsize))/(12*stepsize) ;
16 }
17 double df2(double delta, double x0, double stepsize){
18     return (f2(delta, x0 - 2*stepsize) - 8*f2(delta, x0 - stepsize) + 8*f2(delta, x0 +
stepsize) - f2(delta, x0 + 2*stepsize))/(12*stepsize) ;
19 }
20 double NewtonRaphsonf1(double delta, double x0, double stepsize){
21     double der = df1(delta, x0, stepsize);
22     double x1 = x0 - (f1(delta, x0)/der);
23     while ((x0 - x1) >= pow(stepsize, 8.0)){
24         x0 = x1;
25         der = df1(delta, x0, stepsize);
26         x1 = x0 - (f1(delta, x0)/der);
27     }
28     return x1;
29 }
30 double NewtonRaphsonf2(double delta, double x0, double stepsize){
31     double der = df2(delta, x0, stepsize);
32     double x1 = x0 - (f2(delta, x0)/der);
33     while ((x0 - x1) >= pow(stepsize, 8.0)){
34         x0 = x1;
35         der = df2(delta, x0, stepsize);
36         x1 = x0 - (f2(delta, x0)/der);
37     }
38     return x1;
39 }
40 int main(){
41     const double PI = 3.141592653589793238463;
42
43     double a = 3.0;           // the half width of the well in angstroms
44     double m = 1.0;           // mass of electron in 1 me units
45     double V0 = 10.0;         // height/depth of well in eV
46     double hbar = 1.0;        // hbar
47     double delta = sqrt(2.0*m*V0*pow(a,2.0)/pow(hbar,2.0));
48
49     double even_guess = PI/4.0 ; // Guess for even solution
50     double odd_guess = 0.999*PI ; // Guess for odd solution
51     double even_sol = NewtonRaphsonf1(delta, even_guess, pow(10, -3.0)) ; // Obtaining the solution
using the Newton Raphson method
52     double odd_sol = NewtonRaphsonf2(delta, odd_guess, pow(10, -3.0)) ; // Obtaining the solution using
the Newton Raphson method
53
54     cout << "eta for even sol : " << even_sol << endl;
55     cout << "eta for odd sol : " << odd_sol << endl;
56
57     return 0;
58 }
59

```

The outputs are shown below (values for energy remain the same):

Even solution (η)	Odd solution (η)
1.460	2.922

Plotting the solution and the wavefunctions

