

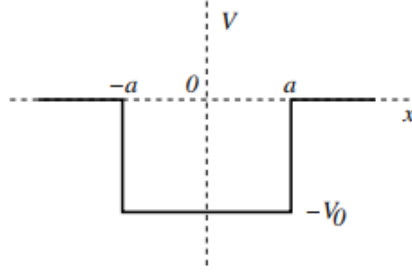
Computational Activity 5
The Energy Levels of the Finite Square Well

Bruce Mvubele - MVBBRU001

14 October 2019

1 Introduction

We will consider an electron in a 1 dimensional finite square with a depth of $-V_0 = -40\text{eV}$ and a width $2a = 0.1\text{nm}$.



The potential for the particle in a box

We want to solve the Schrodinger equation given by:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi_0(x) + V(x)\phi_0(x) = E_0\phi_0(x)$$

for the ground state energy $E_0 = -\epsilon$ and the wave function $\phi_0(x)$.

The mass of the system is $mc^2 = 0.511 \text{ MeV}$.

A useful value is $\hbar c = 197.3 \text{ eV nm}$

The equation to be solved for the 1-d particle in the well is

$$l \tan(la) = k$$

with $l = \sqrt{2m(V_0 - \epsilon)/\hbar^2}$ and $k = \sqrt{2m\epsilon/\hbar^2}$.

The equation can be solved numerically in the form

$$F(\epsilon) = l \tan(la) - k = 0$$

in order to find the bound state energy $E_0 = -\epsilon$.

I shall demonstrate two methods to do this in python namely the Bisection method and the Secant Method.

2 Theory

2.1 Bisection Method

The bisection method is a root finding method that applies to any continuous function. It requires two values of the independent variable which result in two function values of opposite signs which then implies a root in the sub-interval

defined by the two initial values. The bisection method claims that the root is, with some tolerance, at the midpoint of two numbers within the sub-interval .

2.2 Secant Method

For the secant method we need two initial values close to the root we then use the update linear function given by

$$x = x_1 - f(x_1) \frac{x_1 - x_0}{f(x_1) - f(x_0)}$$

to find the roots

3 Results

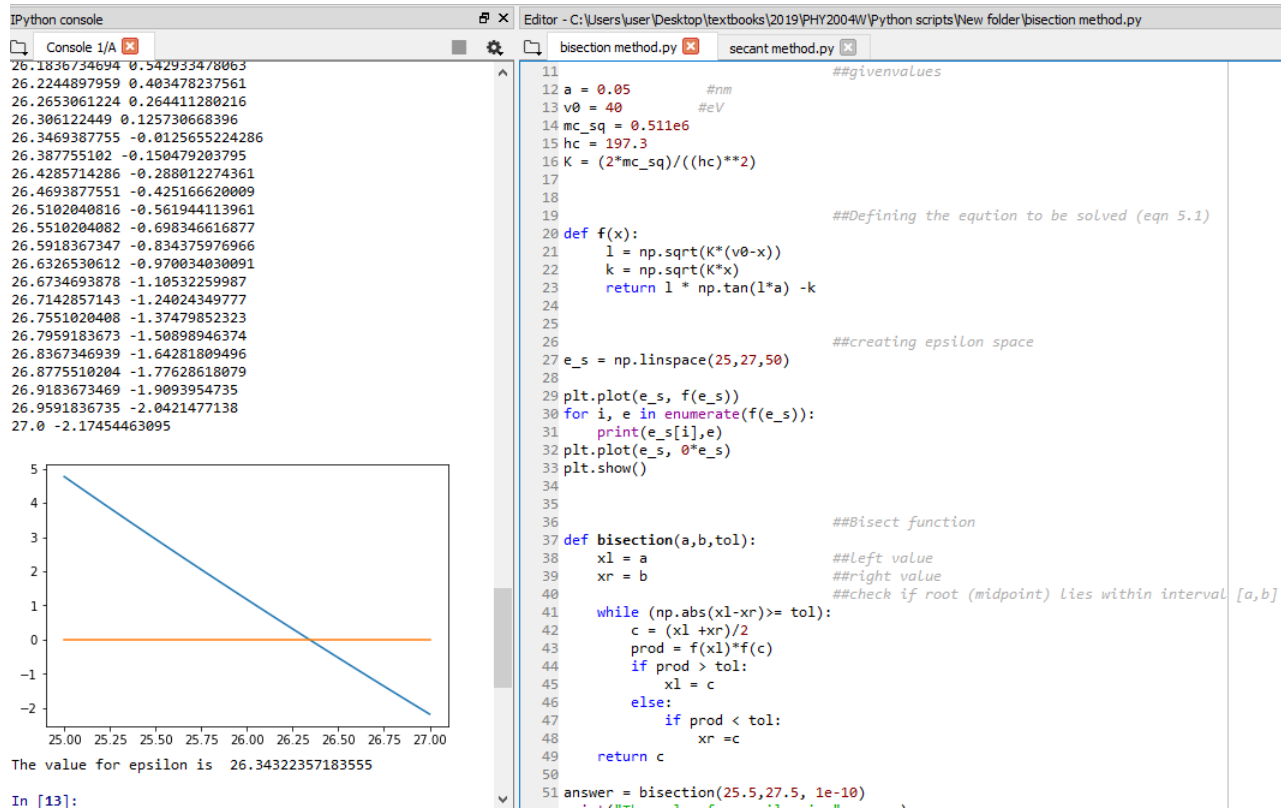


Figure 1: Bisection Method Code

```

Python console
Console 1/A
In [11]: runfile('C:/Users/user/Desktop/textbooks/2019/PHY2004W/Python scripts/New folder/secant method.py',
             wdir='C:/Users/user/Desktop/textbooks/2019/PHY2004W/Python scripts/New folder')
The value for epsilon is 26.3432255481 after 4 iterations
In [12]:

Editor - C:/Users/user/Desktop/textbooks/2019/PHY2004W/Python scripts/New folder/secant method.py
bisection method.py secant method.py
2 """
3 Created on Sat Oct 12 14:38:38 2019
4
5 @author: user
6 """
7 import numpy as np
8 import matplotlib.pyplot as plt
9 from scipy.misc import derivative
10 from scipy import optimize
11
12 def secant(fn,x1,x2,tol,maxiter):    ##Defining secant method form
13     for iteration in range (maxiter):
14         xnew = x2 -(x2-x1)/(fn(x2) - fn(x1)) * fn(x2)
15         if abs(xnew - x2) < tol : break
16     else:
17         x1 = x2
18         x2 = xnew
19
20     else:
21         print("max iter reached")
22     return xnew, iteration
23
24                                     ##Given value
25 a = 0.05          #nm
26 v0 = 40          #eV
27 mc_sq = 0.511e6
28 hc = 197.3
29 K = (2*mc_sq)/((hc)**2)
30
31 def fn(x):
32     l = np.sqrt(K*(v0-x))
33     k = np.sqrt(K*x)
34     return 1 * np.tan(l*a) -k
35
36                                     ## Left and right end points for the root search
37 x1 = 25
38 x2 = 28
39 maxiter = 100
40 r,n = secant(fn,x1,x2,0.000001,100)
41 print("The value for epsilon is", r, "after", n ,"iterations")

```

Figure 2: The Secant Method

Now we look at the strength of the well required to have the same binding energy as the hydrogen atom, $E_0 = -13.6\text{eV}$. To solve this we look at the equation

$$k = l \tan(la)$$

we define $z = la$ and $z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$

$$k^2 + l^2 = \frac{2mV_0}{\hbar^2}$$

which according the prescribed text (Griffith's) can be expressed as

$$ka = \sqrt{z_0^2 + z^2}$$

squaring both sides, substituting for k, z and z_0 and multiplying through by $(\frac{c}{\hbar})^2$ gives

$$\frac{2mc^2 E_0 a^2}{(\hbar c)^2} = \frac{2mc^2 a^2}{(\hbar c)^2} - \frac{2mc^2 (E_0 + V_0) a^2}{(\hbar c)^2}$$

substituting known values then gives

$$-8.92 \times 10^{-19} = 6.56 \times 10^{-20} - 6.56 \times 10^{-20}(E_0 + V_0)$$

which then gives the answer

$$V_0 = 2.06eV$$

4 Discussion and Analysis

From the Bisection Method we arrive at the answer $\epsilon = 26.342235$ which then implies that the energy for the bound state is $E_0 = -26.342235eV$. And from the secant method the epsilon value obtained is $\epsilon = 26.342255$ and so the energy is $E_0 = -26.342255$. From the two results we can see that they agree with each other to four decimal places which is in-bounds for a good approximation. Now since there is a single root for the equation

$$F(\epsilon) = l \tan(la) - k = 0$$

this implies a single state of bound energy and therefore can be no other bound states.

5 Conclusion

The the bisection method yields the energy levels of an electron corresponding to the ground state in a finite potential well of depth -40eV to be $E_0 = -26.342235eV$, the secant method yields the energy to be $E_0 = -26.342255$. The approximations are agreeable with each other to four decimal places. The existence of a single Energy eigenvalue value suggests the existence of a single bound state.

It was also shown that in order for the potential well to have a binding energy equal to the hydrogen atom it has to have the strength of $V_0 = 2.06eV$