Computational Activity 5
The Energy Levels of the Finite Square Well

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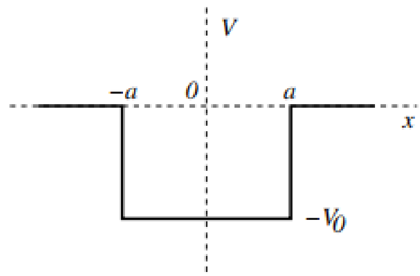
1 Introduction

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



The potential for the particle in a box

W 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 MeV.

A useful value is $\hbar c = 197.3eVnm$

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

$$ltan(la) = k$$

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

The equation can be solved numerica in the form

$$F(\epsilon) = ltan(la) - k = 0$$

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

I shall demonstrate two methods to do this in python namely the 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

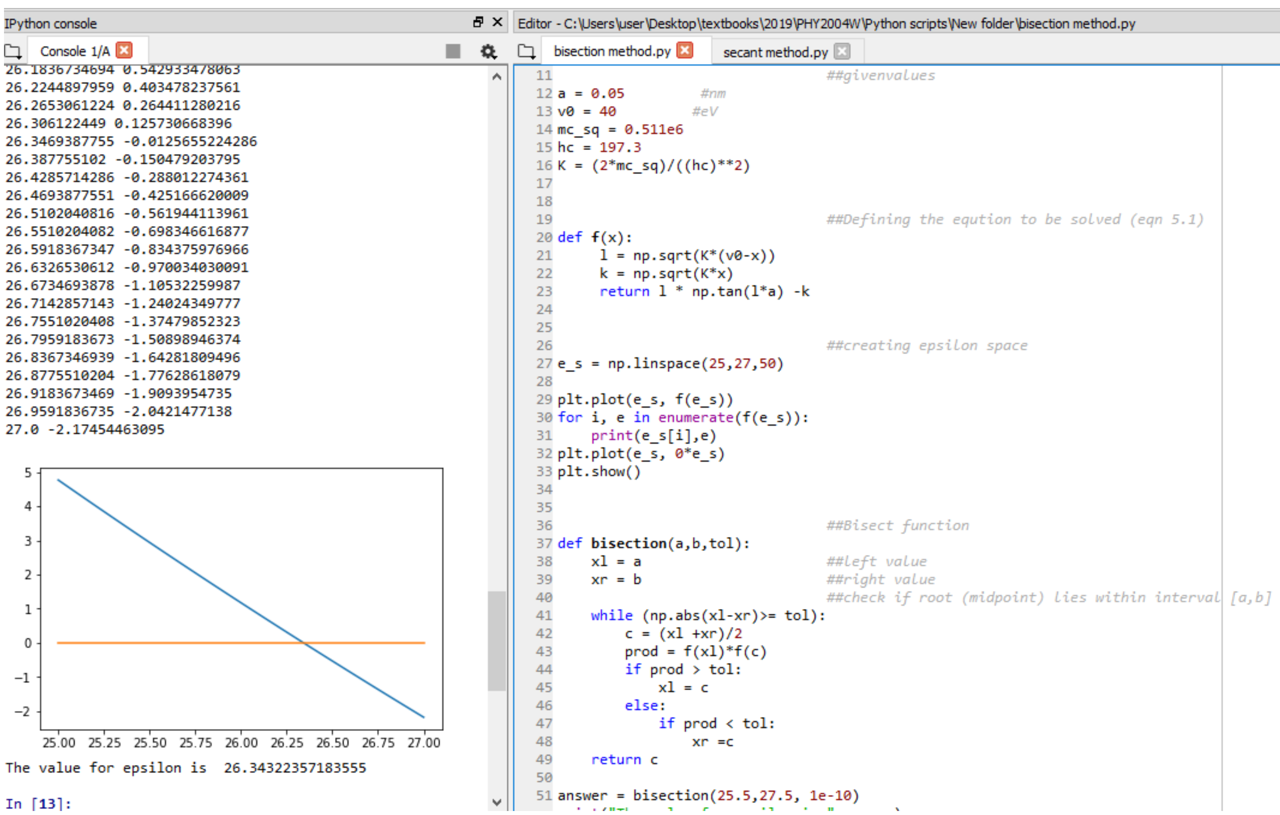


Figure 1: Bisection Method Code

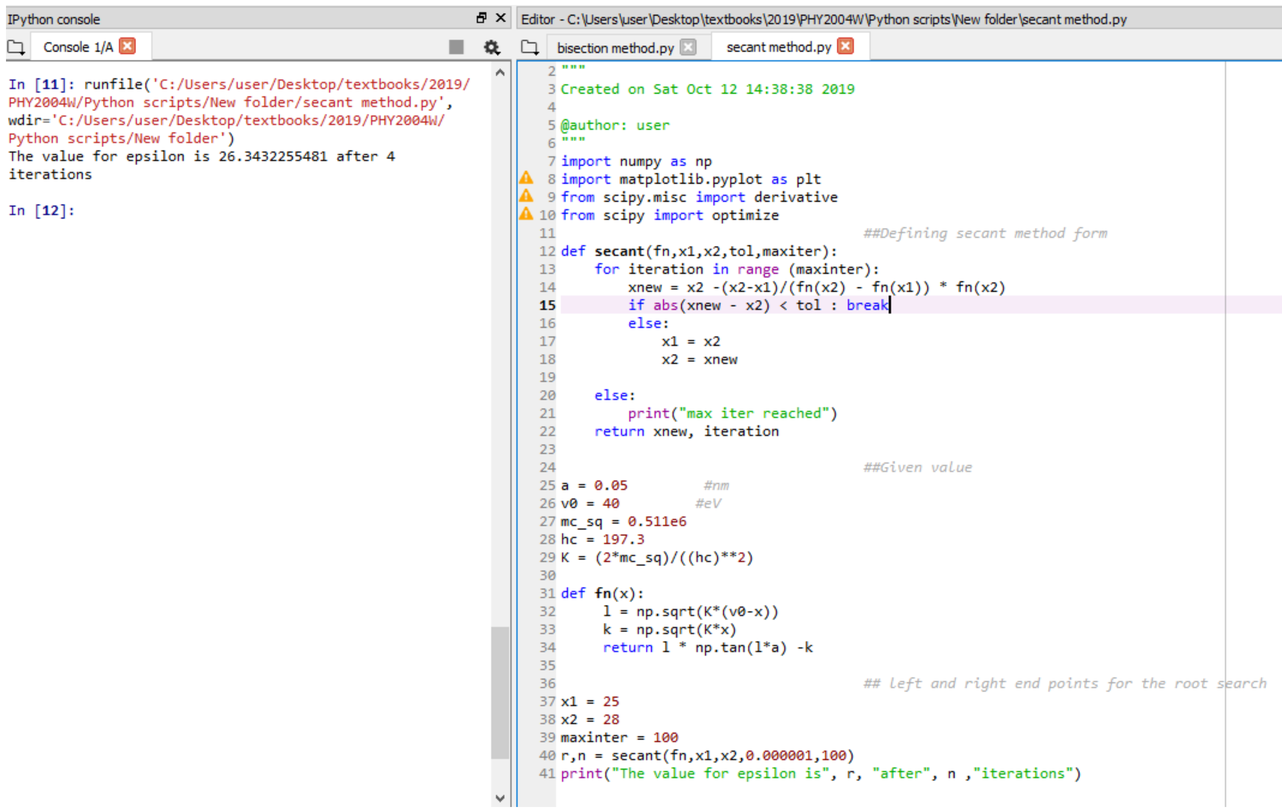


Figure 2: The Secant Method

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

$$k = ltan(la)$$

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 $(\frac{c}{c})^2$ gives

$$\frac{2mc^2E_0a^2}{(\hbar c)^2} = \frac{2mc^2a^2}{(\hbar c)^2} - \frac{2mc^2(E_0+V_0)a^2}{(\hbar c)^2}$$

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 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

$$F(\epsilon) = ltan(la) - k = 0$$

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 $V_0 = 2.06eV$