The *Schrödinger* equation in the motion of electrons

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Abstract

In mathematics, there are some differential equations whose analytical solution cannot be obtained by means of elementary methods. For this, it is necessary to resort to numerical methods that provide us with an adequate approximation of the solutions.
The *Schrödinger*'s equation is an example of this type of equations, since sometimes it is not possible to obtain an analytical solution, so we resort to numerical methods. In this case, we study the half-step method to approximate the solution of the wave equation in the case of simple harmonics.

1 Introduction

The half-increment method consists of making an approximation of the derivative of a function, in order to obtain the numerical values ââof said function and to be able to understand a little the behavior of the function that is being studied.
In the case of the Schrodinger equation, this method gives us the possibility of knowing the behavior of the wave function given some initial established parameters. In addition to them, graphing the wave function allows us to know the proper autofunctions that give us the energy values ââfor which the solutions are maintained.[1]

2 Methods and development

2.1 Finite increment and half increment method

The starting point to understand the numerical method that we will study is the formal definition of a derivative of the first order.

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{y(x+\Delta x) - y(x)}{\Delta x}$$

If instead of taking $\Delta \to 0$ we take finite increments we obtain

$$\frac{dy}{dx} \approx \frac{y(x+\Delta x) - y(x)}{\Delta x}$$

This is

$$y(x+\Delta x) \approx y(x) + \frac{dy}{dx}\Delta x \tag{1}$$

This gives us the value of the function at the point $x + \Delta x$ when we have an expression for the derivative $\frac{dy}{dx}$. In order to give greater clarity, we will do it for two points x_1 and $x_2 = x_1 + \Delta x$, where $\Delta x = x_2 - x_1$

$$y(x_2) \approx y(x_1) + \frac{dy}{dx_1}\Delta x \tag{2}$$

An alternate notation, which results useful when working on several points

$$\Delta x = x_{n+1} - x_n$$

This is

$$x_{n+1} = x_n + \Delta x$$

So (4) is

$$y_{n+1} \approx y_n + \frac{dy}{dx}\Delta x$$

The above is based on the definition of a first-order derivative known as the definition of **Full Increment**. However, there is another definition of a first-order derivative that converges more rapidly.

2.2 Medium-increment

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{y\left(x_1 + \frac{\Delta x}{2}\right) - y\left(x_1 - \frac{\Delta x}{2}\right)}{\Delta x}$$

Taking finite increments we obtain

$$\frac{dy}{dx} \approx \frac{y\left(x_1 + \frac{\Delta x}{2}\right) - y\left(x_1 - \frac{\Delta x}{2}\right)}{\Delta x}$$

With the same reasoning of the finite increment, we obtain the following equations

$$\frac{dy}{dx_{n+(1/2)}} \approx \frac{dy}{dx_{n-1/2}} + C\Delta x \tag{3}$$

Where C corresponds to a function, the assignment of this value depends on the differential equation to be solved

$$y_{n+1} \approx y_n + \frac{dy}{dx_{n+(1/2)}}$$

2.2.1 Example

Consider the second-order differential equation

$$\frac{d^2y}{dt^2} = g \tag{4}$$

This is

$$\frac{d}{dt}\frac{dy}{dt} = g$$

Using finite increments instead of infinitesimals can be considered equivalent to an approximate form

$$\frac{d}{dt}\frac{dy}{dt} \approx \frac{\frac{dy}{dt_{n+1}} - \frac{dy}{dt_n}}{\Delta t}$$

Where n corresponds to a positive integer, with which (4) is of the form

$$\frac{\frac{dy}{dt_{n+1}} - \frac{dy}{dt_n}}{\Delta t} \approx g$$

This is

$$\frac{dy}{dt_{n+1}} - \frac{dy}{dt_n} \approx g\Delta t \tag{5}$$

Secondly

$$\frac{dy}{dt_n} \approx \frac{y_{n+1} - y_n}{\Delta t}$$

So

$$y_{n+1} \approx y_n + \frac{dy}{dt_n}\Delta t \tag{6}$$

Thus, (5) and (6) are the equations that will constitute our iterative method, which we start with an initial value called seed, for which we use n = 0 obtaining a new n + 1 in each step, using the value from n above.

- After selecting Δt reasonably small, starting from initial values (for example $y_0 = 1$, $\frac{dy}{dt_0} = 0$) we use

  $$y_1 \approx y_0 + \frac{dy}{dt_0}\Delta t$$

  Where $t_{n+1} = t_n + \Delta t$

- Then $\frac{dy}{dt_0}$ is used to calculate $\frac{dy}{dt_1}$, like this

  $$\frac{dy}{dt_1} \approx \frac{dy}{dt_0} + g\Delta t$$

- We calculate y_2

  $$y_2 \approx y_1 + \frac{dy}{dt_1}\Delta t$$

- $$\frac{dy}{dt_2} \approx \frac{dy}{dt_1} + g\Delta t$$

This process must be carried out as many times as necessary to generate enough points so that they can be located on a graph. Note that in this case g corresponds to a fixed quantity, however, in the case in which this value is a function of the independent variable, it will be necessary to evaluate said quantity at each new point of the independent variable that is used when evaluating y_k y $\frac{dy}{dt_k}$ with $k = 0, 1, 2, ...$

These steps to follow are for the definition of full increment, modifying it to half increment we obtain

1. After selecting the size of the increment (also called step size) we obtain

   $$\frac{dy}{dt_{1/2}} \approx \frac{dy}{dt_0} + g\frac{\Delta t}{2}$$

   Where $t_{n+1} = t_n + \Delta t$

2. We obtain the value y_1

   $$y_1 \approx y_0 + \frac{dy}{dt_{1/2}}\Delta t$$

3. $$\frac{dy}{dt_{3/2}} \approx \frac{dy}{dt_{1/2}} + g\frac{\Delta t}{2}$$

4. $$y_2 \approx y_1 + \frac{dy}{dt_{3/2}}\Delta t$$

2.3 Program

The previously described process is described in the following code for the solution of the schrodinger equation of a simple harmonic (see results section)

```
import numpy as np
import matplotlib.pyplot as plt
N=100
phi=np.zeros(N)
u=np.zeros(N)
derivada=np.zeros(N)
delta=0.05
phi[0]=1
u[0]=0
derivada[0]=0
e=1
c1=((u[0]**2)-e)*phi[0]
derivada[1]=derivada[0]+(c1*(delta/2))

for i in range(1,N-1):
    u[i]=u[i-1]+delta
    phi[i]=phi[i-1]+(derivada[i]*delta)
    c=((u[i]**2)-e)*phi[i]
    derivada[i+1]=derivada[i]+c*(delta)
phin=np.delete(phi,N-1)
un=np.delete(u,N-1)
plt.plot(un,phin)
```

Figure 1: medium increment method program

3 Results

Next we will use the method described in subsection 2.2 to solve the simple harmonic wave equation, in which the potential satisfies that

$$V(x) = \frac{kx^2}{2}$$

Where k corresponds to the constant of the simple harmonic motion and $\hbar$ corresponds to Dirac's constant or reduced Planck's constant
This potential corresponds to that of a mass connected to a spring. Then the *Schrödinger* equation is of the form

$$\frac{d^2\varphi(x)}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2}kx^2 - E\right)\varphi(x)$$

Before solving this equation by the half-increment method, we will use the following relationship that connects the spring constant k with the oscillation frequency

$$f = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

Then

$$k = 4\pi^2 m f^2$$

With this substitution, the wave equation is:

$$\frac{d^2\varphi(x)}{dx^2} = \frac{2m}{\hbar^2}(2\pi m f^2 x^2 - E)\varphi(x)$$

$$= \left(\frac{4\pi^2 m^2 f^2 x^2}{\hbar^2} - \frac{2mE}{\hbar^2} \right) \varphi(x)$$

So

$$\frac{d^2\varphi(x)}{dx^2} = \left(\left(\frac{2\pi m f}{\hbar} \right)^2 x^2 - \frac{2mE}{\hbar^2} \right) \varphi(x)$$

To simplify the equation do

$$\alpha = \frac{2\pi m f}{\hbar}$$

$$\beta = \frac{2mE}{\hbar^2}$$

We obtain

$$\frac{d^2\varphi(x)}{dx^2} = (\alpha^2 x^2 - \beta)\varphi(x) \tag{7}$$

Consider u a dimensionless variable of the form

$$u = \sqrt{\alpha} x$$

Then

$$\frac{d^2\varphi(x)}{dx^2} = \frac{d^2\varphi(u)}{d(u/\sqrt{\alpha})^2}$$

replacing in (7) we get

$$\alpha \frac{d^2\varphi(u)}{du^2} = (\alpha u^2 - \beta)\varphi$$

Dividing by α

$$\frac{d^2\varphi(u)}{du^2} = \left(u^2 - \frac{\beta}{\alpha} \right) \varphi$$

We can further simplify the equation by defining the first term within the parentheses as a constant e that turns out to be

$$e = \frac{\beta}{\alpha}$$

Because of how the Dirac constant is defined we have

$$e = \frac{\frac{2mE}{\hbar^2}}{\frac{2\pi m f}{\hbar}} = \frac{E}{\pi \hbar f}$$

$$= \frac{E}{\pi f (n/2\pi)} = \frac{2E}{hf}$$

Then the differential equation to solve numerically is

$$\frac{d^2\varphi}{du^2} = (u^2 - e)\varphi$$

Defining the right side of the equality as C

$$C = (u^2 - e)\varphi$$

The we get

$$\frac{d^2\varphi}{du^2} = C$$

Thus, we have the steps for the iterative method

- $$u_{n+1} = u_n + \Delta u$$

- $$\frac{d\varphi}{du_{1/2}} \approx \frac{d\varphi}{du_0} + C\frac{\Delta u}{2}$$

- $$\frac{d\varphi}{du_{n+(1/2)}} \approx \frac{d\varphi}{du_{n-(1/2)}} + C\Delta u$$

- $$\varphi_{n+1} \approx \varphi_n + \frac{d\varphi}{du_{n+(1/2)}}\Delta u$$

3.1 Example

Consider

$$\varphi_0 = 1$$
$$u_0 = 0$$
$$\frac{d\varphi}{du_0} = 0$$
$$\Delta u = 0.05$$
$$e = 1$$

To generate the points of the solution of the equation

- $(u_0, \varphi_0) = (0, 1)$

- $$C = (u_0^2 - e)\varphi_0 = -1$$
  $$\frac{d\varphi}{du_{1/2}} = \frac{d\varphi}{du_0} + C\Delta u = -0.025$$
  $$\varphi_1 = \varphi_0 + \frac{d\varphi}{du_{1/2}}\Delta u = 0.99875$$
  $$u_1 = u_0 + \Delta u = 0.05$$

  So $(u_1, \varphi_1) = (0.05, 0.99875)$

- $$C = (u_1^2 - e)\varphi_1 = -0.99625$$
  $$\frac{d\varphi}{du_{3/2}} = \frac{d\varphi}{du_{1/2}} + C\Delta u = -0.07482$$
  $$\varphi_2 = \varphi_1 + \frac{d\varphi}{du_{3/2}}\Delta u = 0.995$$
  $$u_2 = u_1 + \Delta u = 0.10$$

  So $(u_2, \varphi_2) = (0.10, 0.995)$

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$$C = (u_2^2 - e)\varphi_2 = -0.98505$$
$$\frac{d\varphi}{du_{5/2}} = \frac{d\varphi}{du_{3/2}} + C\Delta u = -0.12406$$
$$\varphi_3 = \varphi_2 + \frac{d\varphi}{du_{5/2}}\Delta u = 0.9888$$
$$u_3 = u_2 + \Delta u = 0.15$$

So $(u_3, \varphi_3) = (0.15, 0.9888)$

This process must be carried out repeatedly to generate the graph of the solution of the *Schrödinger* equation, for this we carry out the code described in figure 1 and obtain the following graph As can be seen in the graph, $\varphi(u)$ and $\frac{d\varphi}{du}$ tend to zero when u tends to infinity,

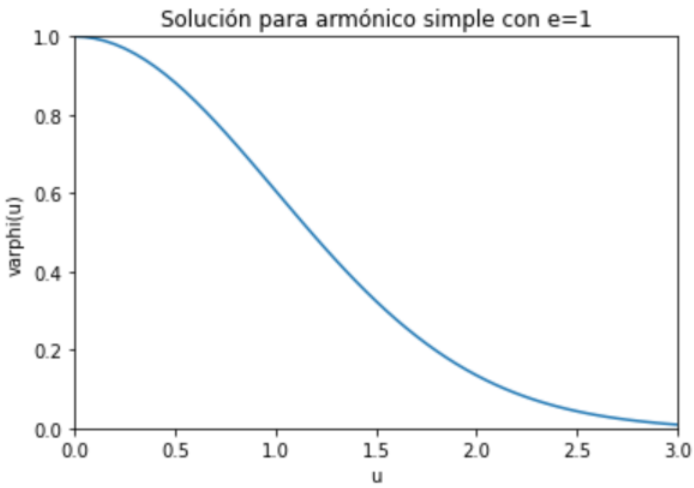

Figure 2: Numerical solution of the simple harmonic for e = 1

in this way, since the criteria of the function are met wave we have found an eigensolution of the equation. That is, e = 1 is an eigensolution for the equation of the *Schrödinger*'s equation Then,as

$$e = \frac{2E}{hf}$$

Then

$$E_1 = \frac{1}{2}hf$$

On the other hand, for e = 3 As in the previous case, we know that e = 3 corresponds to a solution of the equation. Unlike the previous case, where the initial value of the slope is zero, in this case the value must be determined by trial and error since we do not know the analytical solution of the equation.
Performing the same procedure we can verify that e = 5 and e = 7 are critical values, then, we have the following pattern

$$E = \frac{1}{2}hf, \frac{3}{2}hf, \frac{5}{2}hf, \frac{7}{2}hf, ...$$

This is

$$E = \left(n + \frac{1}{2}\right)hf$$

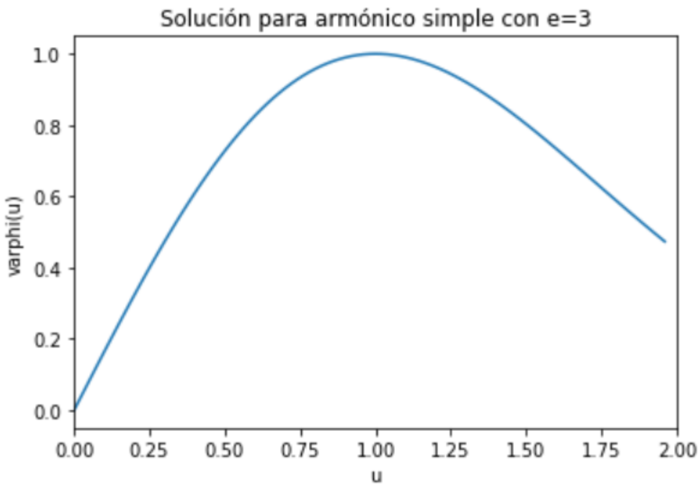

Figure 3: Numerical solution of the simple harmonic for e = 3

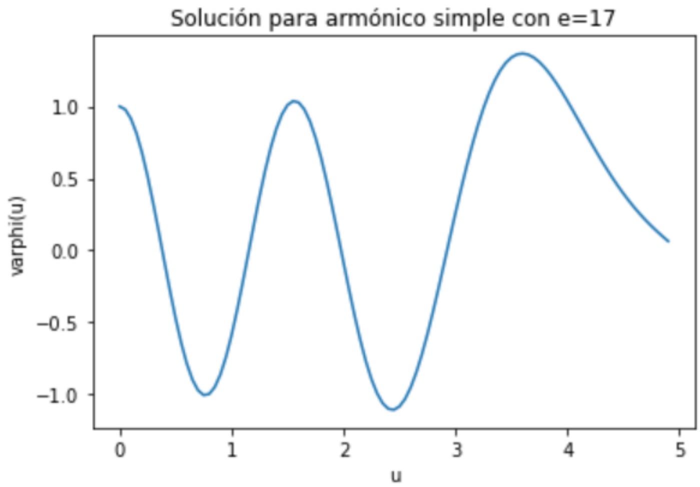

Figure 4: Numerical solution of the simple harmonic for e = 17

Taking this into account, with n = 8, e = 17 would correspond to a critical value Note that in this case, we see that the function does not tend to zero, but that the amplitude of the wave increases along u. This is due to the fact that although e = 17 is a critical value, there is a rounding error when making the approximation by means of the half-increment method, this problem could be solved using a smaller step size, which Which could require more time and computing capacity.

4 Scope

For the third advance, the objective is to carry out the solution for the potential well by means of the half-increment method.

References

[1] Martinez.A.(2009).”Solucion numerica de la ecuacion de SchrÃ¶dinger ”.Recuperado de: http://la-mecanica-cuantica.blogspot.com/2010/11/solucion-numerica-de-la-ecuacion-

de.html

[2] Augustsson,L."Numerical approaches to solving the time-dependent SchrÃ¶dinger equation with different potentials "

[3]

[4] Volkov,M."Solving the quantum scattering problem for systems of two and three charged particles"