

# The *Schrödinger* equation in the motion of electrons

Laura Alejandra Ramos .

e-mail: lramosm@edu.co

## Abstract

The *Schrödinger* equation was developed in 1925 by the Austrian physicist Erwin *Schrödinger*. This equation is of great importance in classical mechanics because it provides the main information about subatomic particles, this through the wave function, whose value describes a possible state of the electron.

In addition to this, the *Schrödinger* equation takes into account different aspects such as: the existence of an atomic nucleus, the energy levels where the electrons are distributed according to their energy, the wave-particle duality, the probability of finding the electron. The following document contains a brief study on the general steps to solve the *Schrödinger* equation and its interpretation in the world of quantum mechanics, in addition, a simple example of how this is done is presented process.

Soon we will proceed with the solution of the equation for the simplest atom: the hydrogen atom.

## 1 Introduction

The *Schrödinger* equation is of vital importance in quantum mechanics, like Newton's equations in classical mechanics. These help us to predict the behavior of subatomic particles, some of which have what is called wave-particle duality, which is that a particle (such as the electron) can behave as a wave and as a particle simultaneously. Thanks to this we obtain what is called the wave function, which will give us information about the behavior of electrons in atoms.[2] It should be noted that the square of this wave function corresponds to the density function that describes the relative probability according to which said random variable will take a certain value.

But ,how is the wave function found? For this, what is known as the *Schrödinger* equation is proposed, which has the wave function as unknown, which can be determined by establishing certain values of border. Furthermore, this wave function is subject to something called the uncertainty principle, which states that it can know the position of the particle, but not its velocity, and vice versa. [1].

## 2 Methods

To properly understand the statement of the *Schrödinger* equation, it was necessary to know the main operator of quantum mechanics called Hamiltonian [3].

On the other hand, basic knowledge was needed on the solution of ordinary differential equations and initial value problems, especially of homogeneous second-order differential equations.

In addition to this, it was necessary to learn about quantum numbers and how it relates to the physical structure of the atom, which is summarized in the following table.

N	l	m	Orbital
1	0	0	1s
2	0	0	2s
2	1	-1,0,+1	2p <sub>x</sub> ,2p <sub>y</sub> ,2p <sub>z</sub>
3	0	0	3s
3	1	-1,0,+1	3p <sub>x</sub> ,3p <sub>y</sub> ,3p <sub>z</sub>
3	2	-2,-1,0,+1,+2	3d <sub>x<sup>2</sup>-y<sup>2</sup></sub> ,3d <sub>xy</sub> ,3d <sub>z<sup>2</sup></sub> ,3d <sub>yz</sub> ,3d <sub>xy</sub>

## 3 Results

### 3.1 General concepts

The *Schrödinger* equation is defined with the following expression

$$H\varphi = ih'\frac{\partial}{\partial t}(\varphi)$$

Where

- $ih$  = constants of nature.
- $H$  = Hamiltonian.
- $\varphi$  = wave function.

The Hamiltonian changes as a function of the system.  $E$  is equal to the mechanical energy of the system

$$H = E_m = E_c + E_p$$

Kinetic energy is that associated with motion.

$$E_c = \frac{1}{2}mv^2$$

But in the case of quantum mechanics this is of the form

$$E_c = \frac{-h^2}{2m}\nabla^2$$

Where

- $h$  = Planck's constant.
- $m$  = mass of the particle.
- $\nabla^2$  = Laplacian.

Potential energy is that associated with force:

$$E_p = K\frac{q_1q_2}{r}$$

Where  $K$  corresponds to Coulomb's constant,  $q_1$  and  $q_2$  are the charges and  $r$  the radius between them.

In the Hydrogen atom, only the interaction between 1 electron and 1 proton occurs, so the Hamiltonian appears as a relatively simple expression

$$H = \frac{-\hbar^2}{2m} \nabla^2 - K \frac{q_e^2}{r}$$

*Schrödinger* equation for the Hydrogen atom.

$$\left( \frac{-\hbar^2}{2m} \nabla^2 - K \frac{q_e^2}{r} \right) \varphi = i\hbar' \frac{\partial}{\partial t} \varphi$$

In the case of having an atom with more electrons, the *Schrödinger* equation becomes more complicated, since the Hamiltonian corresponds to the repulsion between electrons, the attraction between protons and electrons, and the repulsion between electrons that is mitigated by protons. In these cases, the *Schrödinger* equation does not have an analytical solution and it is necessary to resort to numerical methods for its solution.

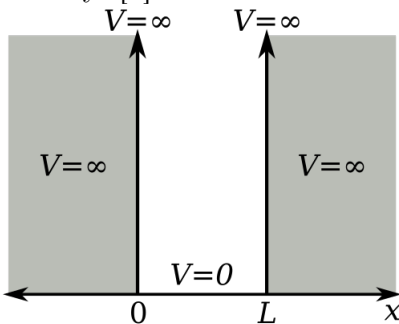
It should be noted that the solution obtained from these equations corresponds to what we call the wave function, this squared function corresponds to the probability density function describing the probability of finding the electron in a certain region of the atom.

On the other hand, certain boundary conditions must be established for the solution of the equation, these boundary values are established by means of the quantum numbers [4] that establish an atomic orbital that encloses 90 % of the probability of finding an electron in that area. This atomic orbital is established thanks to the first 3 quantum numbers  $n, l, m$

- $n$  = principal quantum number, represents the energy level,  $n = 1, 2, \dots$
- $l$  = angular momentum quantum number, set the orbit type (s, p, d, f);  $l = 0, 1, \dots, n-1$ .
- $m$  = magnetic quantum number, sets the orientation of the orbital;  $m = -l, \dots, 0, \dots, l$
- $s$  = spin quantum number  $s = \pm \frac{1}{2}$ , the latter represents the state of rotation of the electron, which can only take two values.

### 3.2 Example 1- Particle in a one-dimensional box

The particle in a box is defined as a point particle, enclosed in a box where it does not experience any type of force, that is, its potential energy is constant, although without loss of generality we can assume that it is zero. On the walls of the box the potential increases to infinity. [5]



$$V(x) = 0 \text{ for } 0 \leq x \leq L$$

$$V(x) = \infty \text{ for } x < 0 \text{ y } x > L$$

1) For this case, we consider the equation *Schrödinger* of independent of time:

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

Where

- $h$  = planck's constant.
- $m$  = mass of the particle.
- $\varphi$  = time independent wave function.
- $E$  = particle energy

2) Since the wave function vanishes out of the box, we set the following boundary conditions:

$$\varphi(0) = 0 \quad (1)$$

$$\varphi(L) = 0 \quad (2)$$

3) Solve the differential equation, using an auxiliary equation

$$\begin{aligned} \frac{-h^2}{2m}\varphi'' - E\varphi &= 0 \\ \varphi &= \frac{\pm\sqrt{0 - 4\left(\frac{-h^2}{2m}\right)(-E)}}{\frac{-2h^2}{2m}} = \frac{\pm\sqrt{\left(\frac{-2h^2E}{m}\right)}}{\frac{-h^2}{m}} = \frac{(\sqrt{2Em}h)i}{-\sqrt{mh^2}} = \frac{-(\sqrt{2Em})i}{h} \end{aligned}$$

**General solution**

$$\varphi(x) = \epsilon^0(A\sin(kx) + B\cos(kx)) \quad (3)$$

Where  $k^2 = \frac{2mE}{h^2}$  and A and B are complex numbers Considering the boundary condition and replacing in the general solution

$$0 = A\sin(0) + B\cos(0) = B$$

Luego

$$\varphi(x) = A\sin(kx) \quad (4)$$

Replacing condition (1) and (2)

$$\varphi(L) = A\sin(kL) = 0$$

This is

$$\sin(kL) = 0 \rightarrow k = \frac{n\pi}{L} \quad (5)$$

With  $n \in \mathbf{Z}^+$ . Note that this consideration does not take into account negative values of  $n$ , since these only represent a change of sign, and do not suggest new states. Likewise, in the calculation of  $E$ , it will be squared, so it is not necessary to consider its negative value.

4) Get A

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\varphi(x)|^2 dx = |A|^2 \int_0^L \sin^2(kx) dx = |A|^2 \int_0^L \frac{1 - \cos(2kx)}{2} dx \\ &= \frac{|A|^2}{2} \left( L - \frac{\sin(2kL)}{2k} \right) = \frac{|A|^2 L}{2} \end{aligned} \quad (6)$$

then

$$1 = \frac{|A|^2 L}{2}$$

then

$$|A| = \sqrt{\frac{2}{L}} \quad (7)$$

Note that the value of A is initially complex, but in this particular case, the imaginary value that meets (7) is taken, which corresponds precisely to this real value. Replacing in (3)

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \operatorname{sen} \left( \frac{n\pi x}{L} \right)$$

5) Find the eigenvalues

We know that  $kL = n\pi$  for  $n \in \mathbf{Z}^+$ , then

$$\frac{\sqrt{2mEL}}{h} = n\pi$$

Solving for E we obtain that for  $n = 1, 2, 3, \dots$

$$E = n^2 \frac{\pi^2 h^2}{2mL^2} \quad (8)$$

This establishes conditions on E for the solutions of the *Schrödinger* equation of the particle in a one-dimensional box. The possible values of E are the eigenvalues or energy levels.

### Conclusions

Self-functions and energies for the problem of the particle in a one-dimensional box

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \operatorname{sen} \left( \frac{n\pi x}{L} \right); \quad (9)$$

$$E_n = n^2 \frac{\pi^2 h^2}{2mL^2} \quad (10)$$

Where n characterizes  $\varphi_n$  and  $E_n$  is the quantum number for the system considered.

## 4 Scope

No updates of the objectives are presented for the second installment, the next step corresponds to analytically solving the *Schrödinger* equation for the Hydrogen atom.

## References

- [1] "Sobre la ecuación de *Schrödinger*"  
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- [2] SANCHÁZ: La ecuación de onda de Schrödinger. 1925  
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- [4] Significado de los números cuánticos  
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- [5] La partícula en una caja  
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