

## Review of the Schrödinger Wave Equation

Celso Luis Levada<sup>(1)</sup>, Huemerson Maceti<sup>(1)</sup>, Ivan José Lautenschleguer<sup>(1)</sup>

(1) Herminio Ometto Foundation – Uniararas- Brazil  
Corresponding Author: Celso Luis Levada

---

**Abstract:** The objective of this work is to investigate the Schrödinger equation, analyzing the mathematical concepts employed and relating them to other areas of knowledge. In quantum mechanics, the Schrödinger equation is a partial differential equation that describes how the quantum state of a physical system evolves over time. It was formulated in late 1925 and published in 1926 by the Austrian physicist Erwin Schrödinger. In quantum mechanics, the analogue of Newton's law is the Schrödinger equation for the quantum system (usually atoms, molecules, and subatomic particles are free, bound, or located). It is not a simple algebraic equation but, in general, a linear partial differential equation. The solutions to the Schrödinger equation describe not only molecular, atomic, and subatomic systems, but also macroscopic systems.

**Keywords:** Schrödinger, Wave Functions, Stationary Waves, Hydrogen Atom

---

Date of Submission: 23-03-2018

Date of acceptance: 07-04-2018

---

### I. Introduction

In the year 1925, Schrödinger began the work to obtain a wave equation in order to apply it to the hydrogen atom. According to FREIRE JR <sup>(1)</sup>, the inspiration for this was De Broglie's doctoral thesis, and his idea was to establish stationary waves in three dimensions, analogous to sound waves in cavities. The Schrödinger equation is an equation used in wave mechanics for the wave function of a particle and allowed the creation of a complete model for the atom. From this point of view, one might think that Schrödinger's theory would be a mere development of De Broglie's theory. However the theory in question can be associated with cases in which De Broglie's theory cannot be applied, such as accelerated motion and rotation. In addition, the model proposed by Schrödinger reconciled the theoretical postulates of De Broglie and Heisenberg, as well as presented a three-dimensional orbital model for each of the energy sub-levels and enabled the determination of the molecular geometry of several chemical substances.

The Schrödinger equation allows computing the associated wave function  $\psi(r, t)$  to a particle moving within a force field described by a potential  $V(r, t)$  (which may depend on the position  $r$  and time  $t$ ). The resolution of the Schrödinger equation <sup>(3)</sup> leads to a set of wave functions and to a set of energies corresponding to the electron states allowed in that atom, since only certain wave functions are allowed as solutions of the equation. As can be seen in the book by Alonso and Finn <sup>(5)</sup>, the mathematical expressions of the wave functions allow us to determine the probability of finding an electron in the vicinity of a point near the nucleus. In the case of the electron of the hydrogen atom in the ground state, this probability depends only on the distance to the nucleus. As it is known <sup>(5)</sup>, quantum mechanics studies the movement of particles that form matter, that is, atoms, molecules and electrons. Microscopic particles, like electrons, do not move following the classical laws of motion, given by Newtonian mechanics. These particles, however, follow other laws that seem to be more appropriate for the propagation of a wave. Thus, a wave motion will be fully known if the spatial and temporal dependence of the wave function is known.

According to ZEILMANN <sup>(2)</sup>, it was from the article by Erwin Schrödinger (1887-1961), titled "An Undulatory Theory of the Mechanics of Atoms and Molecules", that interest arose in investigating the relationship between mathematics and quantum physics referred to in the aforementioned article. Thus, the objective of this work was to investigate the Schrödinger equation, analyzing the mathematical concepts employed and relating them to other areas of knowledge, such as physics and chemistry.

### II. Mathematical Development For The Stationary State

According to KNIGHT <sup>(4)</sup> in the mechanics of oscillations a wave motion can be described by an equation of the type

$$\psi(x, t) = A e^{i(kx - \omega t)} \quad (1)$$

$$\text{where } k = \frac{2\pi}{\lambda} \quad (2)$$

Considering the time independent equation first, we can write

$$\psi(x) = A e^{\frac{i2\pi x}{\lambda}} \quad (3)$$

Then, by making the first derivative of equation (3) with respect to x we have

$$\frac{d\psi(x)}{dx} = \frac{2\pi i}{\lambda} A e^{\frac{2i\pi x}{\lambda}} \quad (4)$$

Now, by making the second derivative with respect to x, it comes

$$\frac{d^2\psi(x)}{dx^2} = -\frac{4\pi^2}{\lambda^2} A e^{\frac{2i\pi x}{\lambda}} \quad (5)$$

By substituting equation (3) into equation (5), we have the following condition

$$\frac{d^2\psi(x)}{dx^2} = -\frac{4\pi^2}{\lambda^2} \psi(x) \quad (6)$$

Taking into account De Broglie's relationship we have

$$\lambda = \frac{h}{mv} \quad \text{and} \quad \lambda^2 = \frac{h^2}{m^2v^2} \quad (7)$$

Substituting (7) into (6) yields the equation

$$\frac{d^2\psi(x)}{dx^2} = -\frac{4\pi^2 m^2 v^2}{h^2} \psi(x) \quad (8)$$

Regrouping the terms of equation (8)

$$\frac{m^2 v^2}{2m} = -\frac{h^2}{8\pi^2 m} \frac{1}{\psi(x)} \frac{d^2\psi(x)}{dx^2} \quad (9)$$

On the other hand, we know that the kinetic energy, T, is given by

$$T = \frac{1}{2} m v^2 = \frac{m^2 v^2}{2m} \quad (10)$$

Substituting equation (9) into equation (10)

$$T = -\frac{h^2}{8\pi^2 m} \frac{1}{\psi(x)} \frac{d^2\psi(x)}{dx^2} \quad (11)$$

Recalling that  $E = T + V$  it results

$$E = -\frac{h^2}{8\pi^2 m} \frac{1}{\psi(x)} \frac{d^2\psi(x)}{dx^2} + V \quad (12)$$

Rearranging the terms of equation (12)

$$\frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 m}{h^2} (E - V)\psi(x) = 0 \quad (13)$$

For the three-dimensional case we have

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - V)\psi = 0 \quad (14)$$

Finally the time-independent Schrödinger equation as a function of the reduced mass ( $\mu$ ) and by considering that  $\hbar = h/2\pi$

$$\frac{-\hbar^2}{2\mu} \nabla^2 \psi(x, y, z) + V \psi(x, y, z) = E \psi(x, y, z) \quad (15)$$

This is the stationary Schrödinger equation for non-relativistic free particles, independent of time, mass  $\mu$  and energy  $E$ . In order to incorporate the time variable, we must consider equation (1) in its complete form, that is,

$$\psi(x, t) = A e^{i(kx - \omega t)}$$

By taking the derivative of  $\psi(x, t)$  with respect to time, we will have

$$\frac{\partial \psi}{\partial t} = -i\omega A e^{i(kx - \omega t)} \text{ or } \frac{\partial \psi}{\partial t} = -i\omega \psi(x, t)$$

On the other hand, we must derive  $\psi(x, t)$  twice with respect to  $x$ . Thus, the first derivative provides

$$\frac{\partial \psi}{\partial x} = ik A e^{i(kx - \omega t)}$$

Meanwhile, the second derivative is given by

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 A e^{i(kx - \omega t)} = -k^2 \psi(x, t)$$

At this point, it is worth recalling some important relations

$$k = \frac{2\pi}{\lambda}; \omega = 2\pi f; \lambda = \frac{h}{p}; v = \lambda f; E = hf; \hbar = \frac{h}{2\pi}$$

Hence we can write

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

This can be rearranged in

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

For the three-dimensional case

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi$$

$$E = T + V = \frac{\mathbf{P}^2}{2m} + V$$

By making the appropriate substitutions, rearranging the terms and, by introducing the reduced mass ( $\mu$ ) into the equation, we can arrive at

$$\frac{-\hbar^2}{2\mu} \left[ \frac{\partial^2 \psi(x, y, z, t)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z, t)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z, t)}{\partial z^2} \right] + V(x, y, z) \psi(x, y, z, t) = i\hbar \frac{\partial \psi(x, y, z, t)}{\partial t} \quad (16)$$

Schrödinger published the paper with the deduction of this equation in 1926 and won the Nobel Prize for this work in 1933, just six years after publication. It is observed that the wave function equation explicitly includes complex numbers that lead to complex wave functions and this is an important fact in quantum mechanics. Complex functions can not represent physical quantities whose measures are real numbers. Even so, complex functions and variables have been used to facilitate algebra and in the end select only the real parts of

the obtained variables. It is not the case for the wave function of quantum mechanics, since it is intrinsically a complex function. However any complex number multiplied by its conjugate complex ( $\psi \psi^*$ ) is a real and positive number.

### III. Meaning Of The Wave Function

After years of discussion about the significance of the wave function involving disputes between Einstein, Bohr, Schrödinger, Heisenberg and others, the Copenhagen interpretation was achieved. The wave function of a system is nothing more than an abstract mathematical representation of the state of the system. It only has meaning in the context of quantum theory. So, what is this function for?

The interpretation that is now accepted for the wave function was formulated by the German physicist Max Born in 1926, who considered it as an amplitude of probability. Max Born interpreted the wave function, considering the square of the absolute value of  $\psi$ ,  $|\psi|^2$ , as the probability density of finding the electron in a given position around the nucleus. If  $\psi(x, t)$  represents a single particle, then  $|\psi(x, t)|^2 dx$  is the probability of finding it in the interval  $(x, x + dx)$  at time  $t$ . So, the term  $|\psi|^2$  is called the probability density, while  $\psi$  is the amplitude of the probability.

The wave function is a complex quantity, it cannot be measured directly by any physical instrument. That means there is no immediate physical sense to this function! Therefore, let us make it well established that, in fact, the wave function of a system is nothing more than an abstract mathematical representation of the state of the system. It only has meaning in the context of quantum theory. So, what is this function for? Can we use it in any way to describe the physical world?

By this interpretation the product  $\psi(x, t)\psi^*(x, t)$ , a real and positive number, represents the probability density function to find the particle at position  $x$  at time  $t$ . In this interpretation the electron would be dispersed by space with a charge density given by  $\rho(x, t) = -e \psi(x, t)\psi^*(x, t)$ . This interpretation also requires that  $\psi(x, t)\psi^*(x, t)$  be continuous.

### IV. Stationary States

A quantum system can remain stationary in certain states in which the energy has a precise value  $E$ . In these stationary states, the wave function assumes a particular simplified form because the wave function does not depend on time. Stationary states are the eigenfunctions of the energy operator or, simply, energy eigenfunctions. The solutions for the stationary state of the wave function can be separated into two functions, one that depends only on spatial coordinates and another that depends only on time. Hence, we will have something of the type  $\psi(x, y, z, t) = \psi(x, y, z) \phi(t)$ . A typical case of this behavior is when the wave function takes the form given by  $\psi(x, y, z, t) = \psi(x, y, z) \exp(-iEt/\hbar)$ . From what it is perceived that every dependence of  $\phi$  in time is associated with the complex factor  $\exp(-iEt/\hbar)$ , whose modulus is unitary. In view of this, we can say that in so-called stationary states the density of probability depends only on position, being independent of time, that is,

$$|\psi(x, y, z, t)|^2 = |\psi(x, y, z)|^2 \quad (17)$$

Stationary states are extremely important in the quantum description of nature, not only because they represent states that have definite energy, but also because the set of Hamiltonian eigenstates, which are stationary states, is complete. This means that any state can be represented as a linear combination of stationary states.

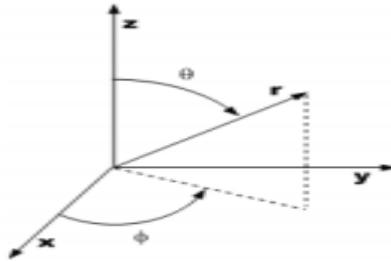
### V. Application For The Hydrogen Atom

The mathematical problem to find the wave functions of the hydrogen atom was to solve the Schrödinger equation with Coulomb potential in the three dimensions

$$\frac{-\hbar^2}{2\mu} \left[ \frac{\partial^2 \psi(x, y, z)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z)}{\partial z^2} \right] - \frac{e^2}{4\pi\epsilon} \frac{\psi(x, y, z)}{\sqrt{x^2 + y^2 + z^2}} = E \psi(x, y, z) \quad (18)$$

This problem has an analytic solution, but requires a completely out-of-context mathematics. However, we will only present the main results.

As Schrödinger did, let's begin by transforming the wave equation expressed in Cartesian coordinates into an equivalent equation in polar coordinates. In this new coordinate system it is possible to separate variables, which means that the function  $\psi(r, \theta, \phi)$  can be decomposed into a product of three functions  $R(r)\Theta(\theta)\Phi(\phi)$ .



The resolution of the radial part of the wave function has solutions that identify with the Laguerre polynomials whose normalization contains the term  $(n-1)!$  which implies that  $n > 1$ . Curiously, in the absence of magnetic fields (internal or external), energy depends only on the quantum number  $n$ , which is why it is called the principal.

$$E = R_H \frac{1}{n^2}$$

The resolution of the azimuth component of the wave function leads to the expression

$$\Phi(\phi) = e^{\pm im\phi} \quad (19)$$

The parameter  $m$  is limited to the set of integers, being known by magnetic quantum number because the energy only depends on it when magnetic fields are considered.

The integer  $m$  is associated with another integer,  $l$ , in determining the acceptable solutions

$$m_l = -l, -l + 1, \dots, 0, \dots, l - 1, l$$

According Eisberg and Resnick <sup>(6)</sup>, we can deduce what comes next. Assuming electron can be described by a wave function of form  $\psi = \psi(x, y, z, t)$ , the Schrödinger equation can be written

$$\frac{-\hbar^2}{2\mu} \left[ \frac{\partial^2 \psi(x, y, z, t)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z, t)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z, t)}{\partial z^2} \right] + V(x, y, z) \psi(x, y, z, t) = i\hbar \frac{\partial \psi(x, y, z, t)}{\partial t}$$

or

$$\frac{-\hbar^2}{2\mu} \nabla^2 \psi + V\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (20)$$

Since  $V(x, y, z)$  does not depend on time,  $\psi(x, y, z, t) = \psi(x, y, z) e^{\frac{-iEt}{\hbar}}$  is a solution to the Schrödinger equation and the eigenfunction  $\psi(x, y, z)$  is a solution of the time-independent Schrödinger equation

$$\frac{-\hbar^2}{2\mu} \nabla^2 \psi(x, y, z) + V\psi(x, y, z) = E \psi(x, y, z)$$

It's convenient to use spherical polar coordinates

$$\frac{-\hbar^2}{2\mu} \nabla^2 \psi(r, \theta, \phi) + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi), \text{ where}$$

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

We can now use separation of variables to split the partial differential equation into set of ordinary differential equations. Then, assuming that the eigenfunction is separable in this form  $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$ , we can write

$$\frac{-\hbar^2}{2\mu} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial (R\Theta\Phi)}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial (R\Theta\Phi)}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 (R\Theta\Phi)}{\partial \phi^2} \right) + V(r)(R\Theta\Phi) = E(R\Theta\Phi) \quad (21)$$

By making the differentiation we conclude that

$$\frac{-\hbar^2}{2\mu} \left( \frac{\Theta\Phi}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{R\Phi}{r^2 \sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) + \frac{R\Theta}{r^2 \sin^2\theta} \frac{d^2\Phi}{d\phi^2} \right) + V(r)(R\Theta\Phi) = E(R\Theta\Phi)$$

Now multiplying by the term  $\frac{-2\mu r^2 \sin^2\theta}{R\Theta\Phi\hbar^2}$  and taking into account the transpose it comes that

$$\frac{1}{\Phi} \frac{d^2\Phi}{d\phi^2} = -\frac{\sin^2\theta}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{\sin\theta}{\Theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) - \frac{2\mu}{\hbar^2} r^2 \sin^2\theta (E - V(r))$$

By making some physical considerations we can replace the original Schrodinger equation in two other equations, namely

$$\begin{aligned} \frac{d^2\Phi}{d\phi^2} &= -m_l^2 \Phi \\ \frac{1}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2\mu r^2}{\hbar^2} (E - V(r)) &= \frac{m_l^2}{\sin^2\theta} - \frac{1}{\Theta \sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) \end{aligned}$$

To be concordant both sides in this last equality must be equal to a constant that, for convenience is chosen as  $l(l+1)$ . This leads to

$$-\frac{1}{\sin\theta} \frac{d}{d\theta} \left( \sin\theta \frac{d\Theta}{d\theta} \right) + \frac{m_l^2 \Theta}{\sin^2\theta} = l(l+1)\Theta \tag{22}$$

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} (E - V(r))R = l(l+1) \frac{R}{r^2} \tag{23}$$

We have now separated the time-independent Schrödinger equation into three ordinary differential equations, which each only associated to  $\Phi$ ,  $\Theta$  and  $R$ . Then we will have as particular solutions the following equations

$$\Phi(\phi) = e^{(im_l\phi)} \text{ where } m_l = 0, \pm 1, \pm 2, \dots$$

In spectroscopy  $m_l$  is called the magnetic quantum number.

By making change of variable  $z = r \cos \Theta$  the equation (22) can be transformed into an associated Legendre equation

$$\frac{d}{dz} \left( (1-z^2) \frac{d\Theta}{dz} \right) + \left( l(l+1) \frac{m_l^2}{1-z^2} \right) \Theta = 0,$$

whose solution is of the type

$$\Theta_{l,|m_l|}(\theta) = \sin^{|m_l|}\theta F_{l,|m_l|}(\cos\theta),$$

where  $F_{l,|m_l|}(\cos\theta)$  represents associated Legendre polynomial functions being

$$m_l = -l, -l+1, \dots, 0, \dots, l-1, l$$

On the other hand, assuming that the ground state is associated to  $n = 1$  and  $l = 0$ , the equation (23) can be written

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} \left( E + \frac{e^2}{4\pi\epsilon r} \right) R = 0$$

In this equation, by making the derivative with respect to the parameter R, it follows that

$$\frac{d^2R}{dr^2} + \frac{2}{r} \frac{dR}{dr} + \frac{2\mu}{\hbar^2} \left( E + \frac{e^2}{4\pi\epsilon r} \right) R = 0 \quad (24)$$

Replacing the solution  $R = A e^{\frac{-r}{a_0}}$  into equation (24), where  $A$  and  $a_0$  are constants

$$\left( \frac{1}{a_0^2} + \frac{2\mu}{\hbar^2} E \right) + \left( \frac{2\mu e^2}{4\pi\epsilon \hbar^2} - \frac{2}{a_0} \right) \frac{1}{r} = 0 \quad (25)$$

In order to satisfy this equation (25) for any  $r$ , both expressions in parentheses must be equal zero, which implies

$$a_0 = \frac{4\pi\epsilon \hbar^2}{\mu e^2} \text{ and } E = -\frac{\hbar^2}{2\mu a_0^2} = -13.6 \text{ eV}$$

It is noticed that the result is in agreement with the results obtained by Bohr. Generalizing this last result we have

$$E_n = -\frac{13.6}{n^2} \text{ eV},$$

where  $n$  represents the principal quantum number, defined by  $n = l + 1, l + 2, l + 3, \dots$

## VI. Final Considerations

The Schrödinger equation is nothing more than a second-order differential equation, which can be applied to a system such as the hydrogen atom, and thus calculate the corresponding energy levels. The Schrödinger equation is easy to use for the hydrogen atom, but when the atomic number is increased, the numerical methods are more effective and facilitate the resolution of the problem. This equation has limitations because it only applies to particles with low velocities. The Schrödinger wave equation can be deduced from De Broglie results, at the classical limit. However, the Schrödinger theory is not a mere application or development of the De Broglie results, since it can be applied to cases in which De Broglie theory cannot be applied, such as accelerated motion and rotation.

## Bibliographic References

- [1]. FREIRE JR, O., PESSOA JR, O. and BROMBERG, JL... Teoria Quântica: estudos históricos e implicações culturais [online]. Campina Grande: EDUEPB; São Paulo: Livraria da Física, 2011. 456 p. ISBN 978-85-7879-060-8. Available from SciELO Books.
- [2]. ZEILMANN, AP, Vetor, Rio Grande, v.18, n.2, p. 34-44, 2008
- [3]. GRIFFITHS, David J.; Quantum Mechanics; 2nd edition - São Paulo. Editora Pearson Prentice Hall, 2011.
- [4]. KNIGHT, R. D., Physics for Scientists and Engineers, 2nd Edition, Person Education Inc., Addison Wesley, Copyright São Paulo 2009, book available in <https://books.google.com.br/books?isbn=8577805972>.
- [5]. ALONSO M. Y FINN E., Física Vol. III Fundamentos Cuánticos Y Estadísticos Edit. Addison- Wesley Iberoamericana (1986)
- [6]. EISENBERG, R. and RESNICK, R. Quantum physics of atoms, molecules, solids, nuclei, and particles, Chapter 7, p.236-238, 1985, book available in [http://www.sicyon.com/resources/library/pdf/eisenbergresnickquantum\\_physics.pdf](http://www.sicyon.com/resources/library/pdf/eisenbergresnickquantum_physics.pdf)

IOSR Journal of Applied Chemistry (IOSR-JAC) is UGC approved Journal with SI. No. 4031, Journal no. 44190.

Celso Luis Levada "Review Of The Schrödinger Wave Equation." IOSR Journal of Applied Chemistry (IOSR-JAC) 11.4 (2018): 01-07.