Derivation and Physical Meaning of the Schrodinger Equation of a Particle in One Dimensional Space

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Received: 29 March 2022; **Accepted**: 14 June 2022; **Published**: 22 June 2022
DOI: http://dx.doi.org/10.29303/jpft.v8i1.3455

***Abstract** - Research has been carried out to determine the physical meaning and derivation of the Schrodinger equation with the literature study research method. Based on the research results obtained through data processing in the form of information obtained from various literature sources, it can be concluded that the general solution of the Schrodinger equation is a wave function. In general, based on mathematical calculations by applying the technique of solving differential equations to the Schrodinger equation, it can be seen that this equation has many solutions, but not all of these solutions can be said to be functions that meet the wave function criteria. This wave function must be able to interpret the real physical criteria of a particle.*

***Keywords**: Schrodinger Equation; Quantum Physics; Wave Mechanics; Particle-Wave Dualism*

INTRODUCTION

In classical physics, the laws that explain the behaviour of waves and particles are fundamentally different. Projectiles obey the law of particle type, such as Newtonian mechanics (Siregar, 2018). Waves undergo interference and diffraction, which Newtonian mechanics with respect to particles cannot explain. The energy carried by a particle is limited to a small region of space; A wave, on the other hand, distributes its energy throughout the space in front of the wave. In describing the behaviour of particles, we often want to determine their location, but this is not easy to do for waves (Feynman, 2010).

In contrast to the obvious differences found in classical physics, quantum physics requires that particles sometimes obey the rules we have previously defined for waves, and we will use some language related to waves to describe particles (Trachanas, 2018).

Experimental evidence accumulated towards the end of the nineteenth century showed that classical mechanics failed when applied to particles as small as electrons. More specifically, careful measurement leads to the conclusion that particles may not have arbitrary energies and that the classical concepts of particles and waves converge (Jun, 2013). This topic shows how these observations set the stage for the development of quantum mechanical concepts and equations in the early twentieth century.

System mechanics related to quantum systems is sometimes called wave mechanics or more specifically quantum mechanics because it deals with the behaviour of particles as waves (Siregar, 2018).

In quantum mechanics, all the properties of a system are expressed in terms of the wave function obtained by solving the equations proposed by Erwin Schrödinger (Krane, 2012). This topic focuses on the interpretation of the wave function, and in particular what it reveals about the location of particles.

In 1926 Erwin Schrödinger proposed an equation for finding the wave function of any system. The time-independent Schrödinger equation for a particle of mass *m* moving in one dimension with energy *E* in a system that does not change with time (volume remains constant) is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi \qquad (1)$$

The value of $\hbar=\frac{h}{2\pi}$ is an easy modification of Planck's constant which is widely used in quantum mechanics. *V*(*x*) is the potential energy of the particle at *x*. Since the total energy *E* is the sum of the potential energy and kinetic energy, the first term on the left must be related (in a way that will be explored later) with the kinetic energy of the particle(Griffiths & Schroeter, 2018). The Schrödinger equation can be considered a basic postulate of quantum mechanics, but its reasonableness can be demonstrated by showing that, for the case of free particles, it is consistent with the de Broglie relation (Susskind & Friedman, 2014)

Quantum mechanics is an abstract concept, such as the concept of waves, probability density, operators, and so on. There are two approaches to the formulation of quantum mechanics, namely the wave mechanics developed by Schrodinger, and the matrix mechanics proposed by Heisenberg. The main difference between classical mechanics and quantum mechanics is in the statement about the dynamic variables that can be measured. Dynamic variables in classical mechanics are expressed by functions, while dynamic variables in quantum mechanics are represented by mathematical operators. Operators in quantum mechanics are applied to wave functions (Griffiths & Schroeter, 2018).

In the quantum approach, the state of a system and can be observed from the results of measurements on the system are generally not identical although they are always related. According to the quantum formulation, the state of a quantum system is described by a state function, which is probabilistic, whereas a certain measurable measurement operation is expressed in the corresponding mathematical operator, regardless of the system under consideration (Krane, 2012).

A classical system, as a simple example of a particle at a potential, is described in classical mechanics by its position and velocity. If the magnitude of the potential affecting the particle is known, as well as the initial position and initial velocity, classically the position and velocity at a later time can be obtained by solving the particle equation. This means that everything about the movement of the particle or system can be known (Sudiarta, 2012).

The development of quantum mechanics started from the wave nature of particles. The wave equations known in classical physics derive the wave equations for particles. This equation is known as the Schrodinger equation (Atkits & Keeler, 2018). The simplest form of this equation is called the eigenvalue equation, which is an energy operator called the particle Hamiltonian which is operated on the particle-wave function (Atkits & Keeler, 2018). The solution to the Schrodinger equation uses boundary conditions that arise from the form of the potential energy of the particle itself. The solution to the equation is the energy and wave function of the particle (Atkits & Keeler, 2018).

Heisenberg's uncertainty principle and the nature of particle-wave duality indicate that the position and velocity of the particle are also waves, so the particle or system must be described using a wave function (Thornton, 2013).

The wave function $\psi(x,t)$. of a system consisting of one particle is usually given by the symbol . This wave function depends on the position *x* and time *t*. Keep in mind that all information about the system is given by a wave function. This also means that the physical properties of the system can be obtained from its wave function (Sudiarta, 2012).

RESEARCH METHODS

This study is research with literature study method. The literature study method is an activity related to the method of collecting library data by reading, analysing, and sorting literature to identify important attributes of the material. The significant difference from other methodologies is that it does not directly relate to the object under study, but indirectly accesses information from various literatures, which are generally referred to as non-contact methods.

The research methodology of literature study includes unstructured qualitative analysis and structured quantitative analysis. This qualitative description rarely shows the relationship of research subject variables, so researchers tend to apply logical reasoning to explore logical relationships between objects rather than quantity relationships. In general, qualitative analysis is to classify the information contained in the literature, to select typical examples to rearrange and arrive at conclusions based on qualitative descriptions. Qualitative analysis of the literature has special value in distinguishing past trends and forecasting future models. Literary qualitative research does not focus on the quantity and completeness of library materials. It focuses on personal literature research and selecting small samples or case characteristics according to research interests and subject requirements.

RESULT AND DISCUSSION

Schrodinger Equation for Potential-Free Particles ($V = 0$)

Consider a particle with a mass m that is contained in a one-dimensional box with the length of L which is free from gravitational fields (g), electric fields (E), magnetic fields (B), and friction. Thus, it can be said that the potential energy V of the particle is zero $(V = 0)$. Apart from this, it can be assumed that the particles in the box are constrained by not being able to leave the box. Such a state allows the particle to only move translationally freely left and right with momentum p_x. The magnitude of the momentum is the same before and after hitting the wall of a one-dimensional box. Furthermore, since the particle can only move freely left and right, the particle only has a kinetic energy of T, where the value is equal to:

$$T = \frac{1}{2} m v_x^2. \tag{2}$$

Since mv_x is the momentum p_x, then equation (2) can be written as $T = \frac{p_x^2}{2m}$. And according to classical mechanics, the total energy of a particle is equal to the sum of its kinetic energy and potential energy $E = T + V$.

Based on the description above, it is known that the potential energy V of the particle is zero $(V = 0)$, so that E can be written even simpler and that the total energy of the particle in the box becomes $E = T$.

This informs us that the most important energy for a particle in a one-dimensional box in the absence of a conservative field is the kinetic energy of the particle only. And by adjusting the equation E using the Hamiltonian quantum operator $\hat{H}$ for the kinetic energy of the particles, the equation can be written as $E = \hat{H}$.

Now, let us consider $\psi(x)$ the wave function of the particle in the box, then E can be written as follows.

$$E\psi(x) = \hat{H}\psi(x) \quad (3)$$

The kinetic energy of the particle T is equal to $\frac{1}{2}mv_x^2$ that used in classical mechanics concepts so if this kinetic energy is substituted into equation (3), it must be converted into the form of a quantum operator. In this case, only momentum p_x and position x have quantum operators $\frac{\hbar}{i}\frac{\partial}{\partial x}$ and x which are actually $\hbar$, and i as the imaginary numbers with a value of $\sqrt{-1}$. Then, the equation for the kinetic energy of the particles can be written as follows:

$$T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad (4)$$

By substituting equation (4) into equation (3), the following equation will be obtained:

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) \quad (5)$$

The negative sign on the right-hand side of the equation is obtained as the result of the square of an imaginary number i of -1. The simplification of equation (5) is:

$$\frac{\partial^2\psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi(x) \quad (6)$$

This is the Schrodinger differential equation or also known as the Schrodinger wave equation. Furthermore, if you pay close attention, the solution for the Schrodinger wave equation can be found. By using the concept of solving differential equations, several solutions are obtained in the form of possible functions $\psi(x)$, such as $\psi(x) = Asin(kx)$, $\psi(x) = Acos(kx)$, $\psi(x) = Ae^{ikx}$, and $\psi(x) = Ae^{-ikx}$. With A as a constant or coefficient of each function. For functions $\psi(x) = Asin(kx)$ and $\psi(x) = Acos(kx)$, this value of A is the amplitude of the sine and cosine wave functions. While the value is a *phase shift* or wave phase shift in the sine and cosine wave functions.

If the four equations above are differentiated twice to get to the second derivative, then the four equations above will give the same result:

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \quad (7)$$

The value of k^2 in equation (7) above is nothing but $-\frac{2mE}{\hbar}$. Thus, it can be written that the value of k is equal to:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (8)$$

According to quantum theory, there are two conditions that must be met by a wave function, namely a wave function must be continuous and a wave function must be differentiable except at the limit of the potential energy value equal to zero or infinity. Thus, to determine the wave characteristics of the particle, it is necessary to set boundary conditions, by setting the value of the boundary conditions $\psi(0) = 0$ and $\psi(L) = 0$. The value of L is the position x $(L = x)$ of the one-dimensional box in which the particle is located which is used as the maximum limit at which the particle will collide and return to translational motion towards position 0 $(x = 0)$.

By applying the value of the boundary conditions that have been determined, it is known that from the four solutions of the Schrodinger differential equation mentioned above, there is only one solution that satisfies this boundary condition, the sine function $\psi(x) = Asin(kx)$. Therefore, based on a simple mathematical calculation by substituting the value $x = 0$ and $x = L$ into the sine function, it is known that the angle kL that satisfies is $\pi, 2\pi, 3\pi, \ldots, n\pi$, so that an equation is obtained to find the value of

k, which is $k = \frac{n\pi}{L}$. And the complete wave function as a solution to the Schrodinger differential equation for this phenomenon is

$$\psi(x) = Asin\left(\frac{n\pi}{L}\right)x \quad (9)$$

with $n = 1, 2, 3, \ldots (n \in \mathbb{N})$.
By applying the boundary conditions as described above, it is generally possible to obtain or prove that there is quantized energy. Then, by combining the two equations of k, we get:

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad (10)$$

By substituting the value of $\hbar = \frac{h}{2\pi}$, then equation (10) can be written as follow

$$E_n = \frac{n^2h^2}{8mL^2} \quad (11)$$

with $n = 1, 2, 3, \ldots (n \in \mathbb{N})$.

Equation (11) is a formulation to determine the amount of quantization energy as described by Niel Bohr. So it can be concluded that the Schrodinger equation for particles in one-dimensional space without being influenced by a conservative field can prove that particles in one-dimensional space have stratified or quantized energy. Or in other words, the particles in a one-dimensional box cannot have the same arbitrary energy levels as hydrogen atoms.

Schrodinger Equation of a Particle with Time Independent

In this second part an assumption is taken that the particles in a one-dimensional box move in translation with the following wave function equation:

$$\psi(x) = Asin(\omega t - kx) \quad (12)$$

with $\psi(x)$ as a wave functions, the angular velocity ω, travel time t, wave vector k, and displacement x. In general, the equation $\psi(x)$ is a sine wave function. If the equation is derived once, it will be obtained:

$$\frac{\partial\psi(x)}{\partial x} = -kAcos(\omega t - kx) \quad (13)$$

And the second derivative of the equation is:

$$\frac{\partial^2\psi(x)}{\partial x^2} = -k^2Asin(\omega t - kx) \quad (14)$$

From equation (14), it can be seen that $Asin(\omega t - kx)$ is $\psi(x)$. Thus equation (14) can be written as:

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0 \quad (15)$$

By substituting the values $k = \frac{2\pi}{\lambda}$ into equation (15), we get:

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{4\pi^2}{\lambda^2}\psi(x) = 0 \quad (16)$$

According to de-Broglie, $\lambda = \frac{h}{mv}$ and by substituting the value of λ into equation (16), we get:

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{4\pi^2m^2v^2}{h^2}\psi(x) = 0 \quad (17)$$

Since the value of $\hbar = \frac{h}{2\pi}$, so it is true that $\frac{1}{h} = \frac{2\pi}{\hbar}$ and $\frac{\partial^2\psi(x)}{\partial x^2} + \frac{4\pi^2}{\lambda^2}\psi(x) = 0$. Therefor $\frac{1}{h^2} = \frac{4\pi^2}{\hbar^2}$ and equation (17) can be written as follow:

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{m^2v^2}{\hbar^2}\psi(x) = 0 \quad (18)$$

From the description in the previous first section, it can be seen that the total energy of a particle is $E = T + V$. So the total energy of the particle is $E = \frac{1}{2}mv^2 + V$. With a little algebraic manipulation, this equation can be written as follow:

$$2m(E - V) = m^2v^2. \quad (19)$$

Furthermore, by substituting equation (19) into equation (18), we get:

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m(E-V)}{\hbar^2}\psi(x)=0 \qquad (20)$$

Equation (20) above is Schrodinger's time-independent equation for a particle in one-dimensional space without neglecting the state of the particle which is affected by a conservative field.

If an analysis is carried out to see how the state of the particles in three-dimensional space with respect to a conservative field, then equation (20) can be written as:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi+\frac{2m(E-V)}{\hbar^2}\psi=0 \qquad (21)$$

where $\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)=\nabla^2$. Then, equation (21) can be stated as:

$$\nabla^2\psi(x,y,z)+\frac{2m(E-V)}{\hbar^2}\psi(x,y,z)=0 \qquad (22)$$

Equation (22) is the Schrodinger equation for particles in time-free three-dimensional space.

Schrodinger Equation of a Particle with Time Dependent

The Schrodinger equation of a particle with time-dependent in one-dimensional space is one of the most important Schrodinger equations used in quantum mechanics. Basically, the time-dependent Schrodinger equation is used to determine and analyse the behaviour of a particle at the atomic and subatomic levels which has the nature of wave-particle duality as proposed by de-Broglie.

In the event of light interference and diffraction, the wave nature of light is more prominent than the particle nature of light. In the case of the photoelectric effect and the Compton effect, the particle nature of light is more prominent than the wave nature of light. This particle property is expressed by the magnitude of momentum p, while the wave property is expressed by λ. The relationship between these two quantities is expressed in the equation $\lambda=\frac{h}{p}$.

According to the theory of classical mechanics, the value is mv. Thus, the above equation can be written as $\lambda=\frac{h}{mv}$ and assuming a particle that is moving freely in the x with the de-Broglie wave function equation $\psi(x)=Asin(\omega t-kx)$. This equation is then reduced to the second derivative, so that it is obtained:

$$\frac{\partial^2\psi(x)}{\partial x^2}=-k^2\psi(x) \qquad (23)$$

with $\omega=2\pi v$ or $\omega=\frac{2\pi E}{h}$ (by recalling $E=hv$), and $k=\frac{2\pi p_x}{h}$.

Then, by inserting both ω and k into equation (23), we obtain:

$$p_x^2\psi(x)=-\hbar^2\frac{\partial^2\psi(x)}{\partial x^2} \qquad (24$$

and

$$\psi(x)=-\frac{\hbar^2}{p_x^2}\frac{\partial^2\psi(x)}{\partial x^2}. \qquad (25)$$

Next, if we try to differentiate the function $\psi(x)=Asin(\omega t-kx)$ with respect to t, obviously we obtain:

$$\frac{\partial\psi(t)}{\partial t}=A\omega cos(\omega t-kx) \qquad (26)$$

The second derivative of function $\psi(x)=Asin(\omega t-kx)$ is:

$$\frac{\partial^2\psi(t)}{\partial t^2}=-A\omega^2 sin(\omega t-kx) \qquad (27)$$

and this can be simplified as follow:

$$\frac{\partial^2\psi(t)}{\partial t^2} = -\omega^2\psi(t) \qquad (28)$$

If we substitute the value of ω into equation (27), then we will obtain:

$$\frac{\partial^2\psi(t)}{\partial t^2} = -\frac{E^2}{\hbar^2}\,\psi(t). \qquad (29)$$

Equation (29) can be stated as follow:

$$E^2\psi(t) = -\hbar^2\frac{\partial^2\psi(t)}{\partial t^2} \qquad (30)$$

and

$$\psi(t) = \frac{-\hbar^2}{E^2}\frac{\partial^2\psi(t)}{\partial t^2} \qquad (31)$$

If we consider $\psi(x) = \psi(t)$, then:

$$\frac{1}{p_x^2}\frac{\partial^2\psi(x)}{\partial x^2} = \frac{1}{E^2}\frac{\partial^2\psi(t)}{\partial t^2} \qquad (32)$$

$$\frac{\partial^2\psi(x)}{\partial x^2} = \frac{p_x^2}{E^2}\frac{\partial^2\psi(t)}{\partial t^2} \qquad (33)$$

$$\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{2m(E-V)}{E^2}\frac{\partial^2\psi(x,t)}{\partial t^2} \qquad (34)$$

where $\psi(x,t)$ is the wave deviation of the particle at the position of x at the time *t*. $\psi(x,t)$ considered as a wave function of particles in one-dimensional space with a fixed energy associated with a fixed frequency.

Solution to Schrodinger Equation of a Particle in One Dimensional Space

Based on the description given beforehand, it can be seen that in equations (7) and (20) there is a wave function $\psi(x)$ of the Schrodinger equation of a particle in one-dimensional space with time-free conditions. With this wave function, the probability of finding a particle at a position x in the interval dx is $\psi^*(x)\psi(x)dx$, and the total probability of finding that particle along the *x*-axis is:

$$\int_{-\infty}^{\infty}\psi^*(x)\psi(x) = \int_{-\infty}^{\infty}|\psi(x)|^2dx = 1 \qquad (35)$$

In equation (35) above, $|\psi(x)|^2$it is called the probability density and $\psi^*(x)$ is the conjugation of the wave function $\psi(x)$. A wave function that satisfies equation (35) is called a normalized function.

A wave function of a particle must have good characteristics so that the properties expressed by equation (35) can be fulfilled. The characteristics that must be considered are:

(a) Not equal to zero, and is *single-valued*, meaning that the wave function $\psi(x)$ has only one value for a value *x*.
(b) The function of its derivative is continuous at all values of *x*, and
(c) Its absolute value function remains finite for *x* towards $\pm\infty$ and in the bound state for the value $\psi^*(x)\psi(x)dx = 0$ at x towards $\pm\infty$.

If the three requirements above are met, then the wave function $\psi(x)$ is considered a function of good behavior.

Suppose the wave function to be normalized is the wave function in equation (10),

$$\psi(x) = A\sin\left(\frac{n\pi}{L}\right)x \qquad (36)$$

The normalization of the wave function must be fulfilled with the integral form $\int_{-\infty}^{\infty}|\psi(x)|^2dx = A^2\int_0^L \sin^2\left(\frac{n\pi}{L}x\right)dx = 1$ and the result of the integration of the wave function above as the result of normalization of the wave function is nothing but $A = \sqrt{\frac{2}{L}}$. Here are the following steps for the integration process:

$$A^2 \int_0^L sin^2\left(\frac{n\pi}{L}x\right)dx = 1 \qquad (37)$$

By taking the value example of $n = 1$ and applying the trigonometric identity $sin^2\theta = \frac{1-cos2\theta}{2}$, then the integration step above becomes:

$$\int_0^L sin^2\left(\frac{\pi}{L}x\right)dx = \frac{1}{A^2}$$

$$\frac{1}{2}\int_0^L \left(1 - cos\left(\frac{\pi}{L}x\right)\right)dx = \frac{1}{A^2}$$

$$\left[x - sin\left(\frac{\pi}{L}x\right)\right]_0^L = \frac{2}{A^2}$$

$$[L - sin(\pi)] - [0 - sin\,(0)] = \frac{2}{A^2}$$

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

and the value of A is:

$$A = \sqrt{\frac{2}{L}} \qquad (38)$$

With the obtained value of A, then the complete normalized function is:

$$\psi(x) = \sqrt{\frac{2}{L}}sin\left(\frac{n\pi}{L}\right)x \qquad (39)$$

Based on the results of the integration above, it can be seen that for the region $x \leq 0$ and $x \geq 0$, the value of $\psi = 0$.

And by taking the example that the length of the one-dimensional space in which the particles are located is equal to $L = 1\,m$, then the normalized equation of the wave function becomes $\psi(x) = \sqrt{2}sin(n\pi)x$ .This condition can be visualized by using the help of the *Mathematica Wolfram* the state of the wave function for different values of n can be described as below.

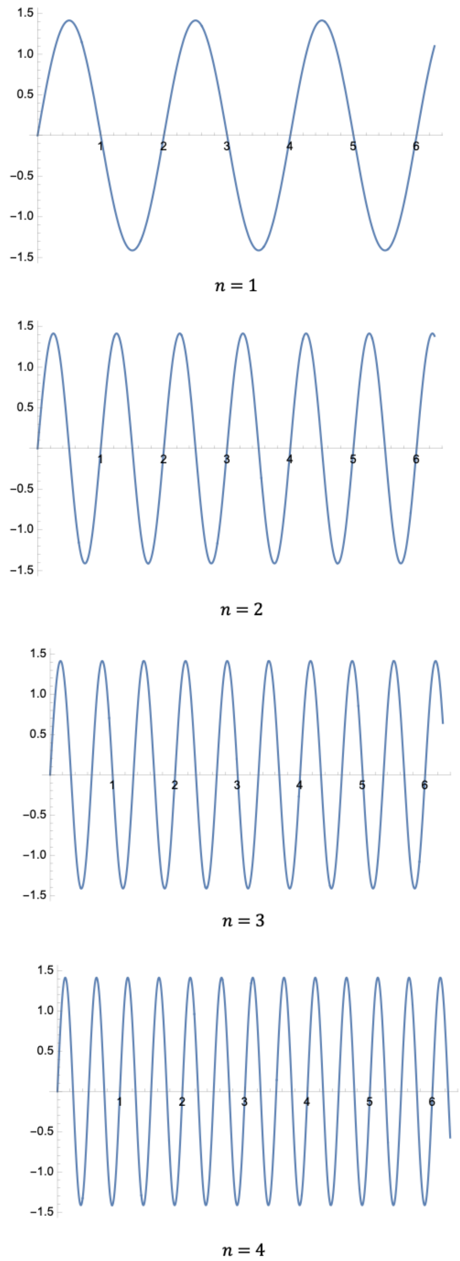

Figure 1. The wave function of a particle in a one-dimensional box with different values of *n*.

Physical Meaning of Schrodinger Equation of a Particle

The wave function $\psi(x)$ basically describes the quantum characteristics or *behaviour* of a particle, such as an electron particle trapped in a one-dimensional space. In addition, the wave function can describe the state of an electron in an atom of a particular element. For example, why an electron that revolves around the nucleus of an atom does not fall into the nucleus of an atom. It can be determined by assuming that electrons are not only particles but also waves so it requires a wave function to describe the *behaviour* of electrons.

According to Schrodinger, the wave function is nothing but charge density by assuming that electrons move in space and their charge spreads to every point in the space. However, the physical meaning of the wave function interpreted by Schrodinger was not entirely correct until finally, Max Born interpreted the wave function by squaring the wave function so that it becomes $|\psi(x)|^2$.

In his interpretation, Max Born considers that the wave function $\psi(x)$ is a way to determine the probability of the position of an electron at a point in space $|\psi(x)|^2$ is nothing but probability density is the probability of finding the position of an electron in one-dimensional space.

In Figure 2 below, it can be seen that when the position of the particle is at $x = 1$ (for $n = 1$), the probability density value obtained based on the graph is 0. This means that at point $x = 1$, the probability of finding electrons at that point is very small. Likewise at point with $x = 0.5$, $x = 1.0$, $x = 1.5$, and $x = 2.0$ with $n = 2$. While at the point where the amplitude of the wave function is very large, the possibility of finding electrons or particles at that point is very large because the probability density value is very large. Thus, it can be concluded clearly that the wave function does not tell the position of electrons or particles in space. , but only shows the probability of the position of the electron or particle.

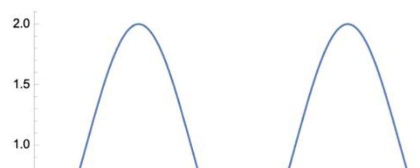

Figure 2. Probability distribution function

CONCLUSION

Based on the description and elaboration of the derivation of the Schrodinger equation for particles in the one-dimensional space above, it can be concluded that the general solution of the Schrodinger equation is a wave function. In general, based on mathematical calculations by applying the technique of solving differential equations to the Schrodinger equation, it can be seen that this equation has many solutions, but not all of these solutions can be said to be functions that meet the wave function criteria. This wave function must be able to interpret the real physical criteria of a particle. One of the criteria that satisfy the solution of the Schrodinger equation is none other than that the function can be normalized. In fact, by normalizing the function which is the solution to the obtained Schrodinger equation, it will obtain a probability value equal to one. If this Max Born’s statistical interpretation can be applied to a function that is a solution to the Schrodinger equation and is successfully normalized, then the function can be used to represent particles realistically. Thus, other functions that cannot be normalized are ordinary mathematical functions that have no physical meaning.

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