

Kurdistan Regional Government-Iraq  
Ministry of Higher Education and Scientific Research  
Salahaddin University-Erbil (<http://www.su.edu.krd> )  
College of Basic Education,  
Department of General Science



## **Quantum Theory and Schrodinger Equation A Literature Review**

The research

Submitted to the College of Basic Education as a part of the requirement of Bachelor Degree in  
General Science

2021-2022

**Prepared by**

Pawan Muhamad Ahmad

Shaima Wahid Salih

**Supervised by**

Dr.Mohammed Azeez Saeed

May 2022 A.D.

Ramadan 1442 H

Gulan 2721 K

**Dedication:**

This research project is the work of one academic year. It is decated to :

- My beloved family
- To all my teachers, who taught me throughout my life, especially assistant professor Dr. Mohammed Azeez Saeed who supervised this research work.

**Acknowledgments:**

I would like to send my warm and endless thanks and gratitude to my family who supported me during all the years of the study without which I was not able to continue my education. Also my special thanks is extended to Assistant Professor Dr. Mohammed Azeez Saeed for supervision of the study. Appreciations are due to the Department of General Science and the College of Basic Education for their support during the four years of the study.

**Table of Content:**

<b>Title</b>	<b>Page</b>
<b>Cover</b>	<b>1</b>
<b>Dedication &amp; Acknowledgment</b>	<b>2</b>
<b>Table of Content</b>	<b>3</b>
<b>Abstract/ Summary</b>	<b>4</b>
<b>Chapter One: Introduction</b>	<b>5</b>
<b>Quantum Theory of Light</b>	<b>5</b>
<b>Blackbody Radiation</b>	<b>6</b>
<b>Photoelectric Effect</b>	<b>7</b>
<b>Compton Effect</b>	<b>9</b>
<b>X-Rays</b>	<b>11</b>
<b>Bragg's Law</b>	<b>12</b>
<b>De Broglie wave-particle duality</b>	<b>12</b>
<b>Heisenberg Uncertainty principle</b>	<b>13</b>
<b>Chapter Two: Schrodinger Equation</b>	<b>14</b>
<b>Time dependent Schrodinger equation</b>	<b>14</b>
<b>Time independent Schrodinger equation</b>	<b>14</b>
<b>Derivation of Schrodinger equation</b>	<b>14</b>
<b>Chapter Three: Solving Schrodinger equation</b>	<b>17</b>
<b>Particle in a 1-dimensional box</b>	<b>17</b>

<b>Define the potential energy</b>	<b>18</b>
<b>Solve the Schrodinger equation</b>	<b>18</b>
<b>Define the wavefunction</b>	<b>19</b>
<b>Determine the allowed energies</b>	<b>20</b>
<b>Chapter four: Discussion</b>	<b>21</b>
<b>Chapter Four : Conclusions</b>	<b>20</b>
<b>Suggestions</b>	<b>21</b>
<b>Conclusions</b>	<b>22</b>
<b>Suggestions for future work</b>	<b>22</b>
<b>References</b>	<b>23</b>

## **Abstract/Summary**

In this research paper a detailed literature review of Quantum mechanics ( theory) was carefully revisited and analysed. All quantum physical phenomena such as photoelectric effect, Compton scattering of photons, X-rays and X- rays diffraction by plane crystals and deBogle wave-particle duality property of photons are stated and analyzed.

The Schrodinger equation for time dependent and independent is also talked and taken into consideration. The derivation of Schrodinger equation is outlined for three dimensional motions. The solution of Schrodinger equation for a particle in one dimensional box is analyzed and the results were tested and established.

It is concluded that the energy of a particle is quantized. This means it can only take one discrete energy values. The lowest possible energy for a particle is not zero (even at 0 K). This means the particle *always* has some kinetic energy.

**Keywords:** Quantum Mechanics, Quantum Theory, Schrodinger equation, Wavfunction

## Chapter One:

### 1.1 Introduction:

The **history of quantum mechanics** is a fundamental part of the history of modern physics. Quantum mechanics' began with a number of different scientific discoveries<sup>[1]</sup>:

- The 1838 discovery of cathode rays by Michael Faraday;
- The 1859–1860 black-body radiation problem by Kirchhoff;
- The 1877 suggestion by Boltzmann that the energy states and radiation law
- The discovery of the photoelectric effect by Heinrich Hertz in 1887
- In 1900 quantum hypothesis by Max Planck that the energy  $E$  is proportional to the frequency  $f$  as defined by the following formula:

$$E = h \times f \quad (1)$$

where  $h$  is called Planck's constant =  $6.63 \times 10^{-34}$  J.S.

### 1.2 Quantum theory of light:

Einstein in 1905, in order to explain the photoelectric effect previously reported by Hertz in 1887, postulated with Max Planck's quantum hypothesis that light itself is made of individual quantum particles, which in 1926 came to be called photons<sup>[1,2]</sup>.

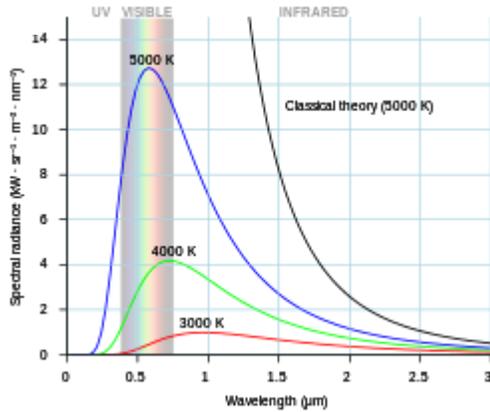
The photoelectric effect was observed upon shining light of particular wavelengths on certain materials, such as metals, which caused electrons to be ejected from those materials only if the light quantum energy was greater than the work function of the metal's surface.

The "quantum mechanics" was explained by the group of physicists including Max Born, Heisenberg, and Pauli, at the University of Göttingen in the early 1920s, and was first used by Born's 1924.

Boltzmann suggested in 1877 that the energy levels of a physical system, such as a molecule, could be discrete.

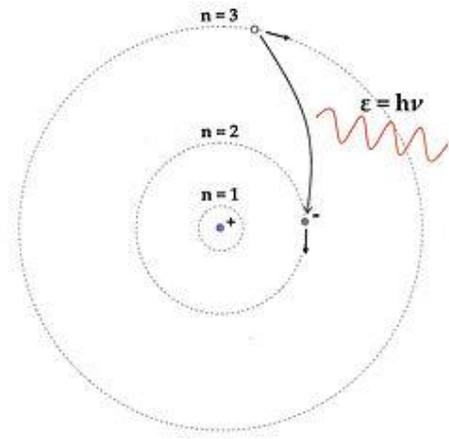
In 1900, the German physicist Max Planck reluctantly introduced the idea that energy is *quantized* in order to derive a formula for the observed frequency dependence of the energy emitted by a black body, called Planck's law.

These *energy quanta* are called "photons". The idea that each photon had to consist of energy in terms of quanta was a remarkable achievement; it effectively solved the problem of black-body radiation energy. In 1913, Bohr explained the spectral lines of the hydrogen atom, again by using quantization.



Figure(1): Blackbody radiation spectrum

With decreasing temperature, the peak of the **blackbody radiation** curve shifts to longer wavelengths and also has lower intensities<sup>[3]</sup>. The blackbody radiation curves (1862) , see figure(1) are also compared with the early, classical limit model of Rayleigh and Jeans (1900) shown on the same graph. The short wavelength side of the curves was already approximated in 1896 by the Wien distribution law.



Figure(2): Bohr quantum model of the Hydrogen atom.

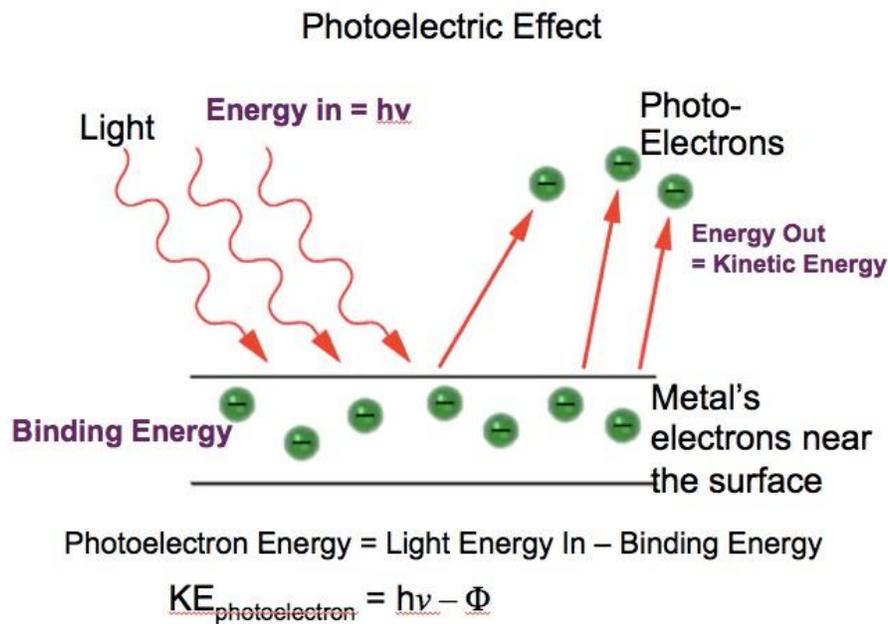
Bohr's 1913 quantum model of the atom, which incorporated an explanation of Rydberg's 1888 formula.

Max Planck's 1900 quantum hypothesis, is that atomic energy radiators have discrete energy values ( $\epsilon=h\nu$ ). Thomson's 1904 model, Einstein's 1905 light quanta postulate, and Rutherford's 1907 discovery of the atomic nucleus.

The electron does not travel along the black line when emitting a photon. It jumps, disappearing from the outer orbit and appearing in the inner one and cannot exist in the space between orbits 2 and 3.

In 1923, the French physicist de Broglie put forward his theory of matter waves by stating that particles can exhibit wave and particle characteristics. This theory was for a single particle and derived from special relativity theory. Quantum mechanics was born in 1925. when Erwin Schrödinger invented wave mechanics and the non-relativistic Schrödinger equation as an approximation to the generalised case of de Broglie's theory. Schrödinger subsequently showed that the two approaches were equivalent.

### 1.3 The Photoelectric Effect:



Figure(3): The photoelectric effect.

The photoelectric effect occurs when light above a certain frequency (the threshold frequency) is shone on metals like zinc, this causes electrons to escape from the zinc. The escaping electrons are called photoelectrons. It was shown in experiments that<sup>[3,4]</sup>;

- the frequency of the light needed to reach a particular minimum value (depending on the metal) for photoelectrons to start escaping the metal
- the maximum kinetic energy of the photoelectrons depended on the frequency of the light not the intensity of the light

The above two observations can only be explained if the electromagnetic waves are emitted in packets of energy (quanta) called photons, the photoelectric effect can only be explained by the particle behaviour of light.

The photoelectric equation involves;

- $h$  = the Planck constant  $6.63 \times 10^{-34}$  J s
- $f$  = the frequency of the incident light in hertz (Hz)
- $\Phi$  = the work function in joules (J) = amount of the energy binding the electron to the metal.
- $E_k$  = the maximum kinetic energy of the emitted electrons in joules (J)

Then  $hf = \Phi + E_k$  (2)

The energy of a photon of light is  $hf$  and the work function ( $\phi$ ) is the minimum energy required to remove an electron from the surface of the material.

So we can see from the equation above that if the light does not have a big enough frequency ( $f$ ) so that the photon has enough energy to overcome the work function ( $\phi$ ), then no photoelectrons will be emitted.

The above equation can be rearranged into the form

$$y = mx + c$$

So plotting a graph of frequency ( $f$ ) on the x-axis and maximum kinetic energy ( $E_k$ ) on the y-axis will give a straight line graph. Where the slope is the Planck constant ( $h$ ) and the y intercept is the work function ( $\phi$ ), the intercept on the x-axis is the threshold frequency  $f_0$ .

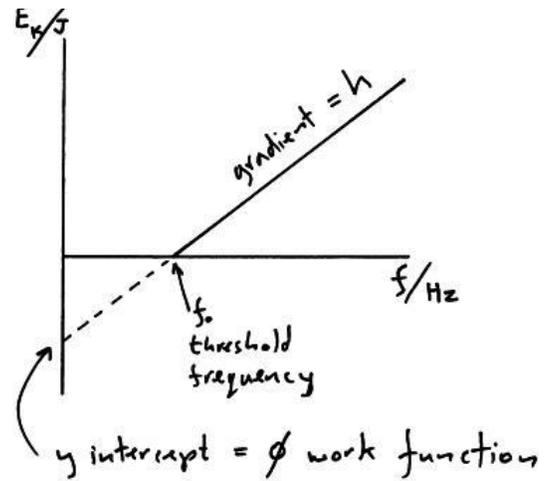
$$hf = \phi + E_k$$

$$hf - \phi = E_k$$

$$E_k = hf - \phi$$

$$y = mx + c$$

1.4  
Compton



scattering(Effect):

Discovered by Arthur Holly Compton, is the scattering of a photon by a charged particle, usually an electron. It results in a decrease in energy (increase in wavelength) of the photon (which may be an X-ray or gamma ray photon), called the **Compton effect**. Part of the energy of the photon is transferred to the recoiling electron. **Inverse Compton scattering** occurs when a charged particle transfers part of its energy to a photon.

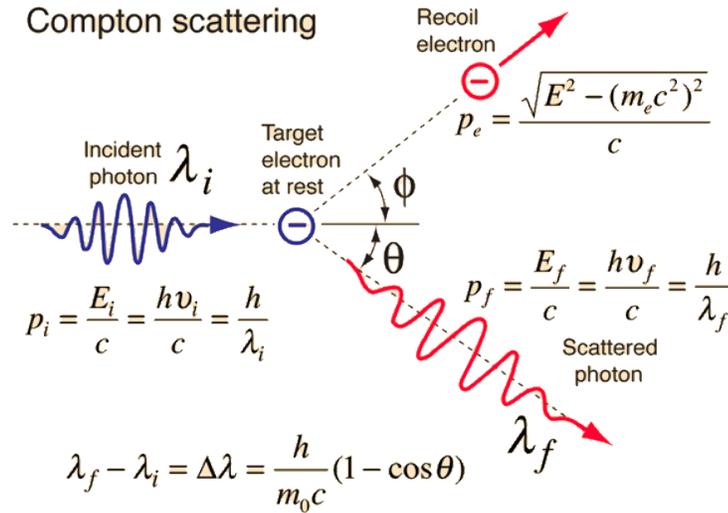
Arthur H. Compton observed the scattering of x-rays from electrons in a carbon target and found scattered x-rays with a longer wavelength than those incident upon the target. The shift of the wavelength increased with scattering angle according to the Compton formula (equation 3) below:

$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_e c} (1 - \cos\theta) \quad (3)$$

Compton explained and modeled the data by assuming a particle (photon) nature for light and applying conservation of energy and conservation of momentum to the collision between the photon and the electron<sup>[5]</sup>. The scattered photon has lower energy and therefore a longer wavelength according to the Planck relationship. Here the quantity  $h/m_e c$  is known as Compton wavelength and equal to

$$\lambda_c = h/m_e c = 2.43 \times 10^{-12} \text{ m} \quad (4)$$

At a time (early 1920's) when the particle (photon) nature of light suggested by the photoelectric effect was still being debated, the Compton experiment gave clear and independent evidence of particle-like behavior. Compton was awarded the Nobel Prize in 1927 for the "discovery of the effect named after him".



Figure(3): Compton scattering(effect) of a photon and a free electron at rest.

### 1.5 X-Rays:

X-rays were discovered in 1895 by Roentgen. He found that a beam of high-speed electrons striking a metal target produced a new and extremely penetrating type of radiation<sup>[5,6]</sup>. Within months of Roentgen's discovery the first medical x-ray pictures were taken, and within several years it became evident that x-rays were electromagnetic vibrations similar to light but with extremely short wavelengths and great penetrating power. Estimates obtained from the diffraction of x-rays by a narrow slit showed x-ray wavelengths to be about  $10^{-10}$  m, which is of the same order of magnitude as the atomic spacing in crystals. William Henry Bragg and William Lawrence Bragg in England suggested using single crystals such as calcite as natural three-dimensional gratings, the periodic atomic arrangement in the crystals constituting the grating rulings. A particularly simple method of analyzing the scattering of x-rays from parallel crystal planes was proposed by W. L. Bragg in 1912.

### 1.5.1 Conditions of producing X-Rays:

1. The three things needed to create x-rays are a source of electrons, a means of accelerating the electrons to high speeds, and a target for the accelerated electron to interact with.
2. X-rays are produced when the free electrons cause energy to be released as they interact with the atomic particles in the target.

X-rays are produced by bombarding a metal target (copper, tungsten) with energetic electrons having energies of 50 to 100 keV<sup>[6]</sup>. The minimum continuous x-ray wavelength,  $\lambda_{\min}$ , is found to depend only on the tube voltage,  $V$ . All of the incident electron's kinetic energy is converted to electromagnetic energy in the form of a single x-ray photon. For this case we have

$$eV = hf = hc / \lambda_{\min}$$

$$\text{Then } \lambda_{\min} = hc / eV$$

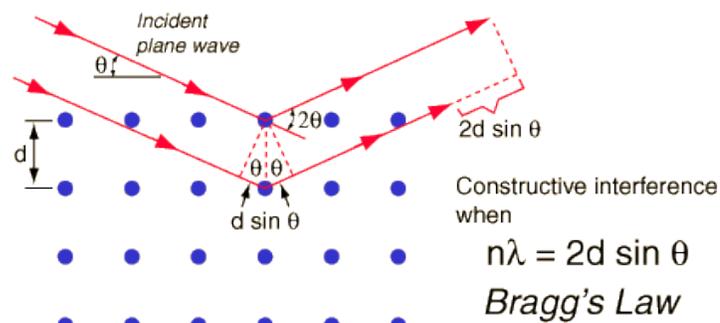
$$\text{Then } \lambda_{\min} = 6.63 \times 10^{-34} \times 3 \times 10^8 / V \times 1.6 \times 10^{-19}$$

$$\lambda_{\min} = 12.4 \times 10^{-7} = 1.24 / MV \quad (4)$$

### 1.6 Bragg's Law ( X-Rays diffraction):

X-Rays are scattered when it falls on a plane of crystal atoms. The equation of the scattering is called Bragg's law<sup>[5,6]</sup>. As shown in figure(4).

$$\text{Then } n \lambda = 2d \sin(\theta) \quad (5)$$



Figure(4) Bragg Diffraction Law

### 1.7 De Broglie particle- wave duality:

By the early 1920s scientists recognized that the Bohr theory contained many

inadequacies:

- It failed to predict the observed intensities of spectral lines.
- It had only limited success in predicting emission and absorption wavelengths for multielectron atoms.
- It failed to provide an equation of motion governing the time development of atomic systems starting from some initial state.
- It overemphasized the particle nature of matter and could not explain the newly discovered wave–particle duality of light.
- It did not supply a general scheme for “quantizing” other systems, especially those without periodic motion.

The first bold step toward a new mechanics of atomic systems was taken by Louis Victor de Broglie in 1923 . He postulated that *because photons have wave and particle characteristics, perhaps all forms of matter have wave as well as particle properties.*

According to de Broglie, electrons had a dual particle–wave nature. Accompanying every electron was a wave. He concluded that the wavelength and frequency of a *matter wave* associated with any moving object were given by

$$\lambda = h/p \text{ and } E = hf$$

Where  $p = mv$  is the momentum of the particle, and  $h$  is Planck’s constant,  $p$  is the momentum, and  $E$  is the total energy of the particle.

$$\text{Thus } \lambda = h/mv \quad (6)$$

### **1.8 Heisenberg uncertainty Principle:**

In 1927 Heisenberg<sup>[6]</sup> developed his idea concerned with the wave-particle duality that:

It is impossible to determine simultaneously the position and momentum of particle.

If a measurement of a position is made with  $dx$  and simultaneously a measurement of the momentum is made with  $dp$  in the  $x$  - direction, the product can never be smaller than  $h/2$  .

Thus

$$\Delta x \cdot \Delta p \geq \hbar/2 \quad (7) \text{ position – momentum uncertainty principle}$$

This means as one uncertainty increase, the other one decrease. And as one uncertainty approaches infinity, the other one must approach zero.

The uncertainty in energy and time is also in the form

$$\Delta E \cdot \Delta t \geq \hbar/2 \quad (8) \quad \text{energy-time uncertainty principle}$$

## Chapter Two:

### 2.1 Schrodinger Equation:

The **Schrödinger equation** is a linear partial differential equation that describes the wave function or state function of a quantum-mechanical system<sup>[7,8]</sup>. It is a key result in quantum mechanics, and its discovery was a significant landmark in the development of the subject. The equation is named after Erwin Schrödinger, who derived the equation in 1925, and published it in 1926.

#### 2.1.1 Time dependent Schrodinger equation is

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[ \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t) \quad (9)$$

#### 2.1.2 Time independent Schrodinger equation is :

$$\left[ \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad (10)$$

### 2.2 Derivation of Schrodinger Equation:

Schrodinger equation is the most important and fundamental equation of the modern physics. Schrodinger equation for a quantum system is a powerful analog of Newton's 2<sup>nd</sup> law of motion for a classical system<sup>[9]</sup>.

Mathematical construction of Schrodinger equation is correct. The establishment of Schrodinger equation is unreasonable in Physics. There is no doubt that the use of Schrodinger equation

violates the law of conservation of energy .Thus Schrodinger equation is unsuitable to be applied to any physical system.

Photon exhibits wave-particle duality. According to Einstein, energy & momentum of a photon is

$$E= h\nu= \hbar\omega , \quad p=E/c = h/\lambda = \hbar k \quad (11)$$

Where  $\omega= 2\pi\nu$ =angular frequency ,  $k= 2\pi/ \lambda =$  wave number and  $\hbar$  equals  $h=2\pi$  = reduced Planck constant

All matter, not only photon, possesses the wave –particle duality. For free material particle, de-Broglie has showed that the frequency and wavelength of the associated wave of the particle are<sup>[10]</sup>:

$$\nu_d =E/h \quad \text{and} \quad \lambda_d= h/p \quad (12)$$

$\lambda_d$  can be obtained, if mass and velocity of the particle are known:

$$\lambda_d =h/p = h/mv \quad \text{and} \quad E=1/2mv^2 \quad \text{then} \quad v= \sqrt{( 2E/m)}$$

$$\text{Thus } \lambda_d = h/m\sqrt{( 2E/m)} = h/\sqrt{( 2mE)} \quad (13)$$

Encouraged by de-Broglie hypothesis, in 1926, Erwin Schrodinger invented an equation to describe the wave behavior of matter particle (electron), as follow:

$$i\hbar \partial \Psi(\mathbf{r},t)/ \partial t = - \hbar^2/2m\nabla^2 \Psi(\mathbf{r},t) + V\Psi(\mathbf{r},t) \quad (14)$$

The operator  $\nabla^2=\partial^2/ \partial x^2 + \partial^2/ \partial y^2 + \partial^2/ \partial z^2$  is the Laplacian in Cartesian coordinates.

$\Psi(\mathbf{r},t)$  is the wavefunction

$V(\mathbf{r},t)$  is the potential energy

$\hbar$  is reduced Planck constant and  $m=$  the mass of the particle

The wavefunction in Schrodinger equation is commonly accepted to be a probability of finding the particle at a certain position.

There have been many attempts to derive the Schrodinger equation from different principles. All these attempts are unsuccessful. They are either mathematically flawed or physically unreasonable. It has been shown that the role of Schrodinger equation is to transform the system into uncertain and unrelated physical system.

Physical research without mathematics is very hard to imagine. Physicists use mathematics as a tool to assist their research and to guide their research. It is a mistake to blindly believe that mathematics can tell everything about the universe.

It is likely that Schrodinger established his equation basing on three main criteria<sup>[11]</sup>;

Criteria 1: Energy and momentum [equation 2] can be expressed in the form of the angular frequency and wave number  $k$  as;

$$E = \hbar\omega, \quad p = \hbar k \quad (15)$$

Criteria 2: The total mechanical energy  $E$  of a material is conserved, that is:

$$E = E_k + E_p$$

$$E = p^2/2m + V(r) \quad (16)$$

$E_k =$  Kinetic energy and  $E_p =$  Potential energy

Criteria 3: In classical physics, the plane wave equation is :

$$A(r,t) = A_0 e^{i(k \cdot r - \omega t)} \quad (17)$$

Schrodinger assumed that matter wave can also be described by plane wave equation. Thus put equation(5) into equation (7), one can get:

$$\Psi(r,t) = \Psi_0 e^{[i/\hbar(p \cdot r - Et)]} \quad (18)$$

Next step. Schrodinger probably multiplied equation (6) by equation (8), thus

$$[p^2/2m + V(r)]\Psi(r,t) = E \Psi(r,t) \quad (19)$$

This operation is allowed in mathematics, but in physics, it is prohibited. At that time Schrodinger must not be able to recognize this problem.

Schrodinger was quite satisfied that energy and momentum in equation (1) can be expressed by the following operators:

$$E = i\hbar \partial / \partial t, \quad p = -i\hbar \nabla \quad (20)$$

Where energy operator correspond to time derivatives and momentum operator correspond to spatial derivatives, thus

$$i\hbar \partial \Psi(r,t) / \partial t = -\hbar^2/2m \nabla^2 \Psi(r,t) + V\Psi(r,t) \quad (21)$$

Which is exactly equation (14), the so-called “an inspired passage”.

The solution of the Schrodinger equation for the Hydrogen atom has always been recognized as the most successful application of quantum mechanics. The physics community believes that all conclusions deduced from the Schrodinger equation are impossible to be the physical facts. Because the application of the Schrodinger equation will eventually cause the change of the physical system. Moreover, the Schrodinger equation may create some man - made physical phenomena, such as the uncertainty of the physical quantities and non-locality of the matter particles. Hence, it is argued that the Schrodinger equation was based upon a misunderstanding

of the real physical world. Without doubt, the physics community must now be aware that it is time to abandon the Schrodinger equation.

## **Chapter Three:**

### **3.1 Solving Schrodinger Equation**

Solution of schrodinger equation is an attempt to find a wave function which satisfy the Schrodinger equation<sup>[11,12]</sup>. A wave function is a mathematical function and it is the solution of the Schrodinger equation. For simplicity, let us consider a particle in one dimensional box.

### **3.2 Particle in a 1-Dimensional box**

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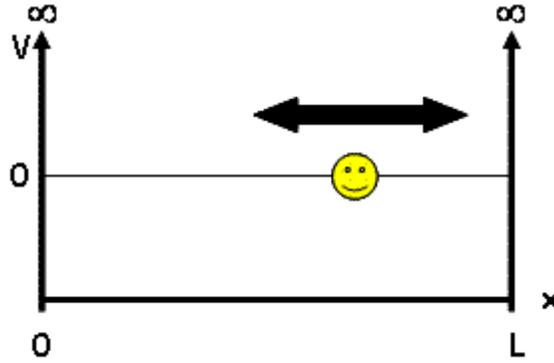
A particle in a 1-dimensional box is a fundamental quantum mechanical approximation describing the translational motion of a single particle confined inside an infinitely deep well from which it *cannot* escape<sup>[12,13]</sup>.

The particle in a box problem is a common application of a quantum mechanical model to a simplified system consisting of a particle moving horizontally within an infinitely deep well from which it cannot escape. The solutions to the problem give possible values of  $E$  and  $\psi$  that the particle can possess.  $E$  represents allowed energy values and  $\psi(x)$  is a wavefunction, which when squared gives us the probability of locating the particle at a certain position within the box at a given energy level.

To solve the problem for a particle in a 1-dimensional box, we must :

1. Define the Potential Energy,  $V$
2. Solve the Schrödinger Equation
3. Define the wavefunction
4. Define the allowed energies

#### **3.2.1 Step 1: Define the Potential Energy $V$**



Figure(5): A particle in a 1D infinite potential well of dimension  $L$ .

The potential energy is 0 inside the box ( $V=0$  for  $0 < x < L$ ) and goes to infinity at the walls of the box ( $V=\infty$  for  $x < 0$  or  $x > L$ ). We assume the walls have infinite potential energy to ensure that the particle has zero probability of being at the walls or outside the box<sup>[13]</sup>. Doing so significantly simplifies our later mathematical calculations as we employ these **boundary conditions** when solving the Schrödinger Equation.

### 3.2.2 Step 2: Solve the Schrödinger Equation

The time-independent Schrödinger equation for a particle of mass  $m$  moving in one direction with energy  $E$  is<sup>[14]</sup>:

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

with

- $\hbar$  is the reduced Planck Constant where  $\hbar = \frac{h}{2\pi}$
- $m$  is the mass of the particle
- $\psi(x)$  is the stationary time-independent wavefunction
- $V(x)$  is the potential energy as a function of position
- $E$  is the energy, a real number

This equation can be modified for a particle of mass  $m$  free to move parallel to the  $x$ -axis with zero potential energy ( $V = 0$  everywhere) resulting in the quantum mechanical description of free motion in one dimension:

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

This equation has been well studied and gives a general solution of:

$$\psi(x) = A\sin(kx) + B\cos(kx) \quad (3)$$

where  $A$ ,  $B$ , and  $k$  are constants.

### 3.2.3 Step 3: Define the wavefunction

The solution to the Schrödinger equation we found above is the general solution for a 1-dimensional system. We now need to apply our **boundary conditions** to find the solution to our particular system<sup>[14]</sup>. According to our boundary conditions, the probability of finding the particle at  $x=0$  or  $x=L$  is zero. When  $x=0$ ,  $\sin(0)=0$  and  $\cos(0)=1$ ; therefore,  $B$  must equal 0 to fulfill this boundary condition giving:

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

We can now solve for our constants (A and k) systematically to define the wavefunction.

#### Solving for k

Differentiate the wavefunction with respect to x:

$$d\psi/dx = kA \cos(kx) \quad (5)$$

$$d^2\psi/dx^2 = -k^2 A \sin(kx) \quad (6)$$

Since  $\psi(x) = A \sin(kx)$ , then

$$d^2\psi/dx^2 = -k^2 \psi \quad (7)$$

If we then solve for k by comparing with the Schrödinger equation above, we find:

$$k = (8\pi^2 m E h^2)^{1/2} \quad (8)$$

Now we plug k into our wavefunction:

$$\psi = A \sin((8\pi^2 m E h^2)^{1/2} x) \quad (9)$$

#### Solving for A

To determine A, we have to apply the boundary conditions again. Recall that the *probability of finding a particle at  $x = 0$  or  $x = L$  is zero*.

When  $x=L$ :

$$0 = A \sin((8\pi^2 m E h^2)^{1/2} L) \quad (10)$$

This is only true when

$$(8\pi^2 m E h^2)^{1/2} L = n\pi \quad (11)$$

where  $n = 1, 2, 3, \dots$

Plugging this back in gives us:

$$\psi = A \sin(n\pi x/L) \quad (12)$$

To determine  $A$ , recall that the total probability of finding the particle inside the box is 1, meaning there is no probability of it being outside the box. When we find the probability and set it equal to 1, we are *normalizing* the wavefunction.

$$\int_0^L \psi^2 dx = 1 \quad \int_0^L \psi^2 dx = 1$$

For our system, the normalization looks like:

$$A^2 \int_0^L \sin^2(n\pi x/L) dx = 1 \quad (10) \quad A^2 \int_0^L \sin^2(n\pi x/L) dx = 1$$

Using the solution for this integral from an integral table, we find our normalization constant,  $A$ :

$$A = \sqrt{2/L} \quad (11) \quad A = \sqrt{2/L}$$

Which results in the normalized wavefunction for a particle in a 1-dimensional box:

$$\psi = \sqrt{2/L} \sin(n\pi x/L) \quad (12) \quad \psi = \sqrt{2/L} \sin(n\pi x/L)$$

### 3.2.4 Step 4: Determine the Allowed Energies

Solving for  $E$  results in the allowed energies for a particle in a box<sup>[15]</sup>:

$$E_n = n^2 h^2 / 8mL^2 \quad (13) \quad E_n = n^2 h^2 / 8mL^2$$

This is an important result that tells us:

1. The energy of a particle is quantized and
2. The lowest possible energy of a particle is **NOT** zero. This is called the **zero-point energy** and means the particle can never be at rest because it always has some kinetic energy.

This is also consistent with the Heisenberg Uncertainty Principle, if the particle had zero energy, we would know where it was in both space and time.

## Chapter Four:

### 4.1 Discussion: What does all this mean?

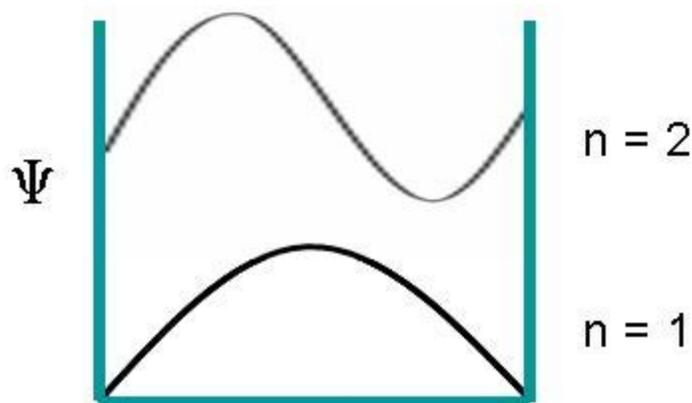
The particle in a box model (also known as the infinite potential well or the infinite square well) describes a particle free to move in a small space surrounded by impenetrable barriers<sup>[14]</sup>. The model is mainly used as a hypothetical example to illustrate the differences between classical and quantum systems.

In classical systems, for example a ball trapped inside a large box, the particle can move at any speed within the box and it is no more likely to be found at one position than another. However, when the well becomes very narrow (on the scale of a few nanometers), quantum effects become important<sup>[15]</sup>. The particle may only occupy certain positive energy levels. The particle in a box model provides one of the very few problems in quantum mechanics which can be solved analytically, without approximations.

This means that the observable properties of the particle (such as its energy and position) are related to the mass of the particle and the width of the well by simple mathematical expressions. Due to its simplicity, the model allows insight into quantum effects without the need for complicated mathematics. It is one of the first quantum mechanics problems taught in undergraduate physics courses, and it is commonly used as an approximation for more complicated quantum systems.

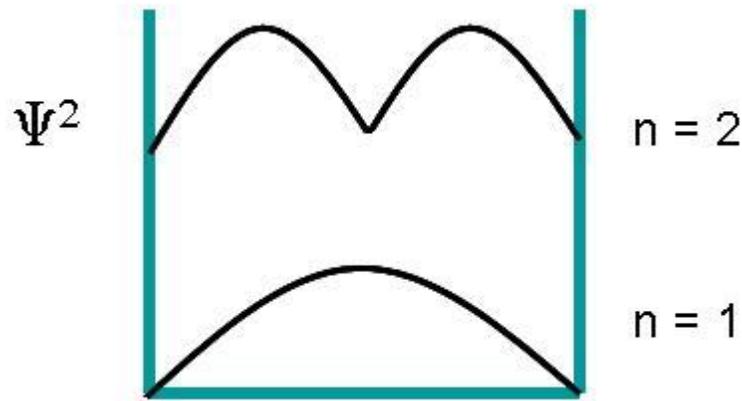
The particle in the box model system is the simplest non-trivial application of the Schrödinger equation, but one which illustrates many of the fundamental concepts of quantum mechanics. The state of lowest energy for a quantum system is termed its ground state<sup>[14,15]</sup>.

The wavefunction for a particle in a box at the  $n=1$  and  $n=2$  energy levels look like figure(6):



Figure(6):

The probability of finding a particle a certain spot in the box is determined by squaring  $\psi$ . The probability distribution for a particle in a box at the  $n=1$  and  $n=2$  energy levels looks like figure(7):



Figure(7)

Notice that the number of **nodes** (places where the particle has zero probability of being located) increases with increasing energy  $n$ . Also note that as the energy of the particle becomes greater, the quantum mechanical model breaks down as the energy levels get closer together and overlap, forming a continuum. This continuum means the particle is free and can have any energy value. At such high energies, the classical mechanical model is applied as the particle behaves more like a continuous wave. Therefore, the particle in a box problem is an example of the wave – particle duality.

#### 4.2 Conclusions:

- It is shown that, even though the mathematical procedure of the construction may be correct, it is evident that the establishment of the Schrödinger equation is unreasonable in physics.
- It is inevitable that the use of the Schrödinger equation will violate the law of conservation of energy.
- Hence, we argue that the Schrödinger equation is unsuitable to be applied to any physical systems
- The energy of a particle is quantized. This means it can only take on discrete energy values.

- The lowest possible energy for a particle is **NOT** zero (even at 0 K). This means the particle *always* has some kinetic energy.
- The square of the wavefunction is related to the probability of finding the particle in a specific position for a given energy level.
- The probability changes with increasing energy of the particle and depends on the position in the box you are attempting to define the energy for
- In classical physics, the probability of finding the particle is independent of the energy and the same at all points in the box

### **Suggestions for future work:**

It is suggested here that more research and scientific explanations should be conducted on how Schrodinger derived and solved his equation in quantum mechanics. The application of mathematical tools and using advanced software in derivation and solving Schrodinger equation are necessary and needed.

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