CHAPTER I
INTRODUCTION

1.1 History of Quantum Mechanics

The history of Quantum Mechanics began essentially with 1838 discovery of cathode ray by Michael Faraday, 1859 statement of Blackbody radiation problem by Gustav Kickoffs, 1877 suggestion by Ludwig Boltzman that energy state could be discrete and 1900 quantum hypothesis by MaxPlank that energy is radiated and absorbed in quantities visible by discrete 'Energy element' E, such that this elements is proportional to the frequency υ with which individually radiated energy as defined by the following formula; $E = h\upsilon = h\omega$, (Zettili, 2007; Wikipedia, free encyclopedia, 07 November 2009; Brown & Rechenberg, 2005).

To be more elaborative, towards the end of nineteenth century, the classical mechanics the theory of electromagnetism and thermodynamics were the main aspect of physics at that time. Classical mechanics was used to predict the dynamics of *material bodies* and Maxwell's electromagnetism provided the proper framework to the study of *radiation*;

matter and *Radiation* were described in terms of *particles* and *waves* respectively. Lorentz force or thermodynamics have explained well, the interactions between matter and Radiation. All these overwhelming successes of classical Physics – classical mechanics, made people to believe that the ultimate description of nature had been achieve. As if all known physical phenomenon could be explained within the general theories of matter and radiation.

At the turn of twenty century, as highlighted by Zettili (2007) however, classical Physics, which had been quite unassailable, was seriously challenged on two front; the first one was the "Relativistic domain" – Einstein's 1905 theory of relativity showed that the validity of Newtonian mechanics ceases at very high speed (i.e at speed comparable to that of light). The second front was the "Microscopic domain" – newly experimental techniques were developed to the point of proving the atomic and subatomic structures. These development shows that the classical physics has fail to provide the proper explanation for several newly discovered phenomena. It thus became evident that the validity of classical Physics ceases at microscopic level and that, new concept had to be invoked to describe, for instant, the structure of atoms and molecules and how light interact with them. Microscopic phenomena such as Blackbody radiation, Photoelectric effect, the atomic stability and microscopy that were not explained by classical Physics had cleared the way for seeking new ideas outside its purview.

In 1900, there comes to the first real breakthrough when MaxPlank introduced the concept of "quantum energy". In his effort to explain the Blackbody radiation, he was able to reproduced experimental results only after postulating that, the energy between radiation and environment takes place in discrete or quantized amounts (Zettili, 2007; Brown & Rechenberg, 2005). He argued that the energy exchange between an electromagnetic waves of frequency υ and matter occurs only in integer multiple of $h\upsilon$ which he called the energy of quantum, where h is a plank constant. This idea posted by plank that gave accurate explanation of Blackbody radiation, prompted new thinking and triggered an avalanche of new discoveries that yielded solutions to the most outstanding problems of the time.

The next major breakthrough was by Einstein in the year 1905 who try to consolidate the work of plank quantum concept. In trying to understand the photoelectric effect, Einstein recognized that, Planck idea of quantization of electromagnetic waves must be valid for light as well. So, following Planck's approach, he postulated that light itself is made up of discrete bits of energy (or tiny particles) called photons each of energy $h\upsilon$, where υ is the frequency of light (Zettili, 2007). The introduction of photons concept enable Einstein to give an elegantly accurate explanation to photoelectric problem, a development that was quite waiting for its solution ever since 1887 when Sir Hertz postulated his first experimental observation.

Furthermore in1913, Neil Bohr, introduced his model of Hydrogen atom. This development came after the experimental discovery of atomic nucleus in 1911 by

Rutherford, and couple with planck's quantum concept and Einstein's photons that Bohr argue that atoms can be found only in discrete energy states and the interaction of atom with radiation takes place only in discrete amount of $h\upsilon$ because it was as a result of transmission of atom between its various discrete energy states. This work provided satisfactory explanation to several outstanding problems such as atomic stability and atomic spectroscopy (Zettili, 2007).

In 1923 Compton came up with a very important discovery which gave the most conclusive confirmation for corpuscular aspect of light. Compton scattered an X-rays with electrons and then gave confirmation that the X-ray photons behave like particle with momenta $\frac{h\upsilon}{c}$; where υ is the frequency of the X-rays and c is the speed.

All these series of breakthrough starting from Planck, then Einstein, then Bohr and to the Compton gave both theoretical foundation as well as experimental confirmation that *waves* exhibit particle behavior at the microscopic scale which classical Physics could not explain, thereby failing not only quantitatively but even qualitatively and conceptually.

Moreover again, in 1923 de Broglie introduced another powerful new concept which could not be reconcile by classical Physicists. De Broglie noted that not only does radiation exhibit *particle-like* behavior but, *material particles* themselves exhibit *wave-like* behavior. This concept was experimentally confirmed by Davisson and Germer in 1927.

Even though the Bohr model of atom was criticized for not following the first principle of a theory, like quantization scheme by Planck, were quite arbitrary. It was this dissatisfaction of the arbitrary nature of Planck's idea and Bohr's postulate as well as the need to fit them within the context of a consistent theory that prompted *Heisenberg Schrödinger* to search for theoretical foundation underlining these new idea and there effort paid off in 1925 when they welded (skillfully) the various experimental findings as well as Bohr's postulates into a refined theory called idea and there effort paid off in 1925 when they welded (skillfully) the various experimental findings as well as Bohr's postulates into a refined theory called "Quantum mechanics". This theory became very reliable and powerful that enable it to explore and unravel many uncharted areas of microphysical world. The theory also has put an end to twenty-five years (1900-1925) of patch work which was dominated by Planck and Bohr and which letter became known as old quantum theory (Zettili, 2007).

1.2 Formulation of Schrödinger equation

Historically, according to Zettili (2007) there were two independent formulations of Quantum mechanics. The first formulation called *Matrix mechanics* was developed by Heisenberg (1925) to describe the atomic structure starting from observed spectral lines. This formulation goes well in that, it provided a good account on the discrete quanta of light emitted and absorbed by atom.

The second formulation as Zettili and Hamdan et al. (2007) highlighted was by Schrödinger (1926) called *Wave Mechanics*; it is a generalization of the de Broglie postulate. This method was more intuitive than matrix mechanics, describes the dynamics of microscopic matter by means of *wave equation* called Schrödinger equation. Schrödinger obtained a differential equation. The solution of this yielded energy spectrum under consideration. These two different formulations – Schrödinger's wave formulation and Heisenberg matrix approach – were shown to be equivalent. Then later came P.A.M Dirac in 1928, (Hotson, 2002; Zettili, 2007 Hamdan et al., 2007; Brown & Rechenberg, 2005) to suggest a more general formulation of quantum mechanics which deals with abstract object such as kets (state vector), brass and operator. Combining special relativity with quantum mechanics, Dirac derived an equation which describes the motion of electron. This equation, known as Dirac's equation predicted the existence of an anti particle the *Positron* which has similar properties but opposite charge with electron; the positron was discovered in 1932 – four years after its prediction by quantum mechanics.

Summarily, we can therefore say that the formulations of quantum mechanics cannot be unconnected with the fact that, the already established *Classical Mechanics* that was known (up to the end of 19th century) fail to explain several microscopic phenomenon such as blackbody radiation, Photoelectric effects and alike. That, quantum mechanics was based on number of observations that defied classical explanation, (Swanson, 2006). We can also say at presence that quantum mechanics remain the only valid framework that described the microphysical world. It is also vital for understanding the Physics of solids, lasers, semiconductor and superconductor devices, plasma etc. In short, quantum mechanics is the founding basis of all modern Physics; Solid-state, nuclear, atomic and particle Physics, Optics, Thermodynamics, Statistical mechanics and so on. Not only that it is also considered to be the foundation of chemistry and Biology (Zettili, 2007).

The Schrödinger equation (Kosloff D & Kosloff R, 1982; Schiesser & Griffith, 2009; Zettili, 2007) is given by;

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x) \qquad (1.2.1)$$

This is the time-dependent Schrödinger equation that we took as our problem in this research work. We used the Method of Lines (MOL) approach and solved the above partial differential equation (PDE). The method involved replacing the spatial (boundary-value) derivatives in the PDE with algebraic approximations and when we do this, the spatial derivatives became no longer stated explicitly in terms of spatial independent variable. We thereby had initial–value variable (time) in the problem to remain. We then used the Mathematical software (MATLAB) specifically used by Schiesser & Griffith (2009) in there effort to solve similar problem. We varied the discretization size (Δx) (at n =201, 251 and 301) and the step size (Δt) (within the intervals $0 \le t \le 35$, $0 \le t \le 32$, and $0 \le t \le 30$,) to see the effect *computational time* and *accuracy of the result* in each case. In the first case, the result indicated that, if we are interested in high accuracy of result then we should increase the number of grids n (i.e. decrease the discretization size Δx) and reduced the step size Δt, because this leads to high accuracy of the result and average computing time (CPU). But when we took the reverse case – that is we reduced the number of grids n (i.e. increase the discretization size Δx) and reduced the step size Δt, the computing time became more faster although the accuracy was not good. The second case was that, we tried maintaining the CPU time and begin to adjust the discretization size Δx while reducing the step size Δt, the result shows the same as in the *first case first problem*. We lastly took the reverse of the case, which is, we tried maintaining the CPU time and begin to adjust the step size Δt while reducing the discretization size Δx, but still the result was the same with that *first case, second problem.*