A MODEL OF THE HYDROGEN ATOM FOR $l = 1$ and $l = 3$ USING THE CAUSAL INTERPRETATION

By

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A DISSERTATION
Submitted to

The University of Zambia in partial fulfilment of the requirements for the degree of
Master of Science in Physics.

THE UNIVERSITY OF ZAMBIA
LUSAKA
2024

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Acknowledgements

I would like to express my gratitude to the individuals whose support and contributions have been instrumental in the completion of this project.

I am grateful to my supervisor, Professor Kaloyerou P. N. for the unwavering guidance, invaluable insights, and continuous availability throughout this research. His expertise and patience enriched the quality of this work.

I would also like to sincerely thank Kamphamba Nyirenda, a Physics Master's student at Jiangsu University (China), for being a source of encouragement and devoting his time to reviewing and improving the quality of this work.

Special thanks go to my parents and dear brothers for the financial support and the love to ensure that this research is completed. Not forgetting my wonderful friends who have always been a source of strength and encouragement throughout this work; Mwendalubi Kambombi, Eness Namwala, Racheal Nyirongo, Viginia Chiposa, Idah Banda, Kelly Zulu, and Tapera Mhoswa among others.

Thank you all for being part of this success.

Abstract

This study presents a model of the hydrogen atom for the orbital angular momentum $l = 1$ and $l = 3$ using the causal interpretation also referred to as the Bohm-de Broglie interpretation of quantum mechanics. The causal interpretation is an alternative interpretation of quantum mechanics that gives a description of underlying physical reality in terms of a single well-defined model which Bohr's principle of complementarity claims to be impossible. This study presents detailed analytical calculations to determine the electron trajectories for the hydrogen atom states ψ_{21m} and ψ_{43m}. Further analytical calculations were made to determine the net force and magnitude of the angular momentum. The model was also extended to determine the trajectory of the rotated wave function. This was done both analytically and numerically using Maple. Maple was also used to plot the trajectories, net force, and angular momentum. The obtained results show that electrons have definite circular paths which are a result of the net force which is always directed to the z-axis. The results for the angular momentum show consistency with quantum mechanics, as the plots show that the angular momentum vector at various positions of the electron for a given value of m form a cone shape in its movement. The results also show that the electron is stationary for $m = 0$, but rotates anti-clockwise for positive values of m and clockwise for negative values of m. From this work, it can be seen that the causal interpretation can be used to make models of quantum experiments/processes. This research therefore brings new light to the behaviour of an electron in atomic systems, thereby making contributions on the effort to develop a physical reality of quantum systems with implications in quantum chemistry and quantum physics. The presentation of this model also shows the effectiveness of Maple in developing computer models, especially in science and mathematics.

Keywords: *Causal interpretation, trajectories, wave function, Maple, hydrogen atom, net force, angular momentum.*

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List of Abbreviations & Symbols

BPC	**B**ohr's **P**rinciple of **C**omplementarity
BPR	**B**orn's **P**robability **R**ule
CE	**C**ontinuity **E**quation
CI	**C**ausal **I**nterpretation
EPR	**E**istein-**P**odolsky-**R**osen Experiment
H-J	**H**amilton-**J**acobi Equation
WKB	**W**entzel-**K**ramers-**B**rillouin approximation

Chapter 1

Introduction

Quantum mechanics is a fundamental branch of physics that deals with the behaviour of matter and light at atomic and subatomic levels. The theory deals with the unusual characteristics of matter that occur below the scale of an atom. Its origin can be traced back to 1900 with the introduction of quantisation of energy by Max Planck in the blackbody radiation problem[1]. The field of quantum mechanics is highly successful with many detailed calculations and technological applications. This success has been based on the Copenhagen interpretation comprising Born's probability rule (BPR) and Bohr's principle of complementarity (BPC).

The Copenhagen interpretation was presented at the 5^{th} physical Solvay Congress which was held from 24^{th} to 29^{th} October 1927 to discuss various interpretations of quantum mechanics[2]. The congress was attended by a group of the world's leading physicists, among whom were Einstein, Lorentz, Born, de Broglie, Dirac, Heisenberg, Pauli and Planck. Among the interpretations presented were de Broglie's pilot wave theory, BPR and BPC. Due to Pauli's objection related to Fermi's rigid rotator (which essentially had to do with the measurement problem of quantum mechanics), de Broglie's interpretation was rejected. By the end of the congress the Copenhagen interpretation was almost universally adopted and has been the dominant interpretation of quantum mechanics to this day. BPR is an essential interpretational element of quantum mechanics which links theory to experiment, while BPC is more of understanding the paradoxical duality revealed in experiments and is not directly linked to the mathematical formalism.

Starting with the measurement quantum postulate, Bohr, in his principle of complementarity, was led to conclude that an experiment should be viewed as an analysable whole. Therefore, to communicate quantum experimental results, classical concepts can be used[3]. He emphasised that, even though these concepts can be used to communicate quantum results, they cannot be attributed to physical reality. Further, Bohr emphasised that concepts of complementary pairs like wave-particle and position-momentum can only be used in two mutually exclusive experiments. This leads to the fundamental conclusion that a description of underlying physical reality is impossible[4]. For this reason, BPC cannot be used to develop computer models of quantum processes/experiments.

In 1952, Bohm[5] independently introduced the causal interpretation (CI) of quantum mechanics. Contrary to BPC, CI provides a single well-defined model of underlying physical reality. It can thus be used to develop mathematical and computer models of quantum processes/experiments. These single, well-defined models can help in avoiding paradoxical and erroneous explanations of quantum processes/experiments. Based on CI, Bohm in his second paper[6], presented the solution to the measurement problem of quantum mechanics, which answered Pauli's objection to de Broglie's pilot wave theory.

In Bohm's approach to quantum mechanics, there exists real fields(R-fields and S-fields) associated with a particle and a particle always has a definite position. A given Hamiltonian and the initial position of the particle yield a unique individual motion for the particle. All that is needed is to assume that the particle actually possesses a definite value of position. Given this value and the wave function the values of the particle's additional dynamical variables like the path, angular momentum and net force can be determined. In this research, this has been dealt with in detail by analytically and numerically determining the equations of motion, the net force and angular momentum for the hydrogen atom.

There is no contradiction with Heisenberg's uncertainty relations in the assumption of definite values for both the position and the momentum of the particle, since the uncertainty relations simply refer to the inevitable statistical scatter in the values obtained for complementary variables in an ensemble of measurements[7]. For Bohm the fundamental interpretation of the wave function is as a type of field which determines particle's motion. Probability is not inherent in the conceptual structure of the theory but arises as a consequence of the necessary lack of knowledge of the precise initial particle's position.

Many detailed calculations have now been carried out to demonstrate exactly how the Bohm approach works in specific cases. In 1955, Bohm, Schiller, and Tiomno extended CI to Pauli's equation, thus providing a model for spin[8]. Using Fortran, Dewdney et.al., were the first to develop computer models based on the causal interpretation[9] [10]. These models include the two-slit experiment, which was developed in 1979[10] and scattering from square potential barriers and square wells (1982)[9]. In 1985, Kaloyerou with Bohm as his supervisor extended CI to boson fields in his PhD thesis and later in two Physics Report papers[11] [12].

The aim of this research is to provide a mathematical and computer model of the hydrogen atom for ψ_{21m} and ψ_{43m} using CI. The solution of the Schrödinger equation for the hydrogen atom yields three quantum numbers n, l, and m which give an infinite number of states of the hydrogen atom[13]. The first quantum number n is the principal quantum number. n determines the energy level of the electron. The second quantum number l is the orbital quantum number which gives the magnitude of the angular momentum. For each value of n there are $n-1$ possible values of l. The third quantum number m is the magnetic quantum number which gives the orientation of angular momentum. The values of m range from $-l$ to l. This gives $2l+1$ values of m for each value of l. In this work, 10 different states of the hydrogen atom have been considered, i.e., three states for $l = 1$ and seven states for $l = 3$. In this model, the spin quantum number m_s has been ignored for simplicity.

Similar work on the hydrogen atom was done by Dewdney and Malik (1993)[14]. Their work gave details on the angular momentum of the electron in the hydrogen atom for $l = 1$ only, but did not treat the electron orbits in detail. They also demonstrated non-locality in the Stern-Gerlach and Einstein-Rosen-Podolsky experiment(EPR). This work differs from the above-mentioned work in the following ways:

1. The wave function of the hydrogen atom has been interpreted differently.
2. The Schrödinger equation has been solved explicitly using CI to obtain the equations of motion of the electron.
3. Plots have been generated to illustrate the relationship between the electron's motion, angular momentum, and the forces producing the motion.
4. Dewdney and Malik only considered the $l = 1$ state, while this work has also been extended to the $l = 3$ state of the hydrogen atom. There is no special reason for the states chosen in this work except to explore the difference in a state with more orientations.

Starting with the wave function of the hydrogen atom, this work presents calculations to determine the trajectories, net force, and angular momentum based on CI. Maple, a modern mathematical software package, has been used to numerically solve the coupled differential equations for the trajectories of the rotated wave function for $l = 1$. Computer plots of the trajectories and the orientation of force and angular momentum at selected points on the trajectories were also provided using maple.

Chapter 2

Literature Review

2.1 Overview

This chapter presents a brief history on development of quantum mechanics around 1900. The details include the beginning of quantisation as introduced by Max Planck, the introduction of the Schrödinger wave equation, and the renown interpretations of quantum mechanics.

The interpretations presented in this chapter are the Copenhagen interpretation, de Broglie's pilot theory, and Bohm's Causal interpretation. The chapter also presents the different responses given to the unanimously accepted interpretation, the Copenhagen interpretation. In this regard, Von Neumman's impossibility proof, EPR experiment, and details of Bohr's principle of complementarity. Further, the chapter highlights the connection of this work to the development of quantum physics and also presents related work that has been done using the causal interpretation and the hydrogen atom.

2.2 The beginning of Quantisation

On April 27, 1900, Lord Kelvin delivered the Friday Evening Lecture at the Royal Institution in London. An extended version of this lecture was submitted to the Philosophical Magazine in February 1901 and published in the July issue under the title 'Nineteenth Century Clouds over the Dynamical Theory of Heat and Light'[15]. In his lecture, he described two clouds over physics (classical physics), which by then was almost viewed to be complete. Cloud one was titled "The Relative Motion of the Ether and Ponderable Bodies". This was discussed in relation to the Michelson-Morley experiment, which showed results that contradicted the hypothesis of the ether by showing that the velocity of light is the same relative to any frame of reference. Cloud two was the Maxwell-Boltzmann doctrine of the partition of energy. The two clouds eventually led to the theories of special relativity and quantum mechanics, respectively.

In line with the second cloud, Wein in 1869 applied the Maxwell-Boltzmann law of partition of energy to solve the blackbody radiation problem. The law he made, worked only for short-wavelength radiation, but it failed to account for long-wavelength radiation. Around the same time, Planck was interested in two domains that were related to the behaviour of light and its interaction with matter. The first was electrodynamics, the theory of electricity, magnetism, and light waves, which was brought to its final form by James Clerk Maxwell in 1865[16]. The second was thermodynamics and statistical mechanics. In this domain, Planck took up a problem on the interaction of an oscillating charge with its electromagnetic field. The oscillating charge behaviour was closer to that of a blackbody. This led Planck to independently reproduce Wein's formula[17].

In 1900, experimenters started finding deviations between the results produced from the Planck-Wein's law and experimental results as wavelengths approached zero. To fix the deviation, Planck in 1900 introduced a new solution to the blackbody radiation by introducing the concept of quantisation of energy[1]. Quantisation was totally different from the classical concept of energy and hence Planck's quantisation marks the origin of quantum mechanics. Later, Einstein (1905)[18] explained the photoelectric effect and was able to apply quantisation of energy to light. He called the quanta of light photons. This was the verification of Planck's radiation law. The next application of the quantisation of energy appeared in Bohr's model of the hydrogen atom[19].

Louis de Broglie in his 1924 PhD thesis[20] brought forth the theory now called de Broglie's hypothesis. In this hypothesis, he asserted that there is always a wave associated with a particle. de Broglie applied Planck's and Einstein's equations of wavelength and wave numbers to particles. Up until this time, atomic models proposed by scientists could only explain the particle nature of electrons but failed to explain the properties related to their wave nature. Clinton Davisson and Ester Germer carried out an experiment, popularly known as Davisson Germer's experiment[21], in which electrons, scattered by the surface of a crystal of nickel metal, displayed a diffraction pattern. This experiment confirmed de Broglie's hypothesis of wave particle duality.

The quest to interpret the concept of quantisation continued with the most renowned physicists of the time, like Bohr, Born, Heisenberg, Pauli and Schrödinger[3,22-25]. In 1925, Heisenberg came up with the idea of representing physical quantities by sets of time-dependent complex numbers[23,26]. A few months later, this new approach was elaborated by Born, Jordan, and Heisenberg himself as matrix mechanics[27]. This was the first consistent theory of quantum mechanics.

In 1926, Schrödinger also published his historical paper, which contained the time-dependent wave equation. This is now referred to as the Schrödinger equation[24]. At that time, physicists were not so familiar with matrix methods but were very familiar with differential equations[28]. Thus, attempts to provide a physical interpretation of quantum mechanics focused on the Schrödinger equation.

2.3 Early Interpretations of Quantum Mechanics

After its formulation in 1926, Schrödinger's wave equation still missed a correct interpretation despite being correct. Physicists started working on the interpretation of the wave equation. In the same year, Born proposed, for the first time, a probabilistic interpretation of the wave function. He interpreted the wave function as a probability amplitude. In his interpretation, the absolute square of the wave function gives the probability of finding a particle at a given location.

Around the same time, Louis de Broglie also developed a theory of the double solution[20]. In this theory, he proposed a version of quantum mechanics in which a particle preserves its classical nature but is guided by a wave Ψ and thus subject to diffraction effects. By this, the wave-particle duality was reduced to a particle guided by a wave.

Another interpretation of quantum mechanics was developed by Bohr. Bohr did not build his interpretation from the mathematical formalism. Instead, he considered complementary pairs of nature. Thus, his interpretation is referred to as Bohr's principle of complementarity[4]. The complementarity principle was first presented at the Como lecture in September 1927, which was attended by renowned physicists of that time except Einstein, who, despite being invited, was not present[29].

A month later, the fifth physical Solvay congress was organised to discuss various interpretations of quantum mechanics and was also attended by many prominent physicists of that time, including Einstein[2]. The first to present was de Broglie who presented his pilot wave theory. De Broglie emphasised that his formula was able to completely determine the motion of a particle if its initial position is known. If the initial position is not known, the probability of the particle's position can be calculated using the wave function Ψ. Thus, de Broglie pointed out that Ψ has two functions. It is a probability wave, but also a pilot wave because it determines the trajectory of the particle. De Broglie's theory was rejected, partially because of the objection raised by Pauli concerning Fermi's rigid rotation.

The Copenhagen interpretation became the unanimously accepted interpretation of quantum mechanics. In 1930, Heisenberg[7] in his lectures emphasised the inseparability of the observer and object in quantum experiments. In this set of lectures, he emphasised that neglecting the interaction between observer and object is not possible because it causes large, uncontrollable changes in the system being observed. This led to more acceptance of the Copenhagen interpretation. Apart from this, Von Neumann's impossibility proof[30] also highly contributed to the establishment of the Copenhagen interpretation.

2.4 The Impossibility Proof

In 1932, Von Neumann in his book which put quantum mechanics on an axiomatic base, provided as a chapter, the "impossibility proof". The proof persuaded the physics community that an interpretation of quantum mechanics in terms of hidden variables is impossible. He concluded at the end of his proof that there is no reason to think causality will be restored[30]. This made the Copenhagen interpretation to gain more favour and its proponents argued that quantum mechanics is therefore complete.

In the real sense, Neumann's proof does not rule out hidden variables in that in his proof he only considered quantum mechanics to be local. In 1952, Bohm in his paper, a suggested interpretation of Quantum theory in terms of hidden variables, introduced CI[5]. In his paper[5], Bohm pointed out that Von Neumann's impossibility proof was not universally true, in that the proof considers hidden variables associated with the system alone and therefore neglects the influence of the measuring apparatus.

Bell in 1966 showed by his inequalities that Von Nuemann's impossibility was not universal[31]. The inequalities also showed that later versions of the impossibility proof by Gleason[32] and Jauch and Piron[33] are equally not valid for the same reasons. He pointed out that the impossibility proof ignores the role of the measuring apparatus in the final measured result, a role emphasised by Bohr in his quantum postulate[34]. Following the development of CI and Bell's work, it can be understood that Von Nuemann, Gleason's and Jauch and Piron's impossibility proofs apply to local hidden variable theories, but not to non-local hidden variable theories such as Bohm's causal interpretation.

2.5 The Einstein–Podolsky–Rosen (EPR) experiment

The famous EPR thought experiment[35] aimed to show that quantum mechanics is an incomplete theory which should be supplemented by additional parameters. The experiment presented a paradox to show that the description of physical reality provided by quantum mechanics is not complete. They argued for the existence of hidden variables which represent physical realities and speculated that it should be possible to construct a theory containing these hidden variables.

The thought experiment involves a pair of particles prepared in what would later become known as an entangled state. Einstein, Podolsky, and Rosen pointed out that, in this state, if the position of the first particle were measured, the result of measuring the position of the second particle could be predicted. If instead the momentum of the first particle were measured, then the result of measuring the momentum of the second particle could be predicted. They argued that no action taken on the first particle could instantaneously affect the other, since this would involve information being transmitted faster than light, which is impossible according to the theory of relativity[36].

The trio invoked a principle, later known as the "EPR criterion of reality". The principle implied that if the value of a physical quantity can be predicted with certainty without, in any way disturbing a system, then there exists an element of reality corresponding to that quantity[35]. From this it can be inferred that the second particle must have a definite value of both position and momentum prior to either quantity being measured. But quantum mechanics considers these two observables incompatible, and thus does not associate simultaneous values for both to any system. Einstein, Podolsky, and Rosen therefore concluded that quantum theory does not provide a complete description of reality[6]. The EPR experiment was shown to be consistent with quantum mechanics by Bohr (based on BPC), and later interpreted as demonstrating non-locality.

2.6 Bohr's Principle of Complementarity

BPC began with the quantum postulate that Bohr first presented at the Como lecture in 1927. The second presentation of BPC was a month later, at the fifth physical Solvay congress, which was organised to discuss various interpretations of quantum mechanics. From the Solvay congress, BPC became famous and unanimously accepted alongside BPR after receiving a favorable response from the congress.

BPC was not built on interpretations of mathematical formalism[4]. Instead, Bohr considered complementary pairs of nature revealed in experiments like the wave-particle duality and 'position and momentum'. Bohr noted that these complementary pairs can only be observed in mutually exclusive experiments and thus referred to as Bohr's principle of complementarity. The details of this postulate and complementarity were also presented in his paper in 1928[3]. The complementarity principle in quantum mechanics leads to the conclusion that the observable events constituting an experience have space-like separation with each other[4]. This seems to contradict the perceived locality of physical laws and encourages the thought that measurement is not a physical process. In the sense the result of a measurement cannot be related to the physical description of the experimenter observed from the outside[6]. There are five main components of complementarity highlighted by Jammer[4]

1. The Quantum of action is indivisible.
2. Discontinuity or the individuality of elementary processes.
3. The interaction between the object under observation and the instrument of observation is uncontrollable.
4. Impossibility of a strict spatio-temporal and at the same time causal description.
5. Classical mode of description should be given up.

This leads to four core tenets of the principle of complementarity which are as follows.

1. The concept of a precisely definable classical state must be given up and a separation of subject object in experiments is impossible. An experiment must therefore be viewed as an analysable whole[5].
2. A single picture is not sufficient to exhaust the description of a quantum system. Rather pairs of complementary concepts are needed. Such concepts can only be used in mutually exclusive experimental arrangements. It is the experimental arrangement which defines the concept to be used.
3. Classical concepts are essential to aid thought and to communicate the results of experiments. However, they cannot be attributed to physical reality.
4. A description of underlying physical reality in terms of a single, well-defined model is not possible.

BPC mainly suffers the following critiques:

1. BPC is not a direct interpretation of mathematical formalism of the quantum theory.
2. ‘Particle and wave’ complementarity is fundamentally different from other complementary concepts like ‘position and momentum’. Bohr however, never accepted the differentiation between the concepts but instead sought a unified view for the complementarity concepts.
3. The denial that a description of underlying physical reality in terms of a single, well-defined model is possible.

It is this last assertion that brings about the main difference of the Copenhagen interpretation and Bohm’s causal interpretation.

Chapter 3

Methodology

3.1 Overview

In this chapter, an outline is made of the methods used to collect, analyse and interpret the data for the model of the hydrogen atom using the causal interpretation. The research design, the formulation of the mathematical model and computer model for the selected hydrogen states, as well as the limitations of the model are explained.

3.2 Research design

The aim of this research is to develop a model of the hydrogen atom using the causal interpretation of quantum mechanics. The methodology employed involves a theoretical, analytical and computational approach. This research does not involve the collection of new experimental data; instead, it relies on existing theoretical and experimental results. A comprehensive literature review was conducted for the development of a theoretical model and identification of research gaps. Relevant books, scientific papers, and articles were accessed mainly through online resources. Key studies consulted during the literature review included Bohm's 1952 paper[5-6], Griffiths' quantum mechanics book[13] and Dewdney and Malik's paper (1993)[14].

The mathematical modelling of the hydrogen atom was based on the causal interpretation of the Schrödinger equation. CI differs from the usual interpretation of quantum mechanics (the Copenhagen interpretation) in that the usual interpretation of quantum mechanics has a component (BPC) which asserts that a description of underlying physical reality in terms of single well-defined model is not possible. On the other hand, CI posits that particles, such as electrons, have definite positions and trajectories even when they are not being observed.

CI is composed of two important functions that represent two fields, the R-field and S-field. The R-field represents the radial coordinate, and the S-field represents the phase or action of the wave function. These fields are not independent, but they co-determine each other. From the Schrödinger equation, CI yields important definitions of S and R in terms of the wave function ψ. Further calculations yield two other important equations, the continuity equation(CE) and the Hamilton-Jacobi equation(H-J), which are defined in comparison with the classical equations. From the continuity equation, the probabilistic interpretation of the wave function $\psi^2 = R^2$ was used to define the initial points of the electron in the trajectory. The H-J equations were used to define the Energy E_n, the momentum $\vec{p}$, the velocity $\vec{v}$, and the extra term, which is the quantum potential Q.

These definitions were later applied to the wave function of the hydrogen atom for the selected states. The definition of momentum p was used to determine the velocity, v, the angle of orientation, θ and the equations of motion. Further calculations were made to determine the angular momentum L and the eigenstates of the hydrogen atom; L^2 and L_z. The extra term Q was then analysed to determine the net force on the electron. From these results, plots to show the orbits, direction of the net force, and the angular momentum were made using Maple.

Furthermore, the calculations were extended to a rotated wave function. Firstly, a wave function rotated at an angle $\beta = 60^{\circ}$ was defined. The momentum, velocity, and quantum potential were also defined for the rotated wave function. Detailed calculations based on these definitions yielded differential equations for the trajectories and the net force. Maple was then used to solve the differential equations using the Fourth Order Runge-Kutta method, and the respective plots were produced. Maple was also used to make animations to illustrate the motion of the electron in the orbit and the vector of angular momentum throughout the orbit.

3.3 Computation Details

Computational simulations were performed using Maple to produce plots for the trajectory, vectors of force and angular momentum. All the plots were done in atomic mass units while the constants used for the plots were obtained from a Handbook of Chemistry and Physics[37]. Firstly, the constants and three equations of motion for the three different states $m=1$, $m=0$ and $m=-1$ were defined. Starting with the initial point, a loop was used to generate data points. From the generated data points, plots and animations for the trajectories were made. Afterwards, the function of net force was defined and was used to generate the vectors by selecting coordinate points on the trajectories. A similar program was written for $l=3$ which required seven equations of motion for the seven different states, $m=3$, $m=2$, $m=1$, $m=0$, $m=-1$, $m=-2$ and $m=-3$. The force vectors were likewise plotted.

For $l=1$, another program was written to show the vectors of the angular momentum. The program involved defining the magnitude of the angular momentum $|L|$ and its components L_x, L_y and L_z as well as plotting. For the rotated wave function, the differential equations were defined and numerically solved using the 4^{th} order Runge-Kutta equation. This was done only for $l=1$. Thus, three differential equations of motion and three differential equations of force were solved and illustrated graphically on plots and animations.

3.4 Analysis

The equations obtained for the trajectories, net force, and angular momentum were compared with their interpretations in quantum mechanics and classical physics. The results from the computational simulations were equally analysed to gain insights into the behaviour of the electron in the hydrogen atom. The plots and animations were compared with existing theoretical and experimental results to validate the accuracy of the model.

3.5 Limitations

The scope of this research cannot be able to capture all the complexities of the hydrogen atom. The model is limited to stationary states, which leaves a lot more work to be developed on the model of the hydrogen atom.

Chapter 4

The Causal Interpretation

4.1 Overview

This chapter presents the details of the causal interpretation. Applying CI to the Schrödinger equation yields two important equations, the continuity equation (CE) and the Hamilton-Jacobi equation (H-J). CE shows that the conservation of probability persists even in CI, whilst the H-J equation contains a very important term known as the quantum potential. The quantum potential accounts for the quantum behaviour of particles. The chapter also shows Bohm's solution to the measurement problem using the causal interpretation. This chapter further presents some of the models of quantum mechanics that have been developed based on the causal interpretation. These include the causal interpretation of stationary states and non-stationary states.

4.2 Interpretation of the Schrödinger Equation

The causal interpretation was introduced independently by Bohm in his 1952 papers[5-6]. CI is an interpretation of quantum mechanics in terms of hidden variables. In the first paper[5] Bohm introduced the causal interpretation. He later learnt that it is equivalent to de Broglie's pilot-wave theory. Thus, CI is also known as the Bohm-de Broglie causal interpretation. In the second paper[6] Bohm provided a solution to the measurement problem of quantum mechanics which addressed Pauli's objection on the fermi rigid-rotator at the 1927 Solvay congress[2].

Bohm got the idea of the causal interpretation when he was writing the chapter on the Wentzel-Kramers-Brillouin(WKB) approximation for his Quantum Mechanics book[38]. He made an approximation to the wave function

$$\Psi(x,t) = R(x,t)\exp\left(i\frac{S(x,t)}{\hbar}\right), \tag{4.1}$$

where R and S are real fields; substituting the wave function into the Schrödinger equation,

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t), \tag{4.2}$$

to get

$$i\hbar\frac{\partial}{\partial t}R\exp\left(\frac{iS(x,t)}{\hbar}\right) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial^2 x}R\exp\left(\frac{iS(x,t)}{\hbar}\right)\right] + V(x)R\exp\left(\frac{iS(x,t)}{\hbar}\right). \tag{4.3}$$

Differentiating gives:

$$\begin{aligned} & i\hbar\frac{\partial}{\partial t}R.\exp\left(\frac{iS(x,t)}{\hbar}\right) + i\hbar R\left(\frac{i}{\hbar}\frac{\partial S}{\partial t}\right)\exp\frac{iS(x,t)}{\hbar} \\ & = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left[\frac{\partial R}{\partial x}\exp\left(\frac{iS}{\hbar}\right) + \frac{i}{\hbar}R\frac{\partial S}{\partial x}\exp\left(\frac{iS}{\hbar}\right)\right] + VR\exp\left(\frac{iS}{\hbar}\right), \end{aligned}$$

$$\begin{aligned} \left[ih\frac{\partial R}{\partial t} - R\frac{\partial S}{\partial t}\right]\exp\left(\frac{iS}{\hbar}\right) = & -\frac{\hbar^2}{2m}\left[\frac{\partial^2 R}{\partial x^2}\exp\left(\frac{iS}{\hbar}\right) + \left(\frac{2i}{\hbar}\frac{\partial R}{\partial x}\frac{\partial S}{\partial x}\right)\exp\left(\frac{iS}{\hbar}\right)\right. \\ & \left. + \left(\frac{i}{\hbar}R\frac{\partial^2 S}{\partial^2 x}\right)\exp\left(\frac{iS}{\hbar}\right) + R\left(\frac{i}{\hbar}\frac{\partial S}{\partial x}\right)^2\exp\left(\frac{iS}{\hbar}\right)\right] \\ & + VR\exp\left(\frac{iS}{\hbar}\right). \end{aligned} \tag{4.4}$$

We now divide through by $\exp(\frac{iS}{\hbar})$ and rearrange, which gives us:

$$i\hbar\frac{\partial R}{\partial t} - R\frac{\partial S}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 R}{\partial x^2} - \frac{i\hbar}{m}\frac{\partial R}{\partial x}.\frac{\partial S}{\partial x} - \frac{ih}{2m}R\frac{\partial^2 S}{\partial x^2} + \frac{R}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + VR. \tag{4.5}$$

When the real and imaginary terms are equated, we get:

$$\frac{\partial R}{\partial t}=-\frac{1}{m}\frac{\partial R}{\partial x}\frac{\partial S}{\partial x}-\frac{1}{2m}R\frac{\partial^2 S}{\partial x^2} \tag{4.6}$$

$$R\frac{\partial S}{\partial t}=\frac{\hbar^2}{2m}\frac{\partial^2 R}{\partial x^2}-\frac{R}{2m}\left(\frac{\partial S}{\partial x}\right)^2-VR \tag{4.7}$$

Similarly, Eqs. (4.6) and (4.7) above can be obtained in 3 dimensions, respectively, as;

$$\frac{\partial R}{\partial t}=-\frac{1}{m}\nabla R\nabla S-\frac{1}{2m}R\nabla^2 S \tag{4.8}$$

and

$$R\frac{\partial S}{\partial t}=\frac{\hbar^2}{2m}\nabla^2 R-R\frac{(\nabla S)^2}{2m}-VR. \tag{4.9}$$

Rearranging Eq. (4.8) gives

$$\frac{\partial R}{\partial t}=\frac{-1}{m}\left[\nabla R\nabla S+\frac{1}{2}R\nabla^2 S\right]. \tag{4.10}$$

Now, we can express Eq. (4.10) in terms of R^2 using the relation

$$\frac{\partial R^2}{\partial t}=R\frac{\partial R}{\partial t}+R\frac{\partial R}{\partial t}=2R\frac{\partial R}{\partial t} \tag{4.11}$$

which gives

$$\frac{\partial R}{\partial t}=\frac{1}{2R}\frac{\partial R^2}{\partial t}. \tag{4.12}$$

Similarly in 3 dimensions, $\nabla R^2=R\nabla R+\nabla R.R=2R\nabla R$, hence

$$\nabla R=\frac{\nabla R^2}{2R}. \tag{4.13}$$

Substituting Eqs. (4.12) and 4.13 into Eq. (4.10) gives

$$\frac{1}{2R}\frac{\partial R^2}{\partial t}=\frac{-1}{m}\left[\frac{\nabla R^2}{2R}\nabla S+R\frac{\nabla^2 S}{2}\right]. \tag{4.14}$$

Then, multiplying by $2R$ yields:

$$\frac{\partial R}{\partial t} = \frac{-1}{m}[\nabla R^2 \nabla S + R^2 \nabla^2 S]. \tag{4.15}$$

The term in the square brackets can be simplified using

$$\nabla.(R^2 \nabla S) = \nabla R^2 \nabla S + R^2 \nabla^2 S. \tag{4.16}$$

This gives the continuity equation:

$$\frac{\partial R^2}{\partial t} = \frac{-1}{m}\nabla.(R^2 \nabla S), \tag{4.17}$$

or

$$\frac{\partial R^2}{\partial t} + \nabla\left(R^2.\frac{\nabla S}{m}\right) = 0. \tag{4.18}$$

Dividing Eq. (4.9) by R yields a Hamilton-Jacobi equation with an extra term,

$$\frac{-\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} \tag{4.19}$$

The extra term, $\frac{-h^2}{2m}.\frac{\nabla^2 R}{R}$ was called the quantum potential by Bohm.

4.2.1 The Hamilton-Jacobi Equation

As earlier mentioned, Eq. (4.19) is the Hamilton-Jacobi equation, noting thoroughly that it differs from the original Hamilton-Jacobi equation by one extra term[39]. By analogy with the classical H-J equation, Bohm gave the following definitions[5]:

Energy E:

$$E = \frac{-\partial S}{\partial t} \tag{4.20}$$

momentum $\vec{p}$:

$$\vec{p} = \nabla S \tag{4.21}$$

From the definition of the directional derivative, it can be shown that ∇S is perpendicular to surfaces of constant S. It therefore follows from Eq. (4.20) that the momentum $\vec{p}$, velocity $\vec{v}$ and trajectory $\vec{r}$ are also perpendicular to surfaces of constant S. Therefore, the velocity can be given by

Velocity $\vec{v}$:

$$\vec{v} = \frac{d\vec{r}}{dt} = \frac{\nabla S}{m} \tag{4.22}$$

and hence the trajectory $\vec{r}$ by

$$\vec{r} = \int \frac{\nabla S}{m} dt. \tag{4.23}$$

Then, we have the extra term, which is the quantum potential Q being given by

$$Q = \frac{-\hbar^2}{2m} \frac{1}{R} \frac{\partial^2 R}{\partial x^2}. \tag{4.24}$$

In classical mechanics, H-J equation describes a particle moving in a potential[39]. Similarly, the H-J equation given by CI can be interpreted as describing a particle moving in a potential. The extra term Q modifies the particle's behaviour so that it is consistent with quantum mechanics. Therefore, the H-J equation yielded from CI gives an interpretation of quantum mechanics in terms of a single well-defined model. Thus, CI asserts that quantum objects described by the Schrödinger equation, such as electrons, neutrons, and protons are always particles guided by the quantum potential Q.

The quantum potential is responsible for the wave behaviour of particles, such as interference effects. Classically, particles cannot give rise to wave patterns such as the interference fringes in Young's two-slit experiment[40]. Because of the H-J equation, the quantum behaviour of particles can be attributed only to the quantum potential Q, which depends only on the R-field. Hence we might as well say the R-field gives rise to the quantum behaviour of particles.The quantum behaviour can also be determined from the S-field because the R-fields and S-fields co-determine one another[5].

4.2.2 The Continuity Equation

Eq. (4.17) is the continuity equation that expresses the conservation of probability. This can be seen from the terms of the equation; From the BPR, we can see that the probability density will be R^2 that is,

$$|\Psi|^2 = R^2 \tag{4.25}$$

With the definition $v = \frac{\nabla S}{m}$ we see that the term $R^2.\frac{\nabla S}{m}$ is the probability current

Thus, even in the causal interpretation the probability element of quantum mechanics persists. The probability aspect comes into play because in a given state the initial position of a particle cannot be precisely determined, but only with the probability determined from R^2. Although from a state Ψ only initial positions can be determined with some probability, particles in nature have definite initial positions and from those positions follow causally determined trajectories which can be calculated using the causal interpretation from the differential equation

$$\frac{d\vec{r}}{dt} = \frac{\nabla S}{m}. \tag{4.26}$$

4.3 The Measurement Theory

In quantum physics, a measurement is the testing or manipulation of a physical system to obtain a numerical result. A fundamental feature of quantum theory is that the predictions it makes are probabilistic[22]. A measurement of a quantum system will generally result in a change in the quantum state of that system[41-42]. In quantum mechanics, the measurement problem is the problem of definite outcomes. Although quantum systems have superpositions, quantum measurements only give one definite result[43].

Bohm in the second paper on hidden variables presented the measurement theory, which shows the quantum theory of measurements expressed in terms of CI[6]. In his paper, he considered an experiment designed to measure an arbitrary Hermitian observable Q associated with an electron. Let $\vec{x}$ represent the position of the electron and y the significant variables of the apparatus. It is enough to consider an impulsive measurement, a strong interaction measurement lasting only for a short time, such that the changes in the system and apparatus that would have taken place prior to the interaction can be neglected. This means that the unperturbed Hamiltonian can be ignored, and therefore only the interaction part of the Hamiltonian needs to be retained.

Let the interaction part of the Hamiltonian be denoted by H_I. The Hamiltonian operator is chosen to be a function of quantities that commute with Q, in this case the interaction process will not produce changes that are uncontrollable in the observable Q, but only in the observables that do not commute with Q[38,44]. In order for the apparatus and the system to be coupled, it is necessary that H_1 also depend on the operators involving y. Let us consider the following interaction Hamiltonian for the sake of illustration of the principles involved in measurements.

$$H_I = aQP_y = -i\hbar aQ\frac{\partial}{\partial y} \tag{4.27}$$

where a is a constant and p_y is the momentum conjugate to y. During the interaction, the Schrödinger equation is approximated by,

$$\begin{aligned} i\hbar\frac{\partial\Psi(\vec{x},y)}{\partial t} &= H_x\Psi(\vec{x},y), \\ i\hbar\frac{\partial\Psi}{\partial t} = aQp_y\Psi &= -i\hbar aQ\frac{\partial\psi}{\partial y}, \\ \frac{\partial\Psi}{\partial t} &= -aQ\frac{\partial\Psi}{\partial y}. \end{aligned} \tag{4.28}$$

Let q denote an eigenvalue of Q. For simplicity, we assume that the eigenvalues, q, are discrete, although the results can be easily generalised to a continuous spectrum.

Expanding $\psi(\vec{x}, y)$ in terms of the eigenfunctions $\Psi_q(\vec{x})$ of Q we get

$$\Psi(\vec{x}, y, t) = \sum_q f_q(y,t)\psi_q(\vec{x}). \tag{4.29}$$

Substituting Eq. (4.29) into Eq. (4.28) gives

$$\sum_q \psi_q(\vec{x})\frac{\partial f_q(y,t)}{\partial t} = -\sum_k aQ\psi_q(\vec{x})\frac{\partial f_q(y,t)}{\partial y}, \tag{4.30}$$

or

$$\sum_q \psi_q(\vec{x})\frac{\partial f_q(y,t)}{\partial t} = -\sum_q aq\psi_q(\vec{x})\frac{\partial f_q(y,t)}{\partial y}. \tag{4.31}$$

Equating the coefficients of $\psi_q(x)$:

$$\frac{\partial f_q(y,t)}{\partial t} = -aq\frac{\partial f_q(y,t)}{\partial y}. \tag{4.32}$$

By using the transformation of variables and using the initial conditions[45], the solution to equation 4.32 is obtained as

$$f_q(y,t) = f_q^o(y - aqt). \tag{4.33}$$

This solution can be checked by choosing a specific $f_q(y,t)$ at a time t. Thus, every function of $y - aqt$ is a solution. In particular, if the initial form of $f_q(y, 0)$ is a wave packet, then $f_q(y,t)$ at time t will be a wave packet that moves according to aqt, where a is a constant and q is the wave packet that contains the variable of the apparatus, y.

The wave function of the apparatus and the system can be written as a product because they are initially independent. This can be expressed as

$$\Psi_o(\vec{x}, y, 0) = \psi_o(\vec{x})g_o(y) = g_o(y)\sum_q C_q\psi_q(\vec{x}) \tag{4.34}$$

where c_q are unknown expansion coefficients and $g_0(y)$ has the form of a wave packet and can be assumed to be centred at $y = 0$ with width δy, for simplicity. From Eq. (4.33) at $t = 0$ and Eq. (4.34)

$$\Psi(\vec{x}, y, 0) = \sum_q \psi_q(\vec{x}) f_q^o(y) = \sum_q \psi_q(\vec{x}) C_q g_o(y) \tag{4.35}$$

gives,

$$f_q^o(y) = C_q g_0(y), \tag{4.36}$$

which implies that

$$\Psi(\vec{x}, y, t) = \sum_q C_q \psi_q(\vec{x}) g_o(y - aqt). \tag{4.37}$$

Eq. (4.37) shows that the interaction has introduced a correlation between q and the apparatus coordinates y. While the system, which is an electron in this case, interacts with the apparatus, the motion of the electron and the apparatus is very complicated (so is the wave function). This is seen by writing

$$\Psi(\vec{x}, y, t) = R(\vec{x}, y, t) e^{iS(\vec{x}, y, t)}. \tag{4.38}$$

This shows that both $R(\vec{x}, y, t)$ and $S(\vec{x}, y, t)$ undergo rapid oscillations as a function of position and time. From this, it can be deduced that the quantum potential

$$Q = \frac{-\hbar^2}{2mR} \left(\nabla_x^2 R + \frac{\partial^2 R}{\partial y^2} \right) \tag{4.39}$$

similarly undergoes severe fluctuations and so does the momentum[6].

In contrast, when the interaction has taken long enough, the behaviour of the system and the apparatus becomes settled. This is because the wave packets corresponding to different values of q will cease to overlap in the y-space. This can be seen by noting that the centre of the q^{th} packet in y-space is at $y = aqt$ or $q = \frac{y}{at}$. We denote the separation of adjacent values of q by δq, the separation of the centres of adjacent packets, and in the y space as

$$\delta y' = at\delta q. \tag{4.40}$$

When the strength of the interaction a and the duration of the interaction t is large enough, $\delta y'$ can be much larger than the width of δy of the wave packet. The packets corresponding to different values of q cease to overlap in the y-space. Depending on the initial values of the system and apparatus, the apparatus variable will enter one of the packets, while the system enters a corresponding eigenstate. This is because the probability density $|\Psi|^2$ is negligible between the distantly separated wave packets. Both the system and apparatus remain in the active wave packet.

The empty wave packets and the corresponding eigenstates can be ignored because the quantum potential due to the empty packets is negligible at the position of the active wave packet. Neither can the empty wave packets affect the momentum of the system p_x and apparatus P_y. This shows that we can obtain a definite measurement result by observing the state $g_o(y - aqt)$ which is the active packet of the apparatus.Thus, for all practical purposes, the system and apparatus are governed only by the active wave packet

$$\Psi_q(\vec{x}, y, t) = \psi_a(\vec{x}) g_0(y - aqt) \tag{4.41}$$

which can be normalised without affecting the physical quantity. The variable for the apparatus y will inevitably become coupled to a whole host of internal degrees of freedom $y_1, y_2, y_3...$ as a result of Brownian motion[46]. Therefore, interference between wave packets corresponding to different states $q's$ could only occur if the packets overlapped in the $y_1, y_2, y_3...$ space as well as in the y-space. The probability of this happening is absolutely negligible. Therefore, the empty wave packets cannot change the measurement. This shows how a definite measurement is obtained without the collapse of the wave function. This, therefore, is the solution to Pauli's rigid rotator objection to de Broglie at the Solvay congress[2] [6].

4.4 Stationary States

A stationary state is a quantum state with all observables independent of time. In other words, stationary states are solutions of the time-independent Schrödinger equation. For a one-particle Hamiltonian, a stationary state would also mean that the particle has a constant probability distribution for position, velocity, and spin.

The solution of the time independent Schrödinger equation is

$$\Psi(x,t) = \psi_0(r)\exp(-iEt/\hbar). \tag{4.42}$$

Applying the causal interpretation;

$$\psi(x,t) = R(x,t)\exp\left(i\frac{S(x,t)}{\hbar}\right) = \psi_0(r)\exp\left(-iEt/\hbar\right) \tag{4.43}$$

implies,

$$R = \psi_0(r) \tag{4.44}$$

and

$$S = -Et. \tag{4.45}$$

Therefore, the components of the equation can be defined as follows; probability density is R^2

$$R^2 = \psi_0(r)^2, \tag{4.46}$$

from Eq.(4.20)

$$E = -\frac{\partial S}{\partial t}$$

(4.47)

and from Eq.(4.45)

$$-\frac{\partial(-Et)}{\partial t} = E, \tag{4.48}$$

This shows that the energy for stationary states is constant.

The momentum $\vec{p}$:

$$\vec{p} = \nabla S \tag{4.49}$$

and quantum potential Q:

$$Q = \frac{-\hbar^2}{2m}\frac{\nabla^2 R}{R} = -\frac{\hbar^2}{2m}\frac{\nabla^2\Psi_0(r)}{\Psi_0(r)}. \tag{4.50}$$

From these results, we conclude that for a stationary state, the energy is constant, and the quantum potential and the probability density are independent of time. This means that the values of energy in a stationary state and the corresponding eigenfunctions are the same as obtained in the usual interpretation of the theory.

4.5 Non-stationary States

A non stationary state:

$$\Psi = C_1 R_1(\vec{x}) \exp\left(-iE_1\frac{t}{\hbar}\right) + C_2 R_2(x) \exp\left(-iE_2\frac{t}{\hbar}\right), \tag{4.51}$$

where C_1, C_2, R_1 and R_2 are real can also be written as

$$\Psi = \exp -i(E_1+E_2)\frac{t}{2\hbar}\left[C_1 R_1(x)\exp -i(E_1-E_2)\frac{t}{2\hbar} + C_2 R_2(x)\exp i(E_1-E_2)\frac{t}{2\hbar}\right] \tag{4.52}$$

Equating Eq. (4.52) to the causal interpretation gives

$$\begin{aligned} R\exp\left(\frac{iS}{\hbar}\right) = \exp - i(E_1+E_2)\frac{t}{2\hbar}\Big[C_1R_1(x)\exp - i(E_1-E_2)\frac{t}{2\hbar} \\ +C_2R_2(x)\exp i(E_1-E_2)\frac{t}{2\hbar}\Big]. \end{aligned} \tag{4.53}$$

Multiplying Eq. (4.53) by its complex conjugate gives

$$\begin{aligned} R\exp\left(\frac{-iS}{\hbar}\right)R\exp\left(\frac{iS}{\hbar}\right) = \exp i(E_1+E_2)\frac{t}{2\hbar}\Big[C_1R_1(x)\exp i(E_1-E_2)\frac{t}{2\hbar}+C_2R_2(x) \\ \exp - i(E_1-E_2)\frac{t}{2\hbar}\Big] \\ \exp - i(E_1+E_2)\frac{t}{2\hbar}\Big[C_1R_1(x)\exp - i(E_1-E_2)\frac{t}{2\hbar}+C_2R_2(x)\exp i(E_1-E_2)\frac{t}{2\hbar}\Big]. \end{aligned} \tag{4.54}$$

Expanding and simplifying gives

$$R^2 = C_1^2R_1^2+C_2^2R_2^2+C_1R_1C_2R_2\exp\left(i(E_1-E_2)\frac{t}{\hbar}\right)+C_1R_1C_2R_2\exp\left(-i(E_1-E_2)\frac{t}{\hbar}\right) \tag{4.55}$$

or

$$R^2 = C_1^2R_1^2+C_2^2R_2^2+2C_1R_1C_2R_2\cos\left[\left(\frac{E_1-E_2}{\hbar}\right)t\right]. \tag{4.56}$$

S can be calculated as follows: Rearranging Eq. (4.53) we get

$$\begin{aligned} R\exp\left[\frac{i}{\hbar}\left(S+(E_1+E_2)\frac{t}{\hbar}\right)\right] = \Big[C_1R_1(x)\exp\left(-i(E_1-E_2)\frac{t}{2\hbar}\right) \\ +C_2R_2(x)\exp\left(i(E_1-E_2)\frac{t}{2\hbar}\right)\Big]. \end{aligned} \tag{4.57}$$

Simplifying by adding and subtracting each side of the equation by its complex conjugate then dividing by Eq. (4.57) gives: Subtracting the complex conjugate on the left hand side gives;

$$\begin{aligned} R\exp\left[\frac{i}{\hbar}\left(S+(E_1+E_2)\frac{t}{\hbar}\right)\right]-R\exp\left[\frac{-i}{\hbar}\left(S+(E_1+E_2)\frac{t}{\hbar}\right)\right] = \Bigg[&C_1R_1(x)\exp\left(-i(E_1-E_2)\frac{t}{2\hbar}\right) \\ -C_1R_1(x)\exp\left(i(E_1-E_2)\frac{t}{2\hbar}\right)&+C_2R_2(x)\exp\left(i(E_1-E_2)\frac{t}{2\hbar}\right) \\ &-C_2R_2(x)\exp\left(-i(E_1-E_2)\frac{t}{2\hbar}\right)\Bigg] \end{aligned} \tag{4.58}$$

or

$$2Ri\sin\left[S+(E_1+E_2)\frac{t}{\hbar}\right)\right] = (C_1R_1-C_2R_2)2i\sin\left((E_1-E_2)\frac{t}{2\hbar}\right). \tag{4.59}$$

Similarly adding the complex conjugate gives;

$$\begin{aligned} R\exp\left[\frac{i}{\hbar}\left(S+(E_1+E_2)\frac{t}{\hbar}\right)\right]+R\exp\left[\frac{-i}{\hbar}\left(S+(E_1+E_2)\frac{t}{\hbar}\right)\right] = \Bigg[&C_1R_1(x)\exp\left(-i(E_1-E_2)\frac{t}{2\hbar}\right) \\ &+C_1R_1(x)\exp\left(i(E_1-E_2)\frac{t}{2\hbar}\right) \\ +C_2R_2(x)\exp\left(i(E_1-E_2)\frac{t}{2\hbar}\right)&+C_2R_2(x)\exp\left(-i(E_1-E_2)\frac{t}{2\hbar}\right)\Bigg] \end{aligned} \tag{4.60}$$

or

$$2R\cos\left[S+(E_1+E_2)\frac{t}{\hbar}\right)\right] = (C_1R_1+C_2R_2)2\cos\left((E_1+E_2)\frac{t}{2\hbar}\right). \tag{4.61}$$

Dividing Eq. [4.59] by Eq.[4.61] gives

$$\tan\left[S+(E_1-E_2)\frac{t}{\hbar}\right] = \left(\frac{C_2R_2-C_1R_1}{C_2R_2+C_1R_1}\right)\tan\left[\frac{(E_1-E_2)t}{\hbar}\right] \tag{4.62}$$

This shows that the particles experience a quantum force, the negative gradient of the quantum potential Q which fluctuates with a frequency $\omega = \frac{(E_1-E_2)}{\hbar}$. The energy of the particle $E = -\frac{\partial S}{\partial t}$ and the momentum $\vec{P} = \nabla S$ fluctuate with the same frequency. In a region where R is small, Q becomes large, the fluctuation can be quite violent, but since R is small the probability R^2 of a particle being found in the region is small. Therefore, in a non-stationary state, the motion of a particle is very irregular, resembling Brownian motion.

4.6 The Frank-Hertz Experiment

In order for a system to make transition from one stationary state to another it has to exchange energy with some other systems[44]. In the Frank-Hertz experiment the other system is a bombarding particle. Let's consider a hydrogen atom of energy E_0 and wave function $\Psi_0(x)$ bombarded by electrons that can be scattered in-elastically leaving the atom with energy E_n and wave function $\Psi_n(x)$. The electron is then represented by a wave packet

$$f_0(y,t) = \int \exp i\vec{k}.\vec{y} f(\vec{k}-\vec{k_0}) \exp -i\hbar k^2 \frac{t}{2m} d\vec{k} \tag{4.63}$$

The centre of the wave packet occurs when $\vec{y} = \frac{\hbar \vec{k_0} t}{m}$

Therefore, the initial wave function is

$$\Psi_i = \Psi_0(x) \exp\bigg(-iE_0 \frac{t}{\hbar} f_n(\vec{y},t) \bigg). \tag{4.64}$$

Ψ_i, being a product state, shows that the atom and the electron behave independently. We prove this as follows:

$$\Psi_0(x) = R_0(x) \exp\left(\frac{iS_0(x)}{\hbar} \right) \tag{4.65}$$

and

$$f_o(\vec{y},t) = M_0(\vec{y}) \exp\left(\frac{iN_0(\vec{y},t)}{\hbar} \right). \tag{4.66}$$

The particle velocities are $\frac{dx}{dt} = \frac{1}{m}\nabla S_0(x)$, $\frac{dy}{dx} = \frac{1}{m}\nabla N_0(y)$, while the quantum potential is

$$Q = \frac{-\hbar^2}{2m}\frac{\nabla_x^2 R_0 M_0}{R_0 M_0} - \frac{-\hbar^2}{2m}\frac{R_0 \nabla_y^2 M_0}{R_0 M_0}. \tag{4.67}$$

Simplifying gives

$$Q = \frac{-\hbar^2}{2m}\frac{\nabla_x^2 R_0}{R_0} - \frac{-\hbar^2}{2m}\frac{\nabla_y^2 M_0}{M_0} \tag{4.68}$$

This shows that the atom and the electron behave independently since the expressions of the velocities are independent and the quantum potential is expressed as a sum of terms, one involving x and another involving y. Solving the Schrödinger equation for the two interacting systems, the atom and electron after they hit each other gives the following series

$$\Psi = \psi_i + \sum_n \Psi_n(\vec{x}) \exp\left(- iE_n \frac{t}{\hbar}\right) f_n(\vec{y},t), \tag{4.69}$$

with $f_n(\vec{y},t)$ as the expansion coefficients. Substituting the form of $f_n(\vec{y},t)$ given by N.F. Mott and H.S.W Massey[47], we get

$$\Psi = \psi_i(\vec{x},\vec{y}) + \sum_n \Psi_n(\vec{x}) \exp(-iE_n \frac{t}{\hbar}) \int f(\vec{k} - k_0) \frac{\exp\left(i\vec{k}_n.\vec{r} - \frac{\hbar^2 k_n^2 t}{2m}\right)}{r} g_n(\theta,\phi,\vec{k}) dk \tag{4.70}$$

where

$$\frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 k_0^2}{2m} + E_0 - E_n. \tag{4.71}$$

$\Psi(\vec{x},\vec{y})$ represents the possibility that the collision is elastic or inelastic since the atom is left in its initial state[47]. The sum term represents an ongoing electron wave packet correlated with the state of the atom Ψ_n. Rearranging Eq. (4.71) gives

$$E_n - E_0 = \frac{\hbar^2 k_0^2}{2m} - \frac{\hbar^2 k_n^2}{2m}. \tag{4.72}$$

This shows that the electron gives up energy to the hydrogen atom exciting a hydrogen atom electron from the ground state Ψ_0 to an excited state Ψ_n. The sum term therefore corresponds to inelastic collisions.

The centre of the n^{th} packet occurs at

$$\vec{r}_n = \frac{\hbar\vec{k}_n t}{m}. \tag{4.73}$$

Because the speed depends on the quantum number of the hydrogen atom n,[19] every packet will eventually be separated by large distances such that their overlap is negligible (though such wave packets never completely separate because of their infinite tails[47]).

The solution Ψ of Eq. (4.71) shows that R and S can no longer be expressed as a product of terms, one containing $\vec{x}$ and the other containing $\vec{y}$, but instead, must be expressed as non product functions of $\vec{x}$ and $\vec{y}$ as $R = R(\vec{x},\vec{y})$ and $S = S(\vec{x},\vec{y})$. This entails that the two systems no longer behave independently, since

$$\vec{v}_x = \frac{\nabla_x S(\vec{x},\vec{y})}{m}$$

and

$$\vec{v}_y = \frac{\nabla_y S(\vec{x},\vec{y})}{m}.$$

The connection is further seen from the quantum potential which can no longer be expressed as a sum of terms involving $\vec{x}$ and terms involving $\vec{y}$:

$$Q = \frac{-\hbar^2}{2mR(\vec{x},\vec{y})}[\nabla_x^2 R(\vec{x},\vec{y}) + \nabla_y^2 R(\vec{x},\vec{y})]. \tag{4.74}$$

Similarly, the probability density cannot be written as a product.

Comparing with the simpler non-stationary states, it can be seen that the motion of the atom and electron are very complicated during the time of interaction, because the expressions $R(\vec{x},\vec{y},t)$ and $S(\vec{x},\vec{y},t)$ obtained from Eq. (4.70) are very complicated, with $\vec{x}$ and $\vec{y}$ terms interconnected. This means that momentum $\vec{P}_{atom}$ and $\vec{P}_{electron}$ and quantum potential undergo rapid and violent fluctuations.

Because $R(\vec{x},\vec{y})$ appears in the denominator of the quantum potential in a region where $R(\vec{x},\vec{y})$ is small, the fluctuations become very large. If the electron and atom enter such a region, they may exchange large amounts of energy and momentum in a very short time even if the classical potential $V(\vec{x},\vec{y})$ is very small. A small value of $V(\vec{x},\vec{y})$ implies a small amplitude of the scattered wave $f(\vec{y},t)$, which in turn implies that fluctuations are small and so is the probability density $R^2(\vec{x},\vec{y})$.

During the interaction, we see that the behaviour of the atom and electron is very complicated and their motions also fluctuate wildly. However, the wave packets eventually separate by large distances, the electron most likely enters one of the n wave packets and the atom enters the corresponding state ψ_n. This is so because the probability density is largest at the position of peaks of the wave packets. Since $R^2(\vec{x},\vec{y})$ between the wave packets is vanishingly small, the electron remains in this n^{th} wave packet and the atom remains in the respective state. It follows that after the interaction, the atom and electron are described by the wave function

$$\Psi_n = \psi_n(x)\exp(iE_n\frac{t}{\hbar}\int f(\vec{k}-\vec{k}_0)\{\exp\left(i\vec{k}_n.\vec{r}-\frac{\hbar^2k_n^2t}{2m}\right).g_n(\theta,\phi,\vec{k})dk, \qquad (4.75)$$

where n denotes the actual wave packet and state entered by the electron and the atom. Eventually, it can be seen that the atom and the electron can be described by the product wave function of Eq. (4.75) instead of the series wave function of Eq. (4.70). This implies that the state of the atom ψ_n and the electron in the wave packet $f_n(\vec{x},\vec{y})$ behave independently. The product state (Eq. (4.75)), corresponds to the hydrogen atom in state Ψ_n and an outgoing electron with correlated energy $E_n = \frac{\hbar^2k_n^2}{2m}$. It is therefore clear that, although during interaction the atom and electron have a continuous range of energies, the final energy transfer $E_n - E_0$ to the hydrogen atom is discrete. The above provides a description of how the energy is always transferred in quanta of size $E_n - E_0$. It should also be noted that the wave function can be re-normalised, because multiplying Ψ_n by a constant does not change the value of any physical quantity, but is needed for a probability interpretation.

If the initial position of the atom and electron is known, then the actual wave packet entered could be predicted[5]. However, the initial position cannot be precisely determined, which is why the Bohm-de Broglie causal interpretation is called the hidden variable theory.

Chapter 5

The Hydrogen Atom

5.1 Overview

The hydrogen atom is the simplest atom because it's made up of only one electron and one proton. This chapter describes the development of the quantum theory of the atom from the classical description. The chapter also gives a summary of the solution to the Schrödinger equation for the hydrogen atom for $l = 1$ and $l = 2$. The wave functions considered in this case are expressed in spherical polar coordinates and are made up of radial functions and spherical harmonics. Further, details of the orbitals, the stationary states considered in this project and the angular momentum have been presented.

5.2 Theoretical Analysis

Being the simplest atom, the hydrogen atom has been used in the analysis and establishment of quantum composition and theories. The hydrogen atom has one electron that is negatively charged and a nucleus that contains a proton that is positively charged. The proton is massive compared to the electron[13].

Experiments by Ernest Rutherford in 1909 showed that the structure of the atom was a dense, positive nucleus with a tenuous negative charge cloud around it[48]. This immediately raised questions about how such a system could be stable. Classical electromagnetism had shown that any accelerating charge radiates energy, as shown by the Larmor formula[49]. If the electron is assumed to orbit in a perfect circle and radiate energy continuously, the electron would rapidly spiral into the nucleus[50]. This would mean that atoms would instantly collapse. However, atoms seem to be stable. Furthermore, the effect of spiralling inward would release continuous frequencies as the orbit got smaller. Instead, atoms were observed to emit only discrete frequencies of radiation[44]. The resolution of this anomaly was brought about with the development of quantum mechanics[19,24]

According to Bohr's model of the hydrogen atom[19], the electron moves in an orbit about the nucleus because of the Coulomb potential. Each state is associated with a unique energy, E_n where n is called the Principal Quantum number and $n \geq 1$. Later, Anorld Sommerfield realised that the principal quantum number 'n' was insufficient. He thus added the orbital angular momentum number l and the magnetic quantum number m, but these give degenerate states of the electron[51]. Different energies occur for different values of n, but we have degenerate states for the values of l and m associated with the same. Bohr also postulated that an electron in its stationary state does not radiate electromagnetic energy.

The quantum description of the hydrogen atom is given by the Schrödinger equation. The solutions to the Schrödinger equation for hydrogen are analytical, giving a simple expression for the hydrogen energy levels and thus the frequencies of the hydrogen spectral lines. These solutions are consistent with Bohr's model but also yield the other two quantum numbers.[52]

The solution of the Schrödinger equation for the hydrogen atom is a wave function made up of a radial component and spherical harmonics. In the usual interpretation of quantum mechanics, the wave function Ψ is a probability amplitude, so that $|\Psi|^2$ is a probability density[22]. In the case, $|\Psi|^2 dxdydz$ is the probability of finding the electron in a certain volume $dydxdz$.

The full eigenfunctions of the hydrogen atom can be expressed in spherical polar coordinates as follows:

$$\Psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi). \tag{5.1}$$

The spherical harmonics ($Y_l^m(\theta,\phi)$) are constant for all s-orbitals. They are symmetrically constant, independent of θ and ϕ. In the distribution of probability, the electron is most likely to be found at the Bohr radius. The Bohr radius is the distance between the electron and the nucleus. This is the most probable radius where an electron can be found.

In this work, the states n = 2; l =1 and n= 4; l= 3 were considered. As given by Griffiths[13], the radial functions (R_{nl}) and the spherical harmonics ($Y_l^m(\theta,\phi)$) for the states under consideration are shown in Table 5.1.

Radial Functions	
$l = 1$	$R_{21} = \frac{1}{2\sqrt{6}}a^{-3/2}(\frac{r}{a})\exp(-r/2a)$
$l = 3$	$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}(\frac{r}{a})^3\exp(-r/4a)$

Spherical Harmonics		
$l = 1$	$m = 0$	$Y_1^0 = (\frac{3}{4\pi})^{1/2}\cos\theta$
	$m = \pm 1$	$Y_1^{\pm}1 = \pm\pm(\frac{3}{8\pi})^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$
$l = 3$	$m = o$	$Y_3^0 = (\frac{7}{16\pi})^{1/2}(5\cos^3\theta - 3\cos\theta)$
	$m = \pm 1$	$Y_3^{\pm}1 = \mp(\frac{21}{64\pi})^{1/2}\sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
	$m = \pm 2$	$Y_3^{\pm}2 = (\frac{105}{32\pi})^{1/2}\sin^2\theta\cos\theta e^{\pm 2i\phi}$
	$m = \pm 3$	$Y_3^{\pm}3 = \mp(\frac{35}{64\pi})^{1/2}\sin^3\theta e^{\pm 3i\phi}$

TABLE 5.1: Radial functions and spherical harmonics for $l = 1$ and $l = 3$

5.3 Angular Momentum

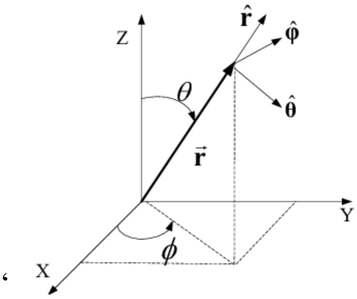
The classical model of the hydrogen atom is one in which an electron moves in a circular planar orbit about the nucleus as earlier discussed. The angular momentum of the electron in such a case would be with respect to an axis. This means that there should be an infinite number of values possible for the component for the angular momentum. The angle between the axis and the vector of the angular momentum will continuously vary from 0° to 180°.

The quantum mechanical angular momentum differs from the classical predictions in two ways. Firstly, the magnitude of the angular momentum is quantized,

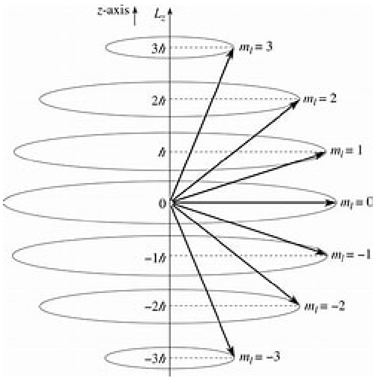
$$|L| = \sqrt{l(l+1)}\hbar. \tag{5.2}$$

Secondly, the angular momentum can only assume $2l+1$ values rather than the infinite number allowed in the classical model.

Figure 5.1a shows the projection of unit vectors in spherical polar coordinates. On the right, Figure 5.1b shows an example of a vector diagram of angular momentum for $l = 3$ and the magnitude of the angular momentum for different values of m. From the Figure 5.1b, it can also be seen that there are 7 values that can be assumed in this state.



(a) Projection of unit vectors in spherical polar coordinates



(b) Quantum mechanics vector diagram for angular momentum of the hydrogen atom for $l = 3$

Chapter 6

The Mathematical Model of the Hydrogen Atom Based on the Causal Interpretation

6.1 Overview

This chapter presents the model of the hydrogen atom. The chapter involves the detailed calculations on the basis of the causal interpretation in order to obtain the trajectories, angular momentum and net force for selected states of the hydrogen atom. The states considered in this model include $l = 1$ and $l = 3$. The calculations to determine the trajectories, angular momentum, and net force, were performed for both states. For $l = 1$, the calculations have also been extended to the rotated wave function. To get the trajectories for the rotated wave function, the differential equations of motion were solved numerically using the fourth order Runge-Kutta method in Maple.

6.2 A Model of the Standard Hydrogen Atom Wave Function for $l = 1$ and $l = 3$

6.2.1 The Wave Functions

In chapter 2, we saw that the causal interpretation yields very important relations that can be used to interpret the Schrödinger equation. From these relations, the trajectory, quantum potential and angular momentum can be determined for the electron in the hydrogen atom.

The wave function of the hydrogen atom is given by[44],

$$\Psi_{nlm}(r,\theta,\phi) = R_{nlm}(r)Y_{lm}(\theta,\phi). \tag{6.1}$$

Here n, l and m represent the principal number, the orbital quantum number and the magnetic quantum number, respectively. As can be seen from Eq. (6.1), the wave function is composed of the radial function and spherical harmonics with respect to the various quantum states of the hydrogen atom. In this research, calculations were performed to determine the trajectory, angular momentum, and the net force on an electron for the cases n = 2, $l = 1$ and n = 4, $l = 3$. The wave functions for the cases n = 2, $l = 1$ and n = 4, $l = 3$ are given in Table 6.1.

6.2.2 The Momentum

In chapter 2 of this work, it was noted that the momentum is given by Eq. (4.21). Therefore, the state $l = 1$ can be determined as follows:

Starting with the causal interpretation, the wave function $\Psi(r,\theta,\phi)$ is given by the expression,

$$\Psi(r,\theta,\phi) = R(r,\theta)\exp\left(i\frac{S(\phi)}{\hbar}\right). \tag{6.2}$$

Conjugating Eq. (6.2) yields,

$$\Psi^*(r,\theta,\phi) = R(r,\theta)\exp\left(-i\frac{S(\phi)}{\hbar}\right). \tag{6.3}$$

Dividing Eq. (6.2) by its conjugate 6.3 gives

$$\frac{\Psi}{\Psi^*} = \frac{R(r,\theta)\exp\left(i\frac{S(\phi)}{\hbar}\right)}{R(r,\theta)\exp\left(-i\frac{S(\phi)}{\hbar}\right)}. \tag{6.4}$$

WAVE FUNCTIONS	
m	Function
***n*=2; *l*=1**	
0	$\Psi_{210} = \frac{1}{\sqrt{3}}(Z/2a_{\mu})^{(}Zr/a_{\mu})\exp(-Zr/2a_{\mu})(\frac{3}{4\pi})^{\frac{1}{2}}\cos\theta$
±1	$\Psi_{21\pm1} = \frac{1}{\sqrt{3}}(Z/2a_{\mu})^{(}Zr/a_{\mu})\exp(-Zr/2a_{\mu})(\frac{3}{8\pi})^{\frac{1}{2}}\sin\theta\exp(\pm i\phi)$
***n* = 4; *l* = 3**	
0	$\Psi_{430} = \frac{1}{768\sqrt{35}}a^{-3/2}(\frac{r}{a})^3\exp(-r/4a)(\frac{7}{16\pi})^{1/2}(5\cos^3\theta - 3\cos\theta)$
±1	$\Psi_{43\pm1} = \mp\frac{1}{768\sqrt{35}}a^{-3/2}(\frac{r}{a})^3\exp(-r/4a)(\frac{21}{64\pi})^{1/2}\sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
±2	$\Psi_{43\pm2} = \frac{1}{768\sqrt{35}}a^{-3/2}(\frac{r}{a})^3\exp(-r/4a)(\frac{105}{32\pi})^{1/2}\sin^2\theta\cos\theta e^{\pm2i\phi}$
±3	$\Psi_{43\pm3} = \mp\frac{1}{768\sqrt{35}}a^{-3/2}(\frac{r}{a})^3\exp(-r/4a)(\frac{35}{64\pi})^{1/2}\sin^3\theta e^{\pm3i\phi}$

TABLE 6.1: List of wave functions for $l = 1$ and $l = 3$

This implies that

$$\frac{\Psi}{\Psi^*} = \frac{\exp\left(i\frac{S(\phi)}{\hbar}\right)}{\exp\left(-i\frac{S(\phi)}{\hbar}\right)}$$

or

$$\frac{\Psi}{\Psi_*} = \exp\left(i\frac{S(\phi)}{\hbar} + i\frac{S(\phi)}{\hbar}\right) = \exp\left(2i\frac{S(\phi)}{\hbar}\right).$$

Introducing the natural log (ln) and solving for S gives

$$S = \frac{\hbar}{2i}\ln\left(\frac{\Psi}{\Psi*}\right). \tag{6.5}$$

Thus, applying Eq. (6.5) to Ψ_{210} (see Table 6.1) gives $S = 0$.

When Eq. (6.5) is applied to Eq. (6.1), for the non-zero values of m (see Table 6.1), the common terms cancel out, leaving the expression,

$$S = \frac{\hbar}{2i} ln(\exp 2im\phi) \tag{6.6}$$

and hence

$$S = m\hbar\phi. \tag{6.7}$$

Since ∇ is given by

$$\nabla = \frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial\theta}\hat{\theta} + \frac{1}{rsin\theta}\frac{\partial}{\partial\phi}\hat{\phi}, \tag{6.8}$$

∇S takes the form

$$\nabla S = \frac{\partial(m\hbar\phi)}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial(m\hbar\phi)}{\partial\theta}\hat{\theta} + \frac{1}{rsin\theta}\frac{\partial m\hbar\phi}{\partial\phi}\hat{\phi}. \tag{6.9}$$

From the fact that S does not depend on r or θ (see Eq. (6.7)), Eq. (6.9) reduces to

$$\nabla S = \frac{m\hbar}{rsin\theta}\hat{\phi}. \tag{6.10}$$

Comparing with Eq. (4.21) from Chapter 4, Eq. (6.10) gives the momentum of the electron.

6.2.3 The Trajectories

From Chapter 4, Eq. (4.22), the velocity of the electron is given by

$$\frac{d\vec{r}}{dt} = \vec{V} = \frac{\nabla S}{m_e}, \tag{6.11}$$

where m_e is the mass of an electron. Consequently, the expression for the trajectory of the electron can be given by

$$\vec{r} = \int \vec{V} dt. \tag{6.12}$$

This implies that

$$\frac{d\vec{r}}{dt} = \frac{m\hbar}{m_e r sin\theta}\hat{\phi}, \tag{6.13}$$

with $\hat{\phi}$ expressed in rectangular coordinates. Eq (6.13) can further be expressed as

$$\frac{d\vec{r}}{dt} = \frac{dx}{dt}\hat{i} + \frac{dy}{dt}\hat{j} + \frac{dz}{dt}\hat{k} = \frac{m\hbar}{m_e r sin\theta}(-sin\phi\hat{i} + cos\phi\hat{j} + 0\hat{k}). \tag{6.14}$$

Equating the corresponding terms gives,

$$\frac{dx}{dt} = -\frac{m\hbar}{m_e r \sin\theta} sin\phi \tag{6.15}$$

$$\frac{dy}{dt} = \frac{m\hbar}{m_e r \sin\theta} cos\phi \tag{6.16}$$

and

$$\frac{dz}{dt} = 0 = constant \tag{6.17}$$

. The angle $\phi(t)$ determines both the motion of the electron orbit and the precession of angular momentum.

6.2.3.1 Equation of Motion ϕ

The angle $\phi(t)$ can be obtained by expressing Eq. (6.13) in spherical polar coordinates, as,

$$\frac{d\vec{r}}{dt} = \frac{dr}{dt}\hat{r} + r\frac{d\theta}{dt}\hat{\theta} + r\sin\theta\frac{d\phi}{dt}\hat{\phi} = \frac{m\hbar}{m_e r\sin\theta}\hat{\phi}. \tag{6.18}$$

The constant r is determined from the probability function[44]. When we compare the coefficients of the unit vectors, we see that $\frac{dr}{dt} = 0$ and $r\frac{d\theta}{dt} = 0$. Hence, r and ϕ are constants of motion and

$$\frac{d\theta}{dt} = 0. \tag{6.19}$$

Therefore, Eq. (6.18) reduces to

$$r\sin\theta\frac{d\phi}{dt}\hat{\phi} = \frac{m\hbar}{m_e r\sin\theta}\hat{\phi} \tag{6.20}$$

or

$$\frac{d\phi}{dt}\hat{\phi} = \frac{m\hbar}{m_e r^2\sin^2\theta}\hat{\phi}. \tag{6.21}$$

Integrating the above equation yields

$$\phi(t) = \frac{m\hbar}{m_e r^2\sin^2\theta}t + \alpha. \tag{6.22}$$

Eq. (6.22) thus gives the direction of motion of the electron orbit and also determines the precession of the angular momentum l.

Substituting into Eq. (6.22) for ϕ and integrating Eq. (6.15) and Eq. (6.16) gives

$$x(t) = r\sin\theta.\cos\left(\frac{m\hbar}{m_e r^2\sin^2\theta}t + \alpha\right) \tag{6.23}$$

and

$$y(t) = r\sin\theta.\sin\left(\frac{m\hbar}{m_e r^2\sin^2\theta}t + \alpha\right) \tag{6.24}$$

Therefore, the trajectory of the electron in the hydrogen atom can generally be given by

$$r(t)=\left[r\sin\theta.\cos\left(\frac{m\hbar}{m_e r^2\sin^2\theta}t+\alpha\right)\right]\hat{i}+\left[r\sin\theta.\sin\left(\frac{m\hbar}{m_e r^2\sin^2\theta}t+\alpha\right)\right]\hat{j}+0\hat{k} \tag{6.25}$$

Eq. (6.25) shows that the motion of the electron is constant with respect to the z-axis.

6.2.3.2 The Angular Momentum

The angular momentum vector is given by the formula,

$$\vec{L}=\vec{r}\times\vec{p}. \tag{6.26}$$

Since Eq. (6.10) gives the linear momentum, we have

$$\vec{L}=r\hat{r}\times\frac{m\hbar}{r\sin\theta}\hat{\phi}, \tag{6.27}$$

giving

$$\vec{L}=\frac{mr\hbar}{r\sin\theta}(\hat{r}\times\hat{\phi}). \tag{6.28}$$

Simplification of Eq. (6.28) results in

$$\vec{L}=-\frac{m\hbar}{\sin\theta}\hat{\theta}. \tag{6.29}$$

In rectangular coordinates, $\hat{\theta}$ is given by the expression

$$\hat{\theta}=\cos\theta\cos\phi\hat{i}+\cos\theta\sin\phi\hat{j}-\sin\theta\hat{k}. \tag{6.30}$$

Substituting Eq. (6.30) into Eq. (6.29) and simplifying gives

$$\vec{L}=-m\hbar(\cot\theta\cos\phi\hat{i}+\cot\theta\sin\phi\hat{j}-\hat{k}). \tag{6.31}$$

Therefore,

$$L_x = -m\hbar \cot\theta \cos\phi, \tag{6.32}$$

$$L_y = -m\hbar \cot\theta \sin\phi, \tag{6.33}$$

and

$$L_z = m\hbar, \tag{6.34}$$

$$L^2 = \vec{L}.\vec{L} = m^2\hbar^2(\cot^2\theta\cos^2\phi + \cot^2\theta\sin^2\phi + 1). \tag{6.35}$$

This simplifies to

$$L^2 = m^2\hbar^2(\cot^2\theta + 1) \tag{6.36}$$

or

$$L^2 = \frac{m^2\hbar^2}{\sin^2\theta} \tag{6.37}$$

The magnitude is therefore given by:

$$|L| = \frac{m\hbar}{\sin\theta} \tag{6.38}$$

6.2.3.3 The Angle θ

By quantum theory[44] the magnitude of the angular momentum is given by

$$|L| = \sqrt{l(l+1)}\hbar. \tag{6.39}$$

Equating Eq. (6.38) to (6.39) gives

$$\sqrt{l(l+1)}\hbar = \frac{m\hbar}{\sin\theta}. \tag{6.40}$$

For l = 1, we have

$$\sqrt{2}\hbar = \frac{m\hbar}{\sin\theta}. \tag{6.41}$$

Solving for θ gives,

$$\theta = \sin^{-1}\left(\frac{m}{\sqrt{2}}\right) \tag{6.42}$$

For l= 3 we have

$$|L| = \sqrt{3(3+1)}\hbar \tag{6.43}$$

therefore

$$\theta = \sin^{-1}\left(\frac{m}{2\sqrt{3}}\right) \tag{6.44}$$

The values of θ obtained for l = 3 are recorded in the Table 6.2.

l	**m**	**Function**	θ
1	-1	$\theta = \sin^{-1}\left(\frac{-1}{\sqrt{2}}\right)$	225°
	0	$\theta = \sin^{-1}\left(\frac{0}{\sqrt{2}}\right)$	0°
	1	$\theta = \sin^{-1}\left(\frac{1}{\sqrt{2}}\right)$	45°
3	-3	$\theta = \sin^{-1}\left(\frac{-3}{2\sqrt{3}}\right)$	240°
	-2	$\theta = \sin^{-1}\left(\frac{-2}{2\sqrt{3}}\right)$	215.26°
	-1	$\theta = \sin^{-}1\left(\frac{-1}{2\sqrt{3}}\right)$	196.77°
	0	$\theta = \sin^{-1}\left(\frac{0}{2\sqrt{3}}\right)$	0°
	1	$\theta = \sin^{-1}\left(\frac{1}{2\sqrt{3}}\right)$	16.77°
	2	$\theta = \sin^{-1}\left(\frac{2}{2\sqrt{3}}\right)$	35.26°
	3	$\theta = \sin^{-1}\left(\frac{3}{2\sqrt{3}}\right)$	60°

TABLE 6.2: Values of θ for l = 3

From Table 6.2, the values of θ for the negative values of m are obtained by subtracting from 180° since $\sin\theta = \sin(180^\circ - \theta)$.

6.2.3.4 The Net Force

From the H-J equation (Eq. (4.19)) in chapter 4, the quantum potential is given by Eq. 4.24. Therefore, Eq. (4.19) can be rewritten in terms of Q as

$$Q = -\frac{\partial S}{\partial t} - \frac{(\nabla s)^2}{2m_e} - V. \tag{6.45}$$

From the definition of energy in Eq. (4.20) and ∇S from Eq. (6.10), Eq.(6.45) can also be expressed as

$$Q = E_n - V - \frac{m^2\hbar^2}{2m_e r^2 \sin^2\theta}. \tag{6.46}$$

Here V is the potential energy of the electron given by

$$V = \frac{-e^2}{(4\pi\varepsilon_0)r}, \tag{6.47}$$

while E_n for the hydrogen atom is given by

$$E_n = -\frac{\mu}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{Z^2}{n^2}, \tag{6.48}$$

where z = 1. The quantum force is given by

$$F = -\nabla Q, \tag{6.49}$$

where the ∇ is given by Eq. (6.8). The energy E_n does not depend on r,θ, and ϕ. Thus, from Eq. (6.45), Q does not depend on ϕ implying that

$$-\nabla Q = \left[\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r^2}\right) + \frac{m^2\hbar^2}{2m_e\sin^2\theta}\left(\frac{-2}{r^3}\right)\right]\hat{r} + \left[\frac{m^2\hbar^2}{2m_e r^2}(-2\cos\theta\sin^{-3}\theta)\right]\frac{\hat{\theta}}{r}. \tag{6.50}$$

From this, we get

$$F_Q = \left[\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{r^2}\right) + \frac{m^2\hbar^2}{2m_e\sin^2\theta}\left(\frac{-2}{r^3}\right)\right]\hat{r} + \left[\frac{m^2\hbar^2}{2m_e r^2}(-2\cos\theta\sin^{-3}\theta)\right]\frac{\hat{\theta}}{r}. \tag{6.51}$$

Simplifying further gives

$$F_Q = \left(\frac{e^2}{4\pi\varepsilon_0 r^2} - \frac{m^2\hbar^2}{m_e \sin^2\theta r^3}\right)\hat{r} - \left(\frac{m^2\hbar^2\cos\theta}{m_e r^3 \sin^3\theta}\right)\hat{\theta}. \tag{6.52}$$

The force due to the classical potential is

$$F_V = -\nabla V = -\nabla\left[-\frac{e^2}{4\pi\varepsilon_0 r}\right] = \left[\frac{e^2}{4\pi\varepsilon_0}\frac{\partial r^- 1}{\partial r}\right]\hat{r}, \tag{6.53}$$

$$F_V = -\frac{e^2}{4\pi\varepsilon_0 r^2}\hat{r}. \tag{6.54}$$

Therefore, the net force of the electron should be given by

$$F_{net} = F_Q + F_V, \tag{6.55}$$

$$F_{net} = \left(\frac{e^2}{4\pi\varepsilon_0 r^2} - \frac{m^2\hbar^2}{m_e \sin^2\theta r^3}\right)\hat{r} - \frac{\cos\theta}{m_e r^3 \sin^3\theta}\hat{\theta} - \frac{e^2}{4\pi\varepsilon_0 r^2}\hat{r}. \tag{6.56}$$

Cancelling the common terms, and simplifying gives

$$\vec{F}_{net} = \frac{-m^2\hbar^2}{m_e r^3 \sin^2\theta}(\hat{r} + \cot\theta\hat{\theta}) \tag{6.57}$$

We express $\vec{F}_{net}$ in rectangular coordinates by first expressing the unit vectors in rectangular coordinate:

$$\begin{aligned}\vec{F}_{net} =& \frac{-m^2\hbar^2}{m_e r^3 \sin^2\theta}[\sin\theta\cos\phi\hat{\imath} + \sin\theta\sin\phi\hat{\jmath} + \cos\theta\hat{k} + \\ & \cot\theta(\cos\theta\cos\phi\hat{\imath} + \cos\theta\sin\phi\hat{\jmath} - \sin\theta\hat{k})].\end{aligned} \tag{6.58}$$

This can be simplified to

$$\vec{F}_{net} = \frac{-m^2\hbar^2}{m_e r^3 \sin^3\theta}(\cos\phi\hat{\imath} + \sin\phi\hat{\jmath}). \tag{6.59}$$

The magnitude of F_{net} is

$$|F_{net}| = \frac{m^2\hbar^2}{m_e r^3 \sin^3\theta}. \tag{6.60}$$

Using the values of θ from Table 6.2, the net force can be deduced as follows from Eq. (6.60) for m = 0, $|F_{net}| = 0$. This shows that the electron will be stationary for $m = 0$. For $m = \pm 1$

$$|F_{net}| = \frac{\hbar^2}{m_e r^3 \sin^3(45)} \tag{6.61}$$

From classical mechanics, the centripetal force is given by

$$|F_C| = \frac{m_e v^2}{r\sin\theta}, \tag{6.62}$$

where

$$|v| = \frac{\vec{P}}{m_e} = \frac{m\hbar}{m_e r\sin\theta}\hat{\phi}. \tag{6.63}$$

Hence

$$|F_C| = \frac{m^2\hbar^2}{m_e r^3 \sin^3\theta}. \tag{6.64}$$

Eq. (6.64) is equal to Eq. (6.60) showing that the centripetal force is the only force acting on the electron in the stationary states of the hydrogen atom. This is the force that keeps the electron orbiting and since their is no loss of energy, the electron does not collapse into the nucleus.

6.3 A model of the Rotated Wave Function for l = 1

6.3.1 The Wave functions

The wave function can be expressed in rectangular coordinates by using Euler's equation. For simplicity, we write the wave function for l =1 given by Table 6.1 as,

$$\psi_{21\pm1} = \pm R_{21} A \sin\theta . \exp(\pm i\phi) \tag{6.65}$$

and

$$\psi_{210} = R_{21} B \cos\theta, \tag{6.66}$$

where

$$A = \left(\frac{3}{8\pi}\right)^{1/2} \tag{6.67}$$

and

$$B = \left(\frac{3}{4\pi}\right)^{1/2}. \tag{6.68}$$

Substituting with Euler's equation

$$\psi_{21\pm1} = \pm R_{21} A (\sin\theta\cos\phi \pm i \sin\theta \sin\phi), \tag{6.69}$$

which in rectangular coordinates becomes

$$\Psi_{21\pm1} = \frac{\pm A R_{21}}{r}(x \pm iy) \tag{6.70}$$

and

$$\Psi_{210} = R_{21} B \frac{z}{r}. \tag{6.71}$$

Considering a case of rotation about the y-axis through the angle $\beta = 60^o$ of the coordinate system, we obtain the following relations for the old and new coordinates.

$$x = z' \sin\beta + x' \cos\beta, \tag{6.72}$$

$$z = z' \cos\beta - x' \sin\beta, \tag{6.73}$$

$$y = y' \tag{6.74}$$

To obtain Ψ_{21m} in terms of x', y' and z', we substitute Eqs. (6.72), (6.74) and (6.73) into Eq. (6.71). Eq. (6.70) to get

$$\Psi_{21\pm1} = \mp\frac{AR_{21}}{r}(z'\sin\beta + x'\cos\beta \pm iy) \tag{6.75}$$

and

$$\Psi_{210} = \frac{BR_{21}}{r}(z'\cos\beta - x'\sin\beta). \tag{6.76}$$

6.3.2 The Trajectory

The trajectory for the rotated wave function can be determined using Eq. (6.5) so that

$$S_{211} = \frac{\hbar}{2i}\ln\left(\frac{\Psi_{211}}{\Psi^*_{211}}\right). \tag{6.77}$$

From Eq. (6.75), the common terms of Ψ and Ψ^* will cancel out, giving

$$S_{211} = \frac{\hbar}{2i}\ln\left(\frac{z'\sin\beta + x'\cos\beta + iy}{z'\sin\beta + x'\cos\beta - iy}\right). \tag{6.78}$$

If $z'\sin\beta + x'\cos\beta + iy = F$, Eq. (6.78) becomes

$$S_{211} = \frac{\hbar}{2i}\ln\left(\frac{F}{F^*}\right). \tag{6.79}$$

The velocity can be determined from ∇S. Starting with the x component,

$$\frac{\partial S}{\partial x'} = \frac{\hbar}{2i}\frac{\partial}{\partial x'}ln\left(\frac{F}{F^*}\right). \tag{6.80}$$

This simplifies to

$$\frac{\partial S}{\partial x'} = \frac{\hbar}{2i}\left(\frac{1}{F}\frac{\partial F}{\partial x'} - \frac{1}{F^*}\frac{\partial F^*}{\partial x'}\right) \tag{6.81}$$

From Eq. (6.78), the differentiation yields

$$\frac{\partial F}{\partial x'} = \cos\beta = \frac{\partial F^*}{\partial x'} \tag{6.82}$$

so that

$$\frac{\partial S}{\partial x'} = \frac{\hbar}{2i}\left(\frac{\cos\beta}{F} - \frac{\cos\beta}{F^*}\right). \tag{6.83}$$

Simplifying further gives

$$\frac{\partial S}{\partial x'} = \frac{\hbar}{2i}\frac{(-2iy'\cos\beta)}{FF^*}, \tag{6.84}$$

$$\frac{\partial S}{\partial x'} = \frac{-\hbar\cos\beta y'}{FF^*} \tag{6.85}$$

or

$$\frac{\partial S}{\partial x'} = \frac{-\hbar y'\cos\beta}{z'^2\sin^2\beta + x'^2\cos^2\beta + y'^2 + 2x'z'\sin\beta\cos\beta}. \tag{6.86}$$

Similarly, the y component can be written as

$$\frac{\partial S_{211}}{\partial y'} = \frac{\hbar z'\sin\beta + \hbar x'\cos\beta}{z'^2\sin\beta + x'^2\cos^2\beta + y'^2 + 2x'z'\sin\beta\cos\beta}. \tag{6.87}$$

and the z component by

$$\frac{\partial S_{211}}{\partial z'} = \frac{-\hbar y'\sin\beta}{z'^2\sin^2\beta + x'^2\cos^2\beta + y'^2 + 2x'z'\sin\beta\cos\beta}. \tag{6.88}$$

The trajectory components, S_{211} are found from Eq. (6.11):

$$\frac{dx'}{dt} = \frac{-\hbar y'\cos\beta}{m_e(z'^2\sin^2\beta + x'^2\cos^2\beta + y'^2 + 2x'z'\sin\beta\cos\beta)}, \tag{6.89}$$

$$\frac{dy'}{dt} = \frac{\hbar(z'\sin^2\beta + x'\cos\beta)}{m_e(z'^2\sin\beta + x'^2\cos^2\beta + y'^2 + 2x'z'\sin\beta\cos\beta)}, \tag{6.90}$$

$$\frac{dz'}{dt} = \frac{-\hbar y' \sin\beta}{m_e(z'^2 \sin^2\beta + x'^2 \cos^2\beta + y'^2 + 2x'z' \sin\beta \cos\beta)}, \tag{6.91}$$

For state Ψ_{210}, it can be deduced that

$$\vec{v} = \frac{\nabla s}{m_e} = 0. \tag{6.92}$$

For state Ψ_{21-1}, similar to state Ψ_{211}, the components of the velocity are as follows:

$$\frac{dx'}{dt} = \frac{\hbar y' \cos\beta}{m_e(z'^2 \sin^2\beta + x'^2 \cos^2\beta + y'^2 + 2x'z' \sin\beta \cos\beta)}, \tag{6.93}$$

$$\frac{dy'}{dt} = \frac{-\hbar(z' \sin^2\beta + x' \cos\beta)}{m_e(z'^2 \sin\beta + x'^2 \cos^2\beta + y'^2 + 2x'z' \sin\beta \cos\beta)}, \tag{6.94}$$

$$\frac{dz'}{dt} = \frac{\hbar y' \sin\beta}{m_e(z'^2 \sin^2\beta + x'^2 \cos^2\beta + y'^2 + 2x'z' \sin\beta \cos\beta)}. \tag{6.95}$$

6.3.2.1 The Net Force

As earlier shown the net force on the electron is obtained as a sum of the quantum potential force F_Q and the electromagnetic force F_V, see Eq. (6.55). We now obtain the net force on the electron for the rotated axes. We begin with the general expression of the force as earlier established,

$$F_{net} = -\nabla E_2 + \frac{\nabla(\nabla S)^2}{2m_e} + \nabla V - \nabla V. \tag{6.96}$$

Since $\nabla E_2 = 0$, the equation above reduces to

$$F_{net} = \frac{\nabla(\nabla S)^2}{2m_e}. \tag{6.97}$$

now

$$(\nabla S)^2 = \left(\frac{\partial S}{\partial x'}\right)^2 + \left(\frac{\partial S}{\partial y'}\right)^2 + \left(\frac{\partial S}{\partial z'}\right)^2 \tag{6.98}$$

Using the components of ∇S for the rotated wave function (Eqs. (6.86), (6.87) and (6.88)), the square of the individual components yields the following expressions: The x - component (See Eq. (6.86))

$$\left(\frac{\partial S}{\partial x'}\right)^2 = \frac{\hbar^2 y'^2 \cos^2\beta}{(FF^*)^2}, \tag{6.99}$$

The y-component (Eq. (6.87))

$$\left(\frac{\partial S}{\partial y'}\right)^2 = \frac{\hbar^2(z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta)}{(FF^*)^2}, \tag{6.100}$$

and the z-component

$$\left(\frac{\partial S}{\partial z'}\right)^2 = \frac{\hbar^2 y'^2 \sin^2\beta}{(FF^*)^2}. \tag{6.101}$$

Giving

$$(\nabla S)^2 = \frac{\hbar^2 y'^2 \cos^2\beta}{(FF^*)^2} + \frac{\hbar^2(z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta)}{(FF^*)^2} + \frac{\hbar^2 y'^2 \sin^2\beta}{(FF^*)^2} \tag{6.102}$$

and

$$\begin{aligned}\nabla(\nabla S)^2 = {} & \frac{\partial}{\partial x}\left[\frac{\hbar^2 y'^2 \cos^2\beta}{(FF^*)^2} + \frac{\hbar^2(z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta)}{(FF^*)^2} + \frac{\hbar^2 y'^2 \sin^2\beta}{(FF^*)^2}\right] \\ & + \frac{\partial}{\partial y}\left[\frac{\hbar^2 y'^2 \cos^2\beta}{(FF^*)^2} + \frac{\hbar^2(z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta)}{(FF^*)^2} + \frac{\hbar^2 y'^2 \sin^2\beta}{(FF^*)^2}\right] \\ & + \frac{\partial}{\partial z}\left[\frac{\hbar^2 y'^2 \cos^2\beta}{(FF^*)^2} + \frac{\hbar^2(z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta)}{(FF^*)^2} + \frac{\hbar^2 y'^2 \sin^2\beta}{(FF^*)^2}\right]\end{aligned} \tag{6.103}$$

expanding

$$\begin{aligned}
\nabla(\nabla S)^2 = \hbar^2 \Bigg[& \frac{1}{FF*}\frac{\partial}{\partial x'}(y'^2\cos^2\beta + z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta + y'^2\sin^2\beta) \\
& + y'^2\cos^2\beta + z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta + y'^2\sin^2\beta\left(\frac{\partial(FF*)}{\partial x'}\right)\Bigg] \\
+\hbar^2 \Bigg[& \frac{1}{FF*}\frac{\partial}{\partial y'}(y'^2\cos^2\beta + z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta + y'^2\sin^2\beta) \\
& + y'^2\cos^2\beta + z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta + y'^2\sin^2\beta\left(\frac{\partial(FF*)}{\partial y'}\right)\Bigg] \\
+\hbar^2 \Bigg[& \frac{1}{FF*}\frac{\partial}{\partial z'}(y'^2\cos^2\beta + z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta + y'^2\sin^2\beta) \\
& + y'^2\cos^2\beta + z'^2\sin^2\beta + 2z'x'\sin\beta\cos\beta + x'^2\cos^2\beta + y'^2\sin^2\beta\left(\frac{\partial(FF*)}{\partial z'}\right)\Bigg]
\end{aligned} \tag{6.104}$$

and then differentiating gives

$$\begin{aligned}
&\nabla(\nabla S)^2 = \\
&\qquad \hbar^2\Bigg[\Bigg[\frac{1}{FF*}(2z'\sin\beta\cos\beta + 2x'\cos^2\beta) \\
&\qquad + \frac{\partial(FF*)^{-2}}{\partial x'}(y'^2\cos^2\beta + z'^2\sin^2\beta + 2x'\sin\beta\cos\beta + x'^2\cos^2\beta + y^2\sin^2\beta)\Bigg] \\
&\qquad + \Bigg[\frac{1}{FF*}(2y'\cos^2\beta + 2y'\sin^2\beta) \\
&\qquad + \frac{\partial(FF*)^{-2}}{\partial y'}(y'^2\cos^2\beta + z'^2\sin^2\beta + 2x'\sin\beta\cos\beta + x'^2\cos^2\beta + y^2\sin^2\beta)\Bigg] \\
&\qquad + \Bigg[\frac{1}{(FF*)^2}(2z'\sin^2\beta + 2x'\sin\beta\cos\beta) \\
&\qquad + \frac{\partial(FF*)^{-2}}{\partial z'}(y'^2\cos^2\beta + z'^2\sin^2\beta + 2x'\sin\beta\cos\beta + x'^2\cos^2\beta + y^2\sin^2\beta)\Bigg]\Bigg]
\end{aligned} \tag{6.105}$$

where

$$FF^* = z'^2\sin\beta + x'^2\cos^2\beta + y'^2 + 2x'z'\sin\beta\cos\beta. \tag{6.106}$$

Squaring Eq. (6.106) gives

$$\begin{aligned}(FF*)^2 =& z'^4\sin^4\beta + 2x'^2z'^2\sin^2\beta\cos^2\beta + 2y'^2z'^2\sin^2\beta \\ &+ 4z'^3x'\sin^3\beta\cos\beta + x'^4\cos^4\beta + 2y'^2x'^2\cos^2\beta + 4z'x'^3\sin\beta\cos^3\beta \\ &+ y'^4 + 4y'^2z'x'\sin\beta\cos\beta + 4z'^2x'^2\sin^2\beta cos^2\beta.\end{aligned} \tag{6.107}$$

Differentiating $(FF*)^2$ gives the formulae:

$$\begin{aligned}\frac{\partial(FF*)^{-2}}{\partial x} =& \frac{-2}{(FF^*)^3}(12x'z'^2\sin^2\beta\cos^2\beta + 4z'^3\sin^3\beta\cos\beta \\ &+ 4x'^3\cos^4\beta + 4y'^2x'\cos^2\beta + 12z'x'^2\sin\beta\cos^3\beta + 4y'^2z'\sin\beta\cos\beta),\end{aligned}$$

$$\frac{\partial(FF*)^{-2}}{\partial y} = \frac{-2}{(FF^*)^3}(4y'z'^2\sin^2\beta + 4y'x'^2\cos^2\beta + 4y'^3 + 8y'z'x'\sin\beta\cos\beta),$$

and

$$\begin{aligned}\frac{\partial(FF*)^{-2}}{\partial z} =& \frac{-2}{(FF^*)^3}(4z'^3\sin^4\beta + 12x'^2z'\sin^2\beta\cos^2\beta \\ &+ 4y'^2z'\sin^2\beta + 12z'^2x'\sin^3\beta\cos\beta + 4x'^3\sin\beta\cos^3\beta + 4y'^2x'\sin\beta\cos\beta).\end{aligned}$$

From Eq.(6.97) and Eq.(6.105) we obtain the net force as;

$$
\begin{aligned}
F_{net} = \frac{\hbar^2}{2m_e}\Bigg[\bigg[&\frac{2z'\sin\beta\cos\beta + 2x'\cos^2\beta}{(FF^*)^2} + (y'^2\cos^2\beta + z'^2\sin^2\beta + 2x'\sin\beta\cos\beta \\
&+ x'^2\cos^2\beta + y^2\sin^2\beta)\frac{\partial(FF*)^{-2}}{\partial x'}\bigg]\hat{i} \\
&+ \bigg[\frac{2y'\cos^2\beta + 2y'\sin^2\beta}{(FF*)^2} + (y'^2\cos^2\beta + z'^2\sin^2\beta + 2x'\sin\beta\cos\beta + x'^2\cos^2\beta \\
&+ y'^2\sin^2\beta)\frac{\partial(FF*)^{-2}}{\partial y'}\bigg]\hat{j} \\
&+ \bigg[\frac{2z'\sin^2\beta + 2x'\sin\beta\cos\beta}{(FF^*)^2} + (y'^2\cos^2\beta + z'^2\sin^2\beta + 2x'\sin\beta\cos\beta \\
&+ x'^2\cos^2\beta + y'^2\sin^2\beta)\frac{\partial(FF*)^{-2}}{\partial z'}\bigg]\hat{k}\Bigg].
\end{aligned}
\tag{6.108}
$$

Eq.(6.105) gives the components of the net force acting on the electron when the axes are rotated. The equation shows that the force on the electron acts in all the directions x, y and z. We want to see from this equation whether rotating the axes affects the direction of the force and be able to compare with the plots that will be yielded from the ordinary axes in Eq.(6.59).

Chapter 7

A Computer Model of the Hydrogen Atom

7.1 Overview

In this chapter, we present the computer model of the hydrogen atom. The plots were made based on the calculations in chapter 6 using Maple. The plots presented show the trajectories of the electron, the direction of force at various points of the trajectory, and the angular momentum vector. All the plots were done in atomic mass units, and the constants used for the plots were obtained from CRC Handbook of Chemistry and Physics[37].

The radius r = bohr radius $a_o = 5.291772107 \times 10^{-11} m$

The electron Mass $m_e = 9.10938356 \times 10^{-31} kg$

Reduced Plank's constant $\hbar = 1.0545871800 \times 10^{-34} J.s$

7.2 The Trajectories

The trajectories of the electron for the stationary states of the hydrogen atom have been obtained from the equations of motion Eq.(6.25). From the equation we can see that the electron moves in the xy- plane as the z-component is constant. From Eq. (6.29), it can also be seen that for positive values of m, the angular momentum will point in the opposite direction of the unit vector $\hat{\theta}$, and will point in the same direction for negative values of m. This implies that the trajectories will be on the positive z-axis for the positive values of m and vice-versa. Therefore, the values of of z can be seen to depend on r and θ which are also constants. This can be deduced from the eigenvalue

$L_z = m\hbar$ and the vector diagram Figure 5.1b, in this case, the values of z are given by

$$z = rcos\theta \tag{7.1}$$

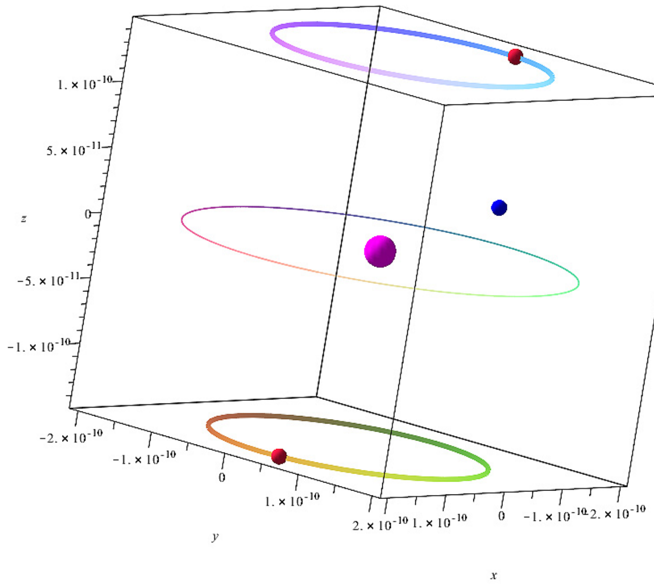
7.2.1 Electron Trajectories for l = 1

From the trajectory (Eqs. (6.25) and (7.1)) and the values of θ presented in Table 6.2, we obtain the trajectories for l=1 as presented in Figure 7.1. The figure shows the two trajectories for the two values of m. The line around the nucleus is not a trajectory, but it is just added for visualisation. We can see that there are two expected orbits for the state, $l = 1$ which are obtained from the two values of m, $m = 1$ and $m = -1$. This model also shows that the electron will remain in the respective path as long as the atom remains in the same state.

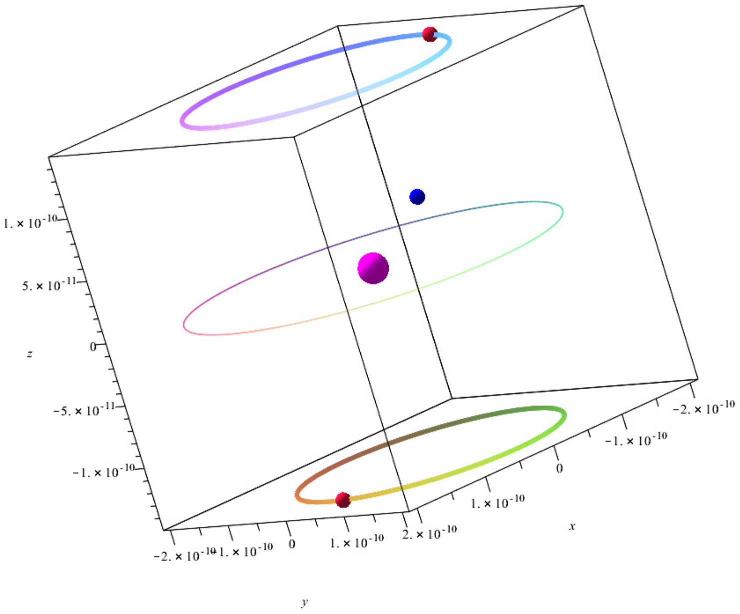
The orbits are at latitude with the nucleus for consistency with the quantum mechanics vector model (Fig. 5.1b) of angular momentum and with the formula $\vec{L} = \vec{r} \times \vec{P}$. This can be seen also from the values of theta in Table 6.2, the values of theta for $m = -1$ and $m = 1$ are 225° and 45°, respectively. These values are measured with reference to the z axis, thus all nonzero values of θ represent a shift from the z axis.

The electron is stationary for $m = 0$, as shown clearly by Eq. (6.11). Its velocity, $v = 0$, because the net force is also zero as can be seen from Eq. (6.56). Therefore, the position of the electron at $m = 0$ can only be fixed by the probability density and it is stationary. Since the $m = 0$ electron is stationary, it cannot be consistent with QM vector model which gives $L_z = 0$ and $|L| = 0$ for $m = 0$. This can also be illustrated from the magnitude of the angular momentum in Eq.6.28 we can see that if $\theta = 0$ the value of the angular momentum L becomes undefined because the denominator becomes zero. Therefore, it is meaningless to discuss the angle θ for $m = 0$. In the vector model of quantum mechanics, the magnitude of angular momentum L is given by $L = \frac{m\hbar}{\cos\theta}$, which gives L = 0 which shows the inconsistency. The middle orbit as shown in the plots is therefore just a reference path around the nucleus.

By use of animations, it can be shown that the electron moves in the clockwise direction when m is negative and in the anticlockwise direction when m positive. The nucleus was fixed at (0,0,0), which is the centre of the atom in this model. The radius r, was defined using the Bohr radius a_o. The results produced are in the scale of an atom as it can be observed from the scales of the axes.



(a) first orientation



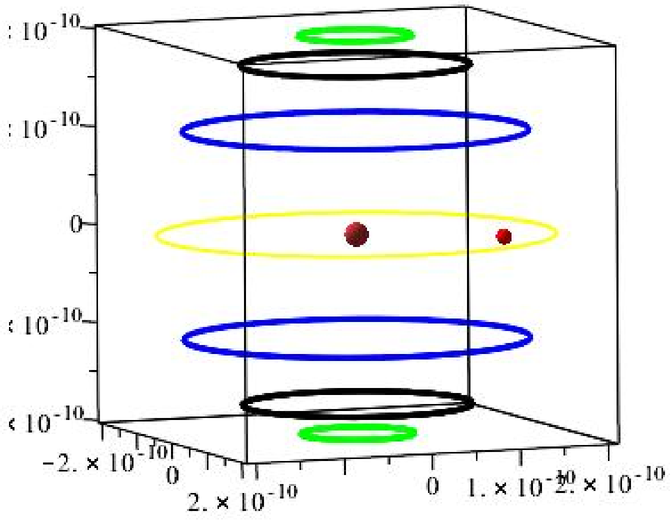
(b) second orientation

FIGURE 7.1: Computer model of electron trajectories for l = 1 plotted using maple, shown at different orientations. The nucleus, in purple, is at the centre of the atom surrounded by three circular orbits of the electron expected for the states m= -1, m=0 and m= 1. The red dots represent the electron in the circular orbit, and the blue dot represents the electron when m= 0.

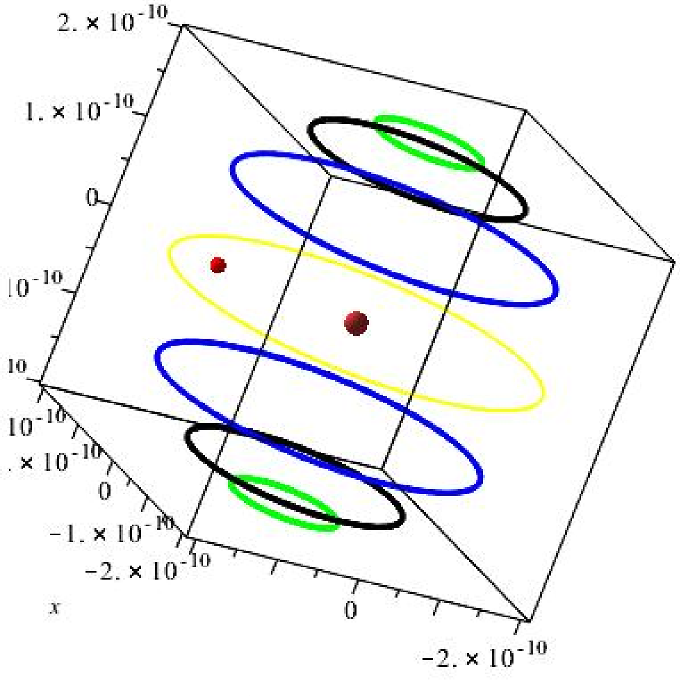
7.2.2 Electron Trajectories for $l = 3$

Similarly, the trajectories for $l = 3$ are presented in Figure 7.2. The figures show the orbits for the different values of m. Since there are seven states for the seven values of m, the seven expected trajectories for the electron in each state are shown below. It is important to note that there is only one electron in the hydrogen atom. Therefore, the trajectories shown in the plots are the seven different possible orbits for the single electron. This means that for each value of m there is only one orbit for the electron. This can also be compared with the vector diagrams of angular momentum in Figure 5.1b. This also shows that the model presented is consistent with quantum mechanics.

As can be seen thus far, different values of m have different radii, which are proportional to the magnitude of m. For a better view of the radii, below is the plot with an orientation which gives a 2-dimensional view. Figure 7.3 also clearly shows that the same values of $|m|$ yield orbits of the same radius, hence they overlap when viewed from the top of the z-axis.



(a) First orientation



(b) Second orientation

FIGURE 7.2: Computer model of electron trajectories for $l = 3$ shown at two different orientations, in meters, illustrating the expected orbits for the 7 different states of $l = 3$ with the nucleus at the centre (big red dot) and the stationary electron (small red dot) for $m = 0$. The orbits above the nucleus represent the positive values of m and vice-versa.

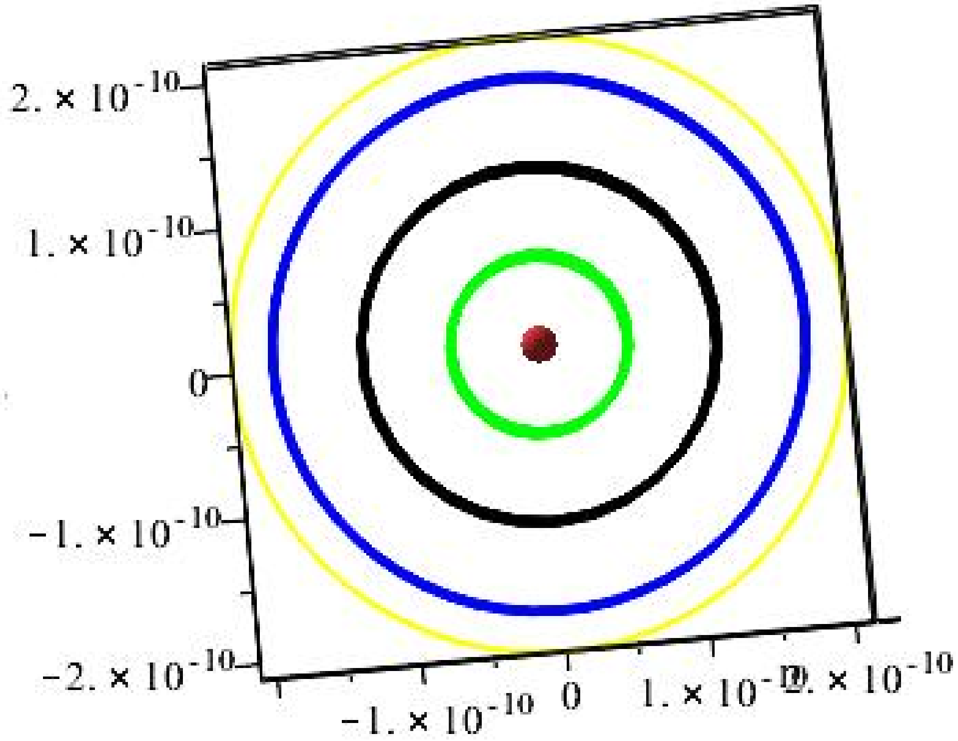
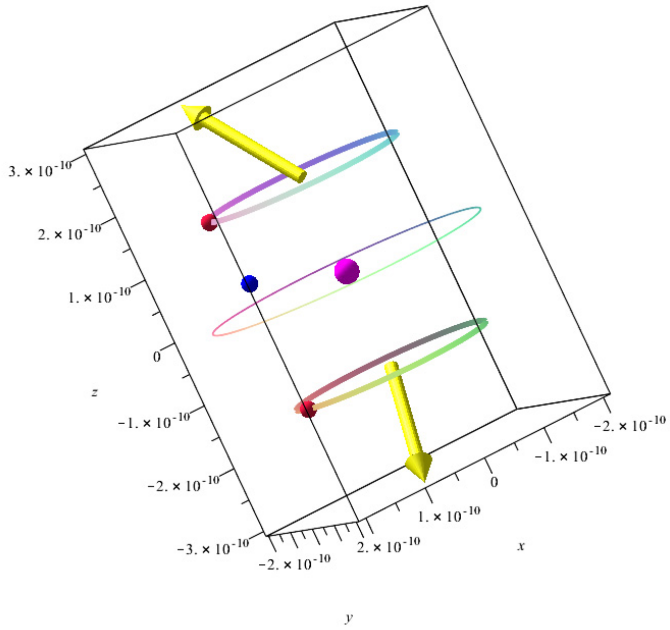


FIGURE 7.3: Electron trajectories for $l = 3$ viewed from the top of the z-axis. The orbits for each value of $|m|$ overlap with the nucleus at the centre with the radius inversely proportional to $|m|$.

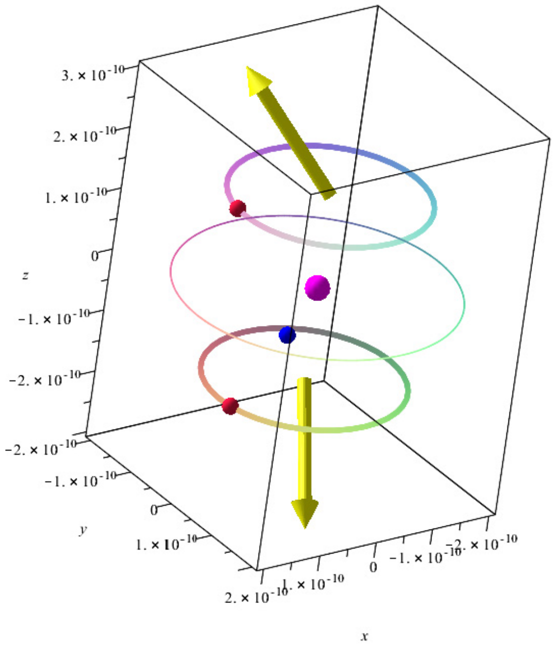
7.3 The Angular Momenta

In CI, the angular momentum is not a statistical property but a real physical attribute of the motion of the particle. The angular momentum is defined by the particle's state. In this case, the angular momentum vector given by Eq. (6.31) depends on both θ and m hence, throughout the motion the angular momentum and the position of the electron are directly linked. The arrows in Figure 7.4 show the direction of the angular momentum vector at selected points of the trajectory. As can be seen, the motion of the electron is in a different direction from that of the angular momentum vector. The plot also suggests that if the angular momentum is animated for all the points of the trajectory, the arrow would sweep through a cone shape as predicted by quantum mechanics.

The projection of the angular momentum vector on the z axis is $m\hbar$ while the projections on the x and y axes are $-m\hbar\cot\theta$ and $m\hbar\cot\theta$, respectively. The plots of angular momentum in figure 7.4 also show that the angular-momentum vector traces out a cone of vertex angle θ about the z axis. The wave functions of the hydrogen atom are eigenstates of L and L_z and their eigenvalues are constants of the motion of an electron.



(a) first orientation

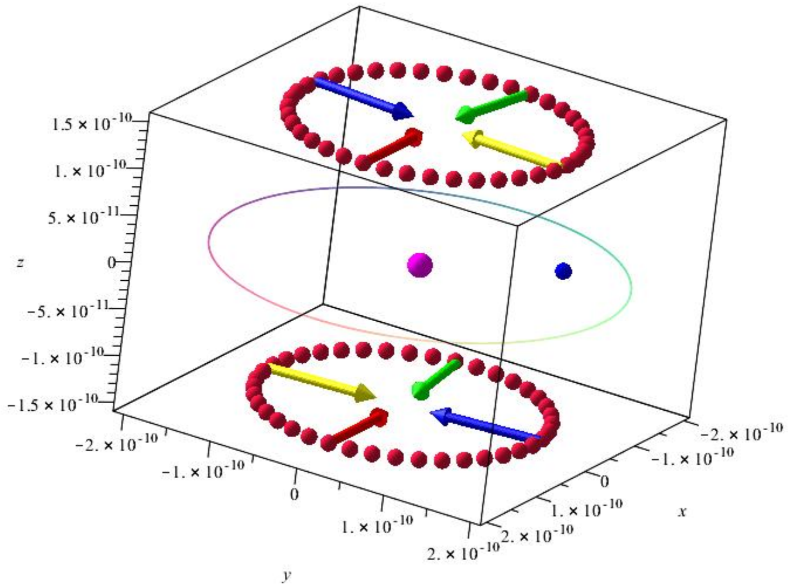


(b) second orientation

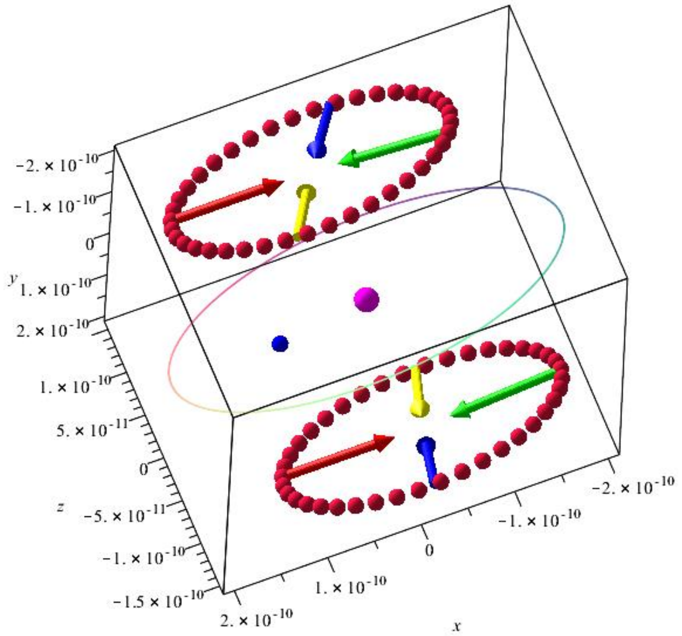
FIGURE 7.4: Angular momentum vector extracted from an animation. The arrows show the direction of the angular momentum when the electron is at the points shown for $m = -1$ and $m = 1$.

7.4 The Net Force

The electron experiences the Coulomb force due to the nucleus of the atom. From the causal interpretation, we see that there is another force on the electron due to the quantum potential Q. Figures 7.5 and 7.6 show that, regardless of the state of the electron, the net force is always directed to the centre of the orbit.



(a) first orientation

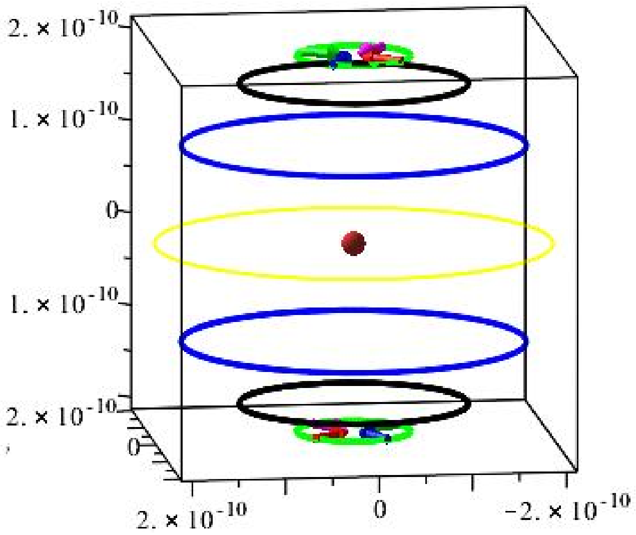


(b) second orientation

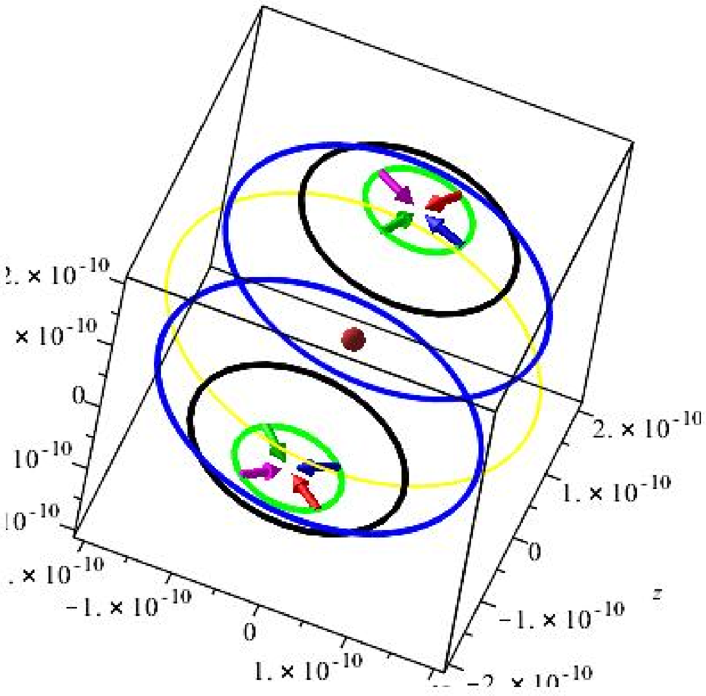
FIGURE 7.5: The direction of force at selected points of the trajectory $l = 1$ in two different plot orientations. The arrows show the direction of the net force on the electron at selected points of the orbits.

From this, we see that the Coulomb force is cancelled out by a term from the quantum potential, leaving a net force that is equivalent to the centripetal force of classical mechanics. It can also be established from Eq. (6.64) and Eq. (6.60) that the magnitude of force obtained from the causal interpretation is equal to the classical centripetal force. This shows that the centripetal force is the only force acting on the electron in the stationary states of the hydrogen atom. This is the force that keeps the electron orbiting and since there is no loss of energy, the electron does not collapse into the nucleus. The plots in Figure 7.5b clearly show the direction of this force.

The plots in Figure 7.5 show, with the use of arrows, that the net force at every point is directed towards the z-axis, hence keeping the electron in constant circular motion. The plots also show no force vectors for $m = 0$. This is because when $m = 0$ it can be seen from Eq. 6.56 that $F = 0$ which implies that the quantum potential completely balances the Coulomb force.



(a) first orientation



(b) Second orientation

FIGURE 7.6: The direction of force at selected points of the trajectory $l = 3$ in two different orientations of the plot. The arrows have been placed on the $m = \pm 3$ orbit only for proper visualisation.

The plot of the force vectors for $l = 3$ have only been shown for the outer trajectories for better visualisation (Figure 7.6). As can be seen, the direction of the force is the same as in Figure 7.5. Figure 7.7 also provides another orientation for the force vectors on the trajectories of $l = 3$.

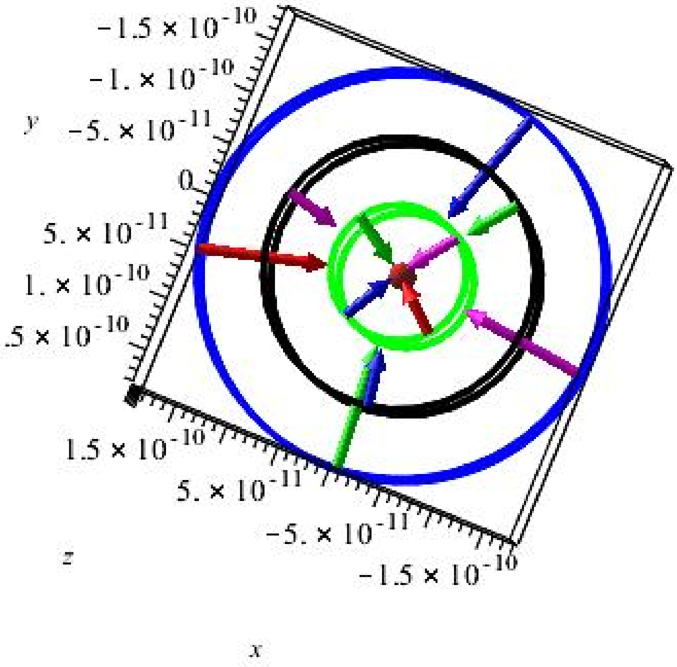
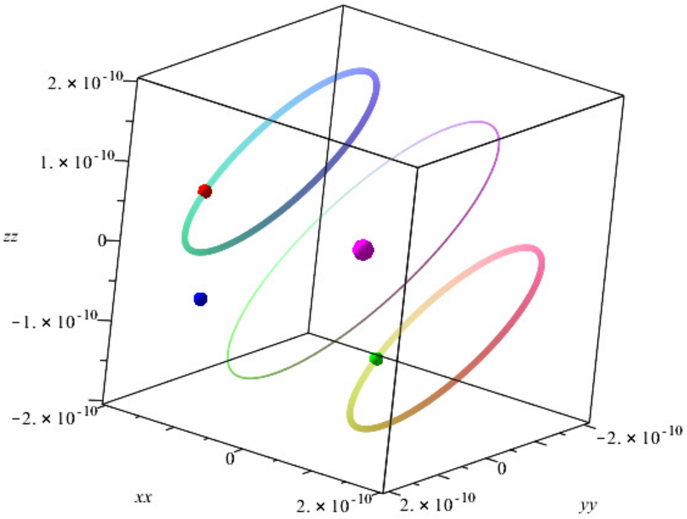


FIGURE 7.7: Force vectors for $l = 3$ viewed from the top of the z-axis showing arrows of the force for the different orbits. The outer orbit represents m = 1, the middle orbit for m = 2 and the inner orbit for m = 3. The respective arrows represent the direction of force on each orbit.

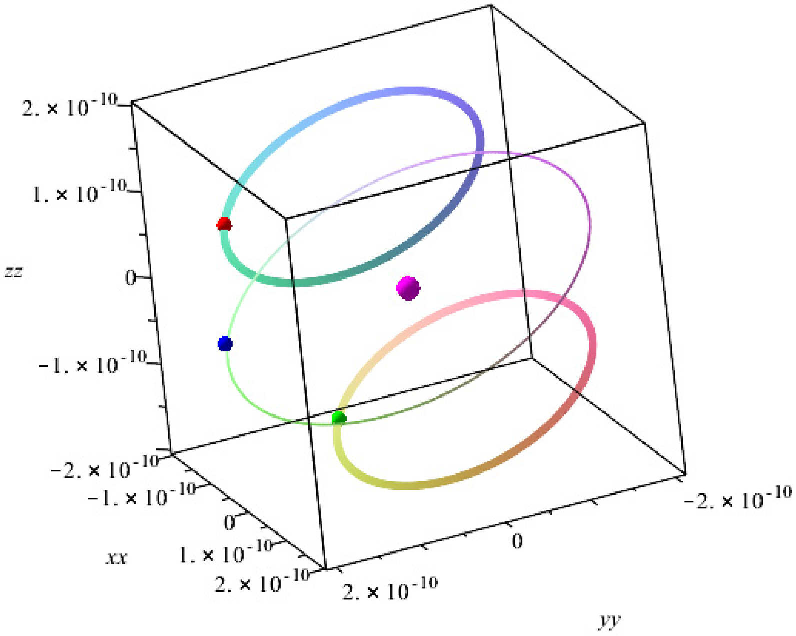
The arrows in Figure 7.7 show the direction of force at selected points on the trajectory. It shows that the force is centripetal for all states and at all points of the trajectory. This clearly shows why the electron keeps orbiting without collapsing into the nucleus. As mentioned earlier, the orbits shown are not equatorial with the nucleus but are given at different latitudes that depend on the angle θ as given by table 6.2.

7.5 The Rotated Wave Function

For a wave function (rotated by angle $\beta = 60^o$ about the y-axis), we want to show that the trajectories and the net force are not altered by the rotation of axes. The plots were obtained by solving the 4^{th} order Runge-Kutta method for differential equations [Eqs. (6.93), (6.94) and (6.95)]. In Figure 7.8, it can be seen that rotating the axis at 60^o yields the same expected trajectories and does not alter the direction of force with respect to the axis of rotation.



(a) First orientation



(b) second orientation

FIGURE 7.8: Electron trajectories for $l = 1$ for the rotated wave function for two different plot orientations. Orbits aligned are to the new axes after rotation. The new axes now labelled as *xx*, *yy* and *zz*.

The results in Figure 7.8 show that only the axis of rotation is changed, while the radius of the orbits remains constant even under rotation. From these results, it can be pointed out that choosing the z-axis to be the arbitrary direction does not have any special significance.

The angular momentum is quantised in its direction and in no other direction. Figure 7.8 shows that despite the quantisation of only one component of the angular momentum, no result of physical significance will depend on which axis happens to have been chosen.

This also shows that one can obtain the same wave function and, therefore, the same probabilities for all physical quantities by working in a system of coordinates in which the axes have been rotated by an arbitrary amount relative to the original axes. For example, for the case of zero angular momentum ($L^2 = 0$), we must also have $L_z = 0$. This means that rotating our coordinate axes leaves the wave function unchanged, so that in the new coordinate system it still corresponds to $L^2 = 0$. It is clear therefore, that for this case no physical results will depend on what axes have been chosen.

The direction of the force is still shown to be towards the centre even for the rotated axes. The force as shown in Eq.(6.108) has a lot of details due to the rotation of the axes. However, Figure 7.9 shows the consistency of the direction of force. This can be seen in detail by comparing Eq.(6.58) with Eq.(6.108 and the plots obtained from the two equations which are Figure 7.5and Figure7.9 respectively.

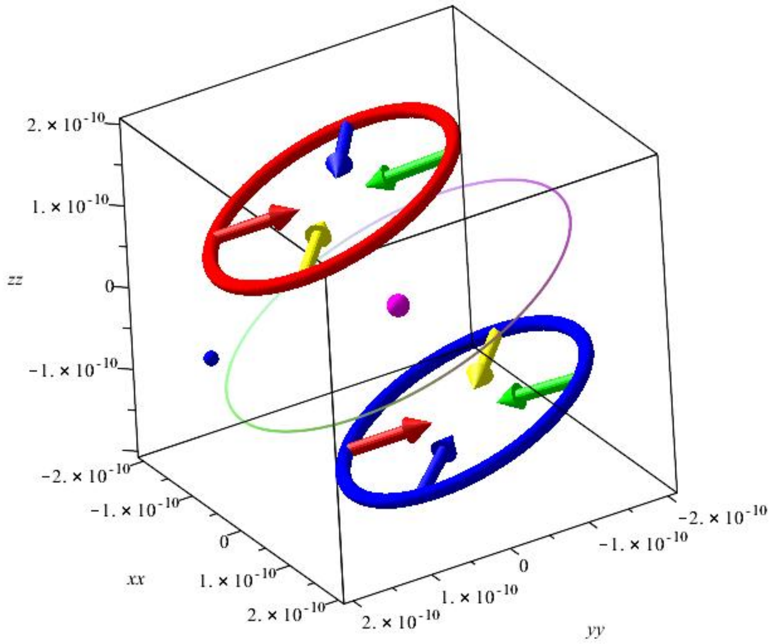


FIGURE 7.9: The direction of force at selected points of the trajectory for $l = 1$ for the rotated wave function. showing the consistence of the direction of the net force.

Chapter 8

Discussion and Conclusions

From the early beginnings of quantum mechanics, there has been a continuous development of theories and interpretations. The unanimously accepted interpretation is the Copenhagen interpretation. Despite its many successes and technological applications, a component of the Copenhagen interpretation, BPC, asserts that a picture of physical reality is impossible and entirely relies on the probability interpretation and classical concepts to explain quantum experiments/processes.

This implies that pictures or models of quantum processes cannot be made using the usual interpretation, which sometimes leads to erroneous and paradoxical interpretations of quantum processes and experiments. On the other hand, Bohm's CI allows us to make models, both mathematical and computer models. From its introduction in 1952[5] [6], CI has been used to make different models of quantum experiments/processes, both relativistic and non-relativistic. Examples of the models presented are the model of Pauli equations[8], the two-slit experiment[10], scattering from square potential barriers and square wells[9] and electromagnetic theory[12].

This research presents a model of the hydrogen atom, the trajectory plots, the direction of force at different points of the trajectory, and the angular momentum using CI. The models presented in this work are consistent with quantum mechanics except for the $m = 0$ case.

Starting with the components of the angular momentum from Eqs. (6.32), (6.33) and (6.34), we can see that CI yields results that are consistent with quantum mechanics[44]. The projection of the angular momentum vector on the z axis is $m\hbar$ while the projections on the x and y axes are $-m\hbar\cot\theta$ and $m\hbar\cot\theta$ respectively. The plots of angular momentum in figure 7.4 also show that the angular-momentum vector traces out a cone of vertex angle θ about the z axis. Since the wave functions of the hydrogen atom are eigenstates of L and L_z and their eigenvalues are constants of the motion of an electron, the obtained values of the observables must correspond to the eigenvalues in quantum mechanics for any valid interpretation of quantum mechanics.

The plots in chapter 7 show that electrons have a definite path. The electron is stationary when $m = 0$, but circling the z axis in an anti-clockwise direction for positive values of m and clockwise for negative values of m. The calculations of the net force also show that the electron in a stationary state experiences two forces: the Coulomb force and the quantum force. A component of the quantum force balances the Coulomb force giving the net force that is equivalent to the classical centripetal force, as can be seen from Eqs. (6.60), (6.61), (6.62), (6.63) and (6.60). This shows that the centripetal force is the only force acting on the electron in the stationary states of the hydrogen atom. This is the force that keeps the electron orbiting and since their is no loss of energy, the electron does not collapse into the nucleus.

The plots(Figures 7.5, 7.6 and 7.9) obtained from the same equations [Eq. (6.60)] clearly show the direction of this force at every point of the trajectory which is towards the centre. The electron is stationary for the $m = 0$ case. This can be seen from Eq. (6.56) which shows that the net force is zero for $m = 0$ because the quantum potential completely balances the electrostatic force. The solutions of the equation of motion (Eq. 6.25) show that if $m = 0$, $x = y = z = constant$.

From the plots in Figure 7.8, we can see that the orbits obtained are the same as the orbits for the standard wave function (Figure 7.1) except for the rotation of the axes. This means that if we rotate our coordinate axes, the wave function is left unchanged. It is therefore clear that, for this case, no physical results will depend on which axes have been chosen. For angular momenta, it will still remain true that $|L|$ is left unchanged by rotation. This follows from the fact that $|L|$ has no dependence on the axes as shown by Eq. (6.38). However, the components of the angular momentum are expected to change. As can be seen in Figure 7.8, the first thing to notice is that the axis of the trajectories is not the z axis, which is the axis of reference in this case. This implies that the components of the angular momentum change.

This research has successfully presented a model of the hydrogen atom using CI.It shows that the electron has a definite trajectory that depends on the state of the hydrogen atom.The net force on the electron is the centripetal force which keeps it revolving around the orbit. Thus, CI gives a description of the underlying physical reality in terms of a single well-defined model.

Chapter 9

Recommendations

This research has provided a model of the hydrogen atom using the causal interpretation. This interpretation helps in developing models/pictures of quantum mechanics which gives better analysis and interpretation of quantum experiments and processes. Currently, the dominating interpretation of quantum mechanics is the Copenhagen interpretation, with which it is impossible to develop pictures of quantum processes. There is therefore a need for students of physics to be exposed even to this alternative interpretation.

In this work, only selected stationary states of hydrogen atom were considered; therefore, researchers can also further this work by extending this model to other stationary states and non-stationary states.

This research advances the understanding of the behaviour of an electron in atomic systems, thereby making contributions on the effort to develop a physical reality of quantum systems with implications in quantum chemistry and quantum physics. The presentation of this model also shows the effectiveness of Maple in developing computer models especially scientific and mathematical.

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Appendix A: Maple program for the electron orbits and angular momentum for the hydrogen atom $l = 1$

Program to plot hydrogen atom orbits for m=1, 0, -1

UNITS=m

```
> restart;
```

> $with(plots)$:

>

Define trajectoriy functions

> $A0 := 5.2917721067\cdot 10^{-11}$

$$A0 := 5.291772107\ 10^{-11} \tag{1}$$

> $mp := 1.672621898\cdot 10^{-27}$

$$mp := 1.672621898\ 10^{-27} \tag{2}$$

> $me := 9.10938356 * 10^{-31}$

$$me := 9.109383560\ 10^{-31} \tag{3}$$

> $\mathrm{mu} := \frac{me\cdot mp}{me + mp}$

$$\mu := 9.104425137\ 10^{-31} \tag{4}$$

> $AMU := \frac{me\cdot A0}{\mathrm{mu}}$

$$AMU := 5.294654095\ 10^{-11} \tag{5}$$

>

> $hb := 1.054571800\cdot 10^{-34}$

$$hb := 1.054571800\ 10^{-34} \tag{6}$$

> $AL := \frac{hb}{me}$

$$AL := 0.0001157676360 \tag{7}$$

> $alpha1 := 0$

$$\alpha 1 := 0 \tag{8}$$

> $alpha2 := 1$

$$\alpha 2 := 1 \tag{9}$$

> $\mathrm{beta} := 0$

$$\beta := 0 \tag{10}$$

> $gammap := 0$

$$gammap := 0 \tag{11}$$

> $\mathrm{theta} := \frac{\mathrm{Pi}}{4}$

$$\theta := \frac{1}{4}\,\pi \tag{12}$$

> $convert\left(\frac{\mathrm{Pi}}{4}, 'units', 'radians', 'degrees'\right)$

$$45 \tag{13}$$

Angle theta to be used for the m = 0 plots and equator plots

> $thetaM0 := \frac{\mathrm{Pi}}{2.5}$

$$thetaM0 := 1.256637062 \tag{14}$$

> $convert\left(\frac{\mathrm{Pi}}{4}, 'units', 'radians', 'degrees'\right)$

$$45 \tag{15}$$

> $thetaEQ := \frac{\mathrm{Pi}}{2}$

$$thetaEQ := \frac{1}{2}\,\pi \tag{16}$$

> $convert(thetaEQ, 'units', 'radians', 'degrees')$

$$90 \tag{17}$$

>

> $r1 := 4 \cdot AMU$

$$r1 := 2.117861638\ 10^{-10} \tag{18}$$

> $r1cos := evalf\left(r1 \cdot \cos\left(\frac{\mathrm{Pi}}{4}\right)\right)$

$$r1cos := 1.497554325\ 10^{-10} \tag{19}$$

> $r1sin := evalf\left(r1 \cdot \sin\left(\frac{\mathrm{Pi}}{4}\right)\right)$

$$r1sin := 1.497554325\ 10^{-10} \tag{20}$$

> $evalf(r1)$

$$2.117861638\ 10^{-10} \tag{21}$$

> $ALRS1 := \frac{AL}{r1^2 \cdot \sin(\mathrm{theta})^2}$

$$ALRS1 := 5.162047460\ 10^{15} \tag{22}$$

Values to be used for the m = 0 plots

$$> \mathit{ALRS1M0} := \frac{\mathit{AL}}{\mathit{r1}^2 \cdot \sin(\mathit{thetaM0})^2}$$

$$\mathit{ALRS1M0} := 2.853509653\ 10^{15} \qquad \textbf{(23)}$$

Values to be used for the equator plots plots

$$> \mathit{ALRS1EQ} := \frac{\mathit{AL}}{\mathit{r1}^2 \cdot \sin(\mathit{thetaEQ})^2}$$

$$\mathit{ALRS1EQ} := 2.581023729\ 10^{15} \qquad \textbf{(24)}$$

Define functions for the orbits

> **for** i **from** 1 **to** 3 **do**

$m[i] := 2 - i$

end do

$$m_1 := 1$$

$$m_2 := 0$$

$$m_3 := -1 \qquad \textbf{(25)}$$

Orbit 1

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx m=-1,0,1
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

$$> \mathit{fx1}[1] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathrm{theta}) \cdot \cos(\mathit{ALRS1} \cdot m[1] \cdot t + \mathit{alpha1}) + \mathrm{beta}$$

$$\mathit{fx1}_1 := t \rightarrow \mathit{r1} \sin(\theta) \cos\left(\mathit{ALRS1}\ m_1\ t + \alpha 1\right) + \beta \qquad \textbf{(26)}$$

$$> \mathit{fx1M0}[2] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathit{thetaM0}) \cdot \cos(\mathit{ALRS1M0} \cdot m[2] \cdot t + \mathit{alpha1}) + \mathrm{beta}$$

$$\mathit{fx1M0}_2 := t \rightarrow \mathit{r1} \sin(\mathit{thetaM0}) \cos\left(\mathit{ALRS1M0}\ m_2\ t + \alpha 1\right) + \beta \qquad \textbf{(27)}$$

$$> \mathit{fx1}[3] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathrm{theta}) \cdot \cos(\mathit{ALRS1} \cdot m[3] \cdot t + \mathit{alpha1}) + \mathrm{beta}$$

$$\mathit{fx1}_3 := t \rightarrow \mathit{r1} \sin(\theta) \cos\left(\mathit{ALRS1}\ m_3\ t + \alpha 1\right) + \beta \qquad \textbf{(28)}$$

$$> \mathit{fx1EQ}[2] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathit{thetaEQ}) \cdot \cos(\mathit{ALRS1EQ} \cdot m[1] \cdot t + \mathit{alpha1}) + \mathrm{beta}$$

$$\mathit{fx1EQ}_2 := t \rightarrow \mathit{r1} \sin(\mathit{thetaEQ}) \cos\left(\mathit{ALRS1EQ}\ m_1\ t + \alpha 1\right) + \beta \qquad \textbf{(29)}$$

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx m=-1,0,1
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

$$> \mathit{fy1}[1] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathrm{theta}) \cdot \sin(\mathit{ALRS1} \cdot m[1] \cdot t + \mathit{alpha1}) + \mathit{gammap}$$

$$\mathit{fy1}_1 := t \rightarrow \mathit{r1} \sin(\theta) \sin\left(\mathit{ALRS1}\ m_1\ t + \alpha 1\right) + \mathit{gammap} \qquad \textbf{(30)}$$

$$> \mathit{fy1M0}[2] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathit{thetaM0}) \cdot \sin(\mathit{ALRS1M0} \cdot m[1] \cdot t + \mathit{alpha1}) + \mathit{gammap}$$

$$\mathit{fy1M0}_2 := t \rightarrow \mathit{r1} \sin(\mathit{thetaM0}) \sin\left(\mathit{ALRS1M0}\ m_1\ t + \alpha 1\right) + \mathit{gammap} \qquad \textbf{(31)}$$

$$> \mathit{fy1}[3] := (t) \rightarrow \mathit{r1} \cdot \sin(\mathrm{theta}) \cdot \sin(\mathit{ALRS1} \cdot m[3] \cdot t + \mathit{alpha1}) + \mathit{gammap}$$

$$\mathit{fy1}_3 := t \rightarrow \mathit{r1} \sin(\theta) \sin\left(\mathit{ALRS1}\ m_3\ t + \alpha 1\right) + \mathit{gammap} \qquad \textbf{(32)}$$

```
> fy1EQ[2] := (t) → r1·sin(thetaEQ)·sin(ALRS1EQ·m[1]·t + alpha1) + gammap
```

$$fy1EQ_2 := t \to r1 \sin(thetaEQ) \sin\left(ALRS1EQ\, m_1\, t + \alpha 1\right) + gammap \tag{33}$$

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx m=-1,0, 1
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

```
> fz1[1] := evalf(m[1]·r1·cos(theta))
```

$$fz1_1 := 1.497554325\ 10^{-10} \tag{34}$$

```
> fz1M0[2] := evalf( m[1]·r1·cos(thetaM0))
```

$$fz1M0_2 := 6.544552367\ 10^{-11} \tag{35}$$

```
> fz1[3] := evalf(m[3]·r1·cos(theta))
```

$$fz1_3 := -1.497554325\ 10^{-10} \tag{36}$$

```
> fz1EQ[2] := evalf( m[1]·r1·cos(thetaEQ))
```

$$fz1EQ_2 := 0. \tag{37}$$

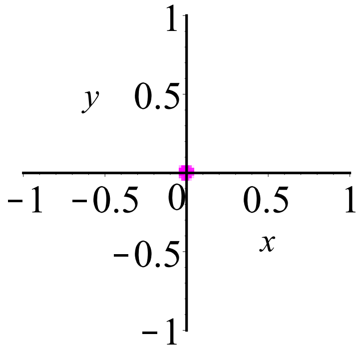
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx m=-1,0,1
xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

Plot of the nucleus

Used in the orbit plots to mnclude the stationary nucleus

```
> nucleus := pointplot3d([0, 0, 0], style=point, symbol=solidcircle, symbolsize=30, color
     ="MAGENTA", orientation = [45, 45, 0], labels=[x, y, z])
```

nucleus :=



```
> display(nucleus) :
```

Create the 3D data array

CORDSi[*j*]:=[x,y,z],are arrays with each cell contaning a triples of data points for an electron trajectory   specified by i=1 to 4.

TRAJi[i] is an array containing all 50 pairs of data points contained in *CORDSi*[*j*] for the *i* th electron trajectory. There are 4 trajectories, i.e., i=1 to 4.

TRAJJi[*j*] is the same as *TRAJN*[*j*], except in contains the data points of *CORDSXYN*[*j*].

xxxxxxxxxxxxxxxxxxxxxx - ORBITS xxxxxxxxxxxxxxxxxxxxx

Coords for orbit 1, m=1

> $evalf\left(\frac{2\cdot \mathrm{Pi}}{49}\right)$

$$0.1282282716 \tag{38}$$

> $t := 0$

$$t := 0 \tag{39}$$

> **for** j **from** 1 **to** 200 **do**

$COORDS1[1][j] := [\ evalf(fx1[1](t)),\ evalf(fy1[1](t)),\ fz1[1]\ ]:$

$t := t + \frac{2\cdot \mathrm{Pi}}{40\cdot ALRS1}$

end do:

Coords for orbit 1, m=0

> $t := 0$

$$t := 0 \tag{40}$$

> **for** j **from** 1 **to** 100 **do**

$COORDS1M0[2][j] := [evalf(fx1M0[2](t)),\ evalf(fy1M0[2](t)),\ fz1M0[2]]:$

$t := t + \frac{2\cdot \mathrm{Pi}}{80\cdot ALRS1}$

end do:

Coords for orbit 1, m=-1

> $t := 0$

$$t := 0 \tag{41}$$

> **for** j **from** 1 **to** 200 **do**

$COORDS1[3][j] := [evalf(fx1[3](t)),\ evalf(fy1[3](t)),\ fz1[3]]:$

$t := t + \frac{2\cdot \mathrm{Pi}}{40\cdot ALRS1}$

end do:

Coords for orbit the equatorial orbit

> $t := 0$

$$t := 0 \tag{42}$$

> **for** j **from** 1 **to** 170 **do**

$COORDS1EQ[2][j] := [evalf(fx1EQ[2](t)),\ evalf(fy1EQ[2](t)),\ fz1EQ[2]]:$

$$t := t + \frac{2\cdot \mathrm{Pi}}{80\cdot ALRS1}$$

end do:

xxxxxxxxxxxxxxxxxxxxxx - ORBIT PLOTS - style = line - xxxxxxxxxxxxxxxxxxxxxx

Orbit plots, m=1

```
> TRAJ[1] := [seq(COORDS1[1][k], k = 1 ..200)] :
```

```
> TRAJJ[1] := pointplot3d(TRAJ[1], style = line, thickness = 5, orientation = [45, 45, 0], labels
        = [x, y, z]) :
```

Orbit plots, m=0

```
> TRAJM0[2] := [COORDS1M0[2][30]] :
```

```
> TRAJJM0[2] := pointplot3d(TRAJM0[2], style = point, symbol = solidcircle, symbolsize = 20,
        color = "Blue", orientation = [45, 45, 0], labels = [x, y, z]) :
```

Orbit plots m=-1

```
> TRAJ[3] := [seq(COORDS1[3][k], k = 1 ..200)] :
```

```
> TRAJJ[3] := pointplot3d(TRAJ[3], style = line, thickness = 5, orientation = [45, 45, 0], labels
        = [x, y, z]) :
```

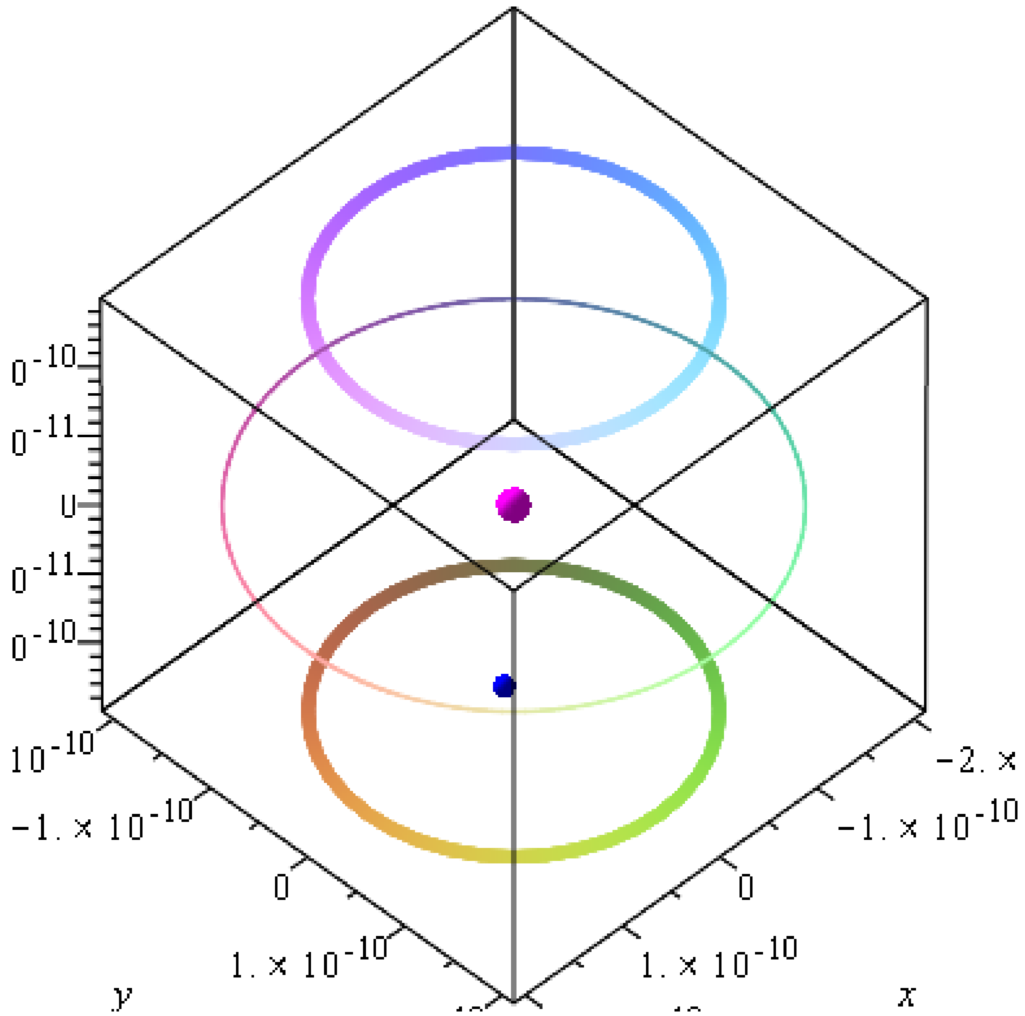
Orbit plot equator

```
> TRAJEQ[2] := [seq(COORDS1EQ[2][k], k = 1 ..170)] :
```

```
> TRAJJEQ[2] := pointplot3d(TRAJEQ[2],  style = line, thickness = 1, orientation = [45, 45, 0],
        labels = [x, y, z]) :
```

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx Display xxxxxxxxxxxxxxxxxxxxxxxxxx

```
> display(TRAJJ[1], TRAJJM0[2], TRAJJ[3],  TRAJJEQ[2], nucleus)
```



xxxxxxxxxxxxxxxxxxxxxx - ORBIT PLOTS - style = point-xxxxxxxxxxxxxxxxxxxxxx

ORBIT[*m*][*j*][*i*] array: The first cell [m] gives m=-1,o,1.The second cell [*j*] indicates orbit *j*, *j*= 1 to 4. The third cell [*i*] contains the ponitplot of orbit *j*.

Orbit plot, m=1

```
> for i from 1 to 200 do
   ORBIT[1][i] := pointplot3d(COORDS1[1][i], style = point, symbol = solidcircle, symbolsize
        = 20, color = "Crimson", orientation = [45, 45, 0], labels = [x, y, z])
   end do:
```

Orbit plot, m=0

```
>  for i from 1 to 200 do
   ORBIT[2][i] := pointplot3d(COORDS1M0[2][30], style = point, symbol = solidcircle,
        symbolsize = 20, color = "Blue", orientation = [45, 45, 0], labels = [x, y, z]) :
   end do:
```

```
> # ORBIT[2][1][10]
```

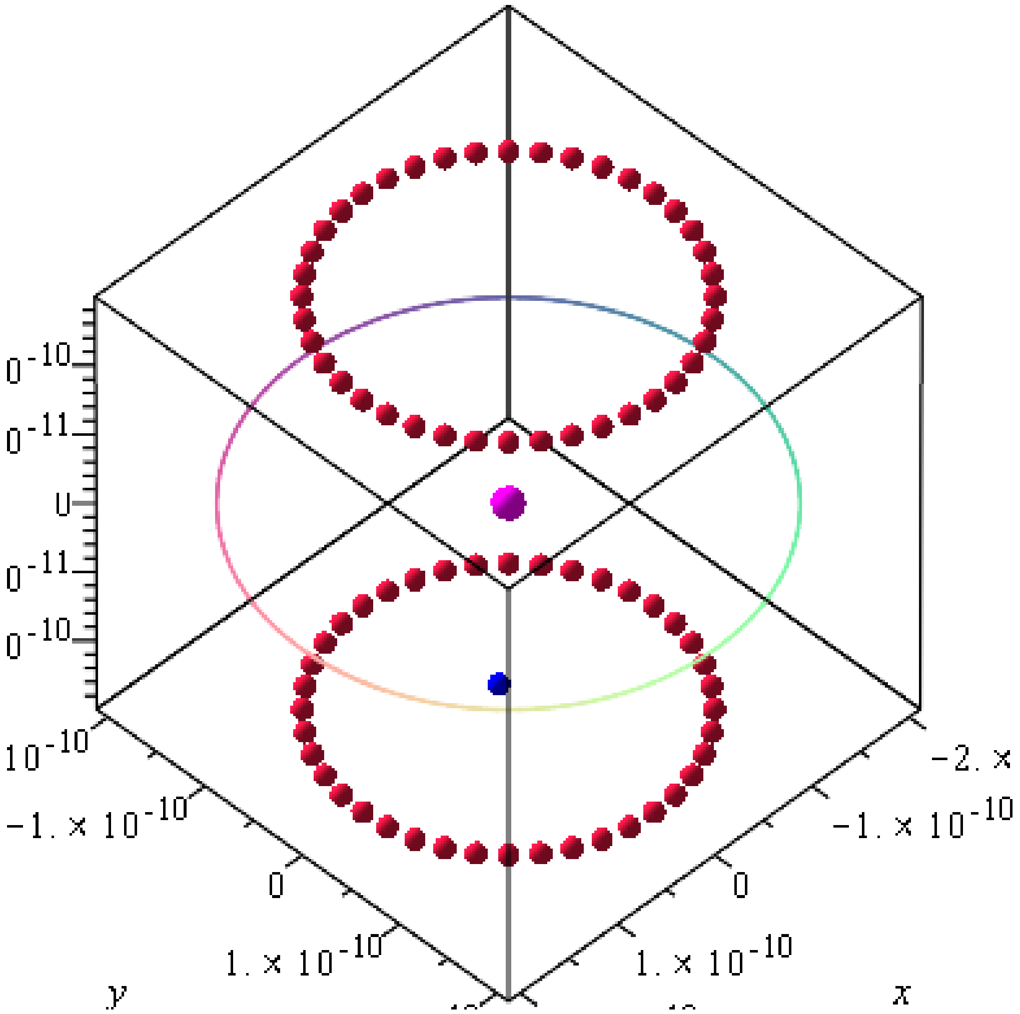
Orbit plot, m=-1

```
> for i from 1 to 200 do
   ORBIT[3][i] := pointplot3d(COORDS1[3][i], style=point, symbol=solidcircle, symbolsize
       =20, color="Crimson", orientation = [45, 45, 0], labels=[x, y, z])
   end do:
```

```
> # ORBIT[3][1][10]
```

xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx Display xxxxxxxxxxxxxxxxxxxxxxxxx

```
> display(seq(ORBIT[1][i], i=1..200),  ORBIT[2][30],  seq(ORBIT[3][i], i=1..200) ,
         nucleus, TRAJJEQ[2])
```



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Animation of the trajectories - style=line

M [i][j] is an array containing j triplets of data points of orbit i (i = 1 to 4). E.g.

M [i][1] = 1 triplet of data points for orbit i, i.e., (x1,y1,z1)

M [i][2] = 2 triplets of data points for orbit i, i.e., (x1,y1,z1), (x2,y2,z2)

M [i][50] = 3 triplets of data points for orbit i, i.e., (x1,y1,z1), (x2,y2,z2), ,,,,, ,,(x50,y50,z50)

....

M [*j*][200] = 2000 triples of data points for trajectory *j*

```
> for i from 1 to 4 do
  M[i] := array(1..200)
  end do:
```

PP [i][j] is an array containing images of j triplets of data points of orbit i (*i* = 1 to 4). E.g.

PP [i][1] = image of 1 triplet of data points for orbit i

PP [i][2] = image of 2 triplets of data points for orbit i

PP [i][3] = image of 3 triplets of data points for orbit i

PP[i][200] = 200 pairs of data points for trajectory i

```
> for i from 1 to 4 do
  PP[i] := array(1..200)
  end do:
```

```
> for j from 1 to 200 do
                          M[1][j] := TRAJ[1][1..j]:
  end do:
```

```
> for j from 1 to 200 do
  M[2][j] := TRAJM0[2]
  end do:
```

```
> for j from 1 to 200 do
                          M[3][j] := TRAJ[3][1..j]:
  end do:
```

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```
> pointplot3d(M[1][200], style=line, thickness=5, orientation = [45, 45, 0], labels=[x, y, z]) :
```

```
> pointplot3d(M[2][200], style=line, thickness=2, orientation = [45, 45, 0], labels=[x, y, z]) :
```

```
> pointplot3d(M[3][200], style=line, thickness=2, orientation = [45, 45, 0], labels=[x, y, z]) :
```

```
> for j from 1 to 200 do
                          PP[1][j] := pointplot3d(M[1][j], style = line, thickness = 5,#  orientation
        = [45, 45, 0], labels = [x, y, z]) :
   end do:
```

```
> display(PP[1][200], nucleus) :
```

```
> for j from 1 to 200 do
          PP[2][j] := pointplot3d(M[2][j], style = point, symbol = solidcircle, symbolsize = 20,
        color = "Blue", orientation = [45, 45, 0], labels = [x, y, z]) :
     end do:
```

```
> display(PP[2][100], nucleus) :
```

```
>    for j from 1 to 200 do
           PP[3][j] := pointplot3d(M[3][j], style = line, thickness = 2, orientation = [45, 45, 0],
        labels = [x, y, z]) :
     end do:
```

```
> display(PP[3][100], nucleus) :
```

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```
> for i from 1 to 3 do
                                for j from 1 to 200 do
                                PPN[i][j] := display(nucleus, PP[i][j]) :
                                end do:
   end do:
```

```
> display(  [seq(PPN[3][i],  i = 1 ..200)] , insequence = true) :
```

SS[*j*] array: Cell j contains j triplets of data points of all 4 trajectories E.g. *SS*[10] contains the first 10 pairs of data points for all 4 trajectories. *SS*[*j*] in the command line
display(*seq*(*SS*[*k*], *k* = 1 ..50) , *insequence* = *true*) will
not display the 4 trajectory simultaneously but, instead,
displays them individually one after the other in the animation.
. Hence the need **for** the *TT*[*k*] *a*rray.

```
> for j from 1 to 200 do

                                    SS[j] := [seq(PP[i][j],  i = 1 ..3)]

   end do:
```

```
> display(SS[200], nucleus) :
```

```
> display( seq(SS[k], k = 1 ..200) , insequence = true) :
```

```
>
```

TT[*k*] = cell j contains the images of *j triplets of data points of all 42 trajectories*. E.g. *TT*[12] contains the images of the first 12 pairs of data points for all 4 trajectories. *TT*[*k*] in the command line *display*(*seq*(*TT*[*k*], *k* = 1 ..50) , *insequence* = *true*) will display the 4 trajectory simultaneously **in** the animation..

```
> for k  from 1 to 200 do
                    TT[k] := display(SS[k], nucleus)
   end do:
```

```
> display( seq(TT[k], k = 1 ..200) , insequence = true) :
```

Animation of the trajectories - style = point

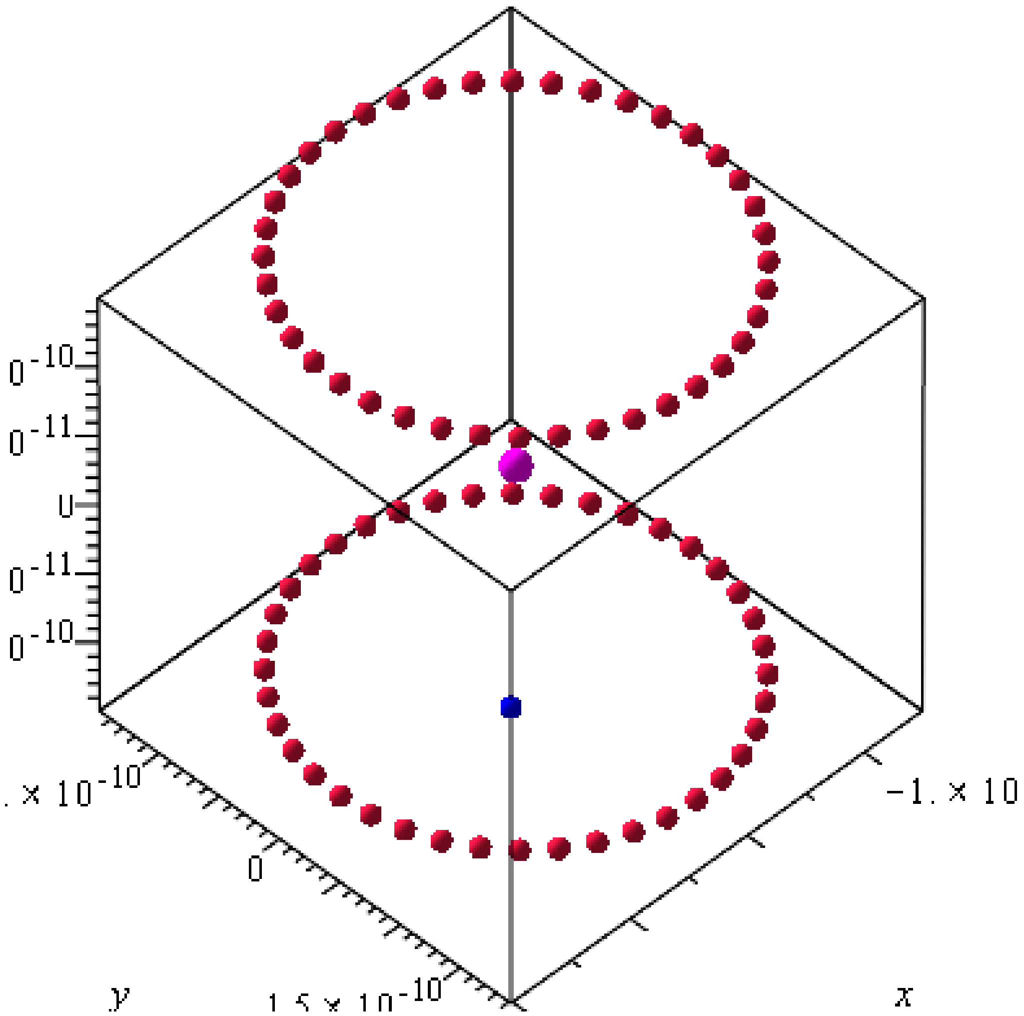
```
> display(nucleus,  seq(ORBIT[1][k], k = 1 ..200) , insequence = true) :
```

```
> display(nucleus, ORBIT[1][10]) :
> display( nucleus, ORBIT[2][30]) :
```

```
> ORBITALL := display(    seq(ORBIT[1][k], k = 1 ..200),  ORBIT[2][30],      seq(ORBIT[3][ k],
        k = 1 ..200),   TRAJJEQ[2] , nucleus,  ) :
> display(ORBITALL) :
```

T|he above coomand can be alternatively, and more compactly, written using the for loop (but excluding PPN[4]). But, displays all possible points for m=0, but which is supposed to be stationary. The aove approach is therfore better.

```
> for i from 1 to 3 do
                    ORBITX[i] := display(seq(ORBIT[i][k], k = 1 ..200))
   end do:
> display(seq(ORBITX[i], i = 1 ..3), nucleus)
```



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Repeat orbit animation using a loop

SSS[*j*] array: Cell i contains j triplets of data points of all 4 orbits E.g. *SS*[10] contains the first 10 pairs of data points for all 4 orbits. *SSS*[*j*] in the command line

display(*seq*(*SS*[*k*], *k* = 1 ..50) , *insequence* = *true*) will **not** display the 4 orbits simultaneously but, instead, displays them individually one after the other **in** the animation. . Hence the need **for** the *TT*[*k*] *a*rray.

```
> for j from 1 to 200 do

                        SSS[j] := seq(ORBIT[i][j], i = 1 ..3)

   end do:
```

```
> SSS[3] := ORBIT[3][30] :
```

```
> SSS[50]:
```

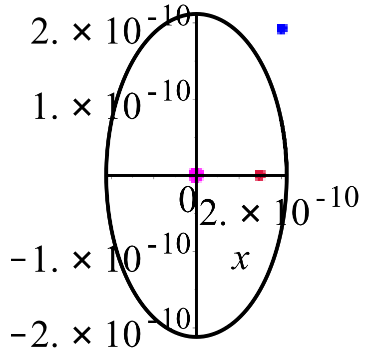
```
> display(SSS[20]):
> display( nucleus, seq(SSS[k], k=1..50), insequence=true):
```

TTT[*k*] = cell j contains the images of *j triplets of data points of all 4 orbits.* E.g. *TTT*[12] contains the images of the first 12 pairs of data points for all 4 orbits. *TT*[*k*] in the command line *display*(*seq*(*TT*[*k*], *k* = 1 ..50) , *insequence* = *true*) will display the 4 orbits simultaneously. **in** the animation.

```
> for k from 1 to 200 do
                    TTT[k] := display(nucleus, SSS[k], SS[k], TRAJJEQ[2], )
  end do:
```

```
> TT3 := display( seq(TTT[k], k=1..200) , insequence=true)
```

TT3 :=



Definition of the angular momentum vectors

Define angular momentum components

```
> magfac := evalf(1.5·10^-34·10^58)
```

$$magfac := 1.500000000\ 10^{24} \tag{43}$$

```
> r := r1sin(theta)
```

$$r := 1.497554325\ 10^{-10} \tag{44}$$

$$> phii[1] := (t) \rightarrow \frac{m[1]\cdot t}{me\cdot r^{2}\cdot \sin(\mathrm{theta})^{2}}$$

$$phii_{1} := t \rightarrow \frac{m_{1}\ t}{me\ r^{2}\ \sin(\theta)^{2}} \tag{45}$$

$$> phii[2] := (t) \rightarrow \frac{m[3]\cdot t}{me\cdot r^{2}\cdot \sin(\mathrm{theta})^{2}}$$

$$phii_2 := t \rightarrow \frac{m_3\, t}{me\, r^2 \sin(\theta)^2} \tag{46}$$

Lx component

```
> Lx[1] := (t) → -hb·m[1]·cot(theta)·sin(phii[1](t))·magfac
```

$$Lx_1 := t \rightarrow -hb\, m_1 \cot(\theta) \sin\left(phii_1(t)\right) magfac \tag{47}$$

```
> seq(evalf(Lx[1](n)), n = 1 ..20)
```

$$\begin{gathered} -1.537381702\ 10^{-10}, -3.956460126\ 10^{-11}, 1.469485269\ 10^{-10}, 7.661417494\ 10^{-11}, \\ -1.276320861\ 10^{-10}, -1.314595305\ 10^{-10}, 3.772789232\ 10^{-11}, 8.483133830\ 10^{-11}, \\ 6.982197718\ 10^{-11}, -1.095106249\ 10^{-10}, 1.388178772\ 10^{-10}, -4.126385954\ 10^{-11}, \\ 1.519242440\ 10^{-10}, -7.327825046\ 10^{-11}, -5.053930514\ 10^{-11}, 1.432024684\ 10^{-10}, \\ 1.350530676\ 10^{-10}, 1.253045098\ 10^{-10}, -1.564012918\ 10^{-10}, 9.108623774\ 10^{-11} \end{gathered} \tag{48}$$

```
> Lx[2] := (t) → -hb·m[3]·cot(theta)·sin(phii[2](t))·magfac
```

$$Lx_2 := t \rightarrow -hb\, m_3 \cot(\theta) \sin\left(phii_2(t)\right) magfac \tag{49}$$

Ly component

```
> Ly[1] := (t) → -hb·m[1]·cot(theta)·cos(phii[1](t))·magfac
```

$$Ly_1 := t \rightarrow -hb\, m_1 \cot(\theta) \cos\left(phii_1(t)\right) magfac \tag{50}$$

```
> Ly[2] := (t) → -hb·m[3]·cot(theta)·cos(phii[2](t))·magfac
```

$$Ly_2 := t \rightarrow -hb\, m_3 \cot(\theta) \cos\left(phii_2(t)\right) magfac \tag{51}$$

Lz component

```
> Lz[1] := hb·m[1]·magfac
```

$$Lz_1 := 1.581857700\ 10^{-10} \tag{52}$$

```
> Lz[2] := hb·m[3]·magfac
```

$$Lz_2 := -1.581857700\ 10^{-10} \tag{53}$$

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

XCOMP array − contains 200 *Lx* components

```
> t := 0
```

$$t := 0 \tag{54}$$

```
> evalf(Pi)
```

$$3.141592654 \tag{55}$$

> **for** j **from** 1 **to** 200 **do**
$XC[1][j] := evalf(Lx[1](t)):$
$t := t + 0.3 \cdot 10^{-51} \cdot evalf(\mathrm{Pi}):\quad :$
end do:

> $t := 0$

$$t := 0 \tag{56}$$

> **for** j **from** 1 **to** 200 **do**
$XC[2][j] := evalf(Lx[2](t)):$
$t := t + 0.3 \cdot 10^{-51} \cdot evalf(\mathrm{Pi})$
end do:

YCOMP array − contains 200 *Ly* components

> $t := 0$

$$t := 0 \tag{57}$$

> **for** j **from** 1 **to** 200 **do**
$YC[1][j] := evalf(Ly[1](t)):$
$t := t + 0.3 \cdot 10^{-51} \cdot evalf(\mathrm{Pi})$
end do:

> $t := 0$

$$t := 0 \tag{58}$$

> **for** j **from** 1 **to** 200 **do**
$YC[2][j] := evalf(Ly[2](t)):$
$t := t + 0.3 \cdot 10^{-51} \cdot evalf(\mathrm{Pi})$
end do:

ZCOMP array − contains 200 *Lz* components

> $t := 0$

$$t := 0 \tag{59}$$

> **for** j **from** 1 **to** 200 **do**
$ZC[1][j] := evalf(Lz[1]):$
end do:

> $t := 0$

$$t := 0 \tag{60}$$

> **for** j **from** 1 **to** 200 **do**
$ZC[2][j] := evalf(Lz[2]):$
end do:

Vector plots

xxxxxxxxx m=1 xxxxxxxxxxxxxxxxxxxx

> $ix[1] := 0$

$$ix_1 := 0 \tag{61}$$

> $jy[1] := 0$

(62)

$$jy_1 := 0 \tag{62}$$

```
> kz[1] := r1·cos(theta)
```

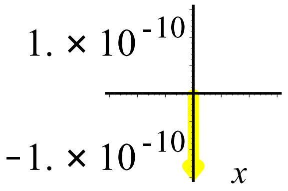
$$kz_1 := 1.058930819\ 10^{-10}\sqrt{2} \tag{63}$$

```
> for n  from 1 to 200 do
  i[1][n] := evalf(XC[1][n])
   end do:
> for n  from 1 to 200 do
  j[1][n] := evalf(YC[1][n])
   end do:
> for n  from 1 to 200 do
  k[1][n] := evalf(ZC[1][n])
   end do:
> for n  from 1 to 200 do
   L[1][n] := arrow(⟨ix[1], jy[1], kz[1]⟩, ⟨i[1][n], j[1][n], k[1][n]⟩, width = [2·10^-11],
         head_length = [4·10^-11], color = yellow, scaling = constrained,  labels = [x, y, z]) :
   end do:

> display(L[1][8], nucleus) :
> VEC[1] := [seq(L[1][n], n = 1 ..10)] :
> display(VEC[1]) :

> TT1 := display( seq(L[1][k], k = 1 ..200) , insequence = true)
```

$TT1 :=$



xxxxxxxxx m=2 xxxxxxxxxxxxxxxxxxxx

```
> ix[2] := 0
```

$$ix_2 := 0 \tag{64}$$

```
> jy[2] := 0
```

$$jy_2 := 0 \tag{65}$$

```
> kz[2] := −r1·cos(theta)
```

$$kz_2 := -1.058930819\ 10^{-10}\sqrt{2} \tag{66}$$

```
> for n  from 1 to 200 do
```

```
 i[2][n] := evalf(XC[2][n])
  end do:
```

```
> for n  from 1 to 200 do
 j[2][n] := evalf(YC[2][n])
  end do:
```

```
> for n  from 1 to 200 do
 k[2][n] := evalf(ZC[2][n])
  end do:
```

```
> for n  from 1 to 200 do
 L[2][n] := arrow(⟨ix[2], jy[2], kz[2]⟩, ⟨i[2][n], j[2][n], k[2][n]⟩, width = [2·10^(-11)],
        head_length = [4·10^(-11)], color = yellow, scaling = constrained,  labels = [x, y, z]) :
  end do:
```

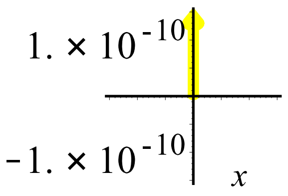
```
> display(L[2][8], nucleus) :
```

```
>  VEC[2] := [seq(L[2][n], n = 1 ..10)] :
```

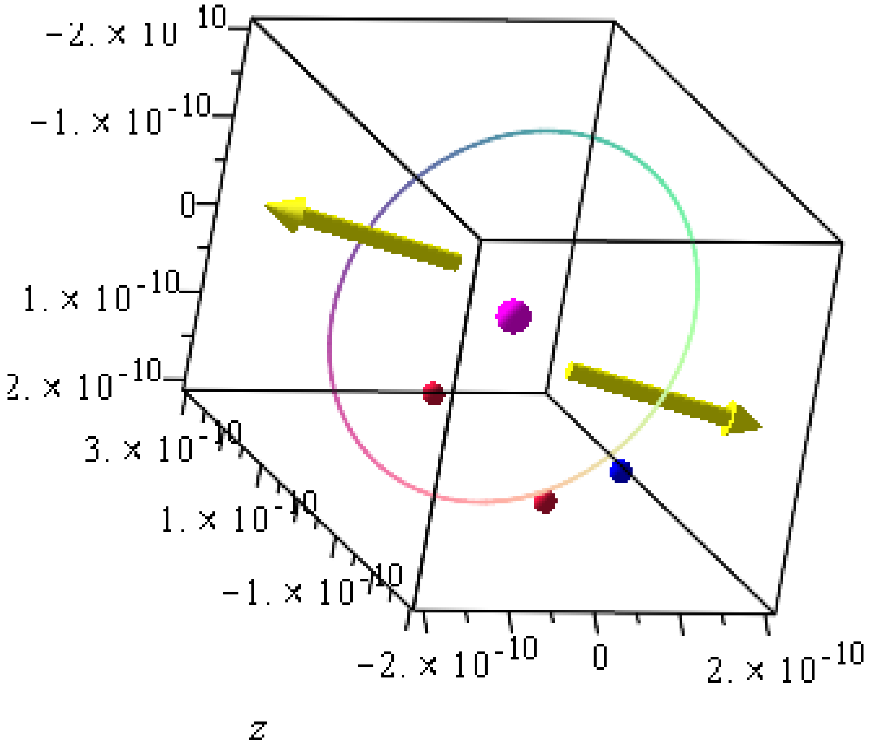
```
> display(VEC[2]) :
```

```
> TT2 := display( seq(L[2][k], k = 1 ..200) , insequence = true)
```

TT2 :=



```
> display( TT1, TT2, TT3)
```


−2. × 10^-10
−1. × 10^-10
0
1. × 10^-10
2. × 10^-10
3. × 10^-10
1. × 10^-10
−1. × 10^-10
−2. × 10^-10
0
2. × 10^-10
z

```
>
>
```