

Dynamic Electron Orbits in Atomic Hydrogen

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Abstract

Even after extensive research in Quantum Mechanics, we are still unable to visualize instant-to-instant motion of an electron in hydrogen atom. That is because in QM treatment, potential energy term has been mistakenly assumed to be time-independent instead of depending on the instant-to-instant varying position of the orbiting electron [1]. This has led to wrong and weird solutions for the electron motion in hydrogen atom. Before the advent of wave mechanics, Sommerfeld model of elliptical electron orbits was able to explain most features of hydrogen spectra, except for the features associated with electron spin and magnetic moment interactions. However, the Sommerfeld elliptical orbits were of kinematic origin and could not provide visualization of instant-to-instant dynamic motion of the orbiting electron. Contrary to the QM perspective, we find that central core of the electron behaves as a classical particle while its electrostatic field behaves as a wave phenomenon. As such an electron under Coulomb force moves strictly in accordance with Newtonian laws of motion. In this paper, we develop dynamic electron orbits in hydrogen atom by using energy and angular momentum conservation principle in central force field. We have shown that during photon emission, angular momentum of the orbiting electron is changed by \hbar due to recoil action. This may be the origin of various quantization rules. During emission of a photon, elliptical orbit transitions are also computed and plotted. Orbit transition time is of the order of 10^{-16} seconds. We have extended this methodology to compute electron orbits in hydrogen molecular bond and computed the H_2 bond energy.

Keywords

Sommerfeld Model, Schrödinger Equation, Dynamic, Electron Orbits, Photon Emission

1. Introduction

1.1. Bohr-Sommerfeld model of Electron Orbits

The structure of hydrogen atom, with just one electron and one proton, is the

simplest of all atoms. Yet the detailed understanding of hydrogen atom has so far proved to be elusive [2]. Even after more than hundred years of persistent struggle, we are neither in a position to understand the physical mechanism of emission of photon from the orbiting electron, nor we can mentally visualize the instant-to-instant orbiting motion of the electron. Development of various models of hydrogen atom during early part of twentieth century, in conjunction with empirical spectroscopy data, has played a crucial role in the development of modern physics. It was largely the effort to explain the hydrogen spectrum that inspired the evolution of quantum mechanics [3]. Before the advent of wave mechanics, developed by Erwin Schrödinger in 1926, Bohr-Sommerfeld model of elliptical electron orbits in hydrogen atom was quite well developed. Calculations based on this model were able to explain most features of the hydrogen spectra [4], except for the features associated with electron spin and corresponding magnetic moment interactions.

Current picture of the hydrogen atom is based on atomic orbitals defined by the solutions of Schrödinger equation for hydrogen atom. Atomic orbitals are bounded regions which describe a specific volume of space where the electron is likely to be located. The solutions of Schrödinger equation for the wave function ψ are interpreted to obtain various significant parameters of the electron motion. The position probability density of an electron is given by $|\psi|^2$ or square of the wavefunction. Thus, as per our current understanding from Schrödinger's wave mechanics, the instantaneous position of an orbiting electron gets smeared over the whole volume of an atomic orbital instead of being a specific point on a well-defined trajectory of its motion [5]. However, this interpretation of distributed position probability of orbiting electron is quite faulty and invalid since a distributed position of the electron will render the Newton's laws of motion as well as the Coulomb's law of electrostatics as inapplicable and redundant.

1.2. Conceptual Mistake in Schrödinger's Equation for Hydrogen Atom

The Schrödinger equation is founded on a conceptual mistake in the representation of Potential Energy. The Coulomb potential energy of the proton electron pair in Hydrogen atom, which is inversely proportional to their instantaneous separation distance, has not been correctly modeled in the Schrödinger equation. The current solutions of Schrödinger's equation for different energy states of electron in Hydrogen atom appear to describe only the time averaged charge density distributions around nucleus and not the trajectories of electrons. That is because the potential energy term V in the equation has been assumed as time invariant and not dependent on the instantaneous position coordinates of the electron. Since the position coordinates of the electron have been wrongly omitted in the input to the equation, naturally the exact position of the electron is lost in the final solution. This has created all the weirdness in subsequent interpretations of QM [1].

However, fundamental problem giving rise to the conceptual mistake in

Schrödinger's Equation is much deeper and intricate which has not been addressed for more than a century. That fundamental problem is the ambiguity in the notion of Fields in general and the electrostatic field in particular. As per the modern concept, a field is a fundamental physical quantity that could independently exist at every point of the space occupied by the field. But Maxwell had supposed that the deformation of luminiferous aether, along with associated stresses and strains, represented various fields of physics including the electromagnetic field.

1.2.1. Intrinsic Electric Field

Consider one electron located at an isolated point P in space, far removed from all other charges. This isolated electron will produce an (intrinsic) electric field around point P that spreads everywhere in surrounding space. This intrinsic electric field or the electrostatic field of an electron is an integral part of the electron charge and does not depend upon the presence or absence of any other charge in its vicinity, not even any test charge. In Maxwell's terminology of "deformations of aether" we might call it "strain field" or "strain wave field" around the electron and consider it as an integral part of the electron structure, whatever it be. However, a significant point to be considered here is that in the entire intrinsic electric field of an isolated electron, there is no potential energy existing anywhere.

1.2.2. Coulomb Field

However, for practical applications we quantify this electric field of the electron by measuring its interaction with a positive test charge positioned at a certain point Q at distance r from point P. The force on second charge or test charge is caused by the mutual interaction between the electric fields of the two charges and is governed by Coulomb's Law of electrostatics. The intrinsic electric field of an electron when quantified with a test charge, using Coulomb's law, may now be termed as Coulomb electric field of the electron. This Coulomb field of the electron will map the force acting on test charge located at Q as well as map the interaction energy released due to the mutual interaction of the superposed intrinsic electric fields of the electron at P and test charge located at Q.

1.2.3. Ambiguity

Mapping of the forces and energies for different locations Q of the test charge through the Coulomb field has introduced a major ambiguity in the notion of Electric Field of the electron. Ambiguity is in the lack of distinction between the intrinsic electric field of isolated electron and isolated test charge and the Coulomb electric field of their interaction forces and energies. Moreover, this mapping of interaction forces and energies cannot represent a physical field since the forces and energies mapped at different field locations Q1, Q2, Q3 etc. do not physically exist when the test charge is physically located at Q. Unfortunately, in Modern Physics the Coulomb electric field is de-facto treated as the Intrinsic electric field of the electron.

1.3. Adopting Best Features from Sommerfeld Model and Wave Mechanics

To fully comprehend and understand any physical phenomenon, we must demand mental visualization of such phenomenon. Due to the conceptual mistake in the Schrödinger's equation for Hydrogen Atom as discussed above, the instantaneous position of the orbiting electron cannot be mentally visualized, but is said to be smeared across atomic orbitals as probability density. In fact, due to this conceptual mistake, the very picture of an electron gets transformed from a real particle with mass m_e and charge "e" to a wave packet whose position and momentum parameters get related through Heisenberg's uncertainty principal. The real electron particle never gets transformed to any wave packet; it is only the intrinsic electric field of the electron which acquires wave-like properties during motion of the electron. Therefore, as in Bohr-Sommerfeld models, we must be able to mentally visualize the instant-to-instant orbiting motion of the electron in hydrogen atom. Hence, we need to adopt best features from both the Bohr-Sommerfeld model as well as the Wave Mechanics that do not contradict empirical spectroscopic data [6].

In order to visualize the instant-to-instant motion of an electron orbiting a proton, we must understand as to how exactly the two charges interact to release potential energy. How released potential energy is transferred to the kinetic energy of interacting particles and how a photon is created. Hence, our basic approach in this paper will be to first make use of some of the most fundamental concepts about electron, nature of charge, field energy and field interaction [7]. With these fundamental concepts, we shall analyze the energy balance of an isolated proton-electron pair and develop the electron trajectory by using energy and angular momentum conservation principle in central force field system. Based on this methodology we improve upon the Bohr-Sommerfeld model to develop dynamic elliptical electron orbits in hydrogen atom.

By treating the physical space as an elastic continuum, the electron structure is found to be of a spherically symmetric standing strain wave core surrounded by a radial phase wave type electrostatic field. About 35% of the total mass energy of the electron (or positron) is distributed in its electrostatic wave field. The Coulomb interaction between two charge particles is effected through superposition of their wave fields. Positive interaction energy between two similar charges implies the transfer of a portion of their kinetic energies to their combined field energy. Negative interaction energy between two dissimilar charges implies the transfer of a portion of their combined field energy to their kinetic energies. Of course, the total energy and momentum of the system is conserved in both cases. Without going into the internal details of the electron structure [8], let us examine the effect of motion on the overall wave field of the electron.

We shall derive a relation from purely classical considerations that by emitting a photon at angular frequency ω , the angular momentum of orbiting electron is changed by \hbar due to mechanical recoil action. This fact will form the basis for

quantization of angular momentum and hence total energy in elliptical electron orbits in hydrogen atom. Further we shall retain the use of quantum numbers n and ℓ , as usual. However, on the considerations of restricting the change in angular momentum to \hbar , we shall associate quantum number ℓ with angular momentum of $(\ell+1/2) \cdot h$ or $k\hbar$ instead of $\sqrt{\ell(\ell+1)} \cdot \hbar$. This will lead to all elliptical electron orbits. During the emission of a photon, the elliptical orbit transitions at constant angular frequency will also be computed and plotted.

1.4. Motion Induced Fields and Kinetic Energy of Orbiting Electron

Let us consider uniform motion of an electron along +x axis, at velocity v . Due to the finite velocity c of the phase waves, the intrinsic wave field of the electron will get deformed. This motion induced field deformation may be considered through the concept of retarded time and retarded position vector. The kinetic energy of the moving particle will be stored in its deformed field. Let the original intrinsic field be deformed such that the change is defined by a motion induced field vector A , that will vanish when the particle velocity becomes zero. The motion induced electric and magnetic fields of the moving charged particle can now be derived from the time derivative and curl of this induced field as:

$$\mathbf{E} = -\frac{1}{\epsilon_0 c} \frac{\partial A}{\partial t} \quad (1)$$

$$\text{and } \mathbf{B} = \mu_0 c \cdot [\nabla \times A] \quad (2)$$

Under certain conditions of motion, like linear acceleration changes, some part of the induced fields could be dissociated from the moving particle, whereas the bound field can never be dissociated unless the particle gets annihilated. The induced fields are an integral part of the moving particle system and it is a matter of interpretation whether the particle motion controls the induced fields or the induced fields govern the particle motion. Even though the ψ wave function of Schrödinger's wave mechanics is purely a mathematical entity, yet it appears quite possible that $|\psi|^2$ may be representing the energy density of motion induced electromagnetic fields accompanying the orbiting electron [9].

2. Motion of an Electron around a Proton

2.1. Isolated Proton—Electron System

Let us consider an isolated proton—electron system with the proton located at the center of chosen coordinate system. Neglecting the motion of proton as too small, we consider the constrained motion of the electron, with mass m_e , under conservation of total system energy and angular momentum. When the electron is far removed from the proton with zero kinetic energy T , we define its electrostatic potential energy V as well as total energy E to be zero. Actually, total energy of the system does include mass energies of the two particles, which is omitted as a constant term by convention. We adopt a sign convention that the

symbols T , V and E representing energy will always be positive. When the electron is brought to a finite radial distance r from the proton, the conventional potential energy ($-V$) of the system gradually changes from zero to $-\frac{e^2}{4\pi\epsilon_0 r}$. The kinetic energy T of the electron simultaneously increases from zero to $\frac{e^2}{4\pi\epsilon_0 r}$. That is, the interaction energy released by the system, keeps getting converted to kinetic energy of the electron on an instant-to-instant basis. Henceforth, we shall replace the term negative potential energy ($-V$) with Coulomb field interaction energy (V) released by the system. If a small part (E_n) of this energy is either emitted out (E_{emt}) as a photon or get stored in other interacting fields (E_{int}) such that $E_n = E_{emt} + E_{int}$, then the system total energy will become $-E_n$ and the remaining K.E. of the electron is given by,

$$T = V - E_n \tag{3}$$

Here the interaction energy E_{int} associated with other interacting fields, like intrinsic spin and orbital magnetic moments or external electric or magnetic fields, may be either positive or negative depending on the type of field interaction.

2.2. Time Invariant Orbital Parameters

Corresponding to the conventional total energy of $-E_n$, let d_n be the radial distance OD at which the K.E. of the electron becomes zero (*i.e.* $V = E_n$), as shown in **Figure 1**. A sphere of radius d_n may be referred as the bounding sphere for the electron. All possible electron orbits for angular momenta $k\hbar$, must be located well within this sphere characterized by principal quantum number n . Let us therefore examine the shape and size of all possible orbits for given orbital quantum numbers n and ℓ .

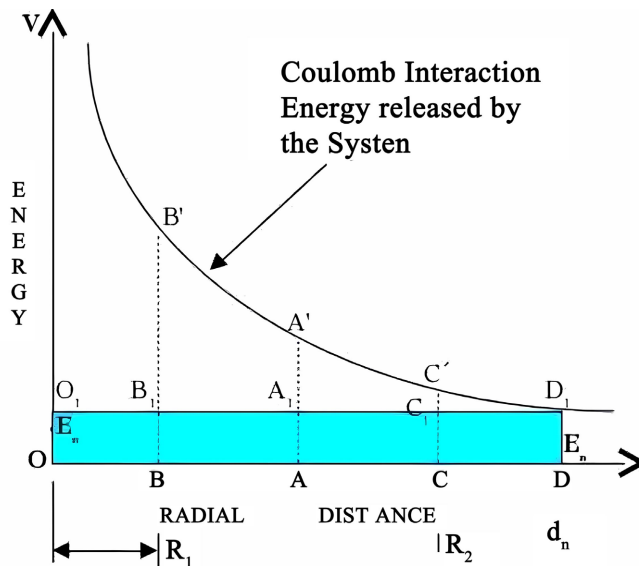


Figure 1. Coulomb interaction energy released (V) by the Electron—Proton system vs. their relative radial distance R . In the elliptical orbital motion of the electron, the relative radial distance oscillates between OC and OB with corresponding K.E. varying between C_1C' and B_1B' .

2.2.1. Nominal Circular Orbit Parameters

Let us consider an electron of mass m_e moving around a proton on a nominal circular orbit of radius a_c , with uniform tangential velocity v_c and kinetic energy T_c . On a circular orbit the Coulomb attractive force is completely balanced by the centrifugal force as,

$$\frac{m_e v_c^2}{a_c} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{a_c^2} = \frac{\eta}{a_c^2} \quad \text{where } \eta = \frac{e^2}{4\pi\epsilon_0} \quad (4A)$$

Equation (4A) directly leads to a relation between kinetic energy T_c and potential energy $-V$ for the circular orbit as.

$$T_c = \frac{m_e v_c^2}{2} = \frac{\eta}{2a_c} = \frac{1}{2}V \quad (4B)$$

From Equations (3) and (4B) we get a unique relation for the total energy ($-E_n$) in circular orbit as,

$$-E_n = T_c - V = -\frac{1}{2}V \quad (4C)$$

Therefore, for a circular orbit of radius $a_c = d_n/2$, angular momentum $L_c = n\hbar$, kinetic energy T_c is always equal to E_n and is half of the Coulomb interaction energy (V) released by the system.

Kinetic energy in circular orbit,

$$T_c = \frac{\eta}{d_n} = E_n \quad (4)$$

Using fine structure constant α as,

$$\alpha = \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{\hbar c} = \frac{\eta}{\hbar c}$$

We get,

$$E_n = \frac{\alpha\hbar c}{2a_c} \quad (5)$$

Also,

$$T_c = \frac{1}{2}m_e v_c^2 = \frac{1}{2} \frac{L_c^2}{m_e a_c^2} = \frac{n^2 \hbar^2}{2m_e a_c^2} \quad (6)$$

From Equations (4)-(6),

$$a_c = \frac{n^2 \hbar}{m_e \alpha c} = \frac{n^2 \hbar^2}{m_e \eta} \quad \text{and} \quad E_n = \frac{m_e \alpha^2 c^2}{2n^2} \quad (7)$$

In the ground state of hydrogen atom, Bohr radius is given by,

$$a_0 = \frac{\hbar^2}{m_e \eta} = 52.92 \text{ pm} \quad (7A)$$

2.2.2. Elliptical Orbit Parameters

However, with the same total energy, there could be many elliptical orbits with their angular momentum $L_e = k\hbar < L_c$ and differing from each other in steps of

\hbar . Since $L_e = 0$ will correspond to head on collision and annihilation of electron, it cannot correspond to any valid orbit. Therefore, as mentioned earlier, we shall take $k = (\ell + 1/2)$ instead of $(\ell(\ell + 1))^{1/2}$. Let the two vertices of the ellipse be identified by subscripts 1 and 2, e.g. radius R_1, R_2 etc. Then, at the vertices:

Angular momentum,

$$L_e = k \cdot \hbar = m_e \cdot v_i \cdot R_i \quad (\text{for } i = 1, 2 \text{ and no summation on } i) \quad (8)$$

From Equations (3) and (4),

$$T_i = \frac{\eta}{R_i} - E_n = E_n \left(\frac{d_n}{R_i} - 1 \right) \quad (9)$$

which gives,

$$R_i = \frac{E_n d_n}{T_i + E_n} = \frac{2a_c E_n}{T_i + E_n} \quad (10)$$

From Equations (8) and (10),

$$L_e^2 = 2m_e T_i R_i^2 = \frac{8m_e a_c^2 E_n^2 T_i}{(T_i + E_n)^2} \quad (11)$$

Using Equations (4) and (6), we can replace $2m_e a_c^2 E_n$ with L_c^2 in Equation (11) to get,

$$L_e^2 = \frac{4L_c^2 E_n T_i}{(T_i + E_n)^2} \quad (12)$$

After substituting $L_e/L_c = k/n$, Equation (12) simplifies to a quadratic in T_i as,

$$T_i^2 - 2 \left[2 \left(\frac{n}{k} \right)^2 - 1 \right] E_n T_i + E_n^2 = 0 \quad (13)$$

Solution of Equation (13) yields two values of T_i that is T_1 and T_2 as given below

$$T_1 = E_n \left(\left(2 \left(\frac{n}{k} \right)^2 - 1 \right) + 2 \frac{n}{k} \cdot \sqrt{\left(\frac{n}{k} \right)^2 - 1} \right) \quad (14)$$

$$T_2 = E_n \left(\left(2 \left(\frac{n}{k} \right)^2 - 1 \right) - 2 \frac{n}{k} \cdot \sqrt{\left(\frac{n}{k} \right)^2 - 1} \right) \quad (15)$$

Using Equations (10), (14) and (15) radius parameters R_1 and R_2 can be computed as,

$$R_1 = \frac{2a_c}{\frac{T_1}{E_n} + 1} = \frac{a_c}{\frac{n}{k} \left(\frac{n}{k} + \sqrt{\left(\frac{n}{k} \right)^2 - 1} \right)} \quad (16)$$

$$R_2 = \frac{2a_c}{\frac{T_2}{E_n} + 1} = \frac{a_c}{\frac{n}{k} \left(\frac{n}{k} - \sqrt{\left(\frac{n}{k} \right)^2 - 1} \right)} \quad (17)$$

From Equations (7), (16) and (17) it can be easily seen that,

Major diameter of the ellipse,

$$R_1 + R_2 = 2a_c = d_n = \frac{2n^2\hbar}{m_e\alpha c} \quad (18)$$

From these values of R_1 , R_2 , T_1 , T_2 , we can compute maximum and minimum values of velocity (V_1 , V_2) and angular velocity $\Omega_1 = V_1/R_1$, $\Omega_2 = V_2/R_2$. From Equations (16) and (17) it can also be shown that the eccentricity e_k of the ellipse is given by,

$$e_k = (R_2 - R_1)/d_n \quad \text{or,} \quad e_k = \frac{R_2 - R_1}{R_2 + R_1} = \sqrt{1 - \left(\frac{k}{n}\right)^2} \quad (19)$$

3. Dynamic Orbit Parameters

After determining the major diameter $2a_c$ the eccentricity e_k & R_2 , V_2 , Ω_2 etc. for the given quantum numbers n , ℓ , we can now compute the instant-to-instant motion of the electron on this orbit. For this purpose, let us introduce Cartesian coordinate system X-Y with origin O at the center of proton as shown in **Figure 2**. The radial position vector \mathbf{R} will be measured from O, the principal focus of the ellipse (proton location). At time $t = 0$ let us start from the outer vertex C, where $R = R_2$, $\theta = 0$, $V_t = V_2$, $V_r = 0$ and $\Omega = \Omega_2$. An analytical orbit equation for a particle in central force field of Coulomb interaction between a proton and electron is given by,

$$R(\theta) = \frac{k^2\hbar}{m_e\alpha c [1 - e_k \cos(\theta - \theta_0)]} = \frac{k^2 a_0}{1 - e_k \cos(\theta - \theta_0)} \quad (20)$$

Orbital angle θ in Equation (20) is measured from outer vertex C (**Figure 2**), k is the angular momentum number given by Equation (8), e_k is the eccentricity of

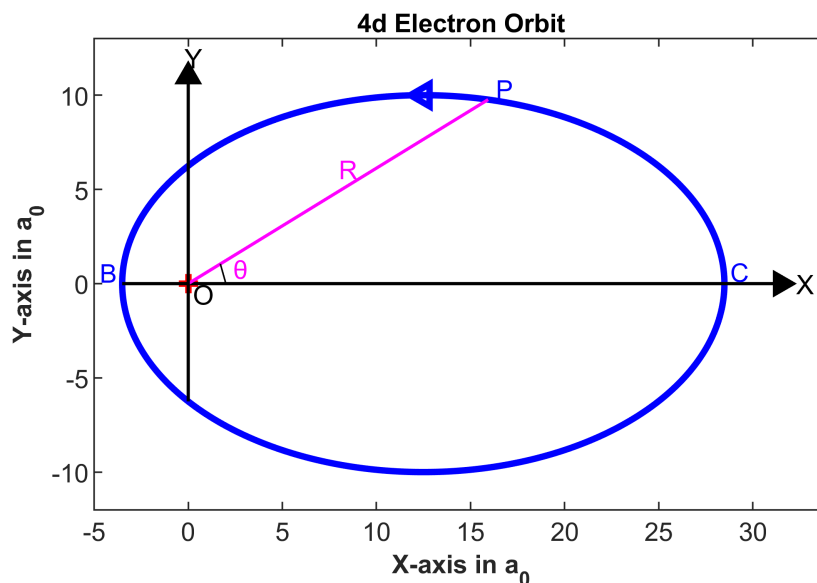


Figure 2. Electron 4d Orbit drawn in the scale of Bohr radius a_0 . In the orbital motion of electron its radial distance R from the Proton O varies between OC to OB.

the orbit given by Equation (19) and a_0 is the Bohr radius. Even though complete electron orbits can be drawn for given angular momentum and principal quantum numbers, k and n by using Equation (20), yet for computing time dependent orbit parameters like velocity, acceleration and kinetic energy we need to resort to numerical computations.

For numerical computations with the aid of a digital computer, we may divide the complete orbit into N (say 10,000) small elements for computing dynamic orbit parameters like angular position θ , radial position R , time t , radial velocity V_r , tangential velocity V_t , total velocity V_e , electron kinetic energy T , angular velocity Ω , radial acceleration A_r , tangential acceleration (∂V_t), and angular acceleration ($\partial \Omega$) at each element. For this purpose, we may take the orbital angle $d\theta$ for each element to be equal to $2\pi/N$. To compute the orbit parameters for the next position (index i) from the old position (index $i-1$), following relations could be used:

$$\text{Orbital angle } \theta(i) = \theta(i-1) + d\theta$$

$$\text{Radial position } R(i) = \frac{k^2 a_0}{1 - e_k \cos(\theta(i) - \theta_0)}$$

$$\text{Kinetic energy } T(i) = \frac{\eta}{R(i)} - E_n$$

$$\text{Tangential velocity } V_t(i) = k * \hbar / (m_e * R(i))$$

$$\text{Angular velocity } \Omega(i) = V_t(i) / R(i)$$

$$\text{Radial acceleration } A_r(i) = -\frac{\eta}{m_e * (R(i))^2} + V_t(i) * \Omega(i)$$

$$\text{Orbital time step } dt = 2 * d\theta / (\Omega(i-1) + \Omega(i))$$

$$\text{Orbital time } t(i) = t(i-1) + dt$$

$$\text{Radial velocity } V_r(i) = V_r(i-1) + (A_r(i-1) + A_r(i)) * dt/2 \quad (21)$$

$$\text{Total velocity } V_e(i) = \sqrt{(V_r(i))^2 + (V_t(i))^2}$$

$$\text{Tangential acceleration } \partial V_t(i) = (V_t(i) - V_t(i-1)) / dt$$

$$\text{Angular acceleration } \partial \Omega(i) = (\Omega(i) - \Omega(i-1)) / dt$$

$$\text{Total acceleration } A_{cc}(i) = \sqrt{(A_r(i))^2 + (\partial V_t(i))^2}$$

$$\text{X-coordinate } X_e(i) = R(i) * \cos(\theta(i))$$

$$\text{Y-coordinate } Y_e(i) = R(i) * \sin(\theta(i)) \quad (22)$$

Implementing these computational steps, through Scilab software, we have obtained instant to instant variation of all dynamic parameters like position, velocity, acceleration etc. and have plotted them against time t or angular position θ . A few typical curves showing trajectories and various dynamic parameters for certain elliptical orbits corresponding to given quantum numbers $[n, \ell]$, are shown in succeeding figures.

For given quantum numbers n and ℓ the instant-to-instant position variation of the orbiting electron describes an elliptical trajectory. The trajectory for 4d electron, with nominal quantum numbers $n = 4$ and $\ell = 2$ is shown in **Figure 2**. On this elliptical trajectory, the radial separation of the electron from the central

proton, varies from about 28.5 times the Bohr radius a_0 at the farthest point, to about 3.5 times a_0 at the nearest point. The eccentricity of this elliptical orbit is about 0.78. The variation of tangential velocity V_t and radial velocity V_r with orbital angle θ , for 2p electron is shown in **Figure 3**.

As expected, the radial velocity V_r is zero at both the nearest point ($\theta = 180^\circ$) and farthest point ($\theta = 0^\circ$) of the electron orbit. The tangential velocity V_t is maximum at the nearest point ($\theta = 180^\circ$) and minimum at the farthest point ($\theta = 0^\circ$) of the orbit. Maximum tangential velocity of the 2p electron is about 2400 km/s. On the other hand, maximum value of radial velocity V_r is just about 1000 km/s. The variation of same tangential and radial velocities with orbital time t in femtoseconds, for 2p electron is shown in **Figure 4**. On the consideration of the frequency of photon likely to be emitted during transition of a 2p electron to its lower orbit 1s, a most probable point for emission of photon is marked as P_{em} in both **Figure 3** and **Figure 4**.

The motion induced electric and magnetic fields accompanying the orbiting electron are expected to be proportional to the radial and tangential velocities V_r and V_t respectively. These motion-induced electric and magnetic fields are likely to get dissociated under appropriate acceleration conditions, within overall constraints of energy and momentum conservation. In this regard, angular acceleration profile of the orbiting electron is quite significant in influencing the emission of induced electric and magnetic fields as a photon.

The variation of orbital angular acceleration $d\Omega/dt$ for 2p electron, plotted against orbital time, is shown in **Figure 5**. The time in this figure is given in femto-seconds and is counted from the electron position at the farthest major

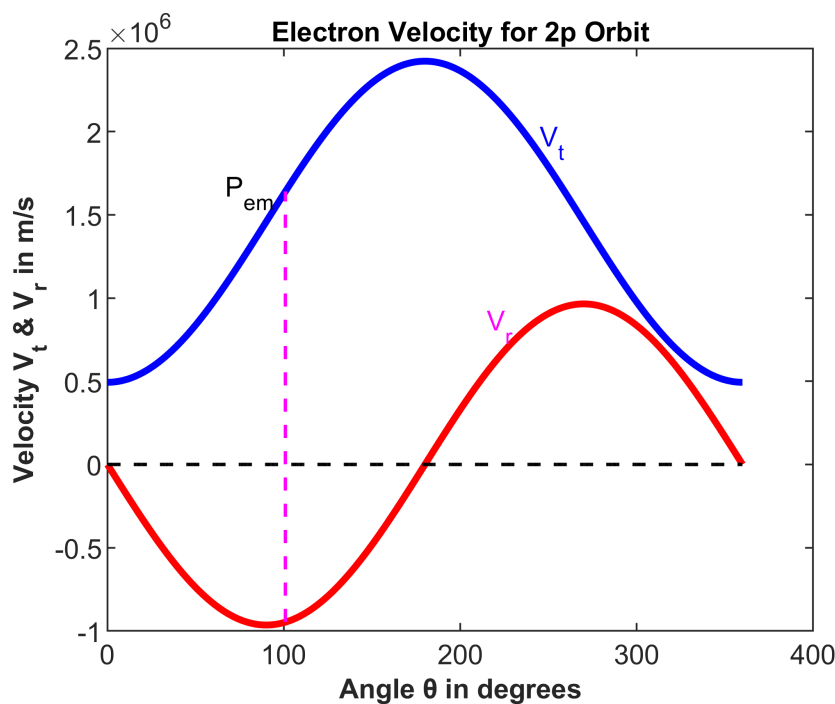


Figure 3. Variation of tangential and radial velocities for 2p electron with orbital angle.

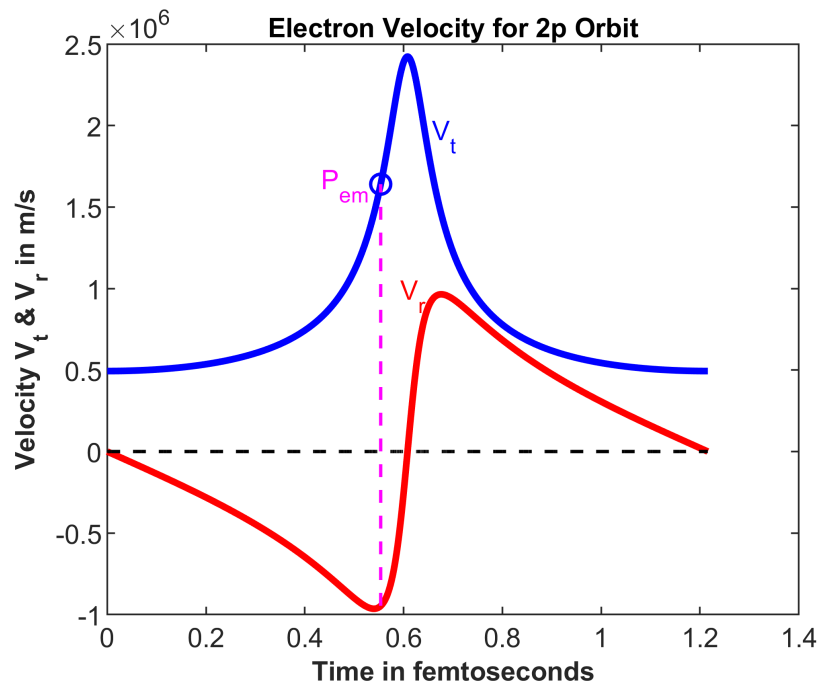


Figure 4. Variation of tangential and radial velocities for 2p electron with orbital time t .

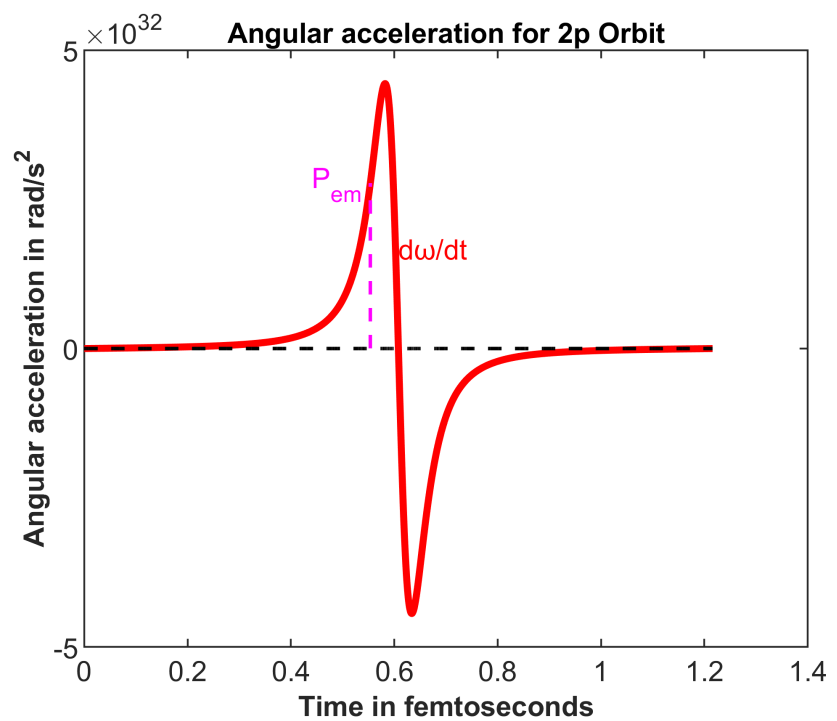


Figure 5. Variation of angular acceleration $d\Omega/dt$ for 2p electron with orbital time t .

vertex. Maximum value of angular acceleration attained while the electron approaches the nearest vertex, is about 4.4×10^{32} rad/s². The angular acceleration profile of an electron in 2p orbit shows steepest rise and fall in the vicinity of the nearest vertex. This region of steepest rise and fall in angular velocity is the

probable region for emission of photon, as depicted by point P_{em} in the figure.

The kinetic energy profile of orbiting electron in 2p orbit is shown in **Figure 6**. Maximum value of kinetic energy of the orbiting electron in 2p orbit is about 16.7 eV which occurs at the nearest vertex. Currently, as per QM interpretations of electron motion in hydrogen atom, only the total energy of about -3.4 eV is associated with the electron in 2p state and there is no mention of any kinetic energy possessed by the orbiting electron. However, total amount of about 3.4 eV has already been emitted out of the system in 2p state, and is no longer available for another photon emission. The energy to be supplied for a new photon to be emitted during transition from 2p state to 1s state will have to be extracted from the electron kinetic energy existing in the motion-induced electric and magnetic fields accompanying the orbiting electron.

The salient orbital parameters for orbiting electron in Hydrogen atom, are given at **Table 1**. One very important parameter to be noted from this table is the time period of the orbital motion, which is independent of ℓ . That is, for a given n the time period of all elliptical orbits is the same as that of a corresponding circular orbit. If $\tau(n)$ is the orbit time period and $S(n, \ell)$ is the total area of the elliptical orbit then the orbital magnetic moment μ_L will be given by,

$$\mu_L = \frac{e \cdot S}{\tau} \quad (23)$$

The orbital magnetic moment μ_L in the units of Bohr magneton μ_B is given in the last column of **Table 1**. It can be easily seen that the ratio of μ_L to μ_B comes out to be equal to total angular momentum number k . Further, maximum velocity and minimum vertex radii are of the same order of magnitude for all s states.

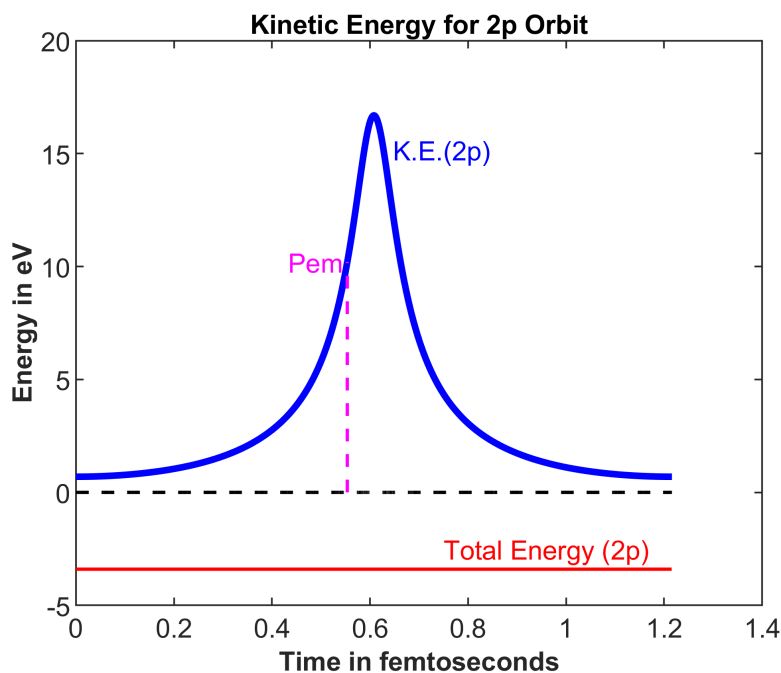


Figure 6. Variation of kinetic energy and total energy for 2p electron with orbital time.

Table 1. Salient orbital parameters.

Orbit No.	Total energy	Eccentricity	Time Period	Vertex-radii		Kinetic Energy Max.	Total Velocity Max	Angular frequency Max.	Angular acceleration Max.	Orbital Magnetic Moment
	ev			fs	Min.					
1s	-13.61	0.866	0.152	0.13	1.87	189.50	8.16e+6	1.15e+18	5.63e+35	0.500
2s	-3.40	0.968	1.216	0.13	7.87	210.83	8.61e+6	1.28e+18	7.20e+35	0.500
2p	-3.40	0.661	1.216	1.35	6.65	16.69	2.42e+6	3.38e+16	4.44e+32	1.500
3s	-1.51	0.986	4.103	0.13	17.87	214.66	8.69e+6	1.30e+18	7.51e+35	0.500
3p	-1.51	0.866	4.103	1.21	16.79	21.05	2.72e+6	4.26e+16	7.72e+32	1.500
3d	-1.51	0.553	4.103	4.03	13.98	5.25	1.36e+6	6.38e+15	1.48e+31	2.500
4s	-0.85	0.992	9.727	0.13	31.88	215.98	8.71e+6	1.31e+18	7.61e+35	0.500
4p	-0.85	0.927	9.727	1.17	30.83	22.45	2.81e+6	4.55e+16	8.97e+32	1.500
4d	-0.85	0.781	9.727	3.51	28.49	6.90	1.56e+6	8.39e+15	2.89e+31	2.500
4f	-0.85	0.484	9.727	8.25	23.75	2.45	9.27e+5	2.12e+15	1.55e+30	3.500

4. Photon Emission from Orbiting Electron

4.1. General Conditions for Emission

In accordance with the foregoing discussions, we may visualize the emission of a photon wave packet from the vicinity of an orbiting electron, under the following general conditions:

- 1) The angular frequency ω , will govern the spatial extension as well as the energy content ($\hbar\omega$) of the emitted photon wave packet.
- 2) The photon will be emitted in the orbital plane of the electron and along tangential velocity vector of the orbiting electron.
- 3) The strength of induced \mathbf{E} and \mathbf{B} fields in the region around relative position vector \mathbf{r} , will be governed by radial and tangential components of the electron velocity (\mathbf{v}_r , \mathbf{v}_t) respectively. The time rate of change of these fields will influence the photon emission process and may be governed by instantaneous time rate of change ($d\omega/dt$) of angular velocity ω of the orbiting electron.
- 4) The direction of emission of the photon may get reversed if the relative phase of induced \mathbf{E} field is opposite at the time of emission. That is, the photon will be emitted in the direction of \mathbf{v}_t if the electron is approaching the nucleus ($-ve \mathbf{v}_r$) and in a direction opposite to \mathbf{v}_t if the electron is receding ($+ve \mathbf{v}_r$) from the nucleus at the time of emission.
- 5) During the photon emission process, the conservation of overall system energy and angular momentum will be ensured.

4.2. Emission Constraints and Characteristics

The electron shells, characterized with principal quantum number n , are depicted with smallest number $n = 1$ for the innermost shell and larger numbers n

= 2, 3, 4 ... etc. for outer shells. When an electron transitions from an outer shell, with quantum number m , to an inner shell with quantum number n , this transition will be accompanied with the emission of a photon of angular frequency ω_{mn} given by Equation (7) as,

$$\omega_{mn} = \frac{m_e \alpha^2 c^2}{2\hbar} \left[\frac{1}{n^2} - \frac{1}{m^2} \right] \quad (24)$$

A photon of angular frequency ω_p will be emitted from the induced field of orbiting electron when the instantaneous angular velocity Ω of the orbital motion is nearly equal to ω_p . Computer simulations of the electron orbit transitions show that most probable zone of photon emissions (in forward direction) is where the orbital angle θ from the outer vertex, is in the range of $\pi/2$ to $3\pi/4$. In this orbital range inward radial velocity (v_r) of orbiting electron is maximum whereas tangential velocity (v_t) is rapidly increasing and the corresponding tangential acceleration is maximum. As such, orbit transitions from any circular orbit appear to be highly improbable. At the instant of photon emission when $\theta = \theta_p$ as the photon is emitted in the direction of tangential velocity vector v_t , the tangential velocity as well as tangential acceleration both are required to be high. However, angular frequency of the emitted photon ω_p must satisfy two conditions, that is, $\omega_p =$ angular velocity Ω and simultaneously $\omega_p = \omega_{mn}$ of Equation (24).

4.3. Photon Emission - Recoil

Let us consider an electron A, with kinetic energy E , orbiting the central proton with tangential velocity \mathbf{v}_t perpendicular to the instantaneous radius r . In view of strong Coulomb bond, we may regard this electron orbiting the central proton as a *coupled rotating body* whose angular momentum and energy content are conserved. The angular momentum of this rotating body can only change if some torque is applied to this coupled rotating body system. During the emission of a photon B in the orbital plane, when a small fraction of kinetic energy δE is being transferred to the photon the orbiting electron will experience some recoil torque T . Let the electron A act on photon B for a small angle $\delta\theta$ to transfer a small fraction of energy δE to photon B. We may assume that the action of recoil torque T , exerted by the photon B under emission, remains constant throughout this energy transfer interaction between A and B. Then the energy transferred from A to B will be given by $\delta E = T \cdot \delta\theta$. If this interaction process lasts for a very small interval of time δt , then an angular momentum impulse of $I_L = T \cdot \delta t$ will be imparted to both A and B in opposite directions. This impulse will imply a small change in angular momentum δL such that,

$$\delta L = I_L = T \cdot \delta t = (\delta E / \delta\theta) \cdot \delta t = \delta E / (\delta\theta / \delta t) = \delta E / \omega \quad (25)$$

The recoil impulse experienced by the electron while transferring a small fraction δE of its K.E. to the photon is therefore given by Equation (25). Hence, the total change in angular momentum ΔL , when a photon of total energy content

$\Delta E = \omega \hbar$ is emitted, will be,

$$|\Delta L| = \Delta E / \omega = \omega \cdot \hbar / \omega = \hbar \quad (26)$$

This is an important result which forms the basis of angular momentum quantization and hence total energy quantization in sub-atomic phenomena. The photon emission recoil phenomenon is unique in two respects. Firstly, the actual recoil interaction between the electron and the photon is affected through the action of released photon fields \mathbf{E}_p and \mathbf{B}_p on the bound -ve electrostatic field of the moving electron. Secondly, the emission phenomenon is unique in the sense that depending on the relative phases of \mathbf{E}_p and \mathbf{B}_p fields, the photon may be emitted by the moving electron either in forward direction or in rearward direction. The photon will be emitted in forward direction when at the time of emission, the electron is approaching the nucleus on its elliptical orbit and the total angular momentum of the orbiting electron will reduce by \hbar . The photon will be emitted in rearward direction when the electron is receding from the nucleus and the total angular momentum of the orbiting electron will increase by \hbar .

5. Orbit Transition Parameters

Let us consider the electron transition from orbit A specified by (n_1, ℓ_1) to orbit B (n_2, ℓ_2) , such that $n_1 > n_2$ and $\ell_2 = \ell_1 - 1$, then from Equations (7) and (18),

$$\begin{aligned} E_1 &= \frac{m_e \alpha^2 c^2}{2n_1^2} \quad \text{and} \quad d_1 = \frac{2n_1^2 \hbar}{m_e \alpha c} = \frac{\alpha \hbar c}{E_1} \\ E_2 &= \frac{m_e \alpha^2 c^2}{2n_2^2} \quad \text{and} \quad d_2 = \frac{2n_2^2 \hbar}{m_e \alpha c} = \frac{\alpha \hbar c}{E_2} \end{aligned} \quad (27)$$

The angular frequency of the photon to be emitted is $\omega_p = (E_2 - E_1)/\hbar$. Angular momentum for orbit A is $L_a = (\ell_1 + 1/2) \cdot \hbar = k_1 \hbar$ and for orbit B is $L_b = (\ell_2 + 1/2) \cdot \hbar = k_2 \hbar$. Therefore, change in angular momentum during the transition from higher orbit A to lower orbit B will be $(k_1 - k_2) \hbar = \hbar$. Corresponding change in total energy during this transition will be $\Delta E = (E_2 - E_1)$. The emission will take place when the electron is approaching the nucleus. The complete orbital parameters for A and B can be worked out as per procedure outlined in Section 3 above. While computing the dynamic parameters of orbit A, we may extract the values of salient parameters at the instant when index $i = I_p$ where the angular speed Ω of orbiting electron just matches the angular frequency ω of the photon under emission as,

$$\Omega(i) = \omega_p = (E_2 - E_1)/\hbar \quad (28)$$

To compute the transition trajectory from A to B we may mark all orbital parameters given by Equations (20) and (21) with index $i = I_p$ as the initial or starting point for the transition trajectory. Divide the transition trajectory path length into N (say 2000) equal steps. With $\delta L = \hbar/N$ or $dk = 1/N$ and $dE = (E_2 - E_1)/N$, let index s represent one of the steps of the transition trajectory such that

s varies from 1 to N . Following relations may be used for step-by-step computation of transition trajectory.

Primary parameters:

$$\Omega(s) = \Omega(I_p); \quad k(s) = k_1 - s * dk; \quad E_n(s) = E_1 + s * dE \quad (29)$$

Associated parameters:

$$\begin{aligned} \text{Instantaneous radius } R(s) &= \sqrt{\frac{k(s) \cdot \hbar}{m_e \cdot \Omega(s)}} \\ \text{Tangential velocity } v_t(s) &= R(s) * \Omega(s) \\ \text{Kinetic energy } T_n(s) &= \frac{\alpha \hbar c}{R(s)} - E_n(s) \\ \text{Total velocity } v_e(s) &= \sqrt{\frac{2T_n(s)}{m_e}} \\ \text{Radial velocity } v_r(s) &= \frac{v_r(s-1)}{\text{abs}(v_r(s-1))} \sqrt{(v_e(s))^2 - (v_t(s))^2} \\ \text{Radial acceleration } A_r(s) &= -\frac{\alpha \hbar c}{m_e (R(s))^2} + v_t(s) * \Omega(s) \\ \text{Time increment } dt &= \text{abs} \left[\frac{2 * (R(s) - R(s-1))}{v_r(s) + v_r(s-1)} \right] \\ \text{Angle } \theta \text{ increment } d\theta &= \Omega(s) * dt \\ \text{Angle } \theta &= \theta(s-1) + d\theta \\ \text{Orbital time } t(s) &= t(s-1) + dt \\ \text{X-axis location } X(s) &= R(s) * \cos \theta(s) \\ \text{Y-axis location } Y(s) &= R(s) * \sin \theta(s) \end{aligned} \quad (30)$$

After repeating these steps N times to compute all orbital parameters, the orbit transition trajectory will join the initial orbit A to the final orbit B. We can now plot the transition trajectory along with orbits A and B. However, special care is required to be taken while joining the transition trajectory to the orbit B. While initial angle θ_0 of Equation (20) is assumed to be zero for orbit A to ensure that major axis of the ellipse is aligned with the X-axis, θ_0 for orbit B is to be computed from $\theta_1 = \theta(s)$ for $s = N$. Let θ_2 be the orbital angle of orbit B when the angular velocity $\Omega(B) = \omega_p$ then the initial angle for orbit B will be given by $\theta_0 = \theta_1 - \theta_2$. With this, major axis of orbit B will get inclined with major axis of orbit A by angle θ_0 . Further, on the considerations of velocity and acceleration constraints discussed above, it is observed that most probable transitions from orbit A specified by (n_1, ℓ_1) to orbit B (n_2, ℓ_2) , are the ones where $n_2 = \ell_1$ and $\ell_2 = \ell_1 - 1$.

A few plots of some typical orbit transitions are shown in **Figures 7-12**. Some of these plots show the variation of some salient orbit parameters during the orbit transition stage. The photon emission time for various transitions is found to be of the order of 10^{-16} seconds which appears to be too small for the actual spatial extension of the photon. This is because the photon is not “created” from a

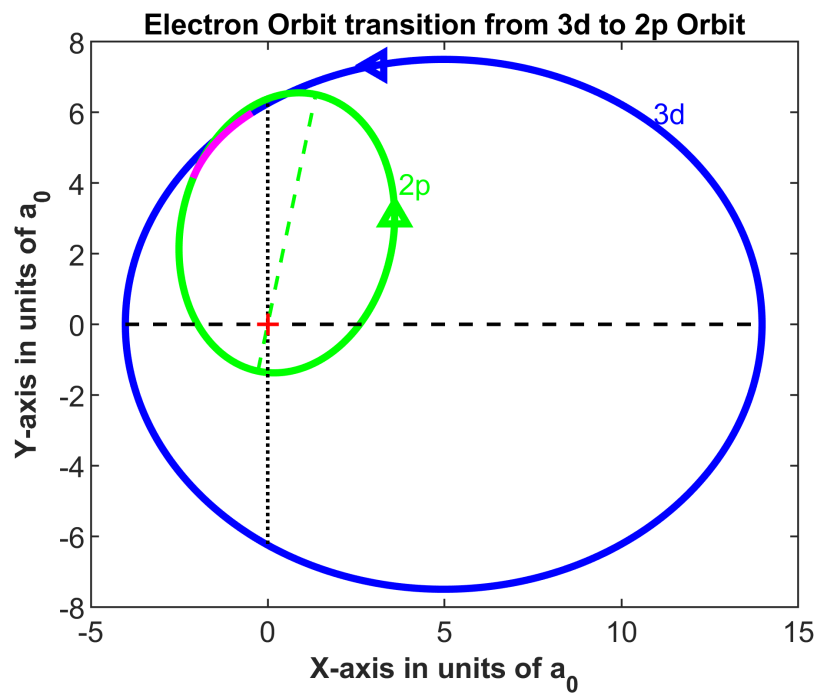


Figure 7. Electron orbit transition from 3d to 2p in which case photon is emitted in the direction of tangential velocity vector.

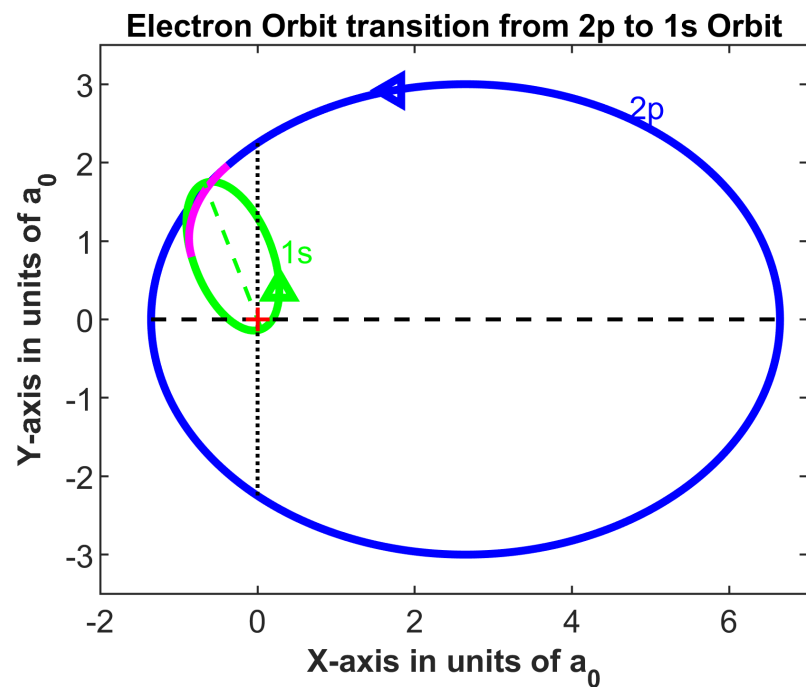


Figure 8. Electron orbit transition from 2p to 1s in which case photon is emitted in the direction of tangential velocity vector.

single point in space, but “released” from the spatially extended induced field of the electron and re-forms to its characteristic shape in accordance with the vector wave equation [8].

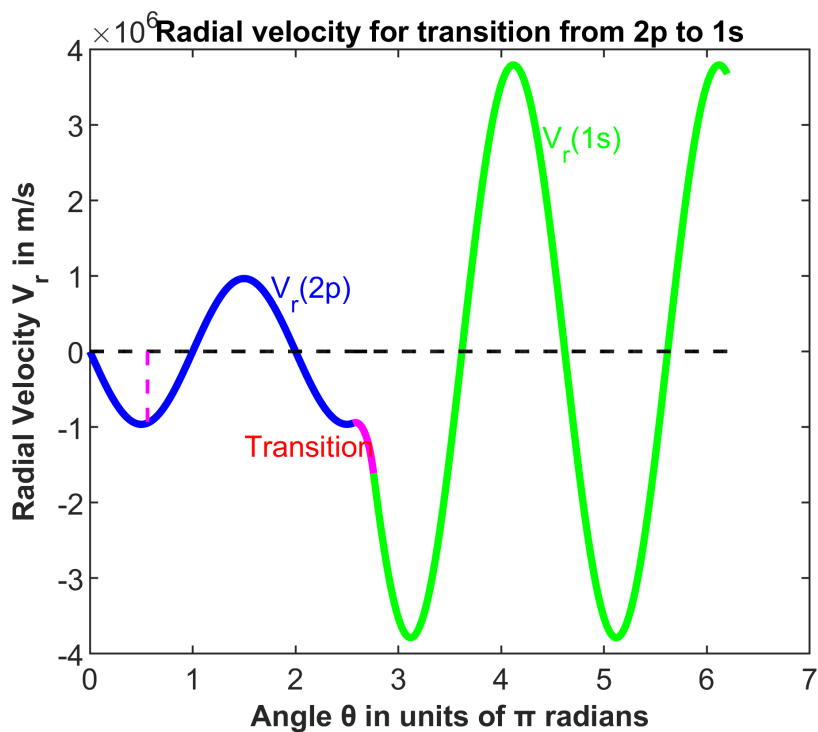


Figure 9. Variation of radial velocity V_r in Orbit Transition from 2p to 1s.

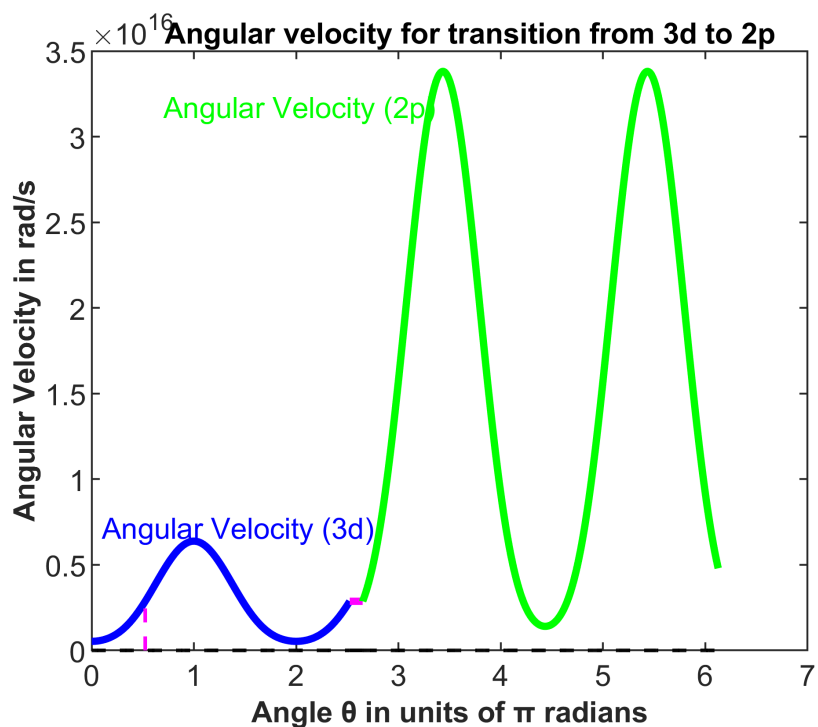


Figure 10. Variation of angular velocity Ω in orbit transition from 3d to 2p.

The transition of a 3d electron orbit to a 2p orbit is shown in **Figure 7**. Both old and new orbits are in the same plane with a common focus at the proton position, which is assumed to be fixed at the origin of the X-Y coordinate system.

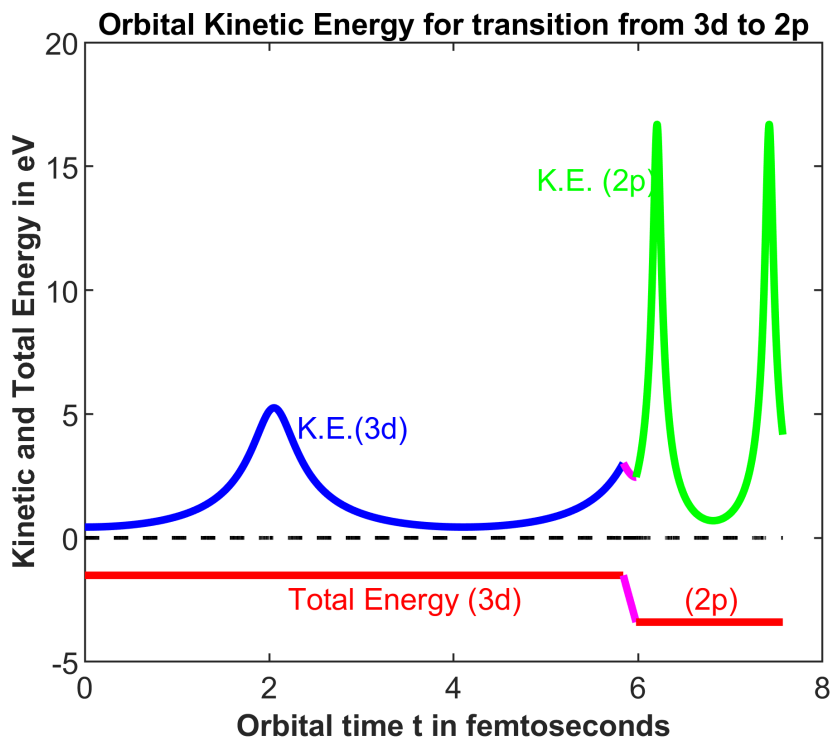


Figure 11. Variation of kinetic and total energy in orbit transition from 3d to 2p.

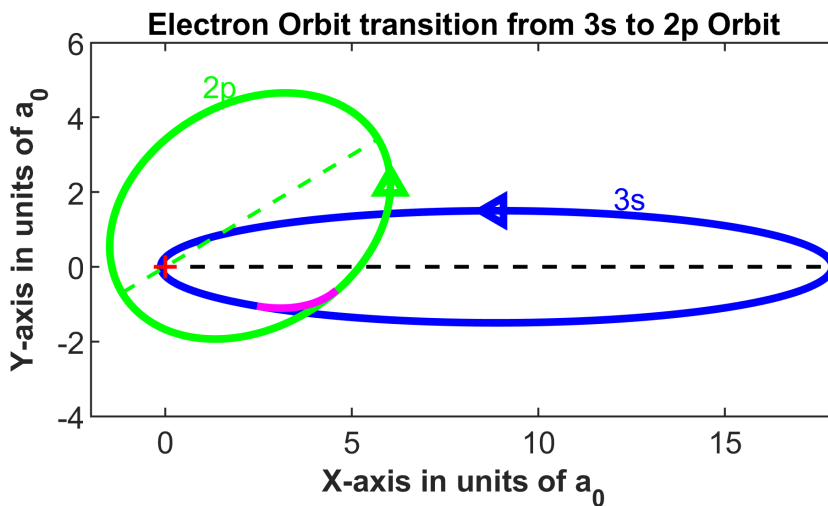


Figure 12. Electron orbit transition from 3s to 2p in which case photon is emitted in a direction opposite to the tangential velocity vector.

Whereas the major axis of old 3d orbit is on the X-axis, the major axis of new 2p orbit gets tilted during transition as shown. Length of major axis also shrinks during transition from $18a_0$ of 3d orbit to $8a_0$ of 2p orbit. Further, in comparison with time period of 4.1 fs for 3d orbit, the time taken by this orbit transition is just about 0.14 fs. Overall, the orbiting electron comes nearer to the central proton after this transition, with minimum vertex radius of $4.03a_0$ in 3d orbit getting reduced to $1.35a_0$ in new 2p orbit. This 3d to 2p orbit transition is associated

with emission of a Balmer series first line of 656.1 nm wavelength.

Similarly, the transition of a 2p electron orbit to a 1s orbit is shown in **Figure 8**. Both orbits are in the same plane with a common focus at the proton position. Whereas the major axis of old 2p orbit is on the X-axis, the major axis of new 1s orbit gets tilted during transition as shown. Length of major axis also shrinks during transition from $8a_0$ of 2p orbit to $2a_0$ of 1s orbit. Further, in comparison with time period of 1.2 fs for 2p orbit, the time taken by photon emission process is just about 0.04 fs. Overall, the orbiting electron comes nearer to the central proton, with minimum vertex radius of $1.35a_0$ in 2p orbit getting reduced to $0.13a_0$ in new 1s orbit. This 2p to 1s orbit transition is associated with emission of a Lyman series first line of 121.5 nm wavelength.

For the electron orbit transition from 2p to 1s orbits, variation of radial velocity V_r has been shown in **Figure 9**. X-axis of this plot depicts orbital angle θ in units of π radians. Whereas maximum radial velocity of the electron in 2p orbit varies between -10^6 to $+10^6$ m/s, corresponding velocity in 1s orbit varies between -3.8×10^6 to $+3.8 \times 10^6$ m/s. Most probable point for emission of a photon from 2p orbit is marked with a vertical dotted line on the 2p V_r curve. At the transition from 2p to 1s orbit, magnitude of radial inward velocity starts shooting up from the transition point onwards as shown in the figure. Similarly, the variation of angular velocity Ω for the electron orbit transition from 3d to 2p orbits has been shown in **Figure 10**. Maximum value of angular velocity in 3d orbit is of the order of 6.5×10^{15} rad/s and corresponding maximum value in 2p orbit is of the order of 3.3×10^{16} rad/s. During the transition from 3d to 2p orbits, the angular velocity is assumed to remain constant for about 0.14 fs. Magnitude of the angular acceleration at the point of probable transition, increases the overall probability of such orbit transition.

Variation of kinetic and total energies of the orbiting electron is shown in **Figure 11** for an orbit transition from 3d to 2p. In accordance with our current understanding, electron transition from 3d to 2p states is only associated with change in total energy from -1.5 eV to -3.5 eV and there is no clarity regarding the instant-to-instant kinetic energy changes in the two states. As seen from **Figure 11**, maximum kinetic energy of the orbiting electron is limited to about 5.3 eV in 3d orbit and it changes to about 16.7 eV in 2p orbit. During the orbit transition stage, after a slight dip in the electron kinetic energy, it suddenly shoots up immediately after entry in the 2p orbit. In contrast to a circular orbit, where the magnitude of total energy is always equal to the kinetic energy, the maximum kinetic energy of electron in an elliptical orbit is always much higher than the magnitude of corresponding total energy.

Variation of electron kinetic energy on elliptical orbit is very significant for emission of a photon from the motion induced electric and magnetic fields accompanying the electron. That is because the variation in kinetic energy of the orbiting electron is associated with variation in magnitude of linear and angular velocities giving rise to the linear and angular acceleration of the electron. Ulti-

mately it is the change in linear and angular acceleration linked with corresponding change in kinetic energy of the orbiting electron that leads to the dissociation of a part of induced electric and magnetic fields in the form of a photon emission. Thus, a photon cannot be emitted from a circular electron orbit. As discussed earlier in Section 4.3, any photon emission from a hydrogen atom will always be associated with a change in electron angular momentum by \hbar during corresponding orbit transition. Therefore, all excited states in hydrogen atom must correspond to all elliptical electron orbits.

Figure 12 shows an unusual type of electron orbit transition where a highly eccentric 3s orbit transitions to a less eccentric 2p orbit on emission of a permissible energy photon. All usual type of orbit transitions occur during acceleration phase of the orbiting electron when the electron is approaching the central proton in hydrogen atom. In this unusual type of orbit transition permissible energy photon is emitted during deceleration phase when the electron is receding from the central proton. In this case, due to opposite sign of radial velocity at the instant of emission, the photon is emitted in a direction opposite to the tangential velocity vector. As such, the angular momentum of orbiting electron increases by \hbar during emission of a permissible energy photon in backward direction. However, due to a relatively lower order of electron velocities and accelerations at the instant of permissible energy photon emission, such unusual orbit transitions are considered quite less probable.

6. Magnetic Moments and Magnetic Interaction Energy

In the foregoing analysis and development of electron orbits in hydrogen atom, we have neglected some small effects for the sake of simplicity because their contribution does not make any significant change in the electron orbits or their dynamic parameters. In that, firstly we have neglected the use of reduced mass of the electron by not considering the electron motion in a Center of Mass coordinate system. By taking into account the reduced mass of the electron we can make fine corrections in the frequency and wavelength of the emitted photons. Secondly, we have so far neglected the contributions of orbital magnetic moment and spin magnetic moments of electron as well as the proton and their associated magnetic interactions. We shall discuss these magnetic interactions in this section and examine their contributions to the refinement of computed frequencies and wavelengths of emitted photons.

6.1. Atomic Magnetic Moments

In a hydrogen atom there are two types of magnetic moments associated with the electron and proton. First one is the orbital magnetic moment μ_L which develops due to the orbiting motion of the electron and is proportional to its angular momentum L . It can be expressed in terms of Bohr Magneton μ_B which is defined by $e\hbar/2m_e$ and equals in magnitude to 9.274×10^{-24} J/T or Am^2 . For any elliptical orbit with angular momentum quantum number $k = \ell + 1/2$ the orbital

magnetic moment can be computed with Equation (23) and as given in the last column of **Table 1**, it comes out to be,

$$\mu_L = -k \cdot \mu_B \quad (31)$$

Second type of magnetic moment is the intrinsic magnetic moment of electron and proton that is associated with their intrinsic spin angular momentum. For the electron this intrinsic magnetic moment is given by $\mu_e = -9.284 \times 10^{-24}$ J/T or Am². For the proton this magnetic moment is given by $\mu_p = 1.41 \times 10^{-26}$ Am². In addition to these three types of magnetic moments there is a magnetic field B_0 induced at the origin or the proton location due to the orbiting motion of the electron. Using Biot-Savart law we get B_0 in terms of electron tangential velocity and angular momentum as,

$$B_0 = -\frac{\mu_0}{4\pi} \cdot \frac{e \cdot V_t}{r^2} = -\frac{\mu_0}{4\pi} \cdot \frac{e \cdot L}{m_e r^3} = -\frac{k\mu_0}{2\pi r^3} \cdot \mu_B \quad (32)$$

6.2. Magnetic Interaction Energy in Electron Orbits

For the sake of simplicity, we assume that the directions of all magnetic moments μ_e , μ_p , μ_L and the orbital magnetic field B_0 are all either parallel or anti-parallel in hydrogen atom [10]. Let us refer the orbiting motion of electron to an XYZ Cartesian coordinate system and select the XY plane as the orbital plane with origin at the proton location. Let us consider positive Z-axis as the positive direction for all spin vectors (S for electron and I for proton), angular momentum vector (L), all magnetic moments (μ_e , μ_p , μ_L) and magnetic field (B_0). When these vectors point in negative Z-axis direction, their values will be considered -ve. By assigning -ve value to the electron spin magnetic moment (μ_e) it is implied that spin angular momentum vector S is +ve. This can be concisely depicted symbolically as ($S\uparrow$, $\mu_e\downarrow$). Similarly for the electron orbit, when the angular momentum vector L is positive, the corresponding orbital magnetic moment will be negative which can be depicted as ($L\uparrow$, $\mu_L\downarrow$). Therefore, the mutual magnetic interaction energies become either positive or negative depending on the relative orientation of the spin and angular momentum vectors. Assuming parallel orientation of all magnetic moments, with r as the instantaneous radial distance of the orbiting electron, $k\hbar$ as the angular momentum of the elliptical orbit and proton spin vector aligned along +Z-axis, three magnetic interaction energies are given below [11].

Proton-electron Spin Interaction with ($I\uparrow$, $S\downarrow$) and ($\mu_p\uparrow$, $\mu_e\uparrow$) is,

$$E_{pe} = -\frac{\mu_0}{4\pi r^3} (\mu_p \mu_e) \quad \text{where } \mu_e \text{ is negative.} \quad (33)$$

Proton Spin-Orbit Interaction with ($I\uparrow$, $L\downarrow$) and ($\mu_p\uparrow$, $\mu_L\uparrow$) is,

$$E_{pL} = -\mu_p \cdot B_0 = \frac{k\mu_0}{2\pi r^3} (\mu_p \mu_B) \quad (34)$$

Electron Spin-Orbit Interaction with ($S\downarrow$, $L\downarrow$) and ($\mu_e\uparrow$, $\mu_L\uparrow$) is,

$$E_{eL} = \frac{\mu_0}{4\pi r^3} (\mu_e \cdot \mu_L) = -\frac{k\mu_0}{4\pi r^3} (\mu_e \cdot \mu_B) \quad \text{where } \mu_e \text{ is negative.} \quad (35)$$

With the above notation, maximum positive magnetic interaction energy for any elliptical electron orbit will be given by $(I\uparrow, S\downarrow, L\downarrow)$ combination of spin and angular momentum vector directions. Corresponding orientation of magnetic moments will be $(\mu_p\uparrow, \mu_e\uparrow, \mu_L\uparrow)$ and will lead to maximum magnetic interaction energy E_{m1} given by sum of Equations (33), (34) and (35) as,

$$E_{m1} = E_{pe} + E_{pL} + E_{eL} \quad (36)$$

On the other hand, maximum negative magnetic interaction energy will be given by $(I\uparrow, S\downarrow, L\uparrow)$ combination of spin and angular momentum vector directions. Corresponding orientation of magnetic moments will be $(\mu_p\uparrow, \mu_e\uparrow, \mu_L\downarrow)$ and will lead to minimum magnetic interaction energy E_{m2} given by,

$$E_{m2} = E_{pe} - E_{pL} - E_{eL} \quad (37)$$

For any electron orbit $[n, \ell]$, it is well known that the conventional total energy $-E_n$ only depends on the principal quantum number “ n ” and is independent of angular quantum number ℓ or its revised form $k = \ell + 1/2$. As such, the energy of emitted photon, being the difference between the total energy levels of initial and final orbits, appeared to depend only on “ n ” in accordance with Bohr model. However, the magnetic interaction energy E_{mi} as given by Equations (36) and (37), does depend on the orbital magnetic moment μ_L which is directly proportional to the orbital angular momentum L and hence to the angular momentum number “ k ”. The magnetic interaction energy E_{mi} directly adds up to the conventional total energy $-E_n$ of the orbiting electron and hence directly influences the energy of emitted photon, though by a very small fraction of an eV. This small contribution of magnetic interaction energy to the conventional total energy $-E_n$ and hence to the energy of the emitted photon, accounts for the so-called fine structure splitting of hydrogen spectrum lines.

In an ensemble of hydrogen atoms in excited states, the conventional total energy of some atoms with spin combination of $(I\uparrow, S\downarrow, L\downarrow)$, will get shifted upwards with the contribution of magnetic interaction energy E_{m1} . On the other hand, conventional total energy of some other atoms with spin combination of $(I\uparrow, S\downarrow, L\uparrow)$, will get shifted downwards with the contribution of magnetic interaction energy E_{m2} . Overall effect of these shifts in energy levels of any electron orbit $[n, \ell]$ will produce the well-known fine structure of hydrogen spectrum. Since the magnetic interaction energies E_{m1} and E_{m2} are proportional to $1/r^3$, their magnitude will vary from instant to instant during orbiting motion of the electron. It appears quite likely that at the instant of orbit transition, the available magnetic interaction energy will be carried along with the emitted photon. The variation of interaction energies E_{m1} and E_{m2} with orbital angle θ is shown in **Figure 13** and **Figure 14** for 3d and 2p orbits respectively. A probable point of photon emission, P_{em} is marked with a vertical dotted line, indicating the magnitude of interaction energies E_{m1} and E_{m2} at emission time, in both **Figure 13** and **Figure 14**.

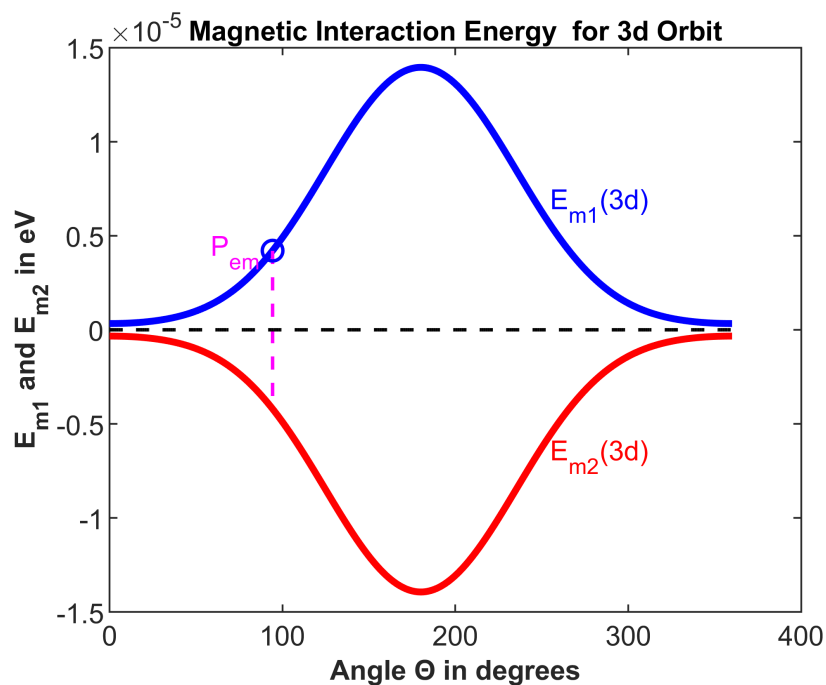


Figure 13. Variation of magnetic interaction energy for 3d orbit with orbital angle θ .

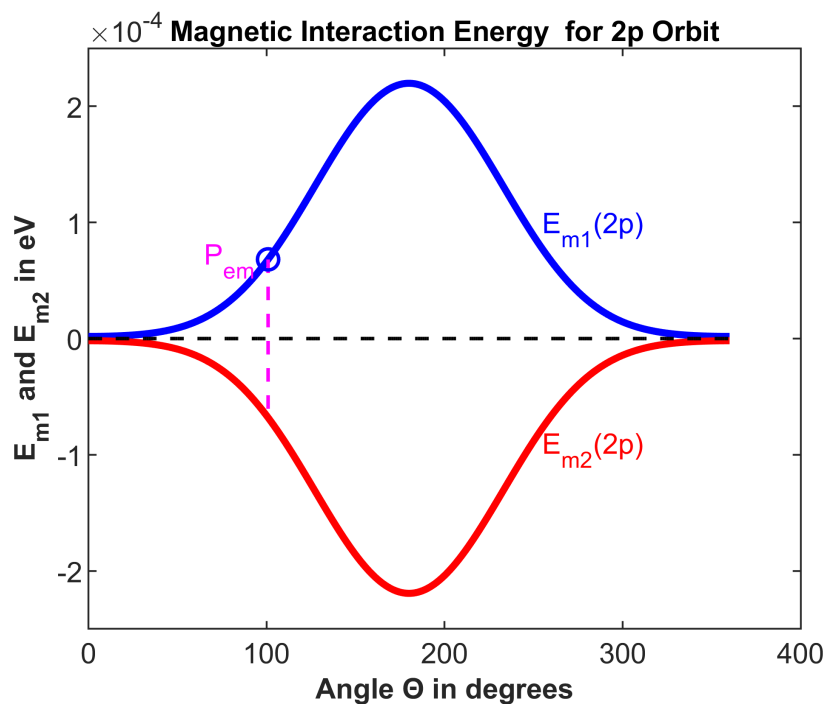


Figure 14. Variation of magnetic interaction energy for 2p orbit with orbital angle θ .

7. Electron Orbits in Molecular Hydrogen Bond

When two hydrogen atoms come close, the two protons will tend to repel each other but their electron orbits will tend to get pulled towards opposite protons. In the process, the two electrons e_1 and e_2 which were earlier orbiting individual pro-

tons P_1 and P_2 , will now start orbiting the line joining P_1P_2 , called bond axis. Finally, when all forces acting on P_1 , P_2 , e_1 and e_2 get dynamically balanced, the configuration of these particles as shown in **Figure 15**, will constitute the hydrogen molecular bond.

For analysis of this bond configuration, let us start with the computation of forces acting on the constituent protons and electrons. If F_{pp} is the Coulomb repulsion force acting on P_1 , P_2 ; F_{pe} is the attraction force acting on any proton-electron pair and F_{ee} is the repulsion force acting on e_1 , e_2 then,

$$F_{pp} = \frac{e^2}{4\pi\epsilon_0 (2a)^2} = \frac{\eta}{(2a)^2} \quad (38)$$

$$F_{ee} = \frac{\eta}{(2r)^2} = \frac{\eta}{12a^2} \quad (39)$$

$$F_{pe} = -\frac{\eta}{(2a)^2} \quad (40)$$

With angle $\theta = \pi/3$, since $F_{pp} + 2F_{pe} \cos\theta = 0$, resultant of all forces acting on each of the two protons vanishes. Similarly, all axial forces acting on two electrons get balanced due to symmetry of the configuration. Regarding the force balance in transverse or radial direction, the resultant of all Coulomb forces on each electron must get balanced with the centrifugal force acting on each orbiting electron. If v_t is the tangential velocity of each electron, then the requirement of force balance in radial direction gives,

$$\frac{\eta}{12a^2} - 2 \cdot \frac{\eta}{4a^2} \cos\left(\frac{\pi}{6}\right) + \frac{m_e v_t^2}{r} = 0$$

which on simplification yields the kinetic energy T_e of one electron as,

$$\frac{(9 - \sqrt{3})\eta}{24a} = \frac{m_e v_t^2}{2} = T_e \quad (41)$$

Next, we need to consider the Coulomb potential energy of two protons and

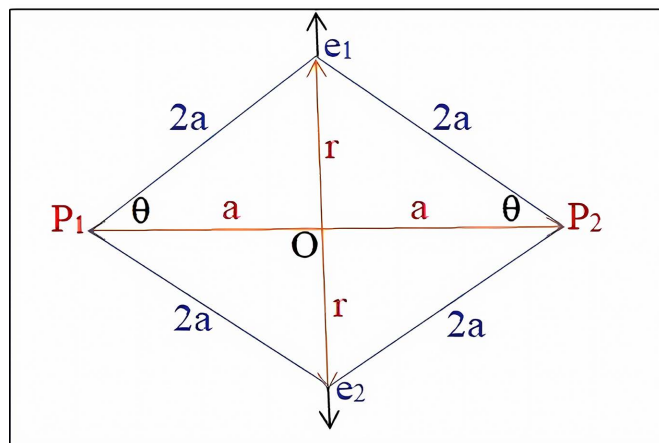


Figure 15. Relative positions of two protons P_1 , P_2 and two electrons e_1 , e_2 in hydrogen molecular bond.

two electrons shown in the hydrogen bond configuration. The potential energy V_{pp} between protons P_1, P_2 ; the potential energy V_{ee} between electrons e_1, e_2 and potential energy V_{pe} between one proton-electron pair (P_1, e_1) is given by,

$$V_{pp} = \frac{\eta}{2a}; \quad V_{ee} = \frac{\eta}{2\sqrt{3}a}; \quad V_{pe} = -\frac{\eta}{2a} \quad (42)$$

Hence, total potential energy of the system configuration V_T is given by,

$$V_T = V_{pp} + V_{ee} + 4V_{pe} = -\frac{(3\sqrt{3}-1)\eta}{2\sqrt{3}a} \quad (43)$$

For the orbiting electrons e_1 and e_2 , on the analogy of hydrogen atom, the angular momentum for a circular orbit can be taken as \hbar . Rewriting Equation (41) in the form of angular momentum and assuming $L = \hbar$ for a circular orbit, we get,

$$\frac{m_e^2 v_i^2 r^2}{2m_e r^2} = \frac{\hbar^2}{6m_e a^2} = \frac{(9-\sqrt{3})\eta}{24a} \quad (44)$$

From Equations (7A) and (44) we get the value of “ a ”, the half bond length as,

$$a = \frac{4\hbar^2}{(9-\sqrt{3})m_e\eta} = \frac{4a_0}{(9-\sqrt{3})} = 29.12 \text{ pm} \quad \text{where } a_0 \text{ is the Bohr radius} \quad (45)$$

The conventional total energy E of the hydrogen molecular bond configuration can now be obtained as a sum of total potential energy V_T and kinetic energy of two orbiting electrons by using Equations (41), (43) and (45) as,

$$E = V_T + 2T_e = -\frac{(3\sqrt{3}-1)\eta}{2\sqrt{3}a} + \frac{(9-\sqrt{3})\eta}{12a} = -\frac{1.1005\eta}{a_0} = -29.95 \text{ eV} \quad (46)$$

Whereas the binding energy of two isolated hydrogen atoms adds up to 27.2 eV, total binding energy of hydrogen molecule is found to be 29.95 eV. This shows that the hydrogen molecular bond configuration discussed above is stable with a dissociation energy of about 2.8 eV. The measured dissociation energy of hydrogen molecular bond may be a little higher due to the kinetic energy of the dissociated atoms. Theoretical bond length of hydrogen bond (2a) of about 58 pm is low in comparison with the measured bond length of about 73 pm. This may be due to axial thermal vibrations of the two protons constituting the bond. In fact, with axial vibrations of the hydrogen bond, the two orbiting electrons may not stay on a common orbit. The orbits of two electrons may get separated and the two orbits may get slightly inclined to the original transverse plane, with two electrons staying in phase opposition to each other.

During the formation of the hydrogen molecular bond, the two hydrogen atoms will usually collide against one another with some initial kinetic energy. The initial kinetic energy of the constituent atoms will have to be dissipated out by some physical mechanism to enable the formation of a stable bond. One physical mechanism that is highly probable in this regard, is the pushing up of one of the orbiting electrons to a higher electronic state, a higher orbit with say $2\hbar$ angular momentum to absorb the available kinetic energy of the collision.

The excited electron may subsequently transition back to the ground state by emitting a photon to dissipate out the excess energy. Hence, the formation of hydrogen molecular bond is associated with emission of a photon from an excited orbiting electron.

8. Summary & Conclusion

In this paper, we have attempted to develop a new model, a new methodology, to compute the detailed instant to instant motion of electron in Hydrogen atom, based on the principle of conservation of energy and momentum. For this, several new basic concepts have been used to develop a better insight and fundamental understanding of the sub-atomic phenomenon. The new concepts include the structure of the electron, Coulomb interaction, potential energy etc. We have also shown that whenever a photon is emitted from an orbiting electron, the angular momentum of that electron is changed by \hbar . This may be seen as the origin of various quantization rules. After introducing several new fundamental concepts, the electron trajectories in the form of elliptical orbits, have been developed and their transitions plotted. The linear velocities, angular velocities, K.E., radial distance r , orbital angle θ and orbital time have been computed and plotted for the instant-to-instant motion of the electron in various electron orbits in hydrogen atom. We have also analyzed magnetic interaction energies associated with electron angular momentum, spin angular momentum of the proton and electron, and plotted their instant-to-instant variation in different electron orbits to explain the fine structure splitting of hydrogen spectrum lines. Finally, we have extended the concept of electron orbits in hydrogen atom to explain the hydrogen molecular bond configuration and to compute its binding energy and bond length. Hopefully, the analysis presented in this paper will enable the scientific community to mentally visualize the instant-to-instant motion of orbiting electrons in hydrogen atoms and their molecular bonds.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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