Modeling Bohr’s Theory of Hydrogen Atom for Physics and Chemistry Education, Computational Physics and Chemistry, and Computer Science Majors

Gurmuhk Singh, Ph.D.

214 Fenton Hall, Department of Computer and Information Sciences
State Univeristy of New York at Fredonia, Fredonia, NY 14063
singh@cs.fredonia.edu

ABSTRACT
This interesting article is primarily targeted for the advanced college undergraduate and first year university graduate students of physics and chemistry education, computational physics and chemistry, and computer science. In the present paper, we are employing an enormous computational power of the second most used and quite versatile software system, the Microsoft Excel 2007, to perform computer simulations to model Bohr’s theory of hydrogen atom in college and university classroom setting of a virtual laboratory. We developed the necessary computer algorithm to compute discrete values of the orbit radius, and stationary energy levels of Bohr’s hydrogen atom. We have performed more than 2000 computer simulations to investigate the model behavior starting from the ground state of H-atom till we reach the energy continuum, where the discrete energy levels begin overlapping. One of the natural consequences of Bohr’s model is that it could provide a perfect corroboration of the experimentally observed spectral lines of H-atom with those empirically obtained from empirical formulas derived by five famous scientists of 19th century, namely, Lyman, Balmer, Paschen, Brackett, Pfund and Humphreys. From the model predictions, it is also feasible to compute very accurately the ionization potential of a singly charged atom such as H, He, Li etc. Using the old theory of classical electro-dynamics, it was not possible to explain the observed line spectrum of hydrogen atom. Bohr’s model of hydrogen atom set the stage for the development of a modern branch of physics and chemistry in microscopic world, the so called quantum mechanics.

1. IISTORICAL BACKGROUND AND NECESSITY OF QUANTUM MECHANICS IN MICROSCOPIC WORLD
Considerable amount of modern scientific progress that took place during 20th century can be summarized in a short list as follows: (i) general theory of relativity [1], (ii) quantum mechanics [2-5], (iii) big bang model of cosmology [6], (iv) the unraveling of the genetic code [7], (v) evolution biology [8], and (vi) may be a few other topics depending on reader’s personal taste and choice. In this short list, quantum mechanics has a unique status due to its profound quality work. Quantum mechanics forced physicists and chemists to change their view points of deterministic reality, and made them to rethink the nature of things at the microscopic level in terms of probabilistic events rather than their deterministic attributes. Therefore, scientists had to revise their classical concepts of position, velocity, momentum as well as their notions of cause and effect in order to understand quantum mechanical implications [9].

Although the prime aim of the formalism of quantum mechanics was to fully describe an abstract microscopic, atomic world far away from realm of daily-life experience, however, its immense impact on human society had been really very pronounced. The spectacular advances in modern physics, chemistry, biology, and medicine, and in essentially every other scientific field, could not have taken place without the tools that quantum mechanics has provided us. Without quantum mechanics it is impossible to talk about global economy, since the electronics revolution that brought us in the extremely fast moving computer age is basically a brain-child of quantum mechanics. In the same way is the photonics revolution that brought us in the Information Age: especially fiber optics, e.g., optical fibers being used for information transmission worldwide and in local communications. The development of quantum physics has transformed our world, bringing with it all the benefits of scientific revolutions and advancements. To get an understanding on the successes of quantum mechanics by an educated layman, a reference may be made to a very recently published, best selling and very inexpensive textbook in which careful explanations of the concepts and details of quantum mechanical phenomena are presented in a nonmathematical form [10].
Unlike the development of general theory of relativity of Einstein [1], which grew out of a brilliant insight into the connection between gravity and geometry, or the deciphering of DNA, which unveiled a new world of biology, quantum mechanics did not evolve from a single easy step. Rather, it was created in one of those rare concentrations of genius that occur from time to time in history. For twenty years after introduction of quantum ideas, they were so confusing to people that there was little basis for its progress and nobody believed it. However, a special mention may be made of a small group of dedicated and really bright young physicists who did major development of quantum mechanics in just three tumultuous years from 1925 to 1928 [3-5, 9]. These scientists were troubled by what they were doing, and in some cases distressed by what they had done. The unique situation of this crucial yet elusive theory is perhaps best summarized by the following observation: Quantum theory is the most precisely tested and most successful theory in the history of science. Nevertheless, not only was quantum mechanics deeply disturbing to its founding fathers, even almost ninety years after the birth of quantum theory essentially in its current form, some of the luminaries of physical sciences remain still dissatisfied with its foundations and its interpretation, even though they acknowledged its stunning mathematical power and elegance.

At the end of 19th century, physicists and chemists had pretty good idea that the electrons resided inside atoms, and that their random motion could give rise to an emission of light in infra red (IR), visible and ultra violet (UV) part of the electromagnetic spectrum, which was thought to be an intrinsic characteristic of each element in the periodic table. However, there was still a big and curious puzzle to solve, i.e., the existence of line spectrum of several elements such as H, He, Ne, Ar, Kr, Xe, Li, Na, K, Rb, Cs, Fe, Co, Ni etc. To obtain line spectrum of a given metallic element, physicists and chemists would heat up different elements using high voltage electric spark until they glowed red hot and then they directed the emitted light from the spark through an optical instrument called diffraction grating or through a prism as was done by Newton in 17th century to investigate the continuous spectrum of ordinary sunlight. The light split by the diffraction grating/optical prism could be analyzed with the help of an optical spectrometer. Newton discovered that the ordinary sunlight was composed of seven continuous colors (more specifically of seven different wavelengths with no well-defined boundaries), and therefore he could explain the formation of rainbow in a direction exactly opposite to Sun’s location on the horizon [11]. Thus, we may conclude that one could observe the whole rainbow of colors, because an optical prism would split up the sunlight into its seven composite wavelengths or colors. However, to investigate the nature of light emitted by atomic gases like H, He, Ne, Ar, Kr etc. under very low pressure, and from metallic elements such as Li, Na, K, Rb, Cs, Fe, Co, Ni etc. at very high temperature, the scientists had to analyze the light emitted by an atomic gas or an element with the help of very high resolution instruments.

In the preceding paragraph, we have just concluded that the sunlight consists of seven rainbow colors, but how about the light emitted by a very hot element of different metals and that of highly excited gaseous atoms. When scientists analyzed the light emitted by the simplest element of periodic table, e.g., hydrogen atom, to their utmost surprise they were unable to observe the whole rainbow of continuous colors. Instead they just observed a few discontinuous bright lines of certain colors, and more specifically of certain wavelengths or frequencies. Actually, we should try to avoid using the term color in our current discussion, because only some of the spectral lines are visible, which is true for white light, but how about the spectral lines in IR and UV region of the electromagnetic spectrum. That would mean that the atoms of a given element were only emitting light waves of certain frequencies or wavelengths in the UV, visible and IR region of the electromagnetic spectrum. Do all atoms radiate the waves of same frequencies or wavelengths? Answer to this question is no. Each atom in periodic table emits a unique set of electromagnetic waves of different frequencies, and consequently of different wavelengths, which are now known as the spectral lines. These spectral lines are a kind of "signature" of the intrinsic nature of each individual atom in the periodic table.

Current article is arranged as follows: We begin, in Section 2, with an introduction to the two atomic models: one was put forward by J. J. Thompson [12] and the other one advocated by Ernest Rutherford [13]. Section 3 discusses fundamental limitations of Rutherford’s model of atom. We present, in Section 4, the theory of Bohr’s model of an atom, and develop its pertinent algorithm. Section 5 discusses the importance of using Microsoft Excel 2007 software system for the current investigation, which could be employed in college and university class-room setting for physics, chemistry and computer science education and computer science majors. Section 6 deals with the actual computer simulations of the hydrogen atom problem and the predictions of Bohr’s model. We will also have a comprehensive discussion on how this simple model could explain the observed spectral lines such as Lyman [14], Balmer [15], Paschen [16], Brackett [17], Pfund [18] and Humphreys [19] series emitted by hydrogen atom in highly excited state. In addition, we would be precisely estimating the value of Rydberg’s constant in two different ways from the predictions of Bohr’s theory of hydrogen atom. Section 7 describes very important outcome of Bohr’s theory the so called correspondence principle. Finally, conclusions and implications of the current investigation will be presented in Section 8 in light of its usefulness for natural science education students and instructors.

2. THE THOMSON AND THE RUTHERFORD MODEL OF ATOM

In 1897, J. J. Thomson discovered an electron, the lowest mass elementary particle. In the early 1900s, it was well known that the atom consisted of subatomic particles called
protons and electrons. However, it was not exactly clear how these protons and electrons were distributed within the tiny volume of an atom. In 1902, Thomson did rigorous mathematical refinement to the atomic model advocated by Lord Kelvin. As Thomson modified the model by putting emphasis on the mechanical and electrical stability of the system, and therefore, in Thomson’s honor the atom was known as the Thomson atom. The atomic model proposed by Thomson was popularly known as the “plum pudding” model [12]. In this model the electrons and protons are assumed to be uniformly distributed throughout the atom just like the plums sitting in the pudding as shown in Fig. 1.

To test Thomson's hypothesis of atom, Rutherford designed his famous "gold foil" experiment [13]. Rutherford argued that if Thomson's model was correct then the mass of the atom should be distributed uniformly throughout the atomic volume. If one fired high speed alpha-particles (helium nuclei emanating from radioactive isotope like $^{241}$Am, $^{210}$Po etc.) at some heavy atomic element, then alpha-particles should pass through the atom without any visible deviation or deflection from their original trajectories. Rutherford decided to test his idea by impinging high speed alpha-particles on a thin gold film. As expected, most of the alpha-particles passed through the gold-foil un-deviated, but to his utmost astonishment a few alpha-particles rebounded almost directly backwards. Rutherford himself made the following remarks: “It was almost as incredible as if you had fired a fifteen-inch bullet at a piece of tissue paper and it came back and it hit you”.

The experimental arrangement to test the predictions of Thomson’s atomic model is depicted in Fig. 2. Rutherford's thin gold-foil experiment, performed by his graduate students, Geiger and Marsden [20], provided concrete evidence for the existence of a minute, positively charged atomic nucleus, from which alpha-particles could scatter in any direction. These experimental observations were not consistent with the predictions of Thomson's model [12]. Therefore, naturally Rutherford discarded the Plum Pudding model and argued that the only way the alpha-particles could be deflected in backward direction was if almost entire mass of an atom were concentrated at the center of its nucleus. Thus, he is given due credit for the development of the planetary model of the atom, in which all the protons are confined to a tiny volume of the nucleus of radius $\approx 10^{-15}$ m, and the electrons orbit around the nucleus like planets orbiting around Sun [13, 20]. A typical radius of the atom is $\approx 10^{-10}$ m, which is 10$^5$ times more than the radius of a nucleus. Thus, the repulsive force
experienced by some of the alpha-particles suggested that the nucleus is positively charged, and this positive net charge must be due to the presence of protons. A diagram of planetary model of an atom with four protons in the nucleus, and four electrons orbiting around the nucleus is displayed in Fig. 3. Further work by Chadwick in 1932 revealed the existence of neutrons within the nucleus of an atom [21] in addition to the protons. The atomic number \( Z \) describes the number of protons in the nucleus. For a neutral atom, atomic number equals the number of electrons outside the nucleus. Subtracting the atomic number \( Z \) from the atomic mass number \( A \) gives the number of neutrons \( (N = A - Z) \) in the nucleus.

3. IMITATIONS OF RUTHERFORD’S MODEL

Although the planetary model of the atom presented by Rutherford was extremely simple to visualize, still it was very successful to explain the scattering of alpha-particles from the nucleus. However, model encountered some intrinsic difficulties for its acceptance among scientists since it had a major drawback. In the planetary model of atom, electrons must orbit around the nucleus in curved or circular paths. This curved/circular motion of electrons should automatically create centripetal acceleration, and hence a centripetal force that must act on an electron directing toward the center of atom. According to classical electrodynamics, any accelerated charged particle must be a source of electromagnetic radiations, which would lead to the decrease in kinetic energy of the electron. As a consequence, an electron radius would decrease and eventually it should spiral around the nucleus at lesser and lesser distance. Ultimately, after sufficient amount of time electron will eventually fall back into the nucleus. Fortunately, to overcome this problem of electron slow fall into the nucleus, a Danish physicist, named Niels Bohr, came up with an interesting solution that led to the development of quantum mechanics.

4. THEORY OF BOHR’S MODEL OF ATOM AND ITS ALGORITHM

Bohr's first model of the atom was developed working in Manchester, England, with Ernest Rutherford, who had proposed a nuclear theory of atomic structure from his work on the scattering of alpha-particles in 1911. It was not, however, understood how electrons could continuously orbit the nucleus without radiating energy, as required by classical electrodynamics. In 1913, Bohr developed his theory of atomic structure by applying quantum theory to the observations of radiation emitted by atoms [22]. Ten years earlier to presenting of Bohr’s model of H-atom, Max Planck had proposed that radiation emitted or absorbed by a perfect black body should always be in discrete amounts or quanta of electromagnetic energy [23]. Bohr postulated that an atom may occupy only a certain number of stable states, each with a certain amount of discrete energy, in which electrons would orbit the nucleus without emitting or absorbing electromagnetic radiation. He proposed that emission or absorption of radiation occurs only if an electron undergoes a transition from one stable atomic state to another stationary state. When an atomic transition occurs, an electron jumping to a higher energy state or orbit should absorb energy in discrete amount. Similarly, an electron jumping from a higher energy state to a lower energy atomic state or orbit must emit energy in discrete amount. During such atomic transitions, an electron will emit or absorb discrete amount of energies corresponding to a particular set of quantum numbers and these quanta of electromagnetic energy are emitted or absorbed at a particular set of frequencies or wavelengths.

Assume an electron in an initial stable state with a larger energy \( E_n \) undergoes a transition to a final stationary state of a lower energy \( E_m \) then according to Einstein [24], energy of a radiated quantum or photon must be equal to the energy difference, \( \Delta E \), between the two stable states,

\[
\Delta E = E_n - E_m = h \nu ,
\]

where \( h \) is called Planck’s constant and \( \nu \) is the frequency of emitted or absorbed electromagnetic radiation. According to dual nature of light, the frequency \( \nu \) of emitted or absorbed photon is related to its wavelength, \( \lambda \), by

\[
c = \lambda \nu ,
\]

where \( c = 2.99792458 \times 10^8 \) m/s is the speed of light in vacuum or free space.

*Fig. 4: An orbiting electron around nucleus of charge \( Z \), for H-atom \( Z = 1 \).*

Let us now apply these above mentioned quantum ideas to the circular electron motion in an atomic nucleus. Assume an electron of mass \( m_e \), charge \( e \), velocity \( v_n \), orbits in a circular orbit of radius \( r_n \) around the nucleus of charge \( Z \).

Total energy of the electron \( E_n \) is sum of its kinetic energy, \( KE \) and potential energy, \( PE \):

\[
E_n = KE + PE = \frac{1}{2} m_e v_n^2 - \frac{Ze^2}{4\pi\varepsilon_0 r_n}
\]

As the electron is orbiting in a circular orbit, centripetal force \( F_p \) must be balanced by the Coulomb force, \( F_C \), between nuclear charge, Ze and electron charge, -e, i.e.

\[
F_p = F_C
\]

\[
\frac{m_e v_n^2}{r_n} = \frac{Ze^2}{4\pi\varepsilon_0 r_n^2}
\]
\[ m_e v_n^2 = \frac{Ze^2}{4\pi\varepsilon_0 r_n} \]  \hspace{1cm} (4) 

From Eq. (3) and Eq. (4), one can easily prove that

\[ E_n = \frac{1}{2} \frac{Ze^2}{4\pi\varepsilon_0 r_n^2} - \frac{Ze^2}{8\pi\varepsilon_0 r_n} = -\frac{Ze^2}{8\pi\varepsilon_0 r_n} \]  \hspace{1cm} (5) 

Thus, the total energy of the electron is negative, indicating that it should confine to a stable orbit around the nucleus through an attractive force. According to Bohr’s postulate, the magnitude of angular momentum, \( L_n \), of an electron in a stationary state should also be quantized

\[ L_n = m_e v_n r_n = \frac{nh}{2\pi} \]  \hspace{1cm} (6) 

where \( r_n \) is the radius of \( n^{th} \) orbit and the allowed values of principal quantum number are \( n = 1, 2, 3, 4, \ldots \), i.e., it can take only integral values and fractional values of \( n \) are not allowed in accordance with quantum theory. Inserting the value of \( m_e v_n \) from Eq. (6) in Eq. (4), we obtain the magnitude of Bohr’s radius for a given stationary orbit:

\[ r_n = \frac{\varepsilon_0 n^2 \hbar^2}{\pi m_e Ze^2} \]  \hspace{1cm} (7) 

This formula will be used to compute the radius of Bohr’s orbit in a given stationary state with principal quantum number \( n \). In a similar manner, Eq. (5) and Eq. (7) can be employed to determine the energy of an electron in any stationary energy state

\[ E_n = -\frac{m_e Z^2 e^4}{8\varepsilon_0^2 \hbar^2 n^2} \]  \hspace{1cm} (8) 

Assume \( n_i \) is quantum number of an electron in its initial or ground energy state and \( n_f \) is that for a higher or an excited state of an atom, we may write Eq. (8) in a more useful fashion:

\[ \Delta E = E_{n_f} - E_{n_i} = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 \hbar^2} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \]  \hspace{1cm} (9) 

Using Eq. (1), Eq. (2) and Eq. (9), we can compute the wavelength of emitted radiation, when an electron undergoes a transition from an excited state to a lower energy state

\[ \frac{1}{\lambda} = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 \hbar^2 c} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \]  \hspace{1cm} (10) 

where Rydberg’s constant for any atom of charge number \( Z \) can be written as

\[ R_E = \frac{m_e Z^2 e^4}{8\varepsilon_0^2 \hbar^2 c} \]  \hspace{1cm} (11) 

Therefore, the theoretical value of Rydberg’s constant for hydrogen atom could be obtained by substituting \( Z = 1 \) in Eq. (11),

\[ R_H = \frac{m_e e^4}{8\varepsilon_0^2 \hbar^2 c} \]  \hspace{1cm} (12) 

For heavy atoms like singly charged He and Li, one should replace the electron mass \( m_e \) with the reduced mass of the atom

\[ \mu = \text{reduced mass} = \frac{(m_e \times m_N)}{(m_e + m_N)} \]  \hspace{1cm} (13) 

where \( m_e \) is the electron mass and \( m_N \) is mass of the atomic nucleus. In scientific literature, \( k \) is also expressed as \( k = 1/4\pi\varepsilon_0 \), where \( \varepsilon_0 \) is called the permittivity of free space.

5. WHY MICROSOFT EXCEL 2007 FOR PRESENT COMPUTATIONAL WORK?

As discussed in our former publication [24], Microsoft Excel 2007 software system has a very user friendly graphical user’s interface (GUI) and can be mastered in a few hours. Another very powerful, salient feature of Excel 2007 is an availability of “Formulas” Tab, which is composed of the following five Groups: (i) “Insert Function”, (ii) “Function Library”, (iii) “Defined Names”, (iv) “Formula Auditing” and (v) “Calculation” Groups. For the present article, we are mainly interested in the first three Groups. “Insert Function” Group is used to insert a given function from “Function Library” for a particular computation or simulation work to be done. “Function Library” Group contains several tailor-made, built-in functions, which could be accessed through nine Dialog Boxes, depending upon what kind of computation is to be performed. These nine Dialog Boxes are listed below: (1) “AutoSum”, (2) “Recently Used”, (3) “Financial”, (4) “Logical”, (5) “Text”, (6) “Date & Time”, (7) “Lookup & Reference”; (8) “Math & Trig”, and (9) “More Functions” Dialog Boxes. The second Group consists of four Dialog Boxes: (1) “Name Manager”, (2) “Define Name”, (3) “Use in Formula”, and (4) “Create from Selection” Dialog Boxes. Now, we discuss the creation and usage of “Range Names”. This provision in Microsoft Excel 2007 software system is quite unique and renders it a very powerful simulation tool for an iterative computational work, which is equivalent to a For loop or Do While loop in Microsoft Visual Studio.Net and a For loop in C++ language. Although, we have performed the present computational work with Excel 2007 software system, it equally good to do the computations with software systems like Mathematica, Maple or Visual Basic Studio.Net 2008, 2010. One may use Unix and Linux based mainframes for the current computational work.
5.1 Creation and Usage of “Range Names” in Microsoft Excel 2007
Using Excel 2007 software system, it is possible to create "Range Name", which can be a single word or a string of a few or several characters that represents of a cell, range of cells or a constant value. “Range Name” for a constant value or a physical constant is just like a defined constant in computing language like Visual Basic (VB) or C++. After creation of a “Range Name” for a cell or a cell range, it can be used in Excel 2007 formulas and functions. A “Range Name” must start with an underscore or an alphabet, but not with a digit, and it can be composed of up to 255 characters. It can consist of a mixture of upper and lower case alphabets, digits, periods, and underscores, which is just like defining a variable or a constant in all other computing languages. However, “Range Name” can not have blank spaces or special characters like $, %, &., @, #, etc. In addition, “Range Name” should not look like the cell address in Excel, C22. “Range Name” can be used in any Excel 2007 formula and function in place of cell addresses or cell references. “Range Name” can also be assigned to the entire database table, when one is interested to compute the information for a subset of data from the entire database. “Range Names” must be unique within an Excel workbook. If a name is created for Sheet1, it can be used in Sheet2 of the same workbook to refer to different cells and vice versa.

5.2 Modifying and Deleting of “Range Names”
It is possible to create multiple “Range Names” in a single step in place of creating one “Range Name” for a given range of cells from the Dialog Box known as “Create from Selection”. It is possible to modify and delete a “Range Name” in case one discovers a typographic error or some mistake has been made, in which case the name is going to be incorrect. In those circumstances, it is good idea to use the “Name Manager” Dialog Box to modify or edit existing “Range Names”, delete them, and even create new “Range Names”. For the current article, we use the following “Range Names” for: electric charge \( e \); an electron volt, \( eV \); Plank’s constant, \( h \); dielectric constant, \( k \); electron mass, \( m \); the value of \( \pi \); speed of light in vacuum, \( c \); charge number \( Z \) of an atom, \( Z \) and these “Range Names” are shown in Fig. 5 through an actual screen-shot of Excel 2007 software system’s “Name Manager” Dialog Box.

6. COMPUTER SIMULATION USING EXCEL SPREADSHEET AND DISCUSSION OF RESULTS
To simulate Bohr’s radius and stationary energy levels for the hydrogen atom, we employ Microsoft Excel 2007 for the current investigation. As mentioned in our previous paper, an Excel spreadsheet is computerized equivalent of a ledger that was used in banks to maintain account information of customers, and further details about the spreadsheet features can be found in that article [25]. Each cell in spreadsheet has a unique cell reference, which is also known as the cell address. Cell reference is designated by column alphabet followed by row number to which the cell belongs. Cell reference may be absolute, relative or a combination of both (called mixed reference), depending on the kind of cell formula to be designed to perform a given simulation or type of built-in function to be used. For the present simulation, we do employ the concept of absolute and mixed cell references. Hidden behind each cell is something known as the cell formula, which can be used to do simulations in terms of some built-in functions in Excel using the Function Wizard or one may design his/her own cell formula using particular cell reference or several references along with usual common mathematical operators: exponentiation, \(^\)\( \); division, \(/\); multiplication, \(\ast\); subtraction \(-\); addition, \(+\). Eq. (7) and Eq. (8) have been used to simulate Bohr’s radius and discrete energy state values with the help of Microsoft software Excel 2007 [26]. The common convention to write a cell formula in Excel software system is to type an equals sign (=) first, and then make use of the defined “Range Names”. Thus, cell formulas corresponding to Eq. (7) and Eq. (8) for the simulation of Bohr’s radius and values of stationary states, respectively, should be typed in Excel spreadsheet as

\[ r_n = \left(\frac{\hbar^2}{4 \cdot \pi^2 \cdot k \cdot m \cdot Z \cdot e^2 \cdot n^2}\right) \]

(14)

\[ E_n = -(2 \cdot \pi^2 \cdot k^2 \cdot m \cdot Z^2 \cdot e^4) / (\hbar^2 \cdot n^2) \]

(15)

One may perceive that the running index in above Eq. (14) and Eq. (15) is the principal quantum number \( n \). These above two equations are used to simulate Bohr’s radius and stationary energy state values by varying the principal quantum number from \( n = 1 \) through \( n = 2100 \) in steps of unity for the hydrogen atom. For \( n = 1 \), one can obtain the radius of hydrogen in its ground state or the lowest energy state. From the current simulation work, the computed radius of H-atom in its ground state is: \( r_1 = 5.3 \times 10^{-11} \) m \( \approx \) \( 10^{-9} \) m, which agrees quite well with the recent determined value for the size of H-atom, indicating that the accuracy in computed value of atomic radius of H-atom is exceedingly good.

In Fig. 6, we plot a graph of electron radius \( r_n \) as a function of the principal quantum number \( n \) on a semi-log scale. For the sake of clarity, only initial 100 values of electron radius are plotted out of a total of more than 2000 simulation performed in the present investigation. Computed values of electron radius have a second degree polynomial behavior. The best-fit second degree polynomial through theoretically computed hydrogen atom radii has the following form: \( y = 5.293 \times 10^{-11}x^2 + 6.659 \times 10^{-23}x - 1.952 \times 10^{-21} \), where the slope of best-fit second degree polynomial is a direct measure of the Bohr radius, \( r_1 = 5.293 \times 10^{-11} \) m.

In Fig. 7, we plot a graph of electron energy, \( E_n \) (in units of eV) as a function of principal quantum number \( n \) for initial 100 values. One can easily perceive an existence of a huge quantum jump of energy, \( \Delta E_2 = - (3.404817 \text{ eV} - 13.619268 \text{ eV}) = 10.214451 \text{ eV} \), between ground energy state with quantum number \( n = 1 \), and the first excited state with quantum number \( n = 2 \). Energy difference between next two successive energy levels with quantum numbers \( n = 2 \) and \( n = 3 \) is \( \Delta E_3 = - (1.513252 \text{ eV} - 3.404817 \text{ eV}) = 1.891565 \text{ eV} \), which is almost five times less than that for...
first two energy states. Furthermore, energy difference between two successive energy states decreases as we approach toward very large value of principal quantum number. When principal quantum number, \( n \to \infty \), the energy difference between two successive energy states becomes almost zero, and theoretically, one approaches an upper limit known as the \textit{continuum}, where the spectral lines of H-atom should overlap. This is, once again, obvious from Fig. 7 in which for quantum number \( n > 30 \), electron energy curve as a function of \( n \) stays almost parallel to the x-axis, which further proves that splitting of energy levels is not possible for very large values of
Fig. 7: Electron energy $E_n$ as a function of principal quantum number $n$ for first 100 simulations.

Fig. 8: Computed spectral lines of H-atom for only three series, i.e., the Lyman, Balmer and Paschen are depicted. The Pfund and Humphrey series are not plotted in this figure for the sake of clarity.
principal quantum number. This is the main reason that we performed more than 2000 simulations for the present research work.

We draw an energy level diagram for the discrete energy states of H-atom in Fig. 8. For the sake of clarity, we depict only transition lines corresponding to three spectral series, namely: the Lyman [14], Balmer [15] and Paschen [16] series. Lyman series [14] lies in the UV region of the electromagnetic spectrum. However, the Paschen [16], Brackett [17], Pfund [18] and Humphrey [19] series are confined to the IR part of the electromagnetic spectrum. Only a few spectral lines of the Balmer series could be seen in the visible part of the electromagnetic spectrum, and those five computed spectral lines are shown Fig. 9 for transition between quantum states with \( n = 2 \) and \( n = 3, 4, 5, \ldots \). Wavelength of each of these lines is computed using Eq. (10) and listed in Table 1. The computed values of spectral lines agree very well with those obtained from the empirical formulas of the Lyman, Balmer, Paschen, Brackett, Pfund and Humphrey (not shown here). Wavelengths of first five spectral lines of the Balmer series are generally represented by \( \lambda_\alpha, \lambda_\beta, \lambda_\gamma, \lambda_\delta \), and \( \lambda_\epsilon \), respectively, which lie in the visible part of the electromagnetic spectrum, and the last spectral line of wavelength \( \lambda_\infty \) lies in the UV region.

Fig. 9: Actual experimentally observed five wavelengths, H-\( \alpha \) (red), H-\( \beta \) (blue-green), H-\( \gamma \) (violet), H-\( \delta \) (violet), and H-\( \epsilon \) (violet) of the Balmer series for H-atom in visible part of the electromagnetic spectrum.

Table 1: Computed values of wavelength, \( \lambda_\alpha, \lambda_\beta, \lambda_\gamma, \lambda_\delta \) and \( \lambda_\epsilon \), for the Lyman, Balmer, Paschen, Pfund and Humphrey series for H-atom.

<table>
<thead>
<tr>
<th></th>
<th>Lyman Series (nm)</th>
<th>Balmer Series (nm)</th>
<th>Paschen Series (nm)</th>
<th>Brackett Series (nm)</th>
<th>Pfund Series (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda_\alpha )</td>
<td>121.545</td>
<td>656.343</td>
<td>1875.266</td>
<td>4051.500</td>
<td>7458.444</td>
</tr>
<tr>
<td>( \lambda_\beta )</td>
<td>102.554</td>
<td>486.180</td>
<td>1281.920</td>
<td>2625.372</td>
<td>4652.895</td>
</tr>
<tr>
<td>( \lambda_\gamma )</td>
<td>97.235</td>
<td>434.089</td>
<td>1093.905</td>
<td>2165.711</td>
<td>3739.846</td>
</tr>
<tr>
<td>( \lambda_\delta )</td>
<td>94.957</td>
<td>410.214</td>
<td>1005.025</td>
<td>1944.720</td>
<td>3296.366</td>
</tr>
<tr>
<td>( \lambda_\epsilon )</td>
<td>93.763</td>
<td>397.047</td>
<td>954.681</td>
<td>1817.565</td>
<td>3038.685</td>
</tr>
<tr>
<td>( \lambda_\infty )</td>
<td>91.159</td>
<td>364.635</td>
<td>820.429</td>
<td>1458.540</td>
<td>2278.969</td>
</tr>
<tr>
<td>( n_f = 2, 3, 4, \ldots )</td>
<td>( n_i = 1 )</td>
<td>( n_f = 3, 4, 5, \ldots )</td>
<td>( n_i = 2 )</td>
<td>( n_f = 4, 5, 6, \ldots )</td>
<td>( n_i = 3 )</td>
</tr>
</tbody>
</table>

Fig. 10: Spectral lines of H-atom plotted on logarithmic scale. Wavelength of first spectral line of Lyman, Balmer, Paschen, Brackett, Pfund and Humphreys series is marked with an arrow. Color shown in this figure does not correspond to actual color of each line.
Table 2: Experimentally determined wavelength, λ, of H-α, H-β, H-γ, H-δ, H-ε spectral lines of the Balmer series of H-atom [26].

<table>
<thead>
<tr>
<th>Transition from $n_i \rightarrow n_f$</th>
<th>3 → 2</th>
<th>4 → 2</th>
<th>5 → 2</th>
<th>6 → 2</th>
<th>7 → 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name of spectral line</td>
<td>H-α,</td>
<td>H-β,</td>
<td>H-γ,</td>
<td>H-δ,</td>
<td>H-ε,</td>
</tr>
<tr>
<td>Wavelength, λ (nm)</td>
<td>656.285</td>
<td>486.133</td>
<td>434.047</td>
<td>410.174</td>
<td>397.007</td>
</tr>
<tr>
<td>Spectral line color</td>
<td>Red</td>
<td>Blue-green</td>
<td>Violet</td>
<td>Violet</td>
<td>Violet</td>
</tr>
</tbody>
</table>

![Graph](image)

$y = 1.096987 \times 10^{-7} x$

Fig. 11: A plot of $1/\lambda$ as a function of $(1/n_i^2 - 1/n_f^2)$ of the Balmer series with quantum numbers, $n_i = 2$ and $n_f = 3, 4, 5, 6 \ldots$. This graph is drawn from initial sixteen data points for the sake of clarity. The best-fit line is used to determine the slope of the graph, which is a theoretical measure of Rydberg’s constant for H-atom.

Experimentally determined wavelengths of these five spectral lines of H-atom are displayed in Table 2. In literature these lines are represented by a special notation: H-α, H-β, H-γ, H-δ, H-ε, H-ζ, H-η, and H-ξ, since these spectral lines are for the H-atom. Experimental value of each wavelength [27] given in Table 2 is very close to the computed value of corresponding wavelength, which indicates Bohr’s model works exceptionally good for explaining the experimental H-atom spectrum. To strengthen our argument, in Fig. 9, we present an actual photograph of the experimental spectrum of H-atom for the first five spectral lines in visible region of the electromagnetic spectrum. First spectral line is of red color, and consequently of longest wavelength. Fifth line is of violet color, and therefore of shortest wavelength among these five theoretically computed and experimentally observed spectral lines in the Balmer series. Last three spectral lines in Table 2 lie in the UV region and their wavelength has been determined with a special instrument called UV Spectrophotometer. To present another perspective of spectral lines, we plot them on log scale in Fig. 10.

From Eq. (10), it is also possible to determine the theoretical value of the Rydberg constant by plugging into the values of fundamental physical constants such as: electric charge, $e = 1.602 \times 10^{-19}$ C, Planck’s constant, $h = 6.626 \times 10^{-34}$ Js and speed of light in free space, $c = 2.99792458 \times 10^8$ m/s. Theoretical value of Rydberg’s constant determined in the present investigation is: $R_\infty = 1.096987 \times 10^7$ m$^{-1}$, which is very near to its corresponding experimentally observed value [26].

Another theoretical technique to determine the fundamental value of Rydberg’s constant is through a graph of $1/\lambda$ as a function of $(1/n_i^2 - 1/n_f^2)$ for any one of the theoretical computed series wavelengths among these five, namely, Lyman [14], Balmer [15], Paschen [16], Brackett [17], Pfund [18] and Humphrey [19] series (not shown here).
When one does that, each plot for a particular series of computed data points, will be a straight line whose slope is a direct measure of the theoretically computed value of Rydberg’s constant. We are planning to determine Rydberg’s constant from the Balmer series, since several spectral lines of this series lie in visible part of the electromagnetic spectrum. Therefore, it is possible that one could determine an independent, experimental value of Rydberg’s constant from the experimental line spectrum of H-atom in laboratory and could compare it with the corresponding theoretically computed value. In Fig. 11, we display a graph of $1/\lambda$ as a function of $(1/n_i^2 - 1/n_f^2)$ for the theoretically computed Balmer series from Eq. (10). One can clearly notice that the plot drawn in Fig. 11 is a straight line. In this graph, we now pass a least squared best-fit linear trend-line, whose equation is $\nu = 1.096987 \times 10^7 \, \text{Hz}$, and putting $n_i = 2$ and after going through some trivial mathematical steps, we get

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{2}{n_f^3} \right)$$

Inserting the values of $\nu$ and $r_n$ from Eq. (4) and Eq. (7), and after going through some trivial mathematical steps, we get

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{2}{n^3} \right)$$

Using $c = \nu \lambda$ and Eq. (1), we can express the frequency of radiation emitted in accordance with Bohr’s quantum model

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Let us assume $n_i = n$ and $n_f = n - m$, where $m = 1, 2, 3, 4, \ldots$ By performing these substitutions in Eq. (18), we get

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{1}{n^2} - \frac{1}{(n-m)^2} \right)$$

This equation can be written as

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{2nm - m^2}{n^2(n-m)^2} \right)$$

Assuming $n >> m$, and putting $m = 1$, we may rewrite Eq. (20) as follows:

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{2}{n^3} \right)$$

One can clearly see that both Eq. (17) and Eq. (21) have exactly the same form, which means in the limit of very large quantum numbers, predictions of quantum mechanics should match with those of the classical mechanics. This is what is known as the correspondence principle, which gave a major boost to the acceptance of Bohr’s model of H-atom among the scientists.

Now, we shall try to compute for H-atom the frequency value, $\nu$ using a very large quantum number, $n = 20,000$, $Z = 1$ and along with values of other fundamental physical constants such as electron mass, $m_e$, electron charge, $e$, permittivity of free space, $\varepsilon_0$ and Planck’s constant, $h$:

$$\nu = \frac{m_e Z^2 \varepsilon^4}{8 \varepsilon_0^2 h^3} \left( \frac{2}{n^3} \right) = 822 \, \text{Hz}$$

This frequency, $\nu = 822$ Hz corresponds to a wavelength of $\lambda = 364635 \, \text{nm} = 0.36 \, \text{nm}$, which can be easily computed and measured in a laboratory.

8. CONCLUSIONS AND IMPLICATIONS OF PRESENT WORK
We may conclude this article with the following noteworthy remarks: We presented a brief historical background of Bohr’s theory of H-atom and its necessary mathematical formulism and algorithm for the college and university students and instructors. We believe that this article would be very beneficial for physics, chemistry education, and computational physics and chemistry and computer science college and university majors. This would also present them with interesting aspects and outcomes of Bohr’s theory in a virtual lab. We employed Microsoft Excel 2007 software system to perform the simulations of Bohr’s theory of an atom. “Range Names” and “Name Manager” Dialog Boxes of Microsoft Excel 2007 were effectively used to perform more than 2000 simulations for the computation of nuclear radius and its corresponding stationary energy value. Two basic assumptions of quantum mechanics have been implemented in the model: (i) In an electronic transition between stationary states, energy of an emitted or absorbed light quantum or photon is quantized and (ii) the angular momentum of an electron in a stationary orbit takes only discrete values. The former assumption was as proposed by Albert Einstein to explain the photoelectric effect [24], whereas the latter one was advocated by Neil Bohr [22]. Bohr's model of the atom successfully described the electron motion in discrete, precisely defined circular orbits around the nucleus. Electrons could only occupy certain allowed energy states called stationary states or orbits. For an electron to occupy an allowed energy state, a certain discrete amount of energy must be imparted to an atom from an external source. Each stationary orbit is assigned a unique quantum number called the principal quantum number, which could take only integral values; the lowest quantum numbers being assigned to those orbits nearest to the nucleus. Only a specified maximum number of electrons can occupy an energy state or an orbital. Under normal circumstances, electrons occupy the lowest energy state or ground state nearest to the nucleus. By absorbing additional amount of energy from an external source, electrons could jump to higher energy states, and release the absorbed energy when they make transitions back to lower energy levels. The Bohr's model of the atom helped to offer one possible explanation for the emission spectrum observed from hydrogen and other atomic gases.

With the help of Bohr’s model, we could predict and compute for the H-atom, wavelengths of many spectral lines such as the Lyman, Balmer, Paschen, Brackett, Pfund, Humphreys series. Since Lyman series lies in the UV region, and whereas Paschen, Pfund and Humphreys series are confined in the IR part of the electromagnetic spectrum, and therefore in laboratory, it will not be feasible to observe the above mentioned line spectra. However, physics and chemistry students and including their instructors would definitely be able to measure experimentally the spectral lines of Balmer series in the visible part of the electromagnetic spectrum for H-atom and several other singly charged ions such as deuteron, helium, Lithium etc., and thus could verify the predictions of Bohr’ model. We compared experimentally determined [27] and theoretically computed values of the wavelengths of five lines of the Balmer series and found an excellent agreement between Bohr’s theory and experimental line spectrum of H-atom, e.g., see Tables 1 and 2 in Section 6.

Using Bohr’s model, it is possible to predict the value of Rydberg’s constant for H-atom, which we did in Section 2 theoretically. We computed its value on the basis of theory in several ways and compared it with the experimentally determined value in Section 6. Once again, an excellent agreement between the computed and experiment value of Rydberg’s constant was found [28]. Therefore, another important outcome of Bohr’s model is to figure out the theoretical value of Rydberg’s constant.

Another major advantage of Bohr’s model of an atom is to predict theoretically the ionization energy or potential of H-atom and its computed value is 13.6 eV, which is very close to its experimentally determined value [27, 28].

Finally, we believe that this current interesting and fascinating article would be appreciated by both university, college instructors as well by graduate and undergraduate students because of the concept of using a widely available software system like Microsoft Excel 2007, which most users these days have installed on their Windows, Mac computers and laptops for scientific and engineering computations. Consequently, we hope this will help make science more accessible to a wider range of college and university students, instructors and members of the general audience. Our user friendly explanations of how to use various built-in Microsoft Excel 2007 functions to carry out numerical calculations that are ordinarily done using computing languages such as Visual Basic (VB), Fortran-2003, C, C++ or Java, will be very helpful to students and instructors alike. The hydrogen spectrum and the Bohr model which explains it with wonderful precision are excellent choices for introducing non-physicists to the basic ideas and methods of quantum physics, and the interplay between experiment, theory, and computation. It is worthwhile to mention here that it is also possible to perform Bohr’s model simulations for H-atom with an exactly same accuracy and precision with a lower of version of Microsoft Excel 2003 software system.

Due to his discovery of the structure of H-atom and the electromagnetic radiation emitted from it, Neils Bohr a Danish physicists was awarded the Nobel Prize for Physics in 1922. He is given credit of pioneering quantum theory, which proved that the nucleus of an atom is surrounded by shells of electrons, each assigned particular sets of quantum numbers according to its orbit. He explained the structure and behavior of the nucleus, as well as the process of nuclear fission, which is widely employed now-a-days for the production of electricity in atomic reactors throughout the entire world. Bohr also put forward an important doctrine of complementarity [29], i.e., a fundamental particle like an electron or a proton is neither a wave nor a particle, because these are complementary modes of particle’s description, which led to the invention of wave mechanics: one of the quantum mechanical formalisms independently developed by Erwin Schrödinger [2]. In wave mechanics, the state of a system is described by a wave function, which is the solution of famous Schrödinger's wave equation in quantum mechanics. On the
other hand, Werner Heisenberg, Max Born and Pascual Jordan [4] independently discovered another version of quantum mechanics, which is known as the matrix mechanics. Both formalisms of quantum mechanics, the matrix mechanics and wave mechanics, apparently incompatible, were proven to be equivalent and correct in explaining several experimental observations and phenomena.

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* Figures marked with an asterisk in the manuscript are taken from http://www.wikipedia.com