

Modeling Bohr's Theory of Hydrogen Atom for Physics and Chemistry Education, and Computer Science Graduates

Gurmukh Singh

Department of Computer and Information Sciences
State University of New York at Fredonia
Fredonia, NY 14063 USA
singh@cs.fredonia.edu

Amitabha Mukhopadhyay

Department of Physics
North Bengal University
Siliguri, West Bengal, India
amitabha82@hotmail.com

ABSTRACT

This article is basically targeted for the advanced university and college undergraduate and graduate students of physics and chemistry education, computational physics and chemistry, and computer science. Here, we employed Microsoft Excel software system to perform computer simulations for modeling Bohr's theory of hydrogen atom in college and university classroom setting. We developed necessary computer algorithm to compute discrete values of orbit radius, energy levels and ionization potential of Bohr's hydrogen atom.

Categories and Subject Descriptors

J.2. [Computer Applications]: Physical Sciences and Engineering – *Physics & Chemistry*.

General Terms and Keywords

Experimental Measurements, Theory, Algorithm, H-atom, Bohr, Thomson and Rutherford Atom, Quantum Mechanics, Monte Carlo Simulations

1. QUANTUM MECHANICS IN THE MICROSCOPIC REALM

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) evolutionary biology [8], and (vi) may be a few other topics depending on reader's 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. 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 provided us. Without quantum mechanics it is impossible to talk about global economy, since the electronics revolution that brought medicine, and in essentially every other scientific field, could not have taken place without the tools that quantum mechanics has 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

Unlike the development of general theory of relativity of Albert Einstein [1], which grew out of a brilliant insight into the connection between gravity and geometry, 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 their introduction, quantum ideas were so confusing 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 physicists who did major development of quantum mechanics in just three years [2-5]. 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 a century after the birth of quantum theory, 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. To get an understanding on the successes of quantum mechanics by an educated layman, a

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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].

Manuscript is arranged as follows: We begin, in Section 2, with an introduction to the two atomic models [11, 12]. Section 3 discusses basic limitations of Rutherford's model. Section 4 presents Bohr's theory of an atom, and develops its pertinent algorithm. Section 5 describes why we use Excel software system for the present work. Section 6 deals with actual computer simulations of the hydrogen atom problem and the predictions of Bohr's model. Finally, conclusions and implications of the current investigation will be presented in Section 7 in light of its usefulness for natural science education students and instructors.

2. THE THOMSON AND RUTHERFORD MODELS

In 1902, J. J. Thomson did rigorous mathematical refinement to the atomic model advocated by Lord Kelvin. The atomic model proposed by Thomson was popularly known as the "plum pudding" model [11] in which electrons and protons are assumed to be uniformly distributed throughout the atomic volume just like plums sitting in a pudding. Rutherford's thin gold-foil experiment, performed by his graduate students, Geiger and Marsden [9], provided a concrete evidence for the existence of a minute, positively charged atomic nucleus, from which alpha particles could scatter in any direction. These observations were not consistent with the predictions of Thomson's model [11]. Thus, naturally Rutherford discarded the plum pudding model and argued that the only way the alpha particles could be deflected in backward direction was if most of the mass in an atom were concentrated at the center called the nucleus.

3. LIMITATIONS OF RUTHERFORD'S MODEL

Although the planetary model of 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. In the planetary model of atom, electrons must orbit around the nucleus in circular paths. This circular electron motion should automatically create centripetal force that must act toward the center of an atom. According to classical electrodynamics, any accelerated charged particle must be a source of electromagnetic radiations, which would lead to the decrease in its kinetic energy. Consequently, electron should spiral around the nucleus at lesser and lesser distance and eventually plunge into the nucleus.

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

Bohr developed his atomic model in 1911 while working in Manchester, UK with Rutherford, who proposed nuclear theory of atomic structure from his work on scattering of alpha particles. In 1913, Bohr refined his atomic theory by applying quantum mechanics to explain the line spectrum of emitted radiations by atoms [14]. Max Planck proposed that radiation emitted or absorbed by a perfect black body should always be in discrete

amounts or quanta. Bohr postulated that an atom may occupy only a certain number of stable states, each one associated with a certain amount of discrete energy, in which electrons would orbit the nucleus without emitting or absorbing electromagnetic radiation. Assume an electron in an initial stable state with a larger energy, E_{n_f} undergoes a transition to a final stationary state of a lower energy, E_{n_i} then according to Einstein [15], energy of a radiated quantum or photon must be equal to the energy difference, ΔE , between the two stable states, $\Delta E = E_{n_f} - E_{n_i} = h\nu$, where h is called Planck's constant and ν is the frequency of emitted or absorbed electromagnetic radiation. According to dual nature of light, the frequency ν of emitted or absorbed photon is related to its wavelength, $\lambda = \nu/c$, where $c = 2.99792458 \times 10^8$ m/s is the speed of light in free space. Let us now apply these quantum ideas to the circular electron motion. 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 Ze . Total energy of the electron E_n is sum of its kinetic energy, KE and potential energy, PE :

$$E_n = \frac{1}{2} \frac{kZe^2}{r_n} - \frac{kZe^2}{r_n} = -\frac{kZe^2}{2r_n} \quad (1)$$

where k is known as the dielectric constant of free space. Eq. (1) shows that total energy of the electron is negative, indicating that it should confine to a stable orbit of the nucleus. According to Bohr's postulate, the magnitude of quantized angular momentum, L_n , of an electron in a stationary state is

$$L_n = m_e v_n r_n = \frac{nh}{2\pi} \quad (2)$$

where r_n is the radius of n th orbit and an allowed value of principal quantum number is $n = 1, 2, 3, 4, \dots$, i.e., it can take only integral values in accordance with quantum theory. Inserting the value of $m_e v_n$ in Eq. (2), we could obtain the magnitude of Bohr's radius for a given stationary orbit:

$$r_n = \frac{n^2 h^2}{4\pi^2 k m_e Z e^2} \quad (3)$$

One may insert r_n from Eq. (3) in Eq. (1) to determine the energy of an electron in any stationary energy state

$$E_n = -\frac{2\pi^2 k^2 m_e Z^2 e^4}{h^2 n^2}. \quad (4)$$

Assume m_i is quantum number of an electron in its initial or ground state and m_f is that for a higher or an excited state of an atom, we may write Eq. (4) in a more useful fashion

$$\Delta E = E_{n_f} - E_{n_i}$$

$$= \frac{2\pi^2 k^2 m_e Z^2 e^4}{h^2} \left(\frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \quad (5)$$

This relationship can be used to compute the transition energy when an electron jumps from one state to another depending on their initial and final quantum numbers, n_i and n_f .

5. WHY EXCEL 2007 FOR PRESENT COMPUTATIONAL WORK?

As discussed in our former publication [18], 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... Next* 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 is equally good to do the computations with software systems like *Mathematica*, *Maple* or *Visual Basic Studio .Net* 2008. One may use Unix and Lynix 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.

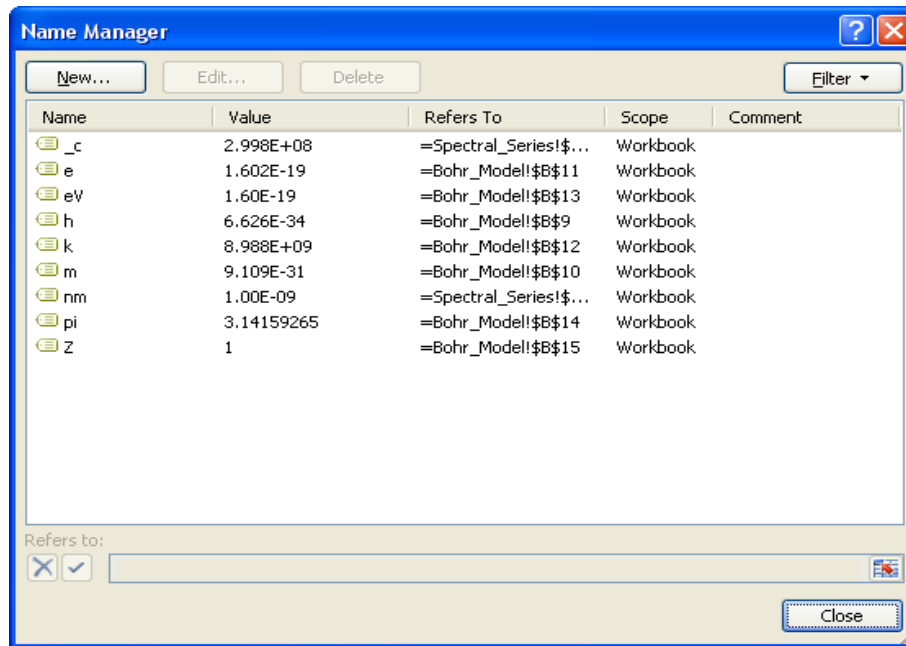


Figure 1: A screen-shot of Microsoft Excel 2007 software system's "Name Manager" Group used to create several named constants whose scope is in the entire workbook.

“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 Name”. 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, π ; speed of light in vacuum, c ; charge number Z of an atom, Z and these “Range Names” are shown in Figure 2 through an actual screen-shot of Excel 2007 software system’s “Name Manager” Dialog Box.

6. COMPUTER SIMULATION WITH EXCEL 2007 SPREADSHEET AND DISCUSSION OF RESULTS

To simulate Bohr’s radius and stationary energy levels for the hydrogen atom, we employ Microsoft Excel 2007 spreadsheet for the current investigation. 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 employed the concept of absolute and mixed cell references [16]. For this article we made use of the defined “Range Names” provision existing in Excel. Thus, cell formulas corresponding to Eq. (3) and Eq. (4) for the simulation of Bohr’s radius and values of stationary states, respectively, should be typed in Excel spreadsheet as

$$r_n = (h^2) / (4 * \pi^2 * k * m * Z * e^2 * n^2) \quad (8)$$

$$E_n = -(2 * \pi^2 * k^2 * m * Z^2 * e^4) / (h^2 * n^2) \quad (9)$$

We performed more than 1500 simulations in the present work to compute r_n and E_n . Now, we draw an energy level diagram for the discrete energy states with quantum number $n = 1, 2, 3, 4 \dots$ etc. of H-atom in Figure 2. For the sake of clarity, we depict only transition lines corresponding to three spectral series, namely: the Lyman ($n_i = 1$ and $n_f = 2, 3, 4, \dots$), Balmer ($n_i = 2$ and $n_f = 3, 4, 5, \dots$) and Paschen series ($n_i = 3$ and $n_f = 4, 5, 6, \dots$). Lyman series lies in the UV region of the electromagnetic spectrum. However, the Paschen, Pfund and Humphrey 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 computed wavelengths of Balmer’s series can be compared with their corresponding experimental values determined in laboratory. Wavelength of each of spectral line could be computed using Eq. (5) and their details will be discussed in a future publication [17].

Ionization energy or potential of an atom is defined as the amount of energy required to dislodge an electron from the outer most orbit of an atom, which can be computed theoretically from Eq. (5) for H-atom by inserting $n_i = 1, n_f = \infty$ and other pertinent physical parameters of H-atom, along with some fundamental physical constants. Once those parameters are plugged in Eq. (5), magnitude of ionization energy or ionization potential for H-atom is computed to be 13.6193 eV, which agrees precisely with that of its corresponding experimental value [18, 19].

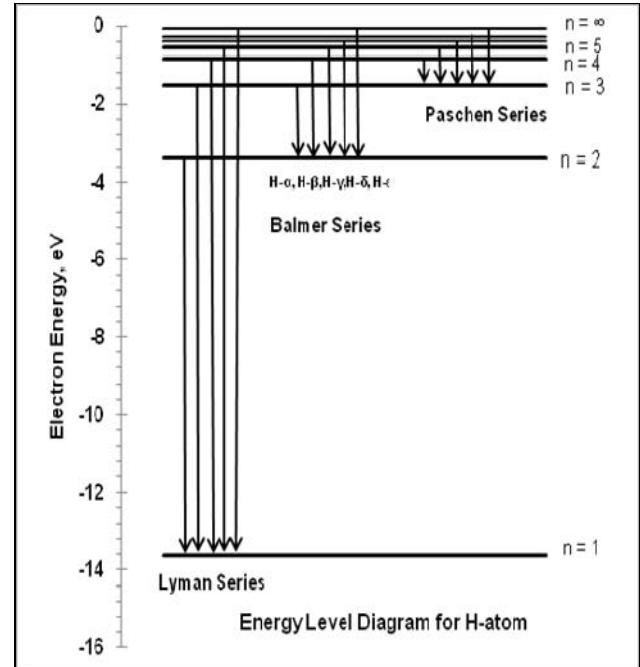


Figure 2: Energy level diagram of H-atom for only the Lyman, Balmer and Paschen series. The Pfund and Humphrey series are not shown for the sake of clarity. are not shown for the sake of clarity.

7. CONCLUSIONS AND IMPLICATIONS OF PRESENT WORK

We may conclude this article with the following noteworthy remarks: 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 to perform more than 2000 simulations for the computation of nuclear radius and it

corresponding stationary energy value. 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.

Finally, we believe that this current interesting and fascinating article would be appreciated by both university, college

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