Research Article

BOHR'S CORRESPONDENCE PRINCIPLE REVISITED USING MS-EXCEL SPREADSHEET SIMULATION

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ABSTRACT

Teaching of quantum physics is a challenging job. However due to the developments in the pedagogical tools, now it has become more effective and learner centric. In this paper, a heuristic approach using MS-Excel spreadsheet software is presented to teach the merger of quantum and classical physics at large energies or quantum numbers. The article illustrates the Bohr's Correspondence principle using H-atom and particle in a box. The energy level spacing is used to demonstrate the quantum and classical behavior of the system. Such a model could be more appropriate for the students of introductory quantum physics.

INTRODUCTION

The teaching of physics becomes a challenge on certain occasions when the teacher thinks of putting the matter across the minds of first level physics learners. This happens so frequently in teaching of "Introductory Quantum Physics" or anything related to it. As all we know that in quantum physics everything is quantized i.e. discrete and there is no space for continuum except near classical limits. That is where historical "Correspondence Principle" comes into scene. Generally, In modern physics literature the Correspondence principle is often defined as the requirement for the quantum theory to go over to the classical theories in the limit of large quantum numbers, or in other words as $h \to 0$, where h is Planck's constant. The correspondence principle establishes the link between classical and quantum physics. The simple statement that quantum mechanics reduces to classical mechanics in the limit where the principal quantum number n approaches infinity, is found in many undergraduate physics text books. Although the statement looks comfortable for reading but it finds the learners in back foot as per conceptual understanding is concerned.

At the time when new theories are developed in physics, it is mandatory in principle that a new theory or model should describe phenomena unexplained by the old one. The new theory must also be consistent with earlier one in the appropriate limit [1]. For example, the limiting case of relativistic mechanics is Newtotnian mechanics.

The Newtonian mechanics can be recovered from relativistic mechanics in the domain of low velocities compared with the speed of light in the vacuum. Since its formulation, quantum mechanics has established itself as the most successful physical theory for the description of sub-atomic systems, such as atoms and elementary particles. Unlike special and general relativity, relations between classical and quantum mechanics are more subtle, given that the conceptual framework of these theories are fundamentally different. While in classical mechanics it is possible to know the exact position and momentum of a particle at any given time, quantum mechanics only specifies the probability of finding a particle at a certain position [2].

The first indication of a mathematical procedure to obtain the classical limit of quantum mechanics can be traced back to Max Planck [3]. He postulated that classical results can be recovered from quantum ones when Planck's constant is taken to zero. Planck originally formulated this limit to show that his energy density for black body radiation approaches the classical Rayleigh Jeans energy density when $h \sim 0$. A different approach is due to Niels Bohr [4]. He postulated that the classical behavior of periodic quantum systems can be determined when the principal quantum number is large. Bohr enunciated it in this way because in his model of the hydrogen atom the transition frequency between two neighboring energy levels tends to the classical orbital frequency of the electron when $n \gg 1$, where n is principal quantum number.

We know that Niels Bohr was a well known physicist. He was born and died in Copenhagen. He is best known as one of the founders of quantum theory and for his work on the structure of atoms, which earned him the Nobel Prize in Physics in

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1922. In the context of his correspondence principle, there are three primary candidate-definitions in the literature. First, there is the *frequency interpretation*, according to which the correspondence principle is a statistical asymptotic agreement between one component in the Fourier decomposition of the classical frequency and the quantum frequency in the limit of large quantum numbers. Second, there is the *intensity interpretation* according to which it is a statistical agreement in the limit of large quantum numbers between the quantum intensity, understood in terms of the probability of a quantum transition, and the classical intensity, understood as the square of the amplitude of one component of the classical motion. Finally, there is the *selection rule interpretation*, according to which the correspondence principle is the statement that each allowed quantum transition between stationary states corresponds to one harmonic component of the classical motion. All these metaphors of Correspondence principle find higher difficulty level among undergraduate physics students. So in this article, energy level spacing is considered to enunciate Correspondence principle.

To illustrate the Correspondence principle, simulation pedagogical tool is employed. The simulation component is achieved through MS-Excel software. Simulation generally refers to mimicing the behaviour of a real world system using computer program. The computer program can be coded in any language such as Fortran, C, C++ and Java. But the versatility offered by MS-Excel spreadsheet is manifold and this spreadsheet software is easily available at economical price. So I restrict myself to spreadsheet simulation of Correspondence principle. In this article, a heuristic tool is presented in a simplified format such that introductory physics learners could understand the transition of certain results obtained in quantum physics to classical physics in the range of large quantum number. To demonstrate the correspondence principle, H-atom and particle in a box are considered [5-7].

Bohr's Model of Atom

Niels Henrik David Bohr's greatest contribution to modern physics was the atomic model. He proposed his atomic model in 1913. He modified the problems and limitations associated with Rutherford's atomic model. In 1913, Bohr refined his atomic theory by incorporating non-classical features such as discrete energy for bound electrons and quantization of their angular momenta. Max Planck proposed that radiation emitted or absorbed by a perfect black body should always be in discrete amounts or quanta. Similarly, Bohr postulated the concept of stationary orbits. According to this assumption an atom will occupy only a fixed number of stable states, each one associated with a certain amount of discrete energy. The orbiting electrons would move in circular paths around the nucleus without emitting or absorbing electromagnetic radiation. Assume an electron in an initial stable state with a larger energy, E_i undergoes a transition to a final stationary state of a lower energy, E_f then according to Einstein, energy of a radiated quantum or photon must be equal to the energy difference, ΔE, between the two stable states, $\Delta E = E_i - E_f = $ hν where h is called Plank's constant and ν is the frequency of emitted electromagnetic radiation. 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:

$$E_n = \frac{1}{2} k \frac{Ze^2}{r_n} - \frac{kZe^2}{r_n}$$
$$\Rightarrow E_n = -\frac{kZe^2}{2r_n} \tag{1}$$

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:

$$L_n = m_e v_n r_n = \frac{nh}{2\pi} \tag{2}$$

where r_n is the radius of nth orbit and an allowed value of principal quantum number is $n = 1, 2, 3, 4, ...$, i.e., it can take only integral values in accordance with quantum theory. The electron is held in a circular orbit by electrostatic attraction. That means centripetal force is equal to the Coulomb force:

$$\frac{m_e v_n^2}{r_n} = \frac{kZe^2}{r_n^2}$$

The above expression will give velocity of orbiting electron as mentioned below:

$$v_n = \sqrt{\frac{kZe^2}{m_e r_n}} \tag{3}$$

Inserting the value of v_n in Eq. (2), we could obtain the magnitude of Bohr's radius for a given stationary orbit:

$$r_n = \frac{n^2 h^2}{4\pi^2 k m_e Z e^2} \tag{4}$$

One may insert r_n from Eq. (4) in Eq. (1) to determine the energy of an electron in any stationary energy state as given below:

$$E_n = -\frac{2\pi^2 k^2 m_e Z^2 e^4}{n^2 h^2} \tag{5}$$

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_1 and n_2.

$$\Delta E = E_{n_2} - E_{n_1} = \frac{2\pi^2 k^2 m_e Z^2 e^4}{h^2} \left\{ \frac{1}{n_1^2} - \frac{1}{n_2^2} \right\} \tag{6}$$

MS-Excel Spreadsheet Organization

To simulate Bohr's Correspondence principle for the hydrogen atom, I made use of most powerful spreadsheet software MS-Excel [8]. MS-Excel is endowed with graphical user interface (GUI) and it has rich library of built in functions. At the same time, it is easier to learn the calculations in Excel and plotting feature make it indispensable learning and pedagogical tool. In general, MS-Excel spreadsheet is collection of cells. 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 used to perform a given simulation or type of built-in function employed. For the present simulation, I employed the concept of relative references and ranges. Thus, cell formulas corresponding to Eq. (6) for the simulation of Bohr's

Correspondence principle is typed in Excel spreadsheet in the cell G8 as:

=(2*pi^2*k^2*me*Z^2*e^4)/h^2 *(1/E8^2-1/F8^2)

The above formula is copied to all the cells from G9 to G8. The constants used in calculations are defined through range names as shown in Figure 2.
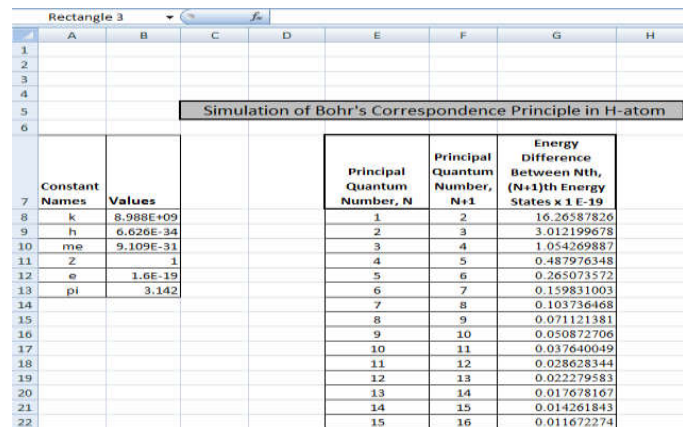

Figure 1 Screenshot of Organization of Spreadsheet.

Using MS-Excel spreadsheet, it is possible to create "Range Name", which can be a single word or a string of a few or several characters that represents a cell, range of cells, a constant value or a formula. By using names, you can make your formulas much easier to understand and maintain. All names have a scope, either to a specific worksheet or to the entire workbook. "Range Name" for a constant value or a physical constant is just like a defined constant in computing language like C or C++. After creation of a "Range Name" for a cell or a cell range, it can be used in Excel 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" [8] can not have blank spaces or special characters like $, %, &, #, @, * etc. "Range Name" can be used in any Excel formula and function in place of cell addresses or cell references in the workbook.
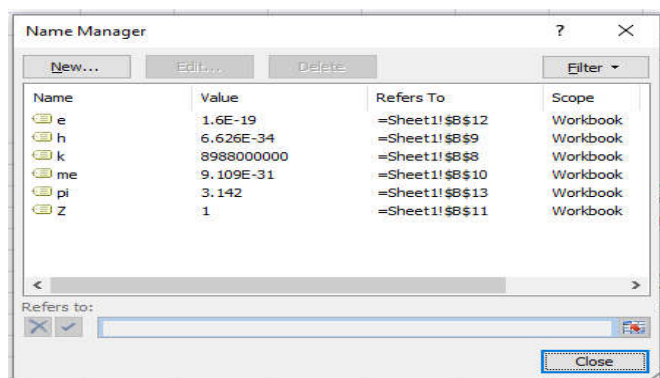

Figure 2 A screen-shot of Microsoft Excel software's "Name Manager

Similarly, we can construct spreadsheet for particle in a box. The concise description of particle in a box is given in the next section.

Particle in a Box

To understand the Quantum Physics, the problem of particle confined to an infinite potential well offers an excellent example. In this case the particle of mass $'m'$ is confined to a box($0 < x < a$). The potential energy, $V(x)$ is assumed to be zero, inside the well and infinite elsewhere. An example of a particle confined to such a potential energy is a bead on a string of length $'a'$. The bead can move freely along the string distance between 0 and 'a', but cannot leave the string.

This particle is described by Schrödinger's Equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

For a free particle, V=0

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \tag{7}$$

The total energy of the particle is purely kinetic and is given as:

$$E = \frac{mv^2}{2} \tag{8}$$

The above expression for energy can be written as:

$\frac{2mE}{\hbar^2} = k^2$, where k $(= \frac{2\pi}{\lambda})$ is wave number.

Solving Eq. (7), we shall obtain $ka = n\pi$ relation from application of boundary conditions, where $n = 1,2,3,4,\ldots\ldots\ldots$ and is called principal quantum number.

Hence the energy of a particle in a box in n^{th} state is:

$$E_n = \frac{n^2\pi^2}{a^2}\frac{\hbar^2}{2m} = \frac{n^2}{a^2}\frac{h^2}{8m} \tag{9}$$

The above expression shows that the energy of the particle is quantized. The energy emitted or absorbed between any two consecutive states can be written as;

$$\Delta E = E_{n+1} - E_n = \frac{h^2}{8ma^2}[(n+1)^2 - n^2] \tag{10}$$

Now fractional change in the energy is computed:

$$\frac{\Delta E}{E_n} = \frac{2n+1}{n^2} \tag{11}$$

DISCUSSION AND RESULTS

Energy difference between consecutive states in H-atom is plotted as a function of principle quantum number n. The plot is shown in Figure 3. It is found that for smaller quantum numbers, the energy states in H-atom are separated considerably thereby exhibiting discreet or quantum nature. As the quantum number increases, the splitting between the energy states decreases almost exponentially and it approaches zero for large quantum numbers, thus resulting in the continuum of energy states. Such a behavior of the H-atom demonstrates the Bohr's Correspondence principle.
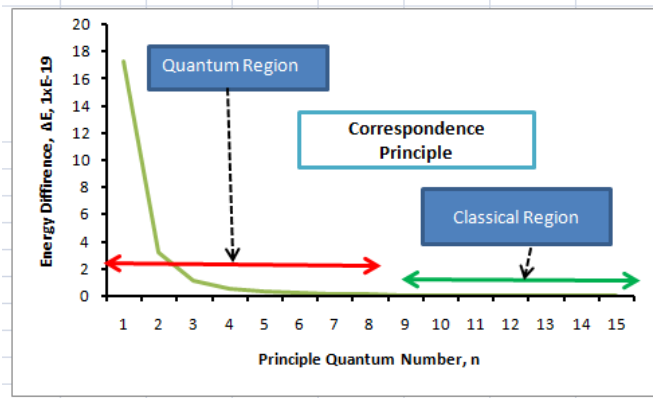
Figure 3 Illustration of Bohr's Correspondence principle in H-atom.

In the case of particle in a box, expression given by Equation (10), $\Delta E = E_{n+1} - E_n = \frac{h^2}{8ma^2}[(n+1)^2 - n^2]$, indicates the spacing between adjacent energy states increases with n. This dependence does predict that the energy spectrum would not become continuous at large quantum numbers – the condition required for quantum mechanical system to approach classical behavior at large energies. However, there is another way of looking at spacing between the energy states i.e. fractional change $(\frac{\Delta E}{E_n} = \frac{2n+1}{n^2})$. A plot is drawn between $\frac{\Delta E}{E_n}$ and principle quantum number n as shown in Figure 4. The plot shows that as $n \to \infty$, the fractional change approaches zero. This is an indication of continuous energy spectrum hence the classical behavior of the quantum mechanical system at large quantum numbers.
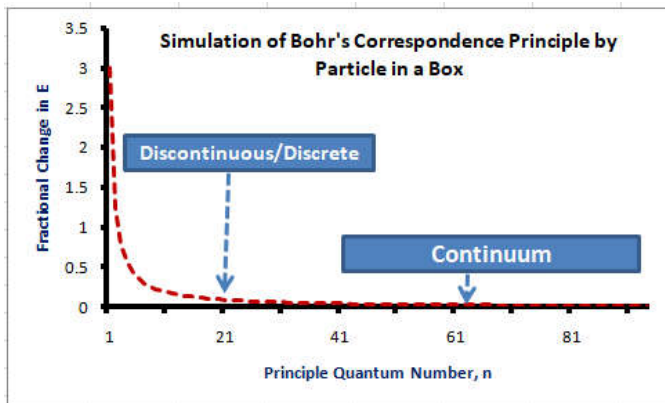

Figure 4 Fractional change as a function of principle quantum number n.

From plots shown in Figures 3 and 4, it is indicative that quantum behavior is prominent feature at small quantum numbers. The energy level spacing is large and it decreases fast in this range. With the increase in quantum number, the level spacing begins to disappear thus resulting in the continuum of the energy. This shows that at large quantum numbers, classical behavior is dominant.

CONCLUSIONS

The teaching of science subjects could be made more effective and result yielding with the judicious use of simulation techniques. The use of MS-Excel spreadsheet software at an early stage of physics education may be productive in enhancing the interest of students to take physics as career. This may horn the programming and computational skills of the students. The inclusion of spreadsheets at introductory level in the physics curriculum is advisable. The simplified picture of Bohr's Correspondence principle may assist the learners to make use of it in other quantum mechanical systems.

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