



Calculation of the Radius for Any Atom Based on the Planck Constant-free Equation, Mathematical Complexity, and Atomism

Ikechukwu Iloh Udema ^{a#*}

^a *Department of Chemistry and Biochemistry, Research Division, Ude International Concepts Ltd. (RC: 862217), B. B. Agbor, Delta State, Nigeria.*

Author's contribution

The sole author designed, analyzed, interpreted and prepared the manuscript.

Article Information

DOI: 10.9734/AJARR/2022/v16i12458

Open Peer Review History:

This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: <https://www.sdiarticle5.com/review-history/94937>

Original Research Article

Received: 17/10/2022

Accepted: 23/12/2022

Published: 27/12/2022

ABSTRACT

Concern has been expressed against the new theories, Heisenberg uncertainty principle (HUP) and Schrödinger wave/quantum mechanics (SE) that are purported to have replaced Bohr's theory and equation. The research was undertaken with the following objectives: 1) to review concerns about atomism; 2) appraise the issues of mathematical complexities in HUP and SE; 3) review criticism against SE and HUP; 4) most importantly derive a Planck constant invariant equation for the calculation of any atomic radii; and 5) re-calculate the radii of selected elements chosen for their biological importance. The theoretical research with calculations, showed that the opposing theories are criticised because, they are obsessed with mathematical complexities with ambiguities without common ground that should usher alternative solution to the problem of the size of atom and thus, they cannot be considered as a valid description of reality. Bohr's equation and variants of it and the Planck constant invariant equation (Eq. (15)) derived in this research are regarded as

ORCID: <https://doi.org/0000-0001-5662-4232>;

*Corresponding author: Email: udema_ikechukwu99@yahoo.com;

deterministic in nature and were capable of reproducing Bohr's radii for any atom; the radii were also capable of reproducing the average ionisation energies of hydrogen and oxygen atoms, chosen for illustration only, when substituted into derived preliminary equation (Eq. (10)).

Keywords: Atomism; Bohr's radii of any element; criticism of Heisenberg and Schrödinger mathematical complexities; deterministic Planck constant free equation; ionisation energy.

1. INTRODUCTION

There is a need to make it abundantly clear unlike almost every other article in the literature, that in this section, every presentation is intended to be comprehensible to all at any level of educational achievement, both formal and informal. Thus, since this research is not intended for those in the field at higher level alone, this section addresses the question of indivisibility of the smallest particle state, even though what may be the smallest cannot for now be strictly defined. A well-known 20th century scientist, Dalton has considered the smallest particle of matter as being the atom including its indivisibility. This is similar to a 21st century observation to the effect that electrons are indivisible at 90 GeV (Laboratoire d'économie de la production et de l'intégration internationale (LEPII)) [1]. Of course this is about electron not the atom, though the issue of indivisibility is pertinent. The atom, hydrogen in particular, and the fundamental particle, the electron, are extremely important biologically and physically. Scholars at the highest level objecting to this position may have to resign; recent challenge to the existence of man was fatally challenged by COVID-19 because the "respiratory chain" where mitochondria are indispensable, was extremely compromised. The hydrogen ion carriers, FADH, NADH, the electron-carriers, the cytochromes and associated enzymes, oxidases and reductases, ensure the generation of molecular energy adenosine triphosphate, ATP, with concomitant release of water vapour. Before this, molecular CO₂ is released. In plants CO₂ is consumed while molecular oxygen is released.

Bohr's model and by extension the associated equation for the determination of the orbital radius of revolving electron had always met criticism; for this reason Heisenberg uncertainty principle (HUP) and Schrödinger wave probability equation (SE) evolved as replacement for Bohr's equation, that was seen to be unable to address multi-electron atoms; but with respect to multi-electron atoms, derived alternative equations [2] whose results that are strictly a function of the ionisation energy, upon evaluation has made

such concerns of no consequence. In this research the concern is to be made of no consequence again by the calculation of the Bohr's radii of any atoms on the basis of Planck constant-free equation to be derived with issue of atomism and concern for mathematical complexities at the background. The HUP and SE models have also met even the harshest informed criticisms as a result of what they stand for and as a result of their misuse [3]. Thus, reaching out to all academic levels, undergraduates, graduates, etc, as a matter of general interest, the objectives of this research are: 1) to carry out an overview of concerns about atomism; 2) to carry out an overview of the issues of mathematical complexities in short theses pertinent to HUP and SE; 3) to carry out an overview of criticism against SE and HUP; 4) most importantly to derive yet again a generalisable Planck constant free alternative equation and 5) re-calculate illustratively the radii of the following atoms: oxygen, hydrogen, carbon, nitrogen, phosphorus, iron, calcium, magnesium, manganese, potassium, sodium, chlorine, fluorine, cobalt, molybdenum, zinc, iodine, and sulphur all being the most abundant elements in the biosphere.

1.1 Atomism

This section begins with issues regarding interest in the smallest possible material existence, abiotic or biotic; the question may be why? The answer shall be self-evidence as time goes own. The concern for the smallest possible existence, biotic or abiotic, has been known to man; the notable example is the mustard seed referred to by head of the Christendom, Jesus Christ, even if it is not necessarily the smallest seed on earth, as to imply that science is actually based on four senses, viz.: sight, smell, touch (irritability), and hearing; even a naïve religious leader cannot stand against this view. Still, the atom could not have been the smallest particle despite the view of Dalton. In line with this view is: According to Mills [3] the Copenhagen interpretation of quantum mechanics is: "it asserts that what we observe is all we can know; any speculation about what an electron, photon, atom, or other

atomic-sized entity really is or what it is doing when we are not looking is just that—speculation. The postulate of quantum measurement asserts that the process of measuring an observable forces it into a state of reality. In other words, reality is irrelevant until a measurement is made". "To see is to believe!" Further to this is: "Quantum mechanical theory is not derived from first principles and relies on faith in the infallibility of the Schrödinger equation since it cannot be directly experimentally confirmed" Mills [3]. All we know today about atoms is due to the pioneering work of others who compulsorily are worth mentioning otherwise, the manuscript cannot make progress, in line with ethics.

Thus without being unnecessarily historical, with due respect to the pioneers of atomic theory, the following personalities are worth remembering (science.com and en.wikipedia.org): Democritus, the ancient philosopher, who opined that all matter is made of atoms; Abu Bakr Muhammad bin Zakariyya who proposed a theory of atom as space occupying object without dimension, yet having magnitude; Amedeo Avogadro who discovered the mole concept and the basis for the notion of the molecules; Millikan Robert Andrew, who determined the charge of an electron; Dmitri Mendeleev who arranged the elements of the periodic table according to the order of atomic weights and discovered the ionisation energy of the atoms of elements; Goldstein Eugen who observed the positive rays leading to the discovery of the subatomic parts of an atom; Thomson JJ who discovered the electrons and proposed the plum pudding or raisin bun model of the atom; Rutherford Ernest who discovered the dense atomic nucleus; Louis de Broglie who theorised that all matter has wave-property duality; Henry Moseley who arranged the elements in the order of their effective atomic number and has Moseley law to his credit; Niels Bohr who defined the equation for the determination of atomic radius restricted to hydrogenic atom and the planetary model of the atom; Johannes Rydberg who discovered the Rydberg constant, valuable in the study of spectroscopy; Johannes Rydberg and Walter Ritz who formulated the Ritz-Rydberg combination principle; Theodore Lyman who discovered the 1st series called Lyman series, of the hydrogen spectrum (HS); Johann Balmer who discovered the 2nd series called Balmer series, of HS-the visible spectrum; Friedrich Paschen who discovered the 3rd series known as Paschen series; Frederick Summer Brackett who

discovered the 4th series known as Brackett series; August Herman Pfund who discovered the 5th series known as Pfund series; Curtis J. Humphreys who discovered the 6th series; Edward Charles Pickering and Alfred Fowler who discovered the 7th series known as the Pickering-Fowler series – the spectral lines arising from He⁺ which according to Bohr originally was attributed to unknown form of hydrogen with half-integer transition level; Erwin Schrodinger who introduced the quantum mechanical model of the atom; and Werner Heisenberg who formulated quantum mechanics based on matrices and the controversial "uncertainty relation". Recent (20th century) concern about Bohr's theory and equation borders on what makes hydrogen atom stable, or rather what constitutes its ground state [3]. The implication is that the time tested "spectroscopic" data (ionisation energy) values are being put to question but not invalidated.

1.2 Concern about Mathematical Complexity

Unlike most research papers in physical sciences, Bohr's equation is regrettably restricted to hydrogen atom and as a consequence other higher elements are left out until recently when modified forms of Bohr's equation [2,4] were derived which satisfactorily reproduced Bohr's radius for hydrogen and there was no reason why those equations cannot be applied to non-hydrogenic atoms. The equations [2,4] in question, Heisenberg's equation of uncertainty principle, Millikan's equation for the calculation of the charge of an electron, equation of mass-energy equivalent by A. Einstein *etc* are all explicit equations showing exact dependent and independent variables. Like in the past, current scientist with interest in most, if not all mathematics based subjects, especially the mathematical fields, e.g., mathematical physics, mathematical chemistry mathematical biology, mathematical economics, *etc* are so imbued with immense knowledge of mathematics beyond mere post graduate level to the point where, a solution to a problem ends up in another problem; this is intended to mean that a lay man may not be able to discern the dependent and independent variable from each other. This is not to say that authors of such papers in those fields containing a lot of mathematical complexities do not know what those variables are, but restriction to them alone is like one "speaking in tongue" which no one but themselves alone understands. Some of those papers can be split into at least three papers, each giving interpretational details

of terms, meaning of mathematical terms or forms, with one or two objectives. “Due regard or highest respect must always be given to scientist and social scientist neck-deep in subjects where “highly advanced mathematics” is the case and to the mathematicians in particular”.

This section is very important because any mention of Bohr’s theory or rather equation often restricted to hydrogenic atom, must take into cognisance of the theories that seem to go against it; it is also instructive to realise that theories that go against Bohr’s equation and theory are also under severe criticism. Any mention of HUP and SE does not necessarily mean that their formal mathematics has to be adopted; doing so would amount to contradictions because as commented elsewhere [3] SE and HUP mathematics and qualitative arguments and Bohr’s mathematics as well as recent extension of Bohr’s mathematical formalism [5] are strange bed fellows. Most of the criticisms against HUP and SE are based on the difficulties and of course the inherent complexities associated with the mathematics applied in those principles or rather concepts [3]. Yet there may be no end to it any time soon as long as there are publishers with preferences for respected scholars and nationalities of choice where those scholars originate. No one in contemporary “cloud of events” from west to east, north to south and *vice versa* should tragically be in doubt about this comment. Honesty demands that, one open up to say that most papers on HUP and SE are replete with very unfamiliar mathematics such as those where complex calculus and set theories play prominent role. Some of the mathematical exposition such as local fractional continuity of function loaded with set theory, theory of local fractional Fourier analysis, the generalised Fourier transforms in fractal space, HUP in local fractional Fourier analysis with set theory, the mathematical aspect of fractal quantum mechanics (QM) *etc*, can be found in work of Yang et al. [6]. A preprint report [7] also showed a lot of mathematics with highly advanced calculus with set theories intended to address what the author felt was vague statements, viz: “It is impossible to prepare states in which position and momentum are simultaneously arbitrarily well localised; it is impossible to measure simultaneously position and momentum, and it is impossible to measure position without disturbing momentum, and vice versa”. In this research those statement are regarded as intelligible.

Again the researcher gave as usual, a complex equation each for uncertainty in position and momentum which specifically defined the standard deviations of position and momentum in a state, ψ [7], usually representing wave function. Once again they presented another definition of HUP viz: “According to the uncertainty principle, the qualitative relationship of a strict mutual exclusiveness of sharp preparations or measurements of position and momentum is complemented with a quantitative statement of a trade-off between competing degrees of the concentration of the distributions of these observables in state preparations or between the accuracies in joint measurements” [7]. This, to the layman is vague and clear example of ambiguity often objected to by Mills [3]; what preparation means is unknown, perhaps, it seems to imply the action or procedure taken to measure either position or momentum which could acceptably make it impossible to define initial position of the electron let alone the final position due to almost infinitesimal size of the electron. Action to be carried out remains perhaps, naively, a qualitative statement of intent, until when such is carried out and measurement of effect or outcome such as change of position and momentum with their errors are determined or measured. This position is however, speculative arising from the statement of ambiguity. By the way it would have been better if statistician devoted to the issue of HUP define clearly error and uncertainty in any of those measurements. This follows from what appears to be two aspect of the same issue given by Mill [3]: The Heisenberg Uncertainty Principle is wrongly interpreted as: The uncertainty in the measured momentum times the uncertainty in the measured position must be no less than \hbar , the reduced Planck constant given as $h/2\pi$ [3]. Perhaps the proper presentation should have been $\Delta x \Delta P \leq \hbar$ (or rather “ $\Delta x \Delta P \lesssim \hbar$; $\Delta x \Delta P \leq \hbar$; $\Delta x \Delta P \approx \hbar$ ”, noting is specified). Perhaps this may be in line with the following assertion by Mill [5]: “The HUP gives a lower limit to the product of the *uncertainty* in the momentum and the *uncertainty* in the position—not the product of the momentum and the position”. “The Heisenberg Uncertainty Principle (HUP) is the mathematical expression for the statistical error in the variables of the wave function such as those assigned to the position and momentum of the electron.

Since the wave function is interpreted as the probability of the position of the electron which puts it everywhere at once with an infinite

number of positions and energies simultaneously including ones with negative kinetic energy, the Heisenberg Uncertainty Principle merely reveals that this model is not a valid physical description of the electron" [3]. Yet an opinion in an old literature [8] posits that the wave description is consistent with uncertainty principle according to which the position of an electron in a given energy level cannot be known exactly. One may wish to know if mathematical expression for the statistical error in the variables of the wave function (or rather its square form) assigned to the position and momentum of the electron equivalent to probability density distribution of electron. In all these issues, one should bear in mind what uncertainty stands for viz: In metrology, measurement uncertainty is the expression of the statistical dispersion of the values attributed to a measured quantity; all measurements are subject to associated uncertainty such as standard deviation. On the other hand, observational (or measurement) error is the difference between a measured value of a quantity and its true value (Wikipedia). This is in the light of view that: "Despite its successes, after decades of futility, quantum mechanics and the intrinsic Heisenberg Uncertainty Principle have not yielded a unified theory, are still purely mathematical, and have yet to be shown to be based in reality [5]. Both are based on circular arguments that the electron is a point with no volume with a vague probability wave requiring that the electron have multiple positions and energies including negative and infinite energies simultaneously" [3]. In other words there appears not be a common ground for both theories. So much about HUP but yet to be exhausted

Next is the Schrödinger theory and associated equation seen to be suitable to hydrogenic atom. "It fails to predict electron spin and leads to models with nonsensical consequences such as negative energy states of the vacuum, infinities, and negative kinetic energy. In addition to many predictions, which simply do not agree with observations, the Schrödinger equation and succeeding extensions predict noncausality, nonlocality, spooky actions at a distance or quantum telepathy, perpetual motion, and many internal inconsistencies where contradicting statements have to be taken true simultaneously" [1]. QM provides an algorithm for computing probabilities for macroscopic events ('detector ticks') that are the consequences of experimental interventions [3].

Concluding in part, probabilities have no place in describing atomic energy levels. "Moreover, quantum theory is incompatible with probability theory since it is based on underlying unknown, but determined outcomes" [3]. This paragraph is considered very important because it gives a clear support for the view that HUP is precluded in the procedure used to derive alternative equation that is generalisation to all atoms in the 1990s but was rejected in a manner that was uncomplimentary and reckless; perhaps precluding HUP and not necessarily typographical errors or grammar per se (the grammar could be described as jargon in the first place) may be the reason for the rejection. The paper [2] has been published elsewhere. The wave function must be real and physical in order for it to be considered a valid description of reality. This view by Hill follows from the observation that electrons formed bubbles in superfluid helium apart from being indivisible at 90 (LEP II). Unfortunately these issues described as being inconsistent with physical laws including those emanating from Feynman's view are largely ignored by the physics community [3]. It may remain so until people like Mills come strongly and until the only motivation to publish for promotion ceases to be.

2. THEORETICAL DEVELOPMENT

In this section equations of the past are re-appraised and any objections against any of them examined *vis-à-vis* alternatives in the literature. Scientific terms are given general definitions or interpretation in line with broad objective, the aim of this research. Phrases such as after some algebra in statements are strictly forbidden; a step-by-step approach is adopted in the derivation of a new equation that is Planck constant invariant mainly for multi-electron atoms.

2.1 Review of Previous Mathematical Models-equations and Results

The research in the past has shown that the computed radii of atoms are found to reproduce the expected periodic variation of size in periods and in groups and nicely reproduced the *d*-block and *f*-block contractions in the respective series [9] similar to the claim in paper one that: the calculated set of theoretical atomic radii of 103 elements of the periodic table using Slater orbitals were found to reproduce the periodic law and reproduced the expected vertical and horizontal trend of variation in atomic size in the

periodic table. Though these finding seem very lofty, it is not subject of verification rather the equations that enabled the calculations may require further clarification. According to the authors [9] the radial charge density distribution function (RCDF, or $\rho(r)$ for the symbol), given below is based on what the author called Slater's analytical form of the radial part of the one-electron function. This is important because it has been an age-long believe in scientific community that, Bohr's equation and SE was more successful with hydrogenic atom. Nonetheless recent research has produced variety of equations that can be used to determine the radii of atoms based on information on the experimentally determined ionisation energies of elements. Nonetheless the equation of $\rho(r)$ given by Ghosh and Biswas, [9] is:

$$\rho(r) = 4\pi r^{2n} (2\xi)^{2n+1} [(2n)!]^{-1} \exp(-2\xi r) \quad (1)$$

In line with broad objective, aim, an explanation to $\rho(r)$ is given herein: As in statistical mechanics applicable to particles in whatever state, including the leptons, but not limited to them, Eq. (1) shows how the density, ρ varies as a function of distance from another preferred particle called reference particle (en.wikipedia.org). After differentiating the equation of RCDF, and after algebraic manipulation or rearrangement, the following result [10] was obtained.

$$n r_{max}^{2n-1} - \xi r_{max}^{2n} = 0 \quad (2)$$

Where r_{max} , n , and ξ are the atomic or ionic radii, principal quantum number (pqn), and orbital exponent given as [10]:

$$\xi = (Z-S) n^* = Z^* n^* \quad (3)$$

Where, Z , Z^* , S , and n^* are the atomic number, effective charge, screening constant and effective pqn. The authors applied slater rule for the determination of S .

From Eq. (1) the authors [10] obtained:

$$r_{max} = n / \xi \quad (4)$$

The concern in this research is that, it is not certain how dimensionless variables such as " ξ ", Z , Z^* , S , and n^* can be used to calculate values such as radii whose SI unit is metres. Noting in papers one and two points to the equation into which the variable can be substituted.

Owolabi et al. [10] explored computer-based programme, otherwise called artificial intelligence using support vector regression that predicts atomic radii of elements above 99 % of accuracy and with associated set theory and matrix formalism were able generate results for many elements. However, the report for hydrogen is far from what Mills [3] says about constant parameters of the hydrogen atom which are known to 10 figure accuracy. The computer "language" and associated mathematics, matrix, set theory etc may be of restricted interest, reserved for high-level specialist.

A hybrid-density functional calculation, perhaps, on atomic scale and Dirac-Breit methods were also explored for the calculation of radii of atoms. According to the authors [11] the results from the two methods were in satisfactory agreement. The Dirac-Breit equation is a relativistic wave equation derived by Breit based on Dirac equation which describes two or more massive spin-1/2 particles (e.g. electrons) interacting electromagnetically to the 1st order in perturbation (or rather, perhaps, during perturbation); this accounts for magnetic interactions. Dirac equation describes all spin-1/2 massive particles such as electrons and quarks (elementary particles that makeup each nucleon) for which parity is a symmetry; it is consistent with both principle of quantum mechanics and theory of special relativity (en.wikipedia.org). Spin being seen as a conserved quantity carried by elementary particles (en.wikipedia.org), is also one of the 2 kinds of angular momentum (the 2nd being orbital angular momentum); it is the rotational motion of electron about its axis passing through its centre of mass, producing in the process, tiny magnetic fields as previously observed by Otto Stern and Walther Gerlach of the University of Hamburg, Germany (Scientific America).

Next in line is the original Bohr's equation which attracted criticism for some reason seen to be unnecessary. The Bohr atomic model or theory considers electrons to have both a known distance from the nucleus – the radius of a circle (or orbit) – and orbit *i.e.* known position and momentum at the same time, which is impossible according to HUP [12]. This shows that one cannot extricate Bohr's original equation from his planetary model: The most important issue is the electrostatic influence of the nucleus on the electron (s), be it oscillatory, vibrational or rotating in motion. This is where Bohr's equation remains very relevant but regrettably he had no

knowledge of how to determine the effective nuclear charge, even if the data for ionisation energies for all elements were available in his days which postdate the days of Dmitri Mendeleev who discovered ionisation energy. "The effective nuclear charge, Z_{eff} , is a measure of the average nuclear charge felt by the outermost electron in the various orbitals, considering the inter-electronic repulsions and its penetration capability" [13]. The only reasonable challenge in old Bohr's equation is the lack of know-how for the determination of effective nuclear charge which however, is not the interest of this research, otherwise with the information about the Z_{eff} of any element the radius of any element can be calculated. Nonetheless there are methods in the literature for calculating Z_{eff} [2]; ionisation energy dependent approach and another approach that relates with the fine structure constant had been derived [14]. This makes Bohr's equation that has the character of specificity, for the calculation of the radius of any atom to assume a universal appeal. Recent researches [2,4] have shown that the radii of all atoms of all elements can be determined.

2.2 Derivation of Yet another Alternative Equation to the Original Bohr's Equation

In this section, another equation which can be used to calculate the radii of some selected elements motivated by their biological importance is to be derived. This is against the backdrop of the description of electron as a wave function, a mathematical description of a quantum state (the mathematical entity that provides a probability distribution for the outcomes of each possible measurement on a system), of an isolated system, instead of a point charge as claimed by Fattah [15] with reference to the literature [16]. The consequence of describing electrons as waveforms is that, it is mathematically impossible to simultaneously derive the position and momentum of an electron [16], a view that has also met opposition [3,17,18]. It seems the "accusers" of Bohr's theory and equation are meeting exceedingly harsher criticism and flawed theories. The first of this Bohr's equation written in different forms is given as:

$$a_0 = \frac{n^2 h^2 \epsilon_0}{\pi m_e e^2 Z_{\text{eff}}} \quad (5)$$

Where, n , h , m_e , e , ϵ_0 and Z_{eff} are the principal quantum number (otherwise called energy level,

pqn), Planck constant, rest mass of an electron, charge of an electron, and permittivity in free space (electric constant) and effective nuclear charge respectively. Most high quality text books [8,19] present Bohr's equation for hydrogen as:

$$a_0 = \frac{h^2 \epsilon_0}{\pi m_e e^2} \quad (6)$$

Guess, simply because the Z_{eff} is = 1 and $n = 1$. Another way is to write the so-called "primitive" equation, the Coulomb equation such as:

$$a_0 = \frac{Z_{\text{eff}} e^2}{8 \pi \epsilon_0 \xi_H} \quad (7)$$

Where ξ_i is average ionisation energy of any atom other than hydrogen.

Again most text books present, Eq. (7) as:

$$a_0 = \frac{e^2}{8 \pi \epsilon_0 \xi_H} \quad (8)$$

Where ξ_H is the average ionisation energy of hydrogen. The reason is as written earlier. It is very clear that the only challenge is the lack of information about Z_{eff} in Eqs (5) and (7) for elements whose Z_{eff} is > 1 and n is ≥ 1 .

Meanwhile, an equation for the determination of the radius of any atom (with due respect for N. Bohr, all radii regardless of element are referred to as Bohr's radii, a_i and a_0 for any other element other than hydrogenic atom or ion and for hydrogen respectively.) had been derived as shown in the literature [2]. The equation is given as:

$$a_i = \frac{n h}{\pi^2 \sqrt{8 m_e \xi_i}} \quad (9)$$

Although Eq. (9) seems to be tied down to heavier atoms, be it hydrogenic and non-hydrogenic, it is nevertheless a general one; substitution of accurate value of the average ionisation energy of say hydrogen gives exactly the same value known in the literature, CODATA [20] for instance. Taking the square of Eq. (9) and rearranging gives:

$$\xi_i = \frac{n^2 h^2}{8 \pi^2 m_e a_i^2} \quad (10)$$

Meanwhile, it has been shown that [15]:

$$\xi_H = \frac{n^2 \xi_i}{Z_{\text{eff}}^2} \quad (11)$$

The equation for Z_{eff} is given as [15]:

$$Z_{\text{eff}} = \sqrt{\left(\frac{8 \xi_i}{m_e}\right) \cdot \frac{nh\epsilon_0}{e^2}} \quad (12)$$

Then, take the reciprocal of Eq. (11) to give:

$$\frac{1}{\xi_H} = \frac{Z_{\text{eff}}^2}{n^2 \xi_i} \quad (13)$$

After substituting Eq. (10) and the square of Eq. (12) into Eq. (13) one gets:

$$\frac{1}{\xi_H} = \frac{8 \pi^2 a_i^2 m_e}{n^4 h^2} \cdot \frac{8 \xi_i n^2 h^2 \epsilon_0^2}{m_e e^4} \quad (14a)$$

Simplification gives:

$$\frac{1}{\xi_H} = \frac{64 \pi^2 \epsilon_0^2 a_i^2 \xi_i}{n^2 e^4} \quad (14b)$$

Making a_i subject of the formula in Eq. (14b) gives:

$$a_i = \frac{e^2 n}{8 \sqrt{(\xi_H \xi_i)} \cdot \pi \epsilon_0} \quad (15)$$

Equation (15) represents an equation independent (or rather free) of Planck constant for the determination of the radius of any atom: Thus if ξ_i and ξ_H are equal, then n should be =1, such that: $a_0 = \frac{e^2}{8 \xi_H \pi \epsilon_0}$. Nonetheless n may be equal to 1 even if ξ_H is not equal to ξ_i as applicable to He and monovalent ion (Li^+). Note however, that n may be = 1 for multi-electron atoms and ions if, ${}^A_Z X$ has only 2 electrons as an atom or as an ion if it has already lost 1 electron leaving behind ($Z - 1$) where $Z = 3$ or 2 electrons leaving behind 2 electrons where $Z = 4$. Thus, with carefulness and deliberate interest one can obtain a well-known Bohr's radius for hydrogen, and consequently there is no justification to stop midway thinking that Eq. (15) should exceptionally yield incorrect value for any multi-electron atom as shown and confirmed in Table 1 for the selected elements. Note however, that the unnumbered equation constitute a reproduction of Eq. (8) because it is unavoidable, in that, Z_{eff} for hydrogen and any other larger hydrogenic ion, ${}^A_Z X^{(Z-1)+}$ is 1. The only innovation lies in Eq. (15) which is generally applicable to higher atoms and non-hydrogenic ions whose ionisation energy and the quantum number of energy level are known for the calculation of the radius

without the need for h . If an atom of higher elements has 2 or more electrons, information about effective nuclear charge is needed for the calculation of the radius; but such information is not applicable to Eq. (15) and, unlike Eq. (9), h is not needed as written earlier.

3. MATERIALS AND METHODS

The research is purely theoretical and calculational without any measurement.

4. RESULTS AND DISCUSSION

A very simple equation such as Eq. (4) does not offer any clue as to how the important periodic property such Bohr's radius for any atom can be calculated; the denominator and nominator are dimensionless. Equations (5) to (16) do not present any dimensional inconsistencies. Of particular interest is Eq. (15) which is the ultimate result of this research. Equation (16) as a corollary validates the procedures of arriving at Eq. (15). The radii of 103 elements as a function of their 1st average ionisation energies had been calculated based on Eq. (9) as in the literature [2] and another equation in the literature [3]. However, in order to evaluate Eq. (15), the radii at the highest energy level of elements commonly encountered in the biosphere were calculated and the values are shown in Table 1.

A close examination of Table 1 reveals that the old result (values of ionisation energies) are very similar to values calculated in this research; differences may be as a result of approximations and the use of fundamental constants whose values were not exactly CODATA [20] values. Typical examples of this issue are the adoption of the following values of fundamental constants, viz: e (1.6021 exp. (-19) C); ξ_H ((1312000 / N_A) J where $N_A = 6.02252 \text{ exp. (23)/mol.}$); ϵ_0 (8.854 exp. (-12) $\text{C}^2/\text{N.m}^2$); the corresponding 2016 CODATA [20] values are: e (1.6021766208 exp. (-19) C); ξ_H ((1312035.26 / N_A) J where $N_A = 6.022140857 \text{ exp. (23)/mol.}$); ϵ_0 (8.854187817 exp. (-12) $\text{C}^2/\text{N.m}^2$). It is pointless recalculating the radii of all the atoms in this research using Eq. (9) except an isolated case in which hydrogen is considered for the purpose of showing that Eq. (9) and Eq. (15) would always give the same value of Bohr's radii. If so, there is no reason whatsoever, why it should not be so for other multi-electron atoms.

Table 1. First Bohr’s radii of selected bioactive elements

S/N	Elements	Electronic configuration	Bohr’s radius* exp. (-11) m	Bohr’s radius# exp. (-11) m
1	H	1s ¹	5.292523983	5.29
2	C	[He] 2s ² 2p ²	11.6319013	11.6
3	N	[He] 2s ² 2p ³	10.2390291	10.2
4	O	[He] 2s ² 2p ⁴	10.57786666	10.6
5	F	[He] 2s ² 2p ⁵	9.351509449	9.4
6	Na	[Ne] 3s ¹	25.82957393	25.8
7	Mg	[Ne] 3s ²	21.17468415	21.2
8	P	[Ne] 3s ² 3p ³	18.08046082	18.1
9	S	[Ne] 3s ² 3p ⁴	18.19046115	18.2
10	Cl	[Ne] 3s ² 3p ⁵	16.25898646	16.3
11	K	[Ar] 4s ¹	37.4707368	37.5
12	Ca	[Ar] 4s ²	31.57498735	31.6
13	Mn	[Ar] 3d ⁵ 4s ²	28.6315694	28.6
14	Fe	[Ar] 3d ⁶ 4s ²	27.76998501	27.8
15	Co	[Ar] 3d ⁷ 4s ²	27.80830482	27.8
16	Zn	[Ar] 3d ¹⁰ 4s ²	25.47039153	25.5
17	Se	[Ar] 3d ¹⁰ 4s ² 4p ⁴	24.99774063	25.0
18	Mo	[Kr] 4d ⁵ 5s ¹	36.6422651	36.7
19	I	[Kr] 4d ¹⁰ 5s ² 5p ⁵	30.18485986	30.2

The average 1st ionisation energies used for calculations were obtained from the literature (en.wikipedia.org/wiki/ionisation energies of the elements); the ionisation energy of hydrogen was however, calculated using 2016, CODATA [20] values of fundamental physical constants. The value calculated for hydrogen using the equation, $\xi_H = Z_{eff}^2 e^4 m_e / 8 \epsilon_0^2 n^2 h^2$ is: 2.179872321 exp. (-18) J (using rest mass) and 2.178685772 exp. (-18) J (using reduced mass = 9.104425137 exp. (-31) kg.). The asterisks (*) and ash (#) denote values calculated using reduced mass in this research and values obtained in earlier research [2,4] respectively

The Coulomb equation ($\xi_i = Z_{eff} e^2 / 8\pi\epsilon_0 a_i$) is one in which *ab initio* the Planck constant does not appear. Where Z_{eff} is equal to one, then hydrogen atom is the case. Since ξ_H is, experimentally determinable, a_0 for hydrogen can be calculated without the Planck constant; but this is not possible if multi-electron atoms are the case because, Z_{eff} should be greater than one and needs to be separately determined. The original Bohr’s equation, Eq. (5) and Eq. (6) contain Planck constant. This is applicable to other variants of the equation given as (en.wikipedia.org/wiki/Bohr’s radius) $a_0 = 4\pi\epsilon_0 \hbar^2 / m_e e^2$; $a_0 = \hbar / m_e c \alpha$ and the equation (Eq. (9)) derived elsewhere [2]. Like the original Bohr’s equation, the presence of reduced Planck constant, $\hbar (= h/2\pi)$, in the latter equations means that the Bohr’s radius of hydrogen and any hydrogenic ion with $Z>1$ cannot be calculated without Planck constant. This is however, unlike Eq. (15).

Worthy of mention is Eq. (10) which shows that if the atomic radius of any atom is determined correctly by experiment or theory, the average ionisation energy of an element can be

determined. Adopting hydrogen and oxygen as reference elements, this assumption is tested as follows: By substituting known values of a_i for multi-electron atom like oxygen and a_0 for hydrogen into Eq. (10) the values of calculated average ionisation energies are respectively, 1313817.284 J/mol. and 1312035.26 J/mol. En.wikipedia.org value is 1313900 and 1312000 J/mol. respectively. Ghosh and Biswas [9] reported radii values equal to 5.292 exp. (-11) m and 4.652 exp. (-11) m for hydrogen and oxygen respectively. Substituting these values into Eq. (15) gives after calculation the following values respectively for hydrogen and oxygen: 1312377.653 J/mol. and 3396636.57 J/mol. The value for hydrogen calculated using radius reported in the literature [9] is very similar to values calculated in this research and recorded elsewhere (en.Wikipedia.org/wiki/ionisation energy). However, the calculated value for oxygen in this research is much more similar to the value elsewhere [4] than the value calculated using the radius determined for oxygen in the literature [9]. The adoption of Slater rule for the determination of effective nuclear charge [9] may account for larger values of the latter leading to

shorter atomic radius. It is interesting to note that the derivation of equations in this research takes its root in the original Bohr's mathematical formalism and there are definite Bohr's equations for the radius of hydrogen and any other hydrogenic multi-electron ion and also for ionisation energy.

5. CONCLUSION

The fact that a material or matter in existence has an infinitesimal magnitude has been reemphasised by evidence from both nonscientific and scientific perspectives. Modern atomic theories, the HUP and SE, that seem to repudiate Bohr's deterministic theory and cognate equation, have been seen to be excessively loaded with mathematical complexities with associated ambiguities without common ground that should usher in alternative solutions to the problem of the size of the atom. From the literature, it is obvious that quantum mechanics (QM) only provides an algorithm for computing probabilities for macroscopic events, though probabilities have no place in describing atomic energy levels. The wave function must be real and physical rather than being mathematical in order for it to be considered a valid description of reality. The derived equation in this research reproduced the values of the radii of atoms, including hydrogen, that were very similar to values reported in the older and much newer literature. The new equation in question is not restricted to multi-electron atoms and ions; it is applicable to hydrogen and other hydrogen-like ions, that is, those ions that possess a single electron. The only experimental variable needed is the average ionisation energy. Substitution of calculated radii for hydrogen (5.292523983 exp. (-11) m) and oxygen (10.57786666 exp. (-11) m) into the derived preliminary equation reproduced after calculation the average ionisation energies for hydrogen (1312035.26 J/mol.) and oxygen (1313817.284 J/mol.). The Bohr's radii of all atoms can be calculated independent of the Planck constant. An alternative method for the determination of the definite three-dimensional space of an atom, excluding interparticle space, should be reserved for future research.

ACKNOWLEDGEMENTS

I appreciate proof-reading service provided by the internet based grammar checker (QuillBot) and the consistent supply of electricity by the management of Royal Court Yard Hotel, Agbor, in Delta State, Nigeria.

COMPETING INTERESTS

Author has declared that no competing interests exist.

REFERENCES

1. Mills RL. The nature of free electrons in superfluid helium-A test of quantum mechanics and a basis to review its foundations and make a comparison to classical theory. *Int. J. Hydrog. Energy.* 2001;26(10):1059–1096.
2. Udema II. Renaissance of Bohr's model via derived alternative equation. *Am. J. Modern Phys.* 2017;6(2):23–31.
3. Mills RL. The fallacy of Feynman's and related arguments on the stability of the hydrogen atom according to quantum mechanics. *Ann. de la Fond. Louis de Broglie.* 2005;30(2):129-149.
4. Udema II. Revisiting Bohr's theory via a relationship between magnetic constant and Bohr radius of any element, *Asian J. Phys. Chem. Sci.* 2018;6(1):1-11.
5. Udema II. A mathematical relationship between hydrogenic periodic property and nuclear properties in furtherance of Bohr's theory. *Asian J. Res. Rev. Phys.* 2022;6(3):1-6.
6. Yang XJ, Baleanu D, Machado JAT. Mathematical aspects of the Heisenberg uncertainty principle within local fractional fourier analysis, *Bound. Value Probl.* 2013;131(2013):1-16.
7. Busch P, Heinonen T, Lahti P. Heisenberg's uncertainty principle. *Phys. Rep.* 2007;452:155-176.
8. Kneen WR, Rogers MJW, Simpson P. *Chemistry, facts, patterns, and principles*, 1st ed. London: The English Language Book Society and Addison-Wesley Publishers Limited; 1972.
9. Ghosh DC, Biswas R. Theoretical calculation of absolute radii of atoms and ions. Part1. The atomic radii. *Int. J. Mol. Sci.* 2002;3:87-113.
10. Owolabi TO, Akande AO, Olatunji SO. Estimation of the atomic radii of periodic elements using support vector machine. *Int. J. Adv. Sci. Technol.* 2014;28:39-49.
11. Duchwicz PR, Castro EA. Comparison between two different approaches toward atomic radii. *Kragujevac J. Sci.* 2005;27: 51-56.
12. Zoolman D. Bohr's model of the atom draws critics. In Kim Rendfeld. *History of Science*; 2016.

13. Sala O, Araki K, Noda LK. A procedure to obtain the effective nuclear charge from the atomic spectrum of sodium. J. Chem. Edu. 1999;76(9):1269-1271.
14. Udema II. Fine structure constant is related to effective nuclear charge and Bohr's radius for any atom. Asian J. Phys. Chem. Sci. 2017;3(4):1-8.
15. Fattah KA. A visualised mathematical model of atomic structure. J. Sci. Technol. Eng. Comp. Sci. 2013;14(3):21-26.
16. Schrödinger E. "Quantization as an eigen value problem". Ann. Phys. 81:109-139.
17. Baek SY, Kaneda F, Ozawa M, Edamatsu K. Experimental violation and reformulation of the Heisenberg's error-disturbance uncertainty relation. Sci. Rep. 2013;3:1-6.
18. Ozawa M. Measurement breaking the standard quantum limit for free-mass position. Phys. Rev. Lett. 1988;60:385-388.
19. Lee JD. A new concise inorganic chemistry. 3rd Ed. New York. Cincinnati. London. Toronto. Melbourne: Van Nostrand Reinhold Company Limited; 1977.
20. Mohr PJ, Newell DB, Taylor BN. CODATA recommended values of the fundamental physical constants. J. Phys. Chem. Ref. Data. 2016;45(4):1-75.

© 2022 Udema; This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Peer-review history:
The peer review history for this paper can be accessed here:
<https://www.sdiarticle5.com/review-history/94937>