Scientific Research Publishing

Journal of Applied Mathematics and Physics, 2018, 6, 1290-1300
http://www.scirp.org/journal/jamp
ISSN Online: 2327-4379
ISSN Print: 2327-4352

The Atom Model of Helium and of Neon Based on the Theorem of Niels Bohr

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How to cite this paper: Allmendinger, T. (2018) The Atom Model of Helium and of Neon Based on the Theorem of Niels Bohr. *Journal of Applied Mathematics and Physics*, **6**, 1290-1300.
https://doi.org/10.4236/jamp.2018.66108

Received: May 8, 2018
Accepted: June 25, 2018
Published: June 28, 2018

Abstract

In a previous, primary treatise of the author the mathematical description of electron trajectories in the excited states of the H-atom could be demonstrated, starting from Bohr's original model but modifying it three dimensionally. In a subsequent treatise, Bohr's theorem of an unalterable angular momentum $h/2\pi$, determining the ground state of the H-atom, was revealed as an inducement by the—unalterable—electron spin. Starting from this presumption, a model of the H_2-molecule could be created which exhibits well-defined electron trajectories, and which enabled computing the bond length precisely. In the present treatise, Bohr's theorem is adapted to the atom models of helium and of neon. But while this was feasible exactly in the case of helium, the neon atom turned out to be too complex for a mathematical modelling. Nevertheless, a rough ball-and-stick model can be presented, assuming electron rings instead of electron clouds, which in the outer shell are orientated as a tetrahedron. It entails the principal statement that the neon atom does not represent a static construction with constant electron distances and velocities, but a pulsating dynamic one with permanently changing internal distances. Thus, the helium atom marks the limit for precisely describing an atom, whereby at and under this limit such a precise description is feasible, being also demonstrated in the author's previous work. This contradicts the conventional quantum mechanical theory which claims that such a—locally and temporally—precise description of *any* atom or molecule structure is generally not possible, also not for the H_2-molecule, and not even for the H-atom.

Keywords

Modified Bohr Model, Electron-Trajectories, Electron-Spin, Three-Dimensional Atom-Models, Confutation of Heisenberg's Uncertainty-Principle

1. Introduction

In 1913, the Dane Niels Bohr published an article entitled "On the Constitution of Atoms and Molecules" [1], focusing on the H-atom. Starting from Rutherford's atom model, which assumed a heavy positively charged nucleus in the centre and a light electronic envelope, and applying Planck's quantum theory of radiation, introduced in 1900 [2] and supplemented by Albert Einstein's photoelectric effect in 1905 [3], he suggested that—as a result of (UV-) radiative excitation—well-defined orbits were occupied by the electron, being associated to enhanced energy levels. His model could widely explain the line-spectrum of hydrogen which had been observed astronomically in certain Space regions as well as in terrestrial experiments using low pressure tubes, and wherein remarkable regularities had been originally found by Balmer [4], later revealed by Rydberg. The essential theorem of his consideration may be expressed by the following statement made in [1]: "In any molecular system consisting of positive nuclei and negative electrons in which the nuclei are at rest relative to each other and the electrons move in circular orbits, the angular momentum of every electron round the centre of its orbit will in the permanent state of the system be equal to $h/2\pi$, where h is Planck's constant." (Therein, "permanent state" means "ground state" of the electron). Moreover, he found that the angular momenta of the excited states are integral multiples of the angular momentum of the ground state. It is worth mentioning that Planck's constant h, which he himself denoted as "elementares Wirkungsquantum" ("elemental action quantum"), represents the product of energy and time (delivering the dimension J·s), being equal to the dimension of an angular momentum. Hence Bohr's atom model may be considered as the outset of modern quantum mechanics.

However, several questions remained: Firstly, the existence of a minimal ground state (permanent state) could not be explained, *i.e.* it was not plausible why the electron does not tumble on the nucleus. Secondly, the intrinsic cause for the existence of such exited—meta-stable—energy states could not be found. Thirdly, Bohr did not deliver a model of a molecule like the H_2-molecule, in contrast to the notification in the title of his article. And fourthly, the structure of atoms with higher atomic number was not given—not even the one of helium—, and likewise the "Aufbau-Principle" of the periodic system of the elements.

A step forward was made in 1924 by Louis De Broglie in his thesis, assuming a *wavy electron motion*, and leading to the term "wave mechanics". It not only explained the deflection of electron beams on thin metal foils (cf. for instance [5]) but also—and in particular—the occurrence of well-defined electron trajectories in the excited states as a result of *standing electron waves*. However, this concept could not be implemented into Bohr's H-atom model comprising such an electron motion and delivering a vivid H-atom model.

An escape from this problem was delivered by Heisenberg postulating the «uncertainty principle» which implied the statement that the location and the

momentum of a particle could not simultaneously be determined. This principle promised to explain the wavy motion of the electron, as well as the fact that it cannot tumble on the nucleus. Based on this theorem, Schrödinger and others developed a complicated theory, based on statistical probability rules, and yielding cloudy orbitals instead of well-defined electron trajectories. In spite of considerable doubts, even expressed by Einstein, this theory was well established and forwarded, in particular implementing the spin phenomenon by Pauli. That was discovered in 1925 by Uhlenbeck and Goudsmith [6] [7], based on the detected multiplicities of spectral lines found in the presence of magnetic fields.

Nevertheless, this conventional theory exhibits crucial contradictions in its terms which already are included within its foundations, and which could not really be cleared away since then. A cardinal intrinsic contradiction is given by Heisenberg's uncertainty principle which is incompatible with De Broglie's standing wave concept implying well-defined electron-trajectories in the excited states. Thereby, the uncertainty of measurability is erroneously equalized to an uncertainty of real states. Moreover, Bohr's hypothesis is not fulfilled for the ground state of the H-atom since a single electron cannot exhibit a constant (vectored) angular momentum when it simultaneously describes a spherical cloudy trajectory, as it would be the case for the s-orbital.

Induced by these contradictions, the author searched and found an H-atom-model implying the De Broglie phenomenon and starting from Bohr's original approach [8]. Thereby, it was needed to assume *three-dimensional wavy electron trajectories* in the excited states, winding up on a surface similar to the one of a hyperboloid (**Figure 1**), whereas at the ground state the electron trajectory is planar. Thereby, the most delicate sticking point was given by the fact that the *partial* horizontal angular momentum (assigned to the rotation axis in **Figure 1**) remains constant even in the exited states, while the *total* angular momentum obeys Bohr's theorem.

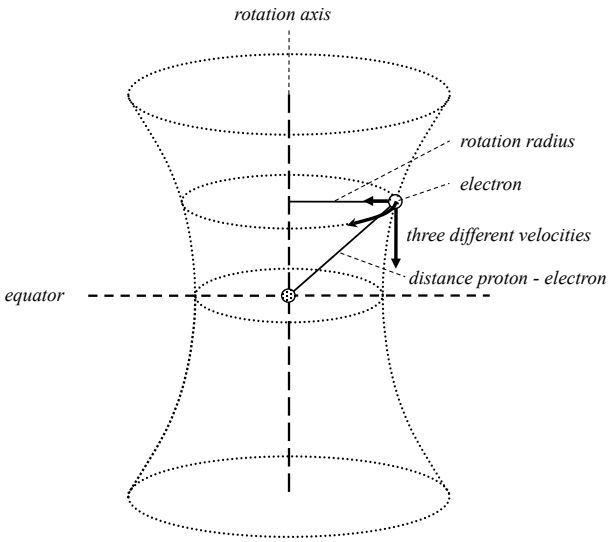

Figure 1. Intermediate position of the electron at the modified model according to [8].

However, the existence of the (stable) planar ground state could not be explained so far. The only plausible explanation appeared when the *spin of the electron* was taken into account, inducing a respective angular momentum leading to the—well-known—spin/orbit coupling. Indeed, the spin hypothesis was known neither to Bohr nor to De Broglie, while the common wave mechanics originally disregarded the spin phenomenon, too. It was solely implemented afterwards, according to the Pauli principle. The electron spin cannot be explained classically, but must be accepted as a natural constant. Since it cannot be annihilated, it delivers the explanation for the ground state at the H-atom (as well as at other atoms or molecules).

Starting from this assumption, it was possible to develop a vivid model for the H_2-molecule, exhibiting planar electron orbits [9]. Analogously to the conventional method of Heitler and London [10] [11], the bond length was computed by searching the total energy minimum (**Figure 2**). Since the bond length can be directly determined by X-ray measurements, verification was possible by empirical evidence, delivering an accurate result (**Figure 3**). In contrast to this, the results of Heitler and London—as well as those of others [12]—, delivered variable and less accurate results. Thus a second proof for the existence of well-defined electron-trajectories could be delivered—namely in the ground-state of the H_2-molecule—, questioning the conventional theory, questioning the conventional theory.

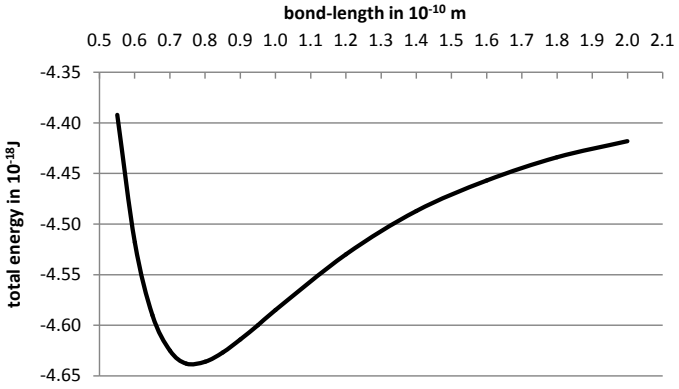

Figure 2. Total energy as a function of the bond-length at the H_2-molecule.

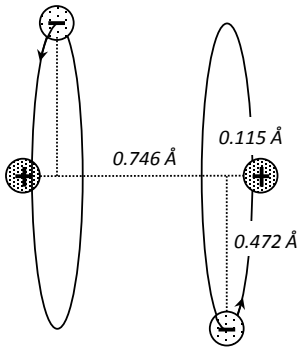

Figure 3. Model of the H_2-molecule (true to scale).

Extending this model-approach, analogous atom models for the noble gases helium and neon are presented here. However, empirical evidence can hardly be delivered, solely plausibility. In view of the complexity of the problem, for neon an exact model computation cannot be delivered, solely an intuitive design.

2. The Three-Dimensional Atom Model of Helium

Starting from Bohr's H-atom model in the ground state, and regarding the constant angular momentum induced by the constant electron spin, for the He-atom the assumption of a simple *concentric* structure according to Figure 4 seems obvious. Using the common physical force laws in combination with the quantum mechanically determined angular momentum, the radius as well as the velocity of the two electrons could easily be computed.

However, the resulting disc-shaped atom structure is not plausible, particularly when the He-atom is taken as the basic model for the atomic core of the higher elements where a tetrahedral array of the external electrons must be assumed, being evident from the CH_4-molecule (methane). Rather a *three-dimensional structure* should be envisaged, potentially enabling a tetrahedral array of the outer electrons. Opposed to this, a spherical, ideally three dimensional structure, as it is claimed within the s-orbital of the conventional quantum mechanics, must be excluded, regarding the above alleged arguments.

Alternatively, the *eccentric* structure shown in Figure 5, where the electron radii describe a *double cone*, appears to be favourable. Indeed, it turned out to be computable, according to the following procedure using the calculation rules given in [9]. Thereby, the special case of a 45˚ eccentric angle is assumed, yielding the geometric relations

$$R = \frac{r}{\sqrt{2}} \tag{1}$$

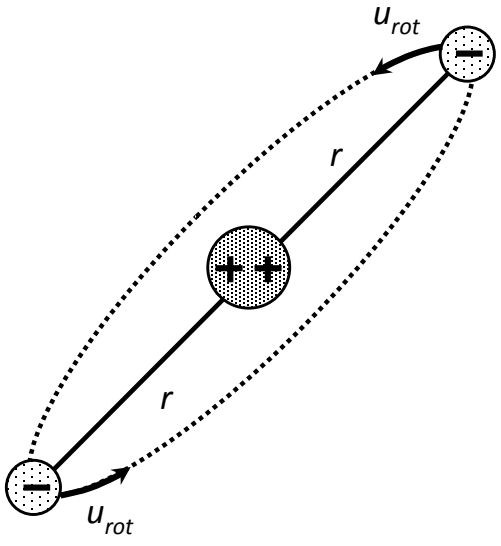

Figure 4. The concentric atom model of helium.

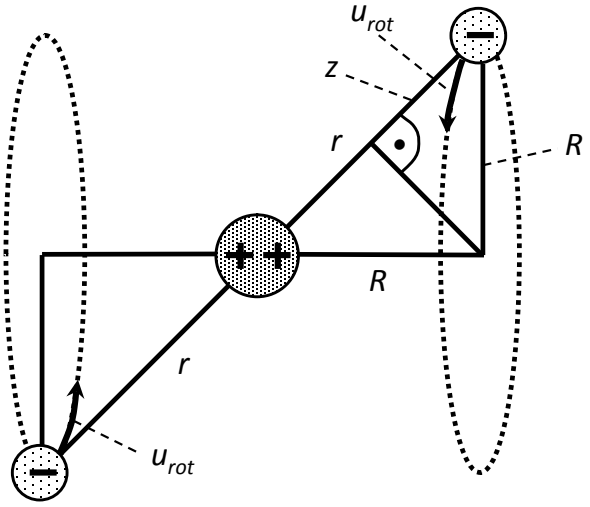

Figure 5. The eccentric atom model of helium.

and

$$z = \frac{r}{2} \tag{2}$$

Moreover, for Coulomb's law the abbreviation

$$K = \frac{e^2}{4\pi\varepsilon_0} \tag{3}$$

is used.

(e = elementary charge, ε_0 = permittivity)

The Coulomb attraction force between each electron and the nucleus is given by the relation $\frac{2K}{r^2}$, while the Coulomb repulsion force between the electrons is $\frac{K}{4r^2}$.

The determination of the concentric centrifugal force of each electron is of particular interest, since—on one hand—it acts in the same direction as the Coulomb forces do, while—on the other hand—solely the eccentric centrifugal force is evident, given by the expression

$$\frac{m_e \cdot u_{rot}^2}{R}$$

(m_e = electron mass, u_{rot} = rotation velocity of the electron)

However, a vector splitting is feasible, delivering the concentric portion of the centrifugal force, namely $\frac{m_e \cdot u_{rot}^2 \cdot z}{R^2}$. When R and z are substituted by r, according to (1) and to (2), the resulting value for the concentric centrifugal force is $\frac{m_e \cdot u_{rot}^2}{r}$ and thus identically equal to the centrifugal force in the concentric model structure according to **Figure 4**. So it is not possible to distinguish com-

putationally between the two variants since they yield the same result with respect to the magnitude of radius *r*.

The balance of forces has to be focused on one electron, related to the nucleus and to the other electron. It is reached when the Coulomb attraction force is equal to the Coulomb repulsion force plus the centrifugal force of the electron, yielding Equation (4):

$$\frac{2K}{r^2} = \frac{K}{4r^2} + \frac{m_e \cdot u_{rot}^2}{r} \rightarrow \frac{7K}{8r} = m_e \cdot u_{rot}^2 \tag{4}$$

Now, the quantum condition has to be regarded, being identically equal for any electron:

$$m_e \cdot u_{rot} \cdot R = \frac{h}{2\pi} \rightarrow m_e \cdot u_{rot}^2 = \frac{h^2}{4\pi^2 \cdot m_e \cdot R^2} = \frac{h^2}{2\pi^2 \cdot m_e \cdot r^2} \tag{5}$$

The combination of (4) and (5) yields the exact value for *r*:

$$r = \frac{8h^2}{7\pi^2 \cdot K \cdot m_e} = \frac{8h^2 \cdot \varepsilon_0}{7\pi \cdot m_e \cdot e^2} = 0.60477 \times 10^{-10}\,\text{m} \tag{6}$$

As a consequence, the distance *R* between the nucleus and the electron rotation centre is $r/\sqrt{2}$ = 0.42767 × 10^{-10} m (10^{-10} m = 1 Å). These values cannot be verified empirically, since the effective atomic radius is not identical with the distance between the nucleus and the electrons. Moreover, this eccentric model is not spherical and thus *anisotropic*, letting assume that both radii—namely *r* and *R*—have to be taken into account. At least it is striking that the average value of these two radii (0.516 Å) is similar to the value of the atomic radius of helium found in the literature (0.49 Å). However, the original sources for the empiric data concerning helium could not be found since they are part of the common physical-chemical data base.

In order to assess the interactions with other He-atoms, *i.e.* the interatomic forces, not only the local positions of these particles are relevant but also their *electric fields*. The electric field-strength distribution around the helium atom—according to this model—is quite complicated, and, because of the rotating electrons, mostly oscillating. A detailed, three-dimensional computation is beyond the scope of this treatise. However, the following special constellation is exemplary and thus worth to be discussed in detail, namely the one along the straight line where the field strength is temporally constant, given by *the line across the nucleus and the rotation centres of the electrons*.

The respective computation is easily feasible according to the schedule given in **Figure 6** where *d* represents the distance between the focused point *P* and the nucleus. Thereof, the distances *a* and *b* can be expressed as functions of *R* and *d*, yielding

$$a^2 = (d - R)^2 + R^2 = d^2 - 2dR + 2R^2,$$

$$b^2 = (d + R)^2 + R^2 = d^2 + 2dR + 2R^2$$

The respective electric field intensities *F* are:

$$F_{\text{nucleus}} = \frac{2K}{e \cdot d^2},\ F_{\text{electron1}} = -\frac{K}{e \cdot a^2},\ F_{\text{electron2}} = -\frac{K}{e \cdot b^2}$$

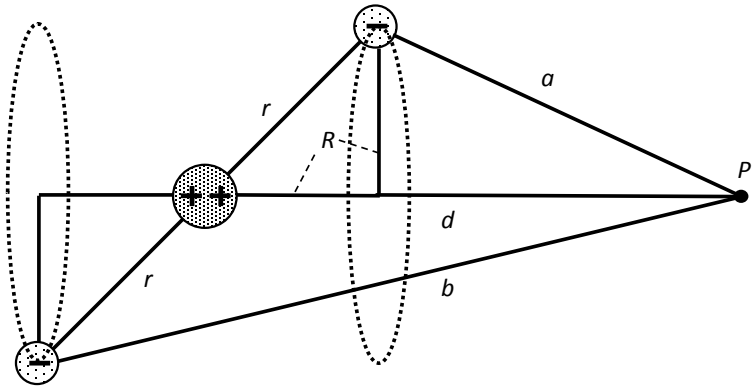

Figure 6. Field strengths of helium along the line *nucleus—electron rotation centre*s.

yielding the total value

$$F_{tot} = \frac{K}{e}\left(\frac{2}{d^2} - \frac{1}{a^2} - \frac{1}{b^2}\right) \tag{7}$$

Thereby, a positive value means that a negative charged particle is attracted, while a positive one is pushed away. According to Formula (7) and assuming invariability of r and R, the relative field strengths can be plotted versus d as a function of a multiple of R (**Figure 7**). Obviously, the total field strength exhibits a minimum which is the precondition for achieving an equilibrium distance.

However, at least two restrictions have to be made: Firstly, this field model is solely valid for dot-like charges but not for whole atoms containing several charged particles, and being three-dimensionally extended. And secondly, it is only valid along the straight line nucleus—rotation centres of the electrons. At any other points, the field strength is temporally not constant, so that temporal fluctuation of the interatomic forces could be expected, which may explain the existence of zero-point-oscillations. Overall, the conditions are too complex for computing intermolecular forces and distances, even if it were possible to use averaged values due to the inertia of the nuclei. As a consequence, distinct coherences between the atom structure and the macro-physical properties such as boiling point (4.215 K), melting point (0.95 K), and the (hexagonal) crystallographic structure (**Figure 8**) cannot be derived.

3. The Three-Dimensional Atom Model of Neon

Neon exhibits the atomic number 10 and thus ten electrons. They are placed within the first and the second atomic shells, comprising 2 and 8 electrons. The former ones represent—together with the nucleus—the core of the atom, while the latter ones are spherically arrayed in a tetrahedron of four electron couples. As an additional condition, for each electron Bohr's theorem of a constant angular momentum $h/2\pi$ must be fulfilled.

In view of the large amount of correlative electrons it does not seem feasible finding an exact mathematical solution for this problem, necessitating at least probability functions due to the perpetually changing situations. Already the fact

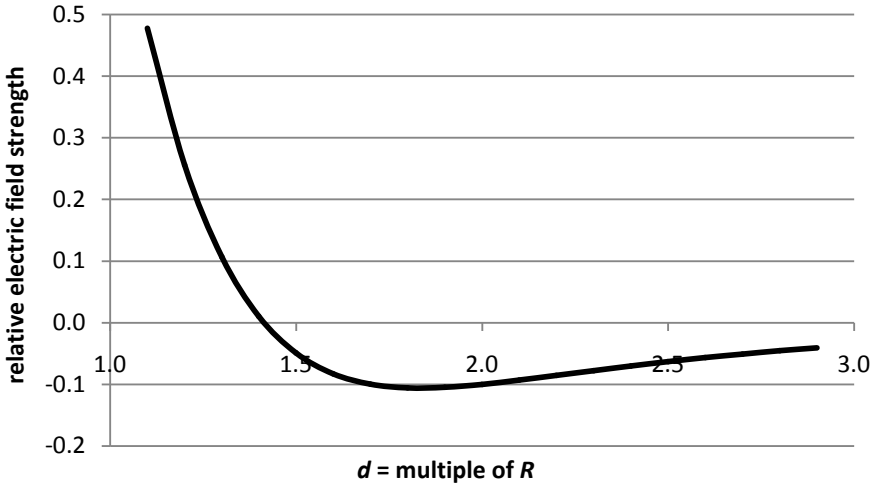

Figure 7. Relative field strength of helium as a function of the distance *d* according to Figure 6.

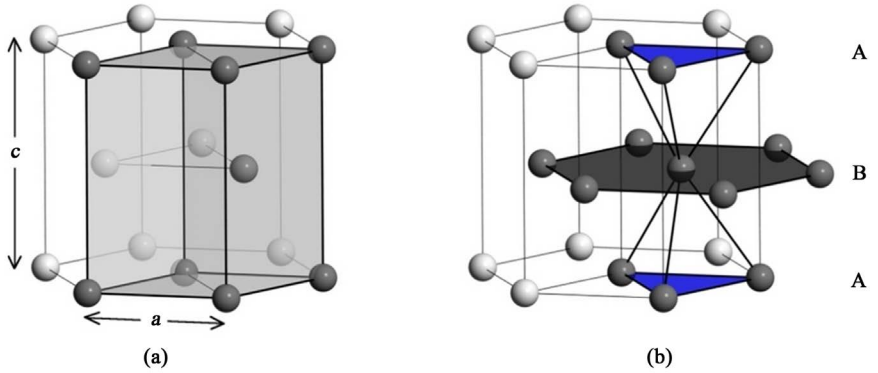

Figure 8. Schematic drafts of the hexagonal close-packing of spheres.

that the Cartesian coordinate system is orthogonal let suppose considerable difficulties for describing the tetrahedral system of the outer electron shelf, while the inner electron shelf—corresponding to the structure of the helium atom—can be described by an orthogonal system. Thus the two coordinate systems are not compatible. But even in case of the inner shelf, considerable difficulties may arise since the respective rotation trajectories of the two electrons are probably not flat but wavy, requiring the introduction of a polar coordinate system. In any case it must be assumed that the neon atom does not represent a static construction with constant electron velocities, but a dynamic one with permanently changing internal distances.

Therefore, within Figure 9 solely an intuitive ball-and-stick model can be presented here, describing a possible snap-shot. From this viewpoint the—blue coloured—two inner electrons rotate within parallel horizontal rings, one electron above and the other below the nucleus (=centre). However, these rings are probably not strictly planar but wavy, due to the—white coloured—rotating outer electron couples, acting as partial obstacles. This model does not deviate significantly from the well-known model of Kimball, but it assumes rotating

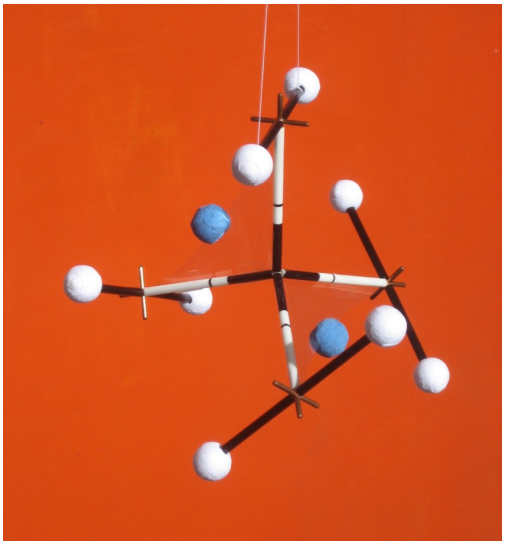

Figure 9. Rough ball-and-stick model for neon with rotating electron couples. (blue: inner shell white: outer shell).

electron rings instead of spherical electron clouds, thus the latter one may still be used for practical purposes in chemistry.

4. Summary and Conclusions

Applying Bohr's theorem of a constant angular momentum $h/2\pi$ for electrons as a consequence of the spin phenomenon, and assuming an eccentric electron rotation instead of a concentric one, the radii for a three dimensional—but not spherical—atom model of helium could easily be computed. The result appears plausible with respect to the known atomic radius even if exact empiric data are not available. Above all, precise statements about *interatomic forces* are not possible. In particular, a stringent reliance between the atomic or molecular structure and the crystallographic structure is not evident.

In contrast to the atom model of helium, the one of neon is not exactly describable and computable since too many interdependencies should be taken into account. It allows solely a rough idea of a vivid model which is characterized by rotating electron rings instead of spherical electron clouds. With respect to a mathematical modelling, one sticking point is founded by the tetrahedral structure of the outer electron shell which cannot be easily described using the orthogonal Cartesian coordinate system. Moreover, the fact that the neon atom does not represent a static construction with constant electron velocities, but a dynamic one with permanently changing internal distances, appears to be considerably complicating. Thus, the helium atom marks the limit for precisely describing an atom, whereby at and under this limit such a precise description is feasible, being also demonstrated in the author's previous work. This contradicts the conventional quantum mechanical theory which claims that such a—locally and temporally—precise description of *any* atom or molecule structure is generally not possible, also not for the H_2-molecule, and not even for the H-atom.

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