

Original Article

About Shape and Size of Atomic Hydrogen

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Abstract - Atoms are usually modeled as spheres, and their radii are often calculated using complex computational methods. This applies to the smallest atom as well as to transuranium elements. However, the smallest atom, hydrogen, occupies a special position among atoms, with only one electron and proton. In this combination, the electron's spin can only be parallel or antiparallel to the proton's spin. Due to these orientation options, the interpretation of a spherical atom appears oversimplified. This article offers an easy-to-calculate approach for the volume of atomic hydrogen. Based on Bohr's atomic model and the electron spin, a conical volume shape is derived classically. For this purpose, the electron's spin is interpreted as intrinsic angular momentum with a defined radius, which can be oriented orthogonally to Bohr's orbital plane and parallel or antiparallel to the proton's spin. The volume of the hydrogen atom determined in this way correlates with the spherical volume, which can be calculated from several literature radii.

Keywords - Bohr's atomic model, Classical calculation, Conical volume, Spin orientation, Spin radius.

1. Introduction

We owe a comprehensive description of the ancient ideas about atomism to the Roman Titus Lucretius Carus, who, in the first century BC, described indivisible primal elements from which all matter was supposed to consist [1]. These primal elements ("rerum primordia") were hard, dense, heavy and different in appearance. According to Lucretius, there are only a limited number of primal forms but an infinite number of similar primal elements. As examples, he named smooth ("levis") and round ("rotundus") primal elements, those with hooks ("hamatus") or pointed ones ("acutus").

In modern times, the smooth, round shape has become increasingly important. In the 18th century, in the transition between alchemy and chemistry, Swedenborg published his ideas about the geometric arrangement of particles in metals, salts and elements [2]. His particles are round. At the beginning of the 19th century, Dalton took up the ancient particle theory and applied it to chemistry [3]. He assigned each chemical element a specific type of primal element with a relative mass.

He chose the ancient Greek term atomos (indivisible) as the name for the primary elements and thus created the modern word atom. In his illustrations, he depicted the atoms as round balls. A hundred years later, Thomson took the theme further and formulated an atomic model consisting of a positively charged sphere with negatively charged particles arranged concentrically and rotating at high speed [4]. According to his calculations, he based the positively charged sphere on a spherical volume.

Bohr also stuck to the round shape [5]. His atom model describes a positively charged nucleus around which electrons rotate in ring orbits. Sommerfeld's extension to the Bohr model increased the atomic structure possibilities beyond the circular shape to include additional elliptical orbits [6]. A short time later, Lande' dealt with the topic of atomic size and assumed that noble gas atoms and the ions of alkali metals and halogens should be viewed as almost spherically symmetrical, or at least cube-symmetrical [7]. With the development of quantum mechanics, the shape of the atom was viewed differently. What was previously clearly defined and preferably round now acquired blur and a probability. Where Bohr and Sommerfeld assumed fixed orbits around the core, quantum mechanics speaks of location probabilities and probability densities [8-11]. There is no longer a firmly defined edge that enables the exact volume calculation. The orbitals result in spherical, dumbbell-shaped or rosette-shaped structures [12].

For our modeling, however, we consider atoms to be round spheres as a first approximation. Moreover, because we see it this way, we define radii for the atomic size. This fully describes a sphere. However, there is no one and only radius for the atoms of an element. Instead, the atomic size depends on the chemical bond between the individual atom and other atoms. As early as 1923, Wyckoff [13] published an article on the subject of atomic radii in which he pointed this out.

In the 19th century, the scientifically based estimation of particle sizes began. Lohschmidt used thermodynamic data to



estimate the diameter of an air molecule at approximately 1000 pm [14]. Thomson used a similar calculation to arrive at a minimum diameter of 20 pm for gas molecules [15]. Meyer used the parameters of density and relative atomic weight to determine a relative atomic volume [16].

With the diffraction of X-rays on crystals [17-20] and the introduction of scattering experiments [21] at the beginning of the 20th century, the direct measurement of atomic radii began. Further calculation variants were developed after the establishment of quantum mechanics. What they all have in common is the implicit question of the most suitable approach that best depicts and describes the natural conditions.

As already mentioned, the literature references differ regarding the atomic radius of an element. They depend on whether the distance between two atomic nuclei was measured or calculated in covalent, ionic or metallic compounds [22-33]. They also depend on which other physical parameters, such as pressure or temperature, are underlying [34-36]. In addition, van der Waals forces act between covalently bound molecules, the radii values of which have also been tabulated [37-39].

For the hydrogen atom, you can find very different atomic radii in the specialist literature, for example, in [22, 23, 26, 28, 29, 30, 32, 33]. Pauling noted that the numerical material for the hydrogen atom has a wider range than the numerical material for the radii of other atoms [32]. In this respect, hydrogen occupies a special position. It also occupies a special position because it consists of only one electron and one proton. For this atom, the average distance between the charges and the orientation possibilities for their spin play a role. The so-called 21 cm line is known from astronomy [40, 41]. This microwave radiation represents the hyperfine structure transition between parallel and antiparallel alignment of the proton and electron spin in atomic hydrogen. The importance of spin orientation also becomes clear using the example of molecular hydrogen. The molecule exists in two different versions [42], ortho- and para-hydrogen. The parallel or antiparallel alignment of the proton spins affects, among other things, the heat of vaporization and chemical reactivity [43].

The hydrogen atom also occupies a special position because it is sometimes used for fundamental models. It, therefore, seems sensible and desirable to extend the geometric interpretation possibilities for this atom and to put them on a basis that is easy to calculate.

Experience teaches us that the bound outer electrons limit atomic volumes. In the case of the hydrogen atom, Bohr's description of the atom offers a simple and clear approach to a geometric shape with a defined boundary [5]. Although we know that this old model does not describe the atomic conditions correctly in all details, it gives us the well-known

Bohr radius (here designated r_{H1}), which Schrödinger also used to calculate eigenfunctions [10].

If we look closer at the hydrogen atom, the spherical approach that is usually used does not seem appropriate in this case. If Bohr's circular plane, in which the electron orbits the center of mass, forms the starting point, then the atomic volume can only run either above or below this plane. The reason for this is the restricted alignment of the proton and electron spins, which can only be parallel or antiparallel. This arrangement can be captured mathematically by applying Bohr's approach in combination with an interpretation of the electron spin as an intrinsic torque with a defined radius. This avoids complex calculations and allows for a geometrically clearly defined and unambiguous result to be achieved.

2. The Electron in Bohr's Atomic Model

To describe the interaction between the proton and electron in the hydrogen atom, Bohr used Coulomb's law, which defines the electrostatic force between charges of magnitude $\pm e_0$ using the electric field constant ϵ_0 [5]. He equated this static force to the centripetal force of the circular motion of an electron with mass m_e on an orbit with radius r_{H1} and orbital velocity v_{H1} around the atomic nucleus:

$$\frac{e_0^2}{4 \pi \epsilon_0 r_{H1}^2} = \frac{m_e v_{H1}^2}{r_{H1}} \quad (1)$$

In addition, he demanded that only integer multiples of Planck's quantum of action h were permitted for the orbital angular momentum L of the electron and introduced the quantum number $n = \{1, 2, 3, \dots\}$ for this purpose:

$$L = n * m_e v_{H1} r_{H1} = n * \frac{h}{2\pi} = n * \hbar. \quad (2)$$

By transforming and combining equations (1) and (2), the smallest permissible orbital radius in the hydrogen atom with the quantum number $n = 1$ is obtained.

$$r_{H1} = 1^2 * \frac{4 \pi \epsilon_0 h^2}{m_e e_0^2} \quad (3)$$

The orbital velocity of the electron v_{H1} is calculated as

$$v_{H1} = \frac{h}{2 \pi r_{H1} m_e} = \alpha c \quad (4)$$

and corresponds to the product of the dimensionless fine structure constant α and the speed of light c .

For the electric field of a hydrogen atom, the potential energy at a distance r is defined as [44]

$$E_{pot} = - \frac{e_0^2}{4 \pi r \epsilon_0} \quad (5)$$

If the proton is considered to be quasi-stationary or slow compared to the electron, only two essential energetic contributions are included in the atomic energy balance according to the Lagrange formalism - the potential energy (5) and the kinetic energy of the electron on its orbit (6)

$$E_{kin.} = \frac{m_e v_{H1}^2}{2} \quad (6)$$

With equation (7)

$$E_{binding} = E_{pot} + E_{kin} = \frac{e_0^4 m_e}{32\pi^2 \epsilon_0^2 \hbar^2} * \frac{1}{n^2}. \quad (7)$$

Bohr obtained the binding energy for the ground state of the hydrogen atom. On closer inspection, it became apparent that similar to the planetary Kepler problem, taking into account the co-motion of the proton led to more precise results.

Therefore, Bohr replaced the mass of the electron with the reduced mass m_r [45]

$$m_r = \frac{m_e * m_p}{(m_e + m_p)} \quad (8)$$

and corrected the binding energy in the hydrogen atom to

$$E_{binding\ H1} = -\frac{e_0^4 m_r}{32\pi^2 \epsilon_0^2 \hbar^2} * \frac{1}{n^2} \quad (9)$$

3. The Spin

In 1925, Uhlenbeck and Goudsmith proposed attributing a further intrinsic property to the electron in addition to its mass and charge [46]. The additional degree of freedom was introduced under the name spin.

This was intended to explain observations such as the splitting of the electron beam in the Stern-Gerlach experiment or the Zeeman effect, which are otherwise incomprehensible.

In 1927, Pauli treated spin mathematically by introducing the spin quantum number $s = 1/2$ and the spin operator.

$$\hat{S} = (\hat{S}_x, \hat{S}_y, \hat{S}_z) \quad (10)$$

whose magnitude is calculated as [48]

$$|\hat{S}| = \sqrt{s(s+1)} \hbar = \sqrt{\frac{3}{4}} \hbar \quad (11)$$

The spin can be aligned parallel or antiparallel to a magnetic field. Therefore, the operator \widehat{S}_{field} has the two eigenstates $\pm \frac{\hbar}{2}$ in the direction of the magnetic field. For the two operators in the orbital plane \hat{S}_1 and \hat{S}_2 , the expected values are zero.

The spin has the properties of an intrinsic angular momentum. Hawking writes that there are particles that only look the same again after two complete rotations. The spin of these particles is given as $1/2$ [48]. These particles include the electron and, since 1927, also the proton, to which Dennison assigned a spin with the quantum number $s = 1/2$ [49].

4. Results and Discussion

In summary, it can be stated that Bohr's considerations in the case of the hydrogen atom describe a circular plane in which the electron and proton move around a common center of gravity - the proton close to the center and the electron at a distance r_{H1} . Suppose you place this circular plane arbitrarily in the x. In that case, in the y plane of a Cartesian coordinate system, the alignment of the proton and electron spins along the z-axis automatically results.

Pauli's derivation of spin seems as if he were describing a moving electron in a magnetic field generated by itself. Such a field would be able to exert a force on the electron. This magnetic force could change the direction of the velocity but not its magnitude.

If the electron's spin is interpreted this way, the amount of momentum remains unchanged at the value.

$$|p_e| = m_e |v_{H1}|. \quad (12)$$

Since the two angular momenta orbital angular momentum and spin are defined by the cross product of momentum and respective radius, the corresponding radii provide the spatial lengths required for the volume calculation. To simplify matters, the spin radius of the electron is required to be orthogonal to the Bohr plane. Its absolute value is calculated using Equations (2), (11) and (12) with the result.

$$r_{SE} = \sqrt{\frac{3}{4}} r_{H1} \quad (13)$$

Therefore, the sphere of influence of the electron extends in the Bohr circle plane over the distance of the orbital radius r_{H1} and in the atomic z-direction in the distance r_{SE} . This situation can be represented in a two-dimensional coordinate system. The abscissa axis is selected for the atomic z-direction. The function values of a linear function $f(r)$ defined by the atomic center of mass at $(0 | 0)$ and the position of the electron at $(0 | 1)$ are plotted on the ordinate axis. The abscissa axis and ordinate axis are divided into multiples of the Bohr radius (r/r_{H1}) so that the distance between the center of mass and the electron on the ordinate axis corresponds exactly to the Bohr radius. As required above, the spin radius r_{SE} of the electron is oriented at right angles to the Bohr radius. The connecting line between the atomic center of mass and the tip of the spin vector lies on a straight line with the functional equation

$$f(r) = \frac{r_{H1}}{r_{SE}} * r \quad (14)$$

The result is a pointed cone with the height r_{SE} , the Bohr circle plane as the base and the volume

By rotating the function $f(r)$ around the r -axis in the interval $[0, \sqrt{\frac{3}{4}}]$ the required volume can be determined as

$$V = \frac{\pi r_{H1}^3}{3} * \sqrt{\frac{3}{4}} \quad (16)$$

$$V = \pi \int_0^{\sqrt{\frac{3}{4}}} (f(r))^2 dr \quad (15)$$

Using the numerical value for the Bohr radius, equation (16) gives the hydrogen atom a volume of $1.35 * 10^{-31} \text{ m}^3$.

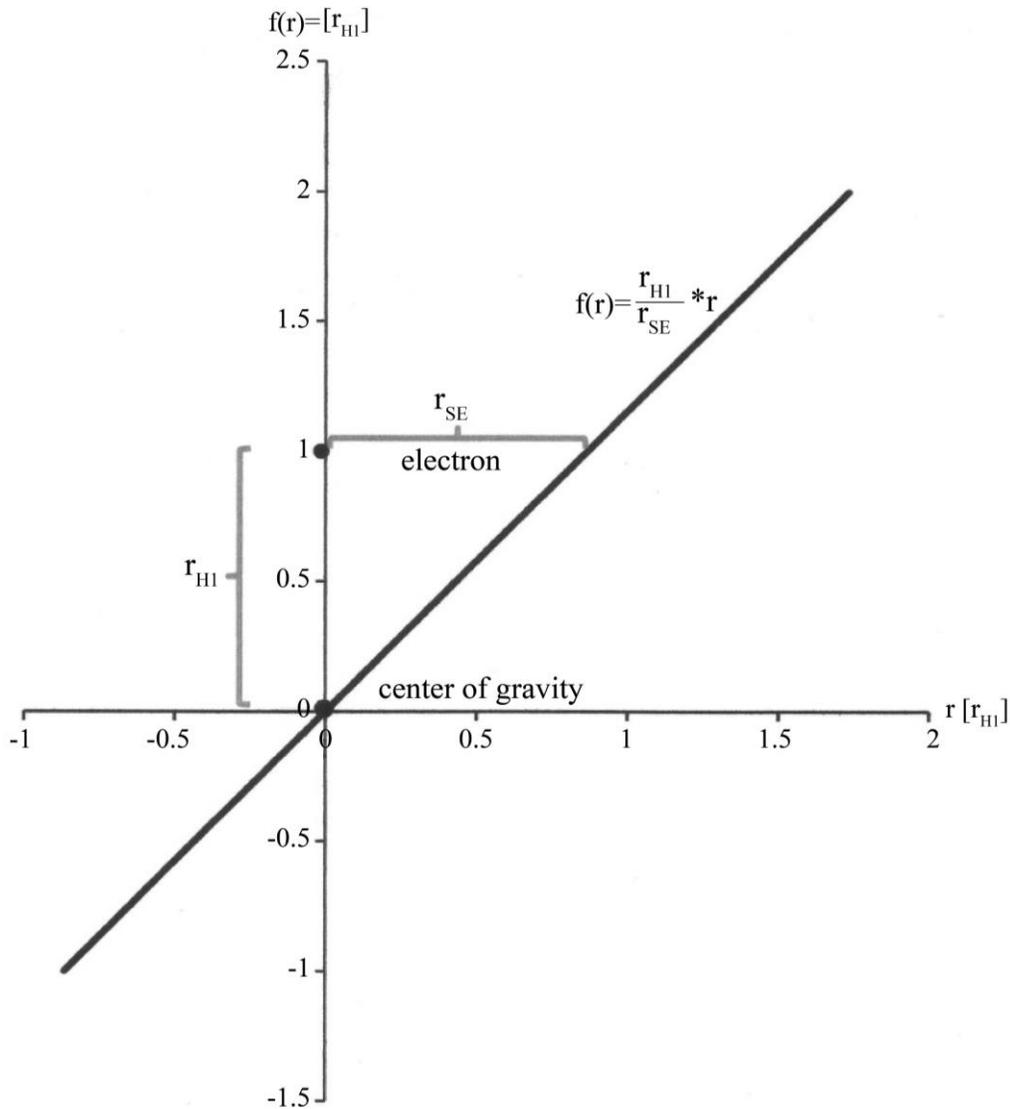


Fig. 1 Graph of the function $f(r)$.

The center of gravity of the atom and the electron are at a distance of r_{H1} (Bohr radius) from each other. The spin radius of the electron is perpendicular to it. The spin radius and the center of gravity of the atom are on the straight line $f(r) =$

$\frac{r_{H1}}{r_{SE}} * r$. The abscissa axis and the ordinate axis are divided into multiples of the Bohr radius r_{H1} .

Table 1. Comparison of calculated volumes for atomic hydrogen

Author	Atomic Shape	Radius r (pm)	Volume V (m ³)
Pauling [32]	sphere	28 to 37	0,9*10 ⁻³¹ to 2,12*10 ⁻³¹
Pyykkö [29]	sphere	32	1,37*10 ⁻³¹
Cordero [28]	sphere	31	1,25*10 ⁻³¹
this work	cone	53	1,35*10 ⁻³¹

No example of a three-dimensional cone with a circular base as the volume of a hydrogen atom could be found in modern technical literature. Therefore, a direct comparison of the radius values is not expedient.

However, a comparison of the calculable atomic volumes can provide clarity about the extent to which the result obtained deviates from the literature values. Therefore, it is compared with the radius data of three authors as an example.

Pauling [32] quotes radius values between 28 pm and 37 pm for the hydrogen atom. The resulting volumes are between 0.9*10⁻³¹ m³ and 2.12*10⁻³¹ m³. Pyykkö and Atsumi [30] state the covalent bond radius to be 32 pm. The associated volume is 1.37*10⁻³¹ m³. Cordero et al. [28] mention 31 pm for the covalent bond radius, from which a volume of 1.25*10⁻³¹ m³ can be calculated. The numerical value of 1.35*10⁻³¹ m³ from this article fits seamlessly into the range specified by the literature data. The outcomes are summarized in Table 1.

5. Conclusion

With the new model of the hydrogen atom presented here, a volume approach has been developed that is both easy to derive and calculate and geometrically unambiguous. The approach combines the influence of the electron via its nuclear distance in Bohr's atomic model with the range of its spin. The influence of the spin radius on the atomic dimensions is thus explicitly taken into account. In the model, the Bohr circle is viewed as an equatorial plane laid out in the x and y directions. Orthogonal to this, the proton and electron spins can only align themselves in two orientations to each other along the z-axis - parallel or antiparallel. This means the electron can only have a spin orientation north or south of the Bohr surface, and a spherical volume is impossible. This is because a single electron cannot adopt both spin orientations simultaneously. In contrast to the usually assumed spherical volume, the geometric result of this work is a cone. Despite the different atomic shapes and the different atomic radii, the atomic hydrogen volume determined in this article correlates with some literature values.

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