How Large Is An Atom?

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Abstract

The atomic radius of a chemical element is a measure of the size of its atoms. Atomic radii represent the sizes of isolated and electrically neutral atoms. In this paper, simple calculations for radii of hydrogen, helium and neon are given. Victor Weisskopf has calculated the radii of different atoms. To calculate the potential energy of electrons due to mutual repulsion among them, Weisskopf has assumed that the effective distance r_{eff} between two electrons is $r/0.6$, where r is the radius of the orbit of electrons. There is a good agreement between the calculated values and the experimentally measured values of the radii of atoms. The atomic radii gradually decrease along each period of the periodic table, from the alkali metals to the noble gases; and increase down each group. The radii of isolated neutral atoms range between 0.3 and 3 angstroms. The radius of an atom is a function of its environment.

1. Introduction

Victor Weisskopf has calculated the radii of different atoms. To calculate the potential energy of electrons due to mutual repulsion among them, Weisskopf has assumed that the effective distance r_{eff} between two electrons is $r/0.6$, where r is the radius of the orbit of electrons. The atomic radius of a chemical element is a measure of the size of its atoms. Atomic radii represent the sizes of isolated and electrically neutral atoms.

The rest of the paper is organised as follows. The sizes of the hydrogen atom, helium atom and neon atom are given in Section 2, Section 3 and Section 4 respectively. General discussion on atomic size is presented in Section 5. Conclusions are given in Section 6.

2. The size of hydrogen atom

According to Bohr, electrons go round the nucleus in certain circular orbits, known as Bohr orbits. The velocity v of the electron in a circular orbit of radius r satisfies the quantization condition

$$m_e v r = n\hbar \qquad (1)$$

where, m_e the mass of the electron is 9.1 x 10^{-31} Kg.

$\hbar = h/2\pi$, h = Planck's constant = 6.62 x 10^{-34} J-s

n = No. of the orbit of the electron = $1, 2, 3, \ldots\ldots$

n is known as *principal quantum number*.

According to (1), the angular momentum of an electron revolving around the nucleus in a circular orbit is an integral multiple of $\hbar$ .Only those circular orbits for which (1) is true are allowed.

Let us find out the radius of first Bohr orbit of hydrogen atom. The kinetic energy K of electron revolving around the proton in hydrogen atom is given by

$$K = \frac{p^2}{2m} \qquad (2)$$

where $p = m_e v$ = the momentum of the electron. Electrons can behave both as particles and waves, known as de Broglie waves. According to de Broglie, the electron wavelength λ is given by

$$\lambda = h/p \qquad (3)$$

Using (3) in (1), we have for first orbit $(n = 1)$

$$r = \frac{\hbar}{m_e v} = \frac{h}{2\pi p} = \frac{\lambda}{2\pi}$$

$$\Rightarrow \lambda = 2\pi r \qquad (4)$$

This equation shows that one electron wave is wrapped around the first orbit. Substituting (3) and (4) in (2), we get

$$K = \frac{h^2}{2m_e\lambda^2} = \frac{\hbar^2}{2m_e r^2} \qquad (5)$$

The potential energy V of the electron is due to electrostatic interaction and gravitational interaction between itself and the proton.

The gravitational potential energy of the electron = $V_g = -\frac{Gm_p m_e}{r}$

The electrostatic potential energy of the electron = $V_e = -\frac{e^2}{4\pi\varepsilon_o r}$

Where, G = gravitational constant = 6.67×10^{-11}m^3/Kg-S^2

m_p= mass of a proton = 1.67 x 10^{-27} Kg

ε = permittivity of free space = 8.85 x 10^{-12} F/m

e = charge of an electron = 1.6 x 10^{-19} C.

Now the ratio

$$\frac{V_g}{V_e} = \frac{4\pi\varepsilon_o G m_p m_e}{e^2} \approx \frac{1}{2.27\times10^{39}}$$

This value shows that the gravitational attraction between proton and electron in hydrogen atom is very much weaker than electrostatic attraction. Hence the gravitational potential V_g can be neglected in comparison with electrostatic potential . The V_g n the potential energy V of the electron is given by

$$V \approx V_e = -\frac{e^2}{4\pi\varepsilon_o r} \qquad (6)$$

The total energy E of the electron is obtained by adding (5) and (6).

$$E = K + V = \frac{\hbar^2}{2m_e r^2} - \frac{e^2}{4\pi\varepsilon_o r} \qquad (7)$$

To find the value of r, when E is minimum, we must set the derivative $\frac{dE}{dr}$ equal to zero.

$$\frac{dE}{dr} = -\frac{\hbar^2}{m_e r^3} + \frac{e^2}{4\pi\varepsilon_o r^2} = 0$$

$$\Rightarrow r = 4\pi\varepsilon_o \frac{\hbar^2}{m_e e^2}$$

This particular value of r when E is minimum is denoted by a_o, known as *Bohr radius*.

$$\therefore\ a_o = 4\pi\varepsilon_o \frac{\hbar^2}{m_e e^2}$$

$$= 0.528\times10^{-10}\text{m} = 0.528\text{Å} \qquad (8)$$

The state of the hydrogen atom corresponding to the orbit with radius equal to *Bohr radius* a_o is called the *ground state*.

Now let us consider the case where the electron is in the second Bohr orbit. Since the energy of this state is higher, it is known as *first excited state*. From (1), we have for the first excited state (n = 2)

$$m_e v r = 2\hbar$$

$$\Rightarrow r = 2\frac{\hbar}{m_e v} = 2\left(\frac{h}{2\pi p}\right)$$

Using (3) in the above expression, we obtain

$$2\pi r = 2\lambda \qquad (9)$$

This equation shows that two wavelengths would be wrapped around the second orbit. Using (9), the kinetic energy of the electron in the second orbit is given by

$$K = \frac{h^2}{2m_e\lambda^2} = 4\left(\frac{\hbar^2}{2m_e r^2}\right) \qquad (10)$$

The potential energy of the electron in the second orbit is given by same equation (6). The energy E of the electron in the second orbit is obtained by adding (6) and (10).

$$E = 4\left(\frac{\hbar^2}{2m_e r^2}\right) - \frac{e^2}{4\pi\varepsilon_o r}$$

Equating $\frac{dE}{dr}$ to zero, we get

$$r_1 = 4\left[4\pi\varepsilon_o\left(\frac{\hbar^2}{m_e e^2}\right)\right] \qquad (11)$$

Where, r_1 = radius of second orbit

Using (8) in (11), we get

$$r_1 = 4a_o = 2^2 a_o \qquad (12)$$

This expression shows that the radius of second orbit is four times the radius of first orbit. So, in general the radius of n th orbit of hydrogen atom is $n^2 a_o$.

3. The size of helium atom

There are two electrons in the helium atom and its nucleus consists of two protons and two neutrons. In the ground state both these electrons rotate in the same orbit around the nucleus.

Using (5) the kinetic energy K of two electrons in helium is given by

$$K = 2\left(\frac{\hbar^2}{2m_e r^2}\right) \qquad (13)$$

The potential energy of the two electrons due to the electrostatic attraction of the nucleus having the charge +2e is

$$V_1 = 2\left(-\frac{2e^2}{4\pi\varepsilon_o r}\right) = -4\left(\frac{e^2}{4\pi\varepsilon_o r}\right) \qquad (14)$$

To calculate the net potential energy of two electrons, we have to take into account the electrostatic repulsion between the electrons also. The minimum distance between the two electrons is zero (Figure 1a), but that would lead to infinite energy, which is unacceptable. The maximum possible distance between the two electrons is $2r$ (Figure 1b).

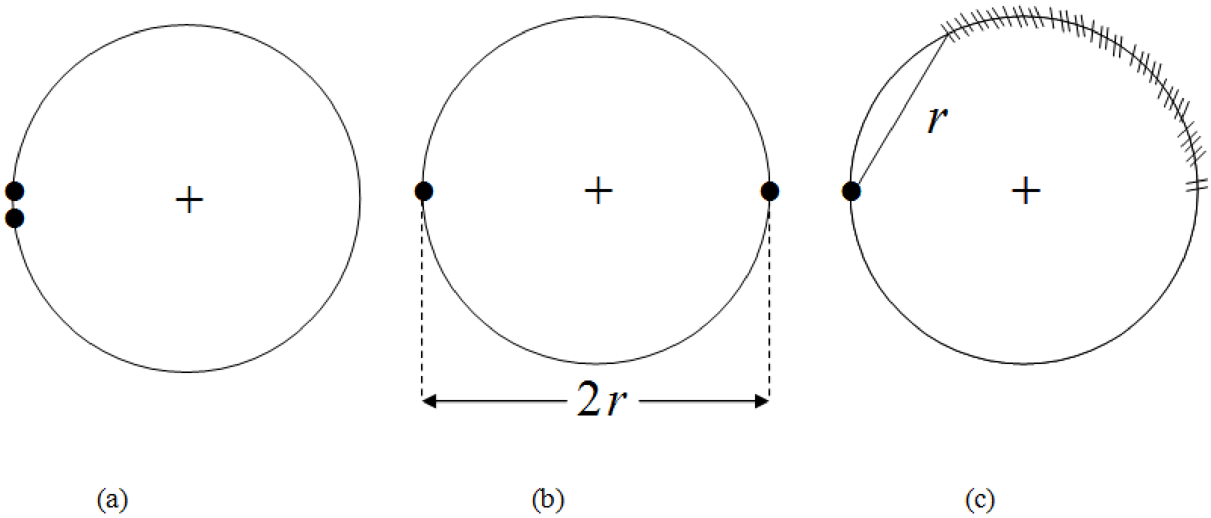

Figure1. Two electrons in the lowest orbit of helium (a) shows a case which is ruled out because of infinite repulsion energy (b) shows the maximum distance between two electrons (c) shows that the second electron is somewhere in the shaded region according to Weisskopf.

According to Weisskopf, the two electrons on the average are at a distance r_{eff} apart (Figure 1c), such that

$$r < r_{eff} < 2r \qquad (15)$$

Weisskopf has assumed that the effective distance r_{eff} between two electrons is $r/0.6$.

$$r_{eff} = \frac{r}{0.6} \qquad (16)$$

Hence, the potential energy of the two electrons due to electrostatic repulsion between them is given by

$$V_2 = \frac{1}{4\pi\varepsilon_o}\left(\frac{e^2}{r_{eff}}\right)$$

Substituting (16) in the above expression, we get

$$V_2 = \frac{0.6}{4\pi\varepsilon_o}\left(\frac{e^2}{r}\right) \qquad (17)$$

Addition of (14) and (17) gives the net potential energy V of two electrons.

$$V = V_1 + V_2 = (-4 + 0.6)\frac{e^2}{4\pi\varepsilon_o r}$$

$$\Rightarrow V = (-3.4)\frac{e^2}{4\pi\varepsilon_o r} \qquad (18)$$

The total energy E of two electrons is found out by adding (13) and (18).

$$E = 2\left(\frac{\hbar^2}{2m_e r^2}\right) - (3.4)\frac{e^2}{4\pi\varepsilon_o r} \qquad (19)$$

Equating $\frac{dE}{dr}$ to zero, the radius of the orbit of two electrons of helium atom in the ground state is given by

$$r = \frac{2}{3.4}\left(4\pi\varepsilon_o \frac{\hbar^2}{m_e e^2}\right)$$

Using (8) for *Bohr radius* in the above expression, we have

$$r \approx 0.588 a_o \approx 0.6 a_o \qquad (20)$$

4. The size of neon atom

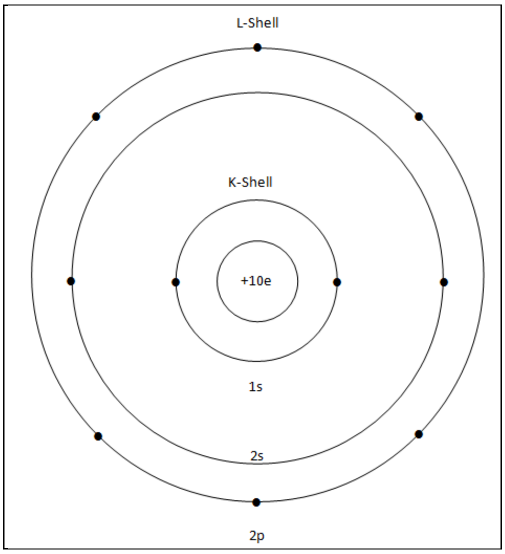

Figure 2. Arrangement of electrons in neon atom.

Neon atom has 10 electrons. These electrons are present in two shells, K-shell and L-shell. K-shell has one sub shell, 1s, and L-shell has two sub shells, 2s and 2p. The electronic configuration of Ne atom is $1s^2$, $2s^2$, $2p^6$. The arrangement of electrons in neon atom is shown in Figure 2.

Weisskopf has calculated the radius of L-shell. The electrons in L-shell see the nucleus which has a charge +10e and also they see the two electrons in K-shell. So,

the net charge seen by electrons of L-shell is +10e - 2e = +8e. The radius L-shell is calculated by taking the effective nuclear charge as Z_{eff} = +8e.

The kinetic energy K of electrons in the L-shell is calculated by taking it as the second orbit of hydrogen atom. As per (10), the contribution of each electron in L-shell to kinetic energy is $4\hbar^2/2m_e r^2$. Since L-shell contains 8 electrons, we have

$$K = 8 \times \left(\frac{4\hbar^2}{2m_e r^2}\right) = 32\left(\frac{\hbar^2}{2m_e r^2}\right) \qquad (21)$$

The potential energy of 8 electrons in L-shell is calculated by taking into account the electrostatic attraction on these electrons by the nucleus with effective charge +8e as well as the repulsive forces among these electrons.

The potential energy of 8 electrons in L-shell due to electrostatic attraction of nucleus having effective charge +8*e* is given by

$$V_1 = 8\times\left(-\frac{8e^2}{4\pi\varepsilon_o r}\right) \qquad (22)$$

The 8 electrons in L-shell are formed into pairs to calculate the potential energy due to repulsive forces among them. The 8 electrons can be formed into $\frac{8x7}{2}$ =28 distinct pairs. As in helium atom, the effective distance r_{eff} between two electrons of a pair is taken as $r/0.6$.Since there are 28 pairs of electrons, the potential energy of electrons in L-shell due to repulsive forces among them is given by

$$V_2 = 28\times\left(\frac{e^2}{4\pi\varepsilon_o r_{eff}}\right)$$

$$= 28\times 0.6\left(\frac{e^2}{4\pi\varepsilon_o r}\right) \qquad (23)$$

The total potential energy *V* of electrons in L-shell is found out by adding (22) and (23),

$$V = V_1 + V_2 = \left(-8^2 + 28\times 0.6\right)\frac{e^2}{4\pi\varepsilon_o r}$$

$$\Rightarrow V = -47.2\times\frac{e^2}{4\pi\varepsilon_o r} \approx -47\left(\frac{e^2}{4\pi\varepsilon_o r}\right) \qquad (24)$$

Addition of (21) and (24) gives the total energy *E* of electrons in L-shell.

$$E = 32\left(\frac{\hbar^2}{2m_e r^2}\right) - 47\left(\frac{e^2}{4\pi\varepsilon_o r}\right)$$

Equating $\frac{dE}{dr}$ to zero, the radius of the orbit of electrons in L-shell of neon atom in the ground state is given by

$$r = \frac{32}{47}\left(4\pi\varepsilon_o\frac{\hbar^2}{m_e e^2}\right)$$

Using (8) in the above expression, we get

$$r = \frac{32}{47}a_o \approx 0.7a_o \qquad (25)$$

Similar calculations can be made for other atoms using very simple physical arguments. In all cases, the effective distance between any two electrons r_{eff} in any orbit of radius *r* is taken as *r*/0.6. There is good agreement between the calculated value of radius of an orbit of an atom and the experimental value.

In general the radius of *n*th shell is given by

$$r = \frac{n^2}{Z_{eff} - \left(Z_{eff} - 1\right)\times 0.3} \qquad (26)$$

Where, Z_{eff} = effective atomic number of the atom

5. General discussion on atomic size

Table 1 compares the calculated values of atomic radii with the measured values for the first ten elements. There is a good agreement between the calculated values and the experimentally measured values of the radii of atoms.

Table1. Atomic radii of first ten elements

Element	***Z***	***Zeff***	***n***	***r* in units of *ao* (calculated)**	***r* in units of *ao* (measured)**
H	1	1	1	1.0	1.0
He	2	2	1	0.6	0.6
Li	3	1	2	4.0	2.8

Be	4	2	2	2.4	2.2
B	5	3	2	1.7	1.6
C	6	4	2	1.3	1.2
N	7	5	2	1.1	1.0
O	8	6	2	0.9	0.8
F	9	7	2	0.8	0.7
Ne	10	8	2	0.7	0.6

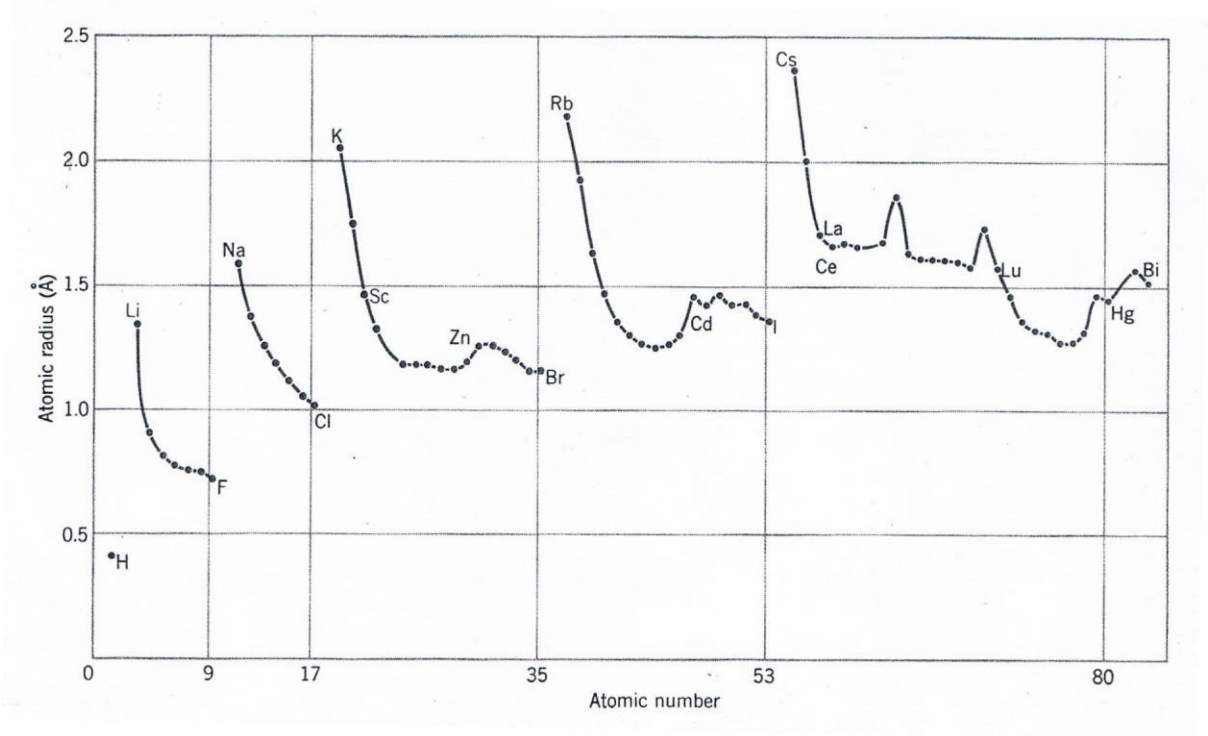

Figure 3. Variation of atomic radius with atomic number.

The variation of atomic radius or atomic size with atomic number for the elements is shown in Figure 3. The following general conclusions can be drawn from this plot.

1. The alkali elements Li, Na,. . . etc., have large radii.
2. Following each alkali element, there is a progressive decrease in atomic radii from left to right along a period in the periodic table.
3. The atomic radius increases sharply between the noble gas at the end of each period and the alkali metal at the beginning of the next period.
4. As we proceed down each group of the periodic table, the atomic radius gradually increases.
5. The variation in atomic size across a period is not always a smooth one, as irregularities are occurring in period 6.

Within a given period, the atomic radius decreases with increasing atomic number owing to the effect of increasing the positive nuclear charge while adding electrons to the same level. Therefore, the effective nuclear charge towards the outermost electrons increases, drawing the outermost electrons closer. As a result, the electrons cloud contracts and the atomic

radius decreases. In a noble gas, the outermost shell is completely filled. Therefore, the addition of electron of next alkali metal will go into a new outer shell, accounting for the sudden increase in the atomic radius.
Within a given group, the atomic radius increases with atomic number because of addition of another level. As we proceed downward from one atom to another within a group, each successive element has its outer electrons in a shell with larger value of *n*. The effective nuclear charge felt by these electrons stays nearly the same, so the dominant effect is an increase in size of the atom that accompanies an increase in the value of the principal quantum number of the outer-shell orbital.

The radii of isolated neutral atoms range between 0.3 and 3 angstroms. Caesium is the largest known atom. The atomic radius of Cs is given variously as 273.1pm, 265pm, 265.5pm or 260pm (1pm $= 1\times10^{-12}$m). Caesium has a large valence shell and relatively low effective nuclear charge. A low nuclear charge means that electrons can wander further, on average, from the nucleus. Rubidium also has large atoms, but its atomic radius is almost 30pm less than that of caesium.
The radius of an atom is a function of its environment. An example is the hydrogen atom, which is assigned with one radius when it combines with itself, a second radius when it combines with the elements of the second period, a third radius when it combines with the elements of the third period, and so on.

6. Conclusion

Victor Weisskopf has calculated the radii of different atoms. The atomic radius of a chemical element is a measure of the size of its atoms. There is a good agreement between the calculated values and the experimentally measured values of the radii of atoms. The atomic radii gradually decrease along each period of the periodic table, from the alkali metals to the noble gases; and increase down each group. The radii of isolated neutral atoms range between 0.3 and 3 angstroms. The radius of an atom is a function of its environment.

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