HELIUM-LIKE ATOMS

Vladislav Konovalov

Abstract

In the article the theory of helium-like atoms is given

The constitution of atom is a corollary of aspiration of any system to a minimum of a potential energy, instead of any selection rules or certain composition of quantum numbers. The aspiration to a minimum of a potential energy is sufficient, exhausting for exposition of atoms.

"In a basis of an operation by notion about the character of a state of an electron in atom with the help of four quantum numbers (n, l, m_l, m_s) lies the principle of the prohibition (or principle of elimination), formulated by Pauli. According to a Pauli's exclusion principle, in atom there can not be two electrons, the state which one would be featured by completely identical combination of values of termed above four quantum numbers; even one of them should accept different values". "About a systematic of particles", M., 1969, page 12. It seemed, the official physics can shout: "Hurrah!" and to figure electronic configurations of all atoms. But is not present! Nothing is gained, will not apply yet rule of Gund: "...the electrons in limits of a given subshell aim to lie so that value of their summary spin was maximal..." (Ibidem, page 14). Feel an inconsistency with a Pauli's exclusion principle? One requires a miscellaneous state of electrons, another - identical. "On the basis of a Pauli's exclusion principle in combination to a rule of Gund it is possible to give the scheme (so-called, ideal scheme), describing allocation of electrons according to values of quantum numbers" (Ibidem, page 14). Well, now that, is possible to shout "hurrah"? Certainly, is not present! The following quotation is rather characteristic for orthodox thinking. "Nevertheless, the tendency was widely spread to consider the ideal scheme just normal, while the actual periodic system was considered as abnormal, as a special case of an abnormal, irregular development of periodicity. This inconsistency, certainly, braked further development of the theory of periodic system. To overcome this inconsistency, it was necessary to refuse not only notion about a dominant role of a main quantum number n (here to you, grandmother, and main quantum number! - V.K.) in definition of sequence of shaping of electronic configurations of multielectronic atoms, but also that generally energy state of an electron in multielectronic atom is always predominantly determined by a main quantum number" (Ibidem, page 21). For the first time a dominant role of a main quantum number has refused V.M. Klechkovsky, by formulating ($n+l$) - rule: "This regularity most clearly is uncovered, if a grouping of quantum levels of electrons in atom to subordinate to a principle grounded at integrating in one group of levels with identical value of the sum main (n) and orbital (l) quantum numbers" (Ibidem, page 22). All this waste of time with a bedding of rules against each other has, at the end, pessimistic finale: "We should, first of all to mark, that the actual scheme of shaping of electronic configurations of atoms in some cases appears not so strictly series, as it should stream from ($n+l$) - rule. Three basic types of discrepancies are watched" - further they are numbered (Ibidem, page 40).
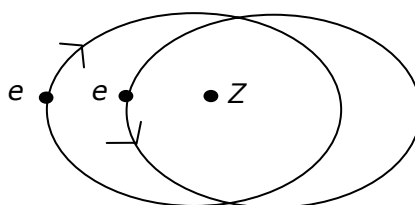

Fig. 1

Let's consider two-electronic atom figured on a figure 1. It is possible to show, that the orbits of electrons are not elliptic, but only ellipsoidal, however, for simplicity of calculations it is possible to accept by their elliptic, exchanging an actual orbit by an equivalent ellipse.

Thus we, naturally, any more can not expect for rigorous quantitative concurrence to experimental data, but those basically is impossible at interaction of many bodies. On a figure mechanical and of the magnet moments of electrons are figured antiparallel, since only at such standing the system will have a minimum potential energy. Interaction of magnet moments to allow here we shall not be. As a first approximation, without them the results will be received quite good as against a quantum mechanics, which one is salvaged only by viewing of this interaction. "The identity of identical particles gives in a quantum mechanics in particular interaction between them, termed by an exchange interaction. ... The exchange energy has not classic analog.... It is impossible to interpret quantities termed sometimes as exchange density, as customary densities of charge: they can be and complex.... The exchange energy is electrostatic - it is proportional to a quadrate of elementary charge.... The more degree of overlapping of wave functions ("of electronic clouds"), the more exchange energy.... Due to an exchange energy in the same system can exists both attractive force and repulsive force". "Physics of a microcosm", "Soviet encyclopedia", M., 1980, page 42-43. In spite of the fact that in this problem of physicists fully darken, as a matter of fact there are only two versions of interpretation of an exchange interaction: or this attractive interaction of antiparallel of magnet moments of electrons (or the repulsion parallel), or is necessary to introduce a new view of interaction. For many reasons both these of version do not approach at all for a quantum mechanics, therefore the exchange interaction has not physical sense.

Position of electrons relevant fig. 1, one in pericentre of an orbit, another - in an apocenter. The blanket binding energy of both electrons $E_{tie1,2}$ is similar to expression (13.1) [1], will make expression:

$$E_{tie1,2} = \frac{m\alpha^2}{2}\left[\frac{1}{(a+C)^2}+\frac{1}{(a-C)^2}\right]-Ze^2\left(\frac{1}{a+C}+\frac{1}{a-C}\right)+\frac{e^2}{2C}-\frac{e^2}{2C} \qquad (1).$$

In (1) last two terms mutual cancel out, since the electrostatic energy interaction of electrons among themselves urges an electron in pericentre "to be attracted" to a nucleus, and electron in an apocenter - "to be repelled". Exchanging in (1) C through eccentricity ℓ, after transformations we shall discover:

$$E_{tie1,2} = \frac{m\alpha^2\left(1+\ell^2\right)}{a^2\left(1-\ell^2\right)^2}-\frac{2Ze^2}{a\left(1-\ell^2\right)} \qquad (2).$$

Differentiating (2) on a and equating a derivative to zero point, we shall discover a semimajor axis of a stationary orbit:

$$a_0 = \frac{m\alpha^2}{Ze^2}\left(\frac{1+\ell^2}{1-\ell^2}\right) \qquad (3).$$

By substituting (3) in (2), we shall discover a binding energy in a ground state:

$$E_{tie1,2}^0 = -\frac{Z^2e^4}{m\alpha^2\left(1+\ell^2\right)} \qquad (4).$$

Apparently, that $E_{tie1,2}^0$ is the sum of the first E_1^0 and second E_2^0 potentials of ionization helium-like of atom. E_2^0 we already know for hydrogen-like atoms, therefore:

$$E_1^0 = -\frac{Z^2e^4}{2m\alpha^2}\left(\frac{1-\ell^2}{1+\ell^2}\right) \qquad (5).$$

From (5) or (4) on experimental potentials of ionization it is easy to find eccentricities of stationary orbits (numeral at e means nuclear charge helium-like of atom): $e_2= 0.6143$, $e_3= 0.4859$, $e_4= 0.4141$, $e_5= 0.3667$, $e_6= 0.3325$, $e_7= 0.3062$, $e_8= 0.2853$, $e_9= 0.2678$, $e_{10}= 0.2534$, $e_{11}= 0.2408$.

In calculation on one electron, is similar (13.4) [1], we shall note:

$$E_{tie1} = \frac{m\alpha^2\left(1+\ell^2\right)}{2a^2\left(1-\ell^2\right)^2}-\frac{Ze^2}{a\left(1-\ell^2\right)}+\frac{mV_c^2}{2} \qquad (6),$$

and designate:

$$E_{tie1} = K \frac{E^0_{tie1,2}}{2} = -\frac{KZ^2 e^4}{2m\alpha^2(1+\ell^2)} \qquad (7),$$

from (6) with the registration (7) we shall discover V_c, differentiated it on a, we shall be convinced, that the maximum value V_c^{max} corresponds $a = a_0$ and we shall discover:

$$V_c^{max} = \frac{Ze^2}{m\alpha} \sqrt{\frac{1-K}{1+\ell^2}} \qquad (8).$$

Allowing, $V_m = V_0 = \frac{Ze^2}{m\alpha}$ and $V_c = \frac{V_0}{n}$ at radiation of photons, comparing with (14.8), we shall discover:

$$K = 1 - \frac{1+\ell^2}{n^2} \qquad (9).$$

By substituting (9) in (7), we shall receive:

$$E_{tie1} = -\frac{Z^2 e^4}{2m\alpha^2(1+\ell^2)} \left(1 - \frac{1+\ell^2}{n^2}\right) \qquad (10),$$

then energy of a photon:

$$h\nu = E'_{tie1} - E''_{tie1} = W\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \qquad (11).$$

The formula (11) is valid for any electron in any atom, if W to consider as function n_1 and n_2. This equation can be received and from more blanket reasons. The radiation of a photon for atoms containing more of one electron though will be determined by transition of a given electron to more low-altitude orbit, but the value of energy of a photon will depend any more only on an difference of a binding energy of a given electron, but also all remaining electrons, as there is a self-acting restructuring of all atom. Besides an electrostatic energy interaction of electrons among themselves simultaneously varies also. Therefore for any electron in any atom:

$$h\nu = E^0\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) + \Delta E \qquad (12),$$

where ΔE - some function from n_1 and n_2, and E^0 - electron-binding energy in a ground state. Equating (12) anyone known semiempirical or absolutely empirical-formula dependences, is successful approaching for exposition of spectrums, we always shall discover ΔE in an explicit view. The known dependences usually enable as a matter of fact not integer values n_1 and n_2. For example, the frequencies of lines in spectrums of alkaline elements are determined by the formula:

$$\nu = Rc\left[\frac{1}{(n_1 - \Delta i_1)^2} - \frac{1}{(n_2 - \Delta i_2)^2}\right],$$

where Δi - correction (so-called quantum defect). For each element of values of the correctionы are various, besides they are various and for the same element depending on value of an orbital quantum number l. R - constant of a Rydberg. G.E. Pustovalov "Atomic and nuclear physics", Publishing House of the Moscow University, 1968, page 118.

We shall not be so was easily, as it is done by a modern physics, to change to idea quantumness at first discrepancies with the test data, though the official physics has occasions to maintain more loyalty, since it considers quantumness as the initial reason of behavior of an electron in atom. The alternate physics considers occurrence quantumness as the inevitable resolution of conflict between aspiration of an electron to a minimum of a potential energy and impossibility of radiation of a nonintegral photon. Not tampering with nonintegral n_1 and n_2 we shall consider W as function n_1 and n_2, then from (12) we shall receive (11). W at $n_2 \to \infty$ and $n_1=1$ numerically is peer to electron-binding energy a nonexcited state (E^0), more correctly, to potential of ionization at removal of a given electron and depends on a degree of excitation of an electron (position of its orbit).

The equation (11), in opinion of the author, is more preferential than any other semiempirical expressions on following circumstances:

1. It has extreme clear physical sense.
2. Integer-valued n_1 and n_2 allows easily interpreting spectral lines.
3. As the change of a binding energy of a given electron imports the solving contribution to energy of a radiated photon, the value W always is close value E^0.

In connection with enunciated, there is a sense to compound the table 1 of values $\Delta = \dfrac{1}{n_1^2} - \dfrac{1}{n_2^2}$, which one is very comfortable for the analysis of spectrums.

Table 1.

n_2 / n_1	1	2	3	4	5	6	7	8	9	10	∞
1	0	0,750	0,889	0,938	0,960	0,972	0,980	0,984	0,988	0,990	1,000
2		0	0,139	0,188	0,210	0,222	0,230	0,234	0.238	0,240	0,250
3			0	0,049	0,071	0,083	0,091	0,095	0,099	0,101	0,111
4				0	0,022	0,034	0,042	0,046	0,050	0,052	0,062
5					0	0,012	0,020	0,024	0,028	0,030	0,040
6						0	0,008	0,012	0,016	0,018	0,028
7							0	0,004	0,008	0,010	0,020
8								0	0,004	0,006	0,016
9									0	0,002	0,012
10										0	0,010

The analysis of spectrums is convenient for conducting under the following scheme: a). We detect electron-binding energy on stationary orbits of given atom. b). Any spectral line of this atom is translated in energy of a photon expressed in electron-volts on the formula: $E(eV) = \dfrac{12397.7}{\lambda\left(\overset{0}{A}\right)}$ and from the formula (11) W is discovered, using the table of values Δ.

The value Δ should be picked from the table so that W was closest value of any electron-binding energy on a stationary orbit. Thus, for each spectral line we shall discover W and values n_1 and n_2.

Usables this scheme for the analysis of spectral lines of helium. Under the formula (4) on one electron in a stationary state the binding energy 39.5 eV is necessary. To receive spectral lines at E^0=39.5 eV, the completely identical and simultaneous excitation of both electrons of helium is necessary, that is very improbable. Other energy state of atom of helium at which one the binding energy of the first electron makes 24.6 eV (first potential of ionization), and second 54.4 eV (second potential of ionization) energy-wise is equivalent binding energies of both electrons on 39.5 eV, since in the sum the energy is identical: 79 eV. We would have completely diverse world, if the magnetic interaction of orbital electronic currents would not steady electrons on an orbit 39.5 eV. Then the electrons have preferred to take miscellaneous orbits: 24.6 eV and 54.4 eV. Therefore excitation of any electron instigates similar reorganization of orbits and in a spectrum of helium we should to observe the relevant series of lines. Besides in anyone it is enough strongly excited atom (at small n_1), we should watch lines relevant $W \approx 13.6$ eV, since from a point of view of an electron on a high-altitude orbit, the atom is represented hydrogen-like. As at removal of an electron from a nucleus there is a reorganization of remaining electronic orbits in structure relevant to atom, engaging the previous standing in the table of elements of the Mendeleyev (at ionization of Zinc the structure will be formed cuprum-like, at ionization of cuprum – nickel-like etc.), in spectrums of elements with sequentially incremented nuclear charge the picture of lines of the previous element with the relevant bias in short-wave area and expansion of a gap between lines is iterated. In table 2 the data of decryption of some lines in a spectrum of helium are given.

Table 2.

n_1	n_2	Wave length of a photon, (A^0)	W,(eV)
1	3	584.33	23.87
3	5	7065.20	24.68
3	6	5875.63	25.32
3	7	5769.60	23.69
3	10	5015.678	24.47
3	4	4685.75	54.00
4	7	5460.73	53.94
4	8	4916.00	53.81
4	8	4960.32	54.33
2	3	6678.149	13.36
2	4	4916.00	13.45
2	4	4960.32	13.29
2	6	4120.82	13.54
2	7	4026.192	13.41
2	8	3888.645	13.60

As well as it was necessary to expect, the values W are close to values 54.4 eV, 24.6 eV and 13.6 eV.

Table 2 displays, that the atom of helium has three systems of spectral lines. The figure 2 explains system of spectral lines of normal atom of helium with E_0=24.6 eV. The systems of spectral lines with E_0=54.4 eV and 13.6 eV concern to abnormal atom of helium. It will be formed as follows. The energy 11 eV (see formula 16.5 in chapter 16) is indispensable for busted of a magnetic attraction of electrons. At deriving this energy the electrons any more can not take a standing relevant to a figure 14.1 and will forms a following configuration: the outside electron takes a quasistationary orbit with a binding energy 24.6–11=13.6 eV, therefore its energy levels practically correspond to levels of atom of hydrogen. The inner-shell electron takes an orbit with a binding energy 54.4 eV, therefore its energy levels correspond to a hydrogen-like atom with nuclear charge +2. Thus, the abnormal helium though and metastable, but is stable enough. It is necessary to allow for it, those spectral lines of neutral helium to not confuse with lines of neutral hydrogen or should be single-pass of ionization helium. The enunciated situation is figured schematically on a figure 2 where the areas of existence of normal and abnormal helium are figured. The outside electron is gone on radius of the first orbit of the Bohr, and interior on an orbit with radius twice smaller.
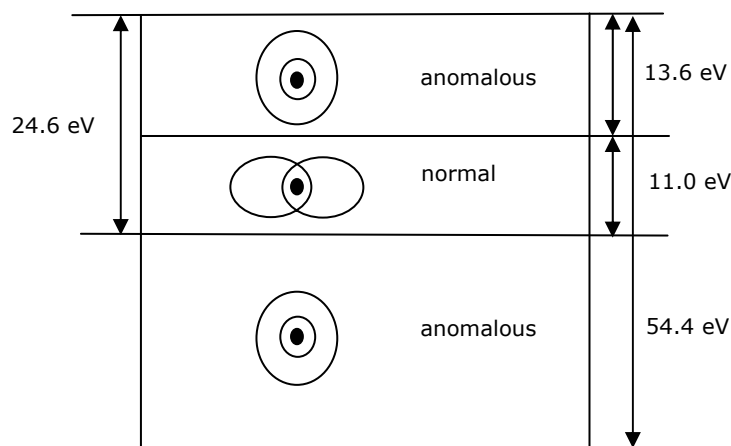

Fig.2

References:

1. http://www.new-physics.narod.ru