THE ENERGY OF THE BINDING OF MULTIELECTRONIC STRUCTURES IN THE FIELD OF BINOMIAL POTENTIAL

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Abstract

We propose a classical procedure to calculate the potential energy of electrons in the ground state of atoms and ions similar to them. It is assumed that the electron-proton and electron-electron interactions are described not by the Coulomb law, but by more complicated binomial potentials.

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1 Introduction

The interest in the theoretical determination of the energy of electrons in atoms and ions similar to them arose from the time moment when Rutherford proposed the model of an atom as a particle consisting of the nucleus and electrons positioned from it at some distances. This interest is conditioned by the hope for that the obtained theoretical results fitting the experimental data will help to reach the understanding the structure of many-electron atoms and ions similar to them.

At present, a lot of different methods of calculations of the binding energies of electrons in atoms is known. One of the examples of such calculations is given by works [1, 2]. However, the attempts to spread the semiclassical and quantum-mechanical methods of calculations used there on the systems with three and more electrons have brought no required results. As an example of such attempts to calculate the energy of electrons in many-electron systems, we mention work [3]. In that work, the quasiclassical and quantum-mechanical ideas were used in the attempt to calculate the ionization energies of 10 lightest elements. Though their numerical values were obtained, a clear model of the electron structure of atoms was not constructed. The structure of the applied formulas and their parameters do not explain the physical, in the common sense of this word, essence of the processes running in an atom.

We consider that we must change our ideas of the nature of the interaction of electrons with a nucleus in order to be successful in the theoretical simulations of many-electron systems. In our opinion, the interaction of electrons with a nucleus in an atom obeys a more complicated law than the Coulomb one. The former is a binomial potential. Just with its help, one can develop such models of atoms, to which the classical methods of calculations will be also applied.

As the basis for such calculations, we take a potential of the binomial form earlier proposed by us in [4, 5] for the interaction of an electron with a proton:

$$V = -\frac{e^2}{r} + \frac{\Gamma}{r^2} \; . \tag{1}$$

.

By using this potential in the study of both the motion of an electron in a hydrogen atom and the scattering of electrons by protons, we were lucky to get the basically new results which change significantly our ideas of the intra-atomic phenomena [4, 6]. Therefore, there is a sense to spread the usage of the binomial potential on the study of many-electron structures. As a result, we will demonstrate the calculation of the ground state energies for six lightest atoms and ions similar to them which are in reasonable agreement with experimental data. By this, we will confirm the correctness of the chosen binomial potentials and models of atoms.

2 Substantiation of the binomial potential of interaction of an electron with a proton

As a basis for the substantiation of the binomial potential [4, 5] of interaction of an electron with a proton, we take the indisputable fact that an electron in an atom is constantly located at some distance from the nucleus. Omitting the discussion of the physical essence of this phenomenon, we can represent the potential energy of the interaction of an electron with a proton in a hydrogen atom by the following function:

$$V = -\frac{e^2}{r} + \frac{\Gamma}{r^x} \ . \tag{2}$$

Here, the first and second terms on the right-hand side correspond, respectively, to the Coulomb interaction and to a hypothetical interaction which counteracts the Coulomb attraction.

In the general case, formula (2) is widely used in the solid-state theory on the description of the interaction of atoms in molecules and crystals [7]. But it was not applied for some reasons to the analysis of the interaction of electrons in an atom. In what follows, we will demonstrate that formula (2) can be very useful also in the modeling of the structure of atoms.

In formulas of the type (2), the constant Γ and the exponent x are unknown, as a rule. But their numerical values can be determined by solving the system of two algebraic equations related to a certain state of the system, for which some experimental data are available [7]. For a hydrogen atom, we can consider its ground state, for which

we obtain the equations

$$-\frac{e^2}{r_0} + \frac{\Gamma}{r_0^x} = E_0 \ , \quad \frac{e^2}{r_0^2} - \frac{x\,\Gamma}{r_0^{x+1}} = 0 \ , \tag{3}$$

where E_0 is the energy of the ground state of a hydrogen atom; r_0 is its equilibrium radius, and e is the electron charge. The second equation in (3) represents the sum of forces acting on the electron.

Rewriting (3) as

$$-\frac{e^2}{r_0} + \frac{\Gamma}{r_0^x} = E_0 \ , \quad \frac{e^2}{xr_0} - \frac{\Gamma}{r_0^x} = 0 \tag{4}$$

and summing the equations, we get the equality

$$-\frac{e^2}{r_0} + \frac{e^2}{xr_0} = E_0 \tag{5}$$

which can be written as

$$\frac{1}{x} - 1 = \frac{E_0 r_0}{e^2} \ . \tag{6}$$

Substituting the numerical values of E_0, r_0, and e^2 in (6), we get $x = 2$. For this value of x, the second equation of system (3) yields

$$\Gamma = \frac{e^2 r_0}{2} \ . \tag{7}$$

Thus,

$$\Gamma = 6.10276 \times 10^{-28} \ \ \text{CGSE} \ \ \text{units and} \ \ x = 2 \ . \tag{8}$$

Let us paid attention to the right-hand side of formula (6)

$$\frac{E_0 r_0}{e^2} = \frac{1}{2} \ . \tag{9}$$

Rewriting relation (9) as

$$E_0 = \frac{e^2}{2r_0} \ , \tag{10}$$

it becomes clear that the last formula defines the ground state energy of a hydrogen atom.

We recall that the Bohr theory gives also the analogous relation [7] but on the basis of the other starting premises: the equality of the centrifugal force and the force of Coulomb attraction.

It is also known that the analogous relation for the ground state energy of a hydrogen atom follows from the solution of the Schrödinger equation. In addition, the Schrödinger equation gives also the relation $r_0 = \hbar^2/me^2$. By substituting the last formula in (7), we get $\Gamma = \hbar^2/2m$.

The above consideration was performed in order to show the logical connection of the binomial potential with the Bohr theory and the Schrödinger theory of a hydrogen atom. In the previous theories, the positive addition to the Coulomb law was also implied, but as some centrifugal force, on the basis of the postulate on a motion of the electron around the nucleus. As known, the hypothesis of the rotational motion of the electron in a hydrogen atom leads to the fundamental difficulties on the interpretation of models of many-electron structures. But our hypothesis of the presence of the repulsive interaction removes the difficulties and is quite suitable in the explanation of many-electron structures.

Let us consider some specific features of results (8). First, we emphasize the small value of the constant Γ relative to e^2 (23.06112×10^{-20}). Therefore, the contribution of the positive term in (2) to the total interaction energy at distances in the scope of two equilibrium radii is negligibly small. Secondly, the integer value of the exponent x ($x = 2$) allows one to carry out analytically, without any difficulties, the integration of equations with this potential. Thirdly, the constant

$$\Gamma = \frac{\hbar^2}{2m} \ , \tag{11}$$

where $\hbar$ is the Planck constant and m is the electron mass, corresponds to the coefficient of proportionality postulated by Schrödinger for his equation.

We also note that formula (2) repeats exactly the potential proposed by Weisskopf [8]. But Weisskopf obtained his formula on the basis of quantum-mechanical premises of the Schrödinger theory, by taking the incompressibility of an atom into account. Such an as-

sumption is also involves the existence of a repulsive force between an electron and a proton. Hence, two basically different approaches (the classical and quantum-mechanical ones) led to the same interaction potential between an electron and a proton. This fact is a corroboration of the logical connection between the theory based on the binomial potential and quantum theory. Therefore, the binomial potential can be considered as a coordinating link between classical theory and quantum mechanics.

But quantum mechanics interprets the positive addition to the Coulomb law as the minimum kinetic energy [8], whereas the classical approach considers it as some counteracting field. The answer to the question about what is more natural will be given by the consideration of many-electron systems. As was mentioned above, the postulation of circular motion of an electron creates the basic difficulties for the theory of many-electron systems. But the assumption on some counteracting potential removes them and opens the possibility to model many-electron systems in the framework of classical mechanics. The positive results of such modeling would be considered as a confirmation of the validity of the interpretation of the new positive term in the electron-proton potential as a certain counteracting potential.

Generally saying, by introducing the binomial potential, we replace, in fact, the postulate of some motion of an electron around the nucleus, which is foreign to classical mechanics, by a more natural hypothesis of the presence of some repulsive potential. We especially emphasize the fact that the proposed binomial potential (1) does not contradict the foundations of quantum mechanics [4, 5] and opens the way for classical mechanics into many-electron systems.

In Fig.1, we show the dependence of the binomial potential of the interaction of an electron with a proton on the distance between them. It is obvious that the Coulomb component dominates in the total interaction energy already at distances of about 2 equilibrium radii ($\sim 1 \times 10^{-8}$ cm). But, at small distances less than a half of the equilibrium radius ($\sim 0.25 \times 10^{-8}$ cm), the positive term in (1) becomes dominant, manifesting the character of a short-range force. Apparently just in such a way, we can explain the circumstance why no deviations from the Coulomb law were noticed at macrodistances, where this law was mainly studied.

As an experimental confirmation of potential (2), we mention the angular distribution on the scattering of electrons by protons [9]. The results of our calculations [10] on the basis of potential (1) coincide completely (Fig.2) with the experimental data [9]. Therefore, we may assert that potential (2) has a direct experimental confirmation.

3 Binomial potential of hydrogen-like ions

Above we have obtained the parameters of the binomial potential (2) (the constant Γ and the exponent $x = 2$) on the basis of only the experimental data on the hydrogen atom. It is natural that the question can arise about how these parameters will agree with the data on hydrogen-like ions. As known, it was experimentally established that the binding energy E_{0z} of an electron with a nucleus in these ions is connected with that of an electron with the proton in a hydrogen atom by the relation

$$E_{0z} = Z^2 E_0 \ , \quad r_{0z} = \frac{r_0}{Z} \ , \tag{12}$$

where Z is the atomic number, E_0 is the binding energy of an electron in the ground state of a hydrogen atom, r_{0z} is the distance of an electron from the nucleus in a hydrogen-like ion, and r_0 is the Bohr radius.

We write the first equation in (3) in the form

$$E_{0z} = Z^2 \left[-\frac{e^2}{r_0} + \frac{\Gamma}{r_0^2} \right] \ , \tag{13}$$

where the expression in the square brackets is the binomial potential in the ground state of a hydrogen atom, or as

$$E_{0z} = -\frac{Zee}{\frac{r_0}{Z}} + \frac{\Gamma}{\left(\frac{r_0}{Z}\right)^2} \ . \tag{14}$$

Formula (14) implies that, in order to calculate the binding energy of an electron with a nucleus in a hydrogen-like ion, we must substitute the nucleus charge Ze and the distance of an electron from the nucleus $r_{0z} = r_0/Z$ in the formula for the binomial potential of

a hydrogen atom in the ground state. Hence, potential (2) remains invariable also on the definition of the binding energy of electrons in hydrogen-like ions.

We can convince themselves in this in another way. Consider the formula

$$E_z = -\frac{Ze^2}{r_z} + \frac{\Gamma}{r_z^x} \ . \tag{15}$$

We assume that the constant Γ and the exponent x are unknown. For their determination, we construct the system of two algebraic equations corresponding to the equilibrium state of a hydrogen-like ion, by following [7]:

$$E_{0z} = -\frac{Ze^2}{r_{0z}} + \frac{\Gamma}{r_{0z}^x} \ , \ 0 = \frac{Ze^2}{r_{0z}^2} - \frac{x\,\Gamma}{r_{0z}^{x+1}} \ . \tag{16}$$

By substituting the experimental values of the energy and the radius from relation (12) in (16), we obtain the system

$$E_0 = -\frac{e^2}{r_0} + \frac{\Gamma}{r_0^x} \ , \ 0 = \frac{e^2}{r_0^2} - \frac{x\,\Gamma}{r_0^{x+1}} \ , \tag{17}$$

analogous to system (4) for a hydrogen atom. Hence, the second method has shown that the parameters of the binomial potential obtained by the experimental values for a hydrogen atom remain valid also for hydrogen-like ions.

It is worth noting one peculiarity of the binomial potential. As follows from (15), the contribution of the positive addition in the binomial potential to the total interaction energy of an electron with a nucleus is independent of the electric charge of a nucleus, i.e. on the number of protons in a nucleus, but depends only on the distance of an electron from the nucleus.

4   The energy of the binding of electrons in two and three electronic atoms

Earlier we determined the law of interaction of one electron with a nucleus. But in order to consider the interaction of two and more electrons with a nucleus, this result is not sufficient. As known, an

electron possesses not only electric properties, but also magnetic ones. Therefore, in the analysis of the systems with at least two electrons, we must take the magnetic interaction into account, in addition to the electrostatic interaction, in order to determine the interaction energy of electrons with one another.

Hence, if we represent a He atom and ions similar to it as the systems consisting of a nucleus and two electrons positioned on a straight line from the nucleus, then the formula for the energy of the binding of the system consisting of two electrons and the nucleus E_{z2} takes the form

$$E_{z2} = -\frac{2Ze^2}{r} + \frac{2\Gamma}{r^2} + \frac{e^2}{R} + \frac{A}{R^2} \,, \tag{18}$$

where Z is the atomic number. On the right-hand side of formula (18), the terms represent, respectively, the Coulomb interaction of electrons with a nucleus, our hypothetic interaction of electrons with a nucleus, the Coulomb interaction of electrons with one another, and the magnetic interaction of electrons, $R = 2r$, and A is the constant characterizing the magnetic interaction.

A lithium atom and ions similar to it can be represented in the form of an equilateral triangle, whose vertices are occupied by electrons, and the nucleus is located at the geometric center. Then the energy of the binding E_{z3} of this system is

$$E_{z3} = -\frac{3Ze^2}{r} + \frac{3\Gamma}{r^2} + \frac{3e^2}{R} + \frac{3A}{R^2} \,, \tag{19}$$

where $R = \sqrt{3}$, and the terms on the right-hand side are analogous to those in (18).

We determined the constant A in (18) and (19) by using the experimental values of the energies of atoms of He and Li. By averaging the obtained values, we take

$$A = 3.107 \times 10^{-28} \ \ \text{CGSE} \ \ \text{units.} \tag{20}$$

The results of the comparison of experimental data [11] with the values calculated by formulas (18) and (19) for He, Li, and ions similar to them with regard for constant (20) are given in Table 1.

The validity of formulas (18) and (19) is supported by the following examples.

It is known that there exist negative ions of hydrogen. We will try to explain the physical nature of this fact with the help of formulas (18) and (19). Let us take a proton and add successively electrons to it. After the next addition, we will construct the curve of the interaction potential of these electrons with the proton. It is seen in Fig. 3 that the proton with two electrons is a stable system, because these potential well is deeper than that of the hydrogen. But the potential wells with three and four electrons become shallower than the potential well of the hydrogen atom. Therefore, two electrons with a proton can else create a stable structure in the form of a negative ion, and the next electrons will be rejected. Thus, our evaluations have shown in agreement with the experimental data that the negative ion of a hydrogen atom is energetically admissible and can be realized with the negative charge equal 1.

We should like to emphasize the difference between the curves of the potential wells of a hydrogen atom and a one-charge negative hydrogen ion. This difference corresponds to the experimental value of the binding energy of an electron with a hydrogen atom which is equal to $0.75eV$. So our result is exactly equal to the experimental value [12], which also confirms the validity of formulas (18) and (19).

The second example of the efficient application of formulas (18) and (19) can be the explanation of the chemical inactivity of a He atom. In Fig. 4, we show the process of successive addition of electrons to the nucleus of He. As seen, the nucleus of He with three electrons is an energetically unstable structure as compared with the "nucleus of He – two electrons" system. The difference in the position of their potential wells is $7.7eV$. This means physically that the presence of the third electron near the nucleus of He is unfavorable by energy. For this reason, the atoms of He do not participate in chemical reactions, which explains its chemical inertness.

Thus, we have proved that formulas (18) and (19) represent quite properly the potential energy of the system including a nucleus and two and three electrons.

5   The energy of the binding of electrons in atom of beryllium and ions similar to it

A Be atom has four electrons. Therefore, the choice of the form of a geometric figure formed by the electrons and the nucleus is a some-

what more complicated problem than in the case of a He or Li atom. Four electrons can be positioned in a plane in the form of a rhomb and in space in the form of a three-dimensional tetrahedron. We will compare these two versions by making calculations of the depth of potential wells. That version will be preferable, whose potential well will be deeper.

Let us represent a Be atom in the form of a tetrahedron, whose vertices are occupied by electrons, and the nucleus is located at its geometric center. In this model, the potential energy of a Be atom is given by the formula

$$E_{z4t} = -\frac{4Ze^2}{r} + \frac{4\Gamma}{r} + \frac{6e^2}{R} + \frac{6A}{R^2} \, , \tag{21}$$

where Z is the atomic number, R is the length of a tetrahedron edge, i.e. the distance between electrons, and r is the distance of electrons from the nucleus, $r = 0.612R$.

If we represent a Be atom in the form of a rhomb, whose vertices are occupied by electrons, and the nucleus is located at its center, then its potential energy is

$$E_{z4r} = -\frac{2Ze^2}{r_1} + \frac{2\Gamma}{r_1^2} - \frac{2Ze^2}{r_2} + \frac{2\Gamma}{r_2^2} + \frac{4e^2}{R} + \frac{e^2}{2r_1} + \frac{e^2}{2r_2} + \frac{4A}{R^2} + \frac{A}{(2r_1)^2} + \frac{A}{(2r_2)^2} \, , \tag{22}$$

where R is the length of a rhomb edge, r_1 and r_2 are two possible distances of electrons from the nucleus. Here, the following relations hold: $r_1 = R \sin \alpha$, $r_2 = R \cos \alpha$, where α is the angle between a rhomb edge and its bisectrix.

The calculations of the potential energies by formulas (21) and (22) have shown that the model of a Be atom in the form of a rhomb with an angle of 30^0 at a vertex is preferable. Figure 5 makes it obvious. The potential well of curve 2 calculated by formula (22) with an angle α of 15^0 is by 2 eV deeper than that of the potential curve of a tetrahedron.

Moreover, the configuration of a Be atom in the form of a rhomb agrees also with the modern quantum-mechanical ideas. Two first electrons ($1s$) are positioned significantly closer to the nucleus than two other ($2s$) electrons. That is, we have obtained a curious situation, where the classical model supplements the quantum-mechanical one.

In Table 1, we present the potential energies of a Be atom and ions similar to it and the relevant experimental data [10]. The good agreement of the calculated values with the experimental data can be considered as a confirmation of the validity of the chosen model of a Be atom.

6 The energy of the binding of electrons of atoms of boron and carbon

As the starting premise for the choice of a geometric model of atoms of boron and carbon, we take the crystal form of these substances into account. Assuming that atoms of B and C admit a close packing, it is natural to assume that these atoms are in the forms of a hexahedron and an octahedron, respectively.

Let us consider a B atom as a hexahedron, whose vertices are occupied by electrons, and the nucleus is located at the geometric center. In such a model, the potential energy is as follows:

$$E_{z5} = -\frac{3Ze^2}{r_1} + \frac{3\Gamma}{r_1^2} - \frac{2Ze^2}{r_2} + \frac{2\Gamma}{r_2^2} + \frac{9e^2}{R} + \frac{e^2}{1.633R} + \frac{9A}{R^2} + \frac{A}{(1.633R)^2} ,$$
(23)

where Z is the atomic number, R is the length of a hexahedron edge, r_1 is the distance of the electrons positioned on the base plane of a hexahedron from the nucleus, $r_1 = R/\sqrt{3}$, and r_2 is the distance of the electrons, which are located at the vertices opposite from the base of a hexahedron, from the nucleus, $r_2 = R/\sqrt{2/3}$.

Let us consider a C atom as a octahedron, whose vertices are occupied by electrons, and the nucleus is located at the geometric center. The potential energy reads

$$E_{z6} = -\frac{6Ze^2}{r} + \frac{6\Gamma}{r^2} + \frac{12e^2}{R} + \frac{3e^2}{\sqrt{2}R} + \frac{12A}{R^2} + \frac{3A}{\left(\sqrt{2}R\right)^2} ,$$
(24)

where Z is the atomic number, R is the length of a octahedron edge, r is the distance of the electrons from the nucleus, $r = R/\sqrt{2}$.

The results of calculations by formulas (23) and (24) are presented in Table 1. We think that the attained accuracy allows us to assert that the proposed models of atoms of boron and carbon are quite adequate to the real situation.

7 Conclusions

The purpose of the given work was to show that if the interaction of electrons in an atom with a nucleus and between themselves is represented in the form of binomial potentials, then the atoms can be modeled by geometric figures (planar or three-dimensional ones), which would give the possibility to calculate the energies of the ground states of atoms and ions.

The results of calculations presented in Table 1 convince us in the validity of the chosen geometric models and the above-presented formulas. The comparison of the theoretical results and experimental data allows us to believe that the proposed approach based on the use of binomial potentials reflects correctly the interactions and the spatial structure of electrons in atoms.

Our formulas allow one to calculate the curve of potential energy for specific systems. This gives the possibility to determine the equilibrium distances between particles and, by comparing the potential wells, to give preference to that or another model. As an example, we mention the choice of the configuration of electrons of a Be atom or the search for the stable negative hydrogen ions.

The energy of the binding of an electron with a hydrogen atom calculated by our formulas coincides exactly with the experimental value $(0.75\ eV)$.

The disagreements seen in Table 1 are apparently conditioned by the neglect of both the interactions of nuclear magnetic moments with electrons and the orientation of electrons as magnets relative to the nucleus and to one another in the calculations. But these errors can be referred to the second-order effects in view of their absolute values.

On the whole, we believe that the purpose of our work is attained.

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Table 1: Comparison of theoretical potential energies of certain atoms and ions with experimental data.

| Number of electrons	Elements	H	He	Li	Be	B	C	N	O
1	E_{exp}, erg 10^{-10}	0.2177	0.871	1.961	3.487	5.449	7.846	10.68	13.953
	E_{theor}, erg 10^{-10}		0.870	1.959	3.483	5.442	7.837	10.66	13.93
	$Error$, %		+0.07	+0.08	+0.11	+0.12	+0.11	+0.12	+0.12
2	E_{exp}, erg 10^{-10}		1.265	3.172	5.951	9.602	14.12	19.53	25.79
	E_{theor}, erg 10^{-10}		1.255	3.097	5.764	9.246	13.55	18.67	24.61
	$Error$, %		+0.8	+2.4	+3.2	+3.9	+4.3	+4.6	+4.8
3	E_{exp}, erg 10^{-10}			3.259	6.243	10.21	15.16	21.1	28.0
	E_{theor}, erg 10^{-10}			3.280	6.546	10.90	16.42	23.06	30.79
	$Error$, %			-0.6	-4.6	-6.3	-7.7	-8.5	-9.1
4	E_{exp}, erg 10^{-10}				6.392	10.61	15.92	22.33	29.83
	E_{theor}, erg 10^{-10}				6.436	10.64	15.99	22.45	30.05
	$Error$, %				-0.7	-0.3	-0.4	-0.5	-0.7
5	E_{exp}, erg 10^{-10}					10.75	16.32	23.08	31.08
	E_{theor}, erg 10^{-10}					10.57	17.00	24.90	34.49
	$Error$, %					+1.1	+1.7	-7.3	-9.9
6	E_{exp}, erg 10^{-10}						16.50	23.56	31.08
	E_{theor}, erg 10^{-10}						15.49	23.59	33.31
	$Error$, %						+6.5	-0.1	-6.0
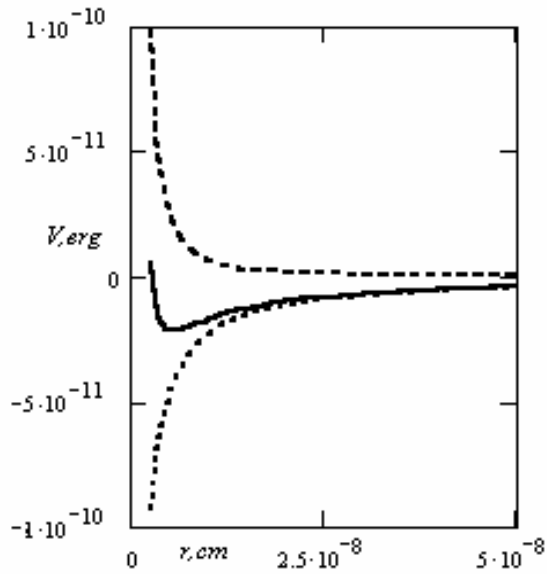
Figure 1: Electron-proton interaction energy versus the distance between particles for the binomial potential (1) ——, for the Coulomb potential - - - , and for their sum − − −.
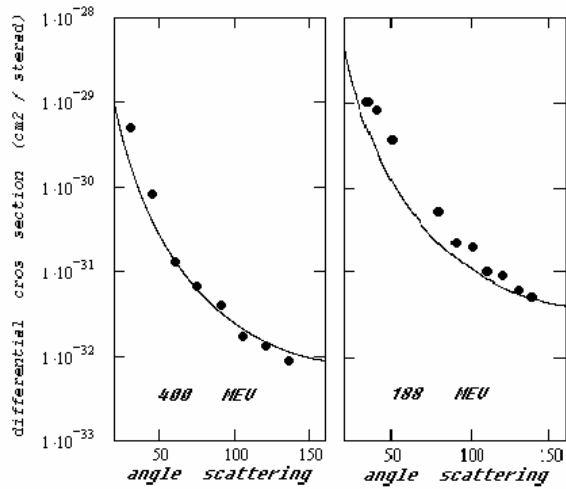
Figure 2: Comparison of the calculated effective scattering cross-sections of electrons with energies of 400 and 188 MeV (the continuous curve) with the experimental data (points) taken from [9].
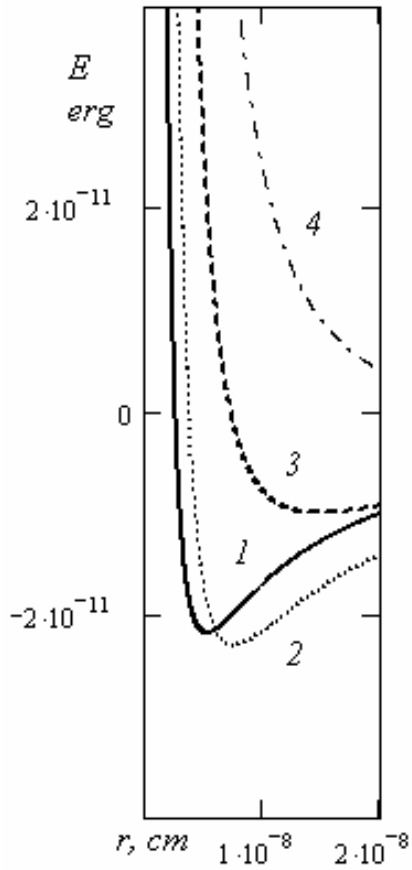
Figure 3: Negative hydrogen ion. The potential energy of one (1), two (2), three (3), and four (4) electrons.
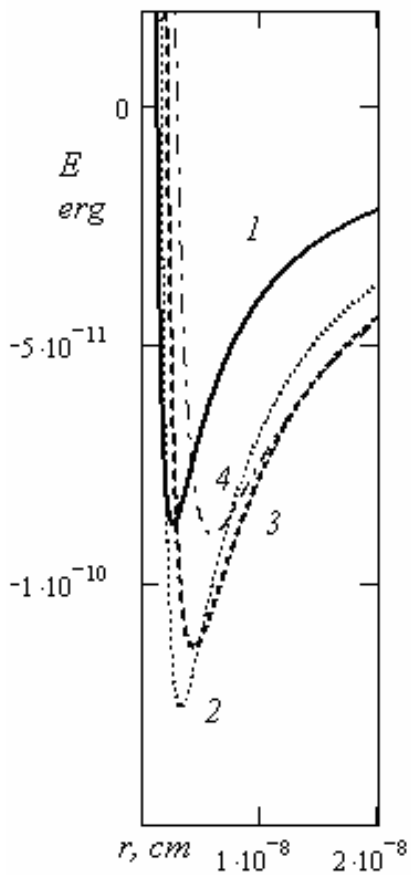
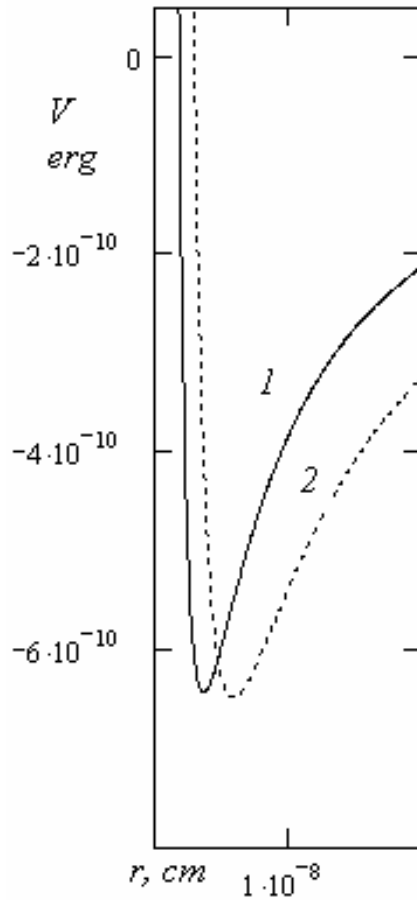Figure 4: Atom of helium. The potential energy of one (1), two (2), three (3), and four (4) electrons.

Figure 5: Potential energies of electrons interacting with the nucleus and with one another in an atom of beryllium: 1 - the model of a tetrahedron, 2 - the model of a rhomb with an angle of 30^0 at a vertex.

Comment on
THE ENERGY OF THE BINDING OF MULTIELECTRONIC STRUCTURES IN THE FIELD OF BINOMIAL POTENTIAL

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The Gudym and Andreeva model belongs to the class of models devised to explain a very narrow set of physical facts. Their model gives binding energies of several atoms and their ions.

Sometimes it may be useful to have a prescription for quick calculation of certain physical characteristics of some system – generalized Balmer's formula for the emission spectrum of hydrogen is an example – especially when it can be derived from a simple unifying idea with minimum number of free parameters. Some of such ideas may be more or less bizarre, sometimes quite interesting, like for example the Kepler's model described in his *Mysterium Cosmographicum* [1], but usually they have no physically important content. Other ideas, such as the Newton's law of gravitation or the Bohr's 'quantum condition', were important for the development of science and our understanding of nature. I am thoroughly convinced that the Gudym and Andreeva phenomenological model belongs to the first

kind of funny toy models which are interesting as such, and, at the same time, carry no interesting message for today's physics.

Gudym and Andreeva propose a classical procedure of modelling binding energies of electrons in the six lightest atoms and their positively charged ions. In my opinion, the Authors' argumentation in many places is vague or thoroughly wrong, at least from the point of view of our understanding of contemporary physics. I discussed some of my objections in my comment to the Authors' previous paper [2] and I refer the interested reader there. I showed that the binomial potential cannot be treated seriously as a replacement for the Coulomb proton-electron interaction: among other things, the predicted emission spectrum of hydrogen atom with the binomial potential would be drastically different from that observed.

I have alluded above to the Kepler model not without cause. In some respects the Gudym and Andreeva model resembles it much. They start their paper with discussion of hydrogen. They consider binomial potential for the interaction of electron with proton, and determine two free parameters of the potential by finding its minimum corresponding to Bohr's atomic units, assuming simultaneously the ground state electron to be at rest with respect to the nucleus. The physical nature of the binomial potential is not explained by the authors. To me, the only reason for using it, is to have the electron's potential energy with a minimum at rest and with the same asymptotics as Coulomb potential. For the other five atoms, by including also Coulomb and 'magnetic' interactions between electrons, and introducing additional two free parameters, they assume that electrons are located at rest on vertices of certain geometric figures that allow for static configurations with minimum energy. These are respectively, a line segment for helium (+1 free parameter measuring 'magnetic' coupling of two electrons), an equilateral triangle for lithium, a rhombus that is energetically more preferred than tetrahedron for beryllium (+ 1 free parameter measuring the rhombus' inclination), hexahedron for boron and octahedron for carbon. In each case the nucleus is located in the center of symmetry and sizes of these atoms are determined by the minimum of energy. The 'magnetic' coupling constant of the 'magnetic' potential is determined by averaging the respective values obtained by comparison with experimental binding energies of electrons in helium and lithium. This

potential has nothing to do with interaction of magnetic dipoles, and has no counterpart in Maxwell's electromagnetic theory. However, this pure phenomenology gives binding energies of electrons in these atoms and ions, which are comparable with the experimental values.

The fact that by a minimization of some ansatz potentials with several free parameters (plus symmetry arguments), one may reconstruct with finite accuracy some set of numbers, should not astonish. That such procedure approximates binding energies of few simple atoms is rather an interesting observation. The Authors have not constructed ground states of other atoms, they tabulated only some numbers for nitrogen and oxygen. It is natural that one would want to see some comparison of prediction of the model with binding energies of other atoms and, more importantly, with their emission spectra. Only such comparison can decide about predictive power of a model. I have an impression that this will be impossible without introducing a very large number of other effective potentials with free parameters – counterparts of 'epicycles'.

From the point of view of quantum chemistry the problem of finding binding energies of electrons in atoms and ions is equivalent to finding energy spectrum of suitable Hamiltonians. The 'only' problem in finding the spectra is of computational nature rather than conceptual. Therefore, there is no need of inventing new physics of ionization energies. At the same time one should not forget that quantum electrodynamics solves these and many other problems of atomic physics with unprecedented precision, and that the only free parameters it requires are: the fine structure constant, two dimensional constants $\hbar$ and c, and masses of the proton and electron (if other kinds of particles are not taken into account).

References

[1] The Kepler model of the planetary system related sizes of six celestial concentric spheres. The idea lying behind this system was the following. At the time six planets had been known. There were six spheres supporting these planets. Six – as being the sum of its divisors – is a perfect number. Spheres, as they are perfect, as well. Five regions in between, as only five regular Platonic solids exist. Inscribed in between these spheres the solids

determine ratios of the spheres' radii – quite convincing idea, isn't it?

[2] Bratek Ł, (2007) Concepts of Physics, Volume IV, No.4, 567

Comment on
THE ENERGY OF THE BINDING OF MULTIELECTRONIC STRUCTURES IN THE FIELD OF BINOMIAL POTENTIAL

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The Gudym and Andreeva model belongs to the class of models devised to explain a very narrow set of physical facts. Their model gives binding energies of several atoms and their ions.

Sometimes it may be useful to have a prescription for quick calculation of certain physical characteristics of some system – generalized Balmer's formula for the emission spectrum of hydrogen is an example – especially when it can be derived from a simple unifying idea with minimum number of free parameters. Some of such ideas may be more or less bizarre, sometimes quite interesting, like for example the Kepler's model described in his *Mysterium Cosmographicum* [1], but usually they have no physically important content. Other ideas, such as the Newton's law of gravitation or the Bohr's 'quantum condition', were important for the development of science and our understanding of nature. I am thoroughly convinced that the Gudym and Andreeva phenomenological model belongs to the first

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