### **The Extended Bohr Theory**

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### Abstract

The Extended Bohr Theory allows calculation of successive ionization
energies (E_ion from I to VIII) for elements $Z = 1$ to $Z = 18$ . Without using the
Schrödinger eqaution it is possible to calculate singular spectral lines for many elements.
For 1-electron systems accuracy is beter than 0.001 eV.
For 2-electron systems accuracy is beter than 0.02 eV.
For 3-electron systems accuracy is beter than 0.02 eV.

I. Introduction.

The ionization energy of hydrogen (13.598433 eV) and the entire hydrogen emission spectrum can be calculated with high accuracy using Bohr's Theory.

Bohr's theory of atomic structure can also be used with good accuracy for the so-called Rydberg atoms, i.e. for hydrogen-like single-electron ions of helium He(+), lithium Li (++), boron B(+++), etc.

For example, for ionized helium He(+) or He(II) the appropriate formula for the potential of the energy levels of the last remaining electron in the cation is :

$$E = -hcR_{He} * Z^{2}(1/k^{2} - 1/n^{2}) \quad (n > k)$$
(1a)  
or:  
$$E = -B_{He} * Z^{2}(1/k^{2} - 1/n^{2}) \quad (n > k)$$
(1b)

where  $B_{He} = 13.60384 \text{ eV} \approx \frac{1}{2}$  Hartree = 1 Rydberg = 1 Ry,

and the minus sign means that when the electron drops from the higher n level to the lower k level, energy is released, i.e. the atom loses energy. In this convention, the ionization energies are positive.

 $B_{He} = 13.60384 \text{ eV}$  differs slightly from  $B_H = 13.5984 \text{ eV}$  because the value of the Rydberg constant differs slightly for hydrogen and helium. This is because a orbiting electron causes the nucleus to vibrate, so both the electron and the nucleus orbit around their common center of mass. In the case of <sup>4</sup>He, the movements of the nucleus are smaller than in the case of <sup>1</sup>H, so that the Rydberg constant is correspondingly higher. Therefore, the largest Rydberg constant occurs for a stationary nucleus and is:

 $R_{\infty} = m e^4 / (8 h^3 \epsilon^2 c) = 10 973 731.568 51 [1/m]$  (2)

Generally, for any mass of the nucleus, using the formula for the total angular momentum - after the transformations, we get that:

 $\begin{array}{ll} R_X = R_\infty \ / \ (1 + \ m/M) & (3) \\ m - electron \ mass & m = 9.109 \ 383 \ 56 \ \ ^* \ 10^{-31} \ \ [kg] \\ M - mass \ of a given nucleus & [kg] \\ R_\infty - Rydberg \ constant \ when \ the \ kernel \ is \ stationary. \\ R_X \ - \ the \ value \ of \ the \ Rydberg \ constant \ for \ the \ X \ atom \ with \ the \ mass \ of \ the \ M \ nucleus. \end{array}$ 

 $\begin{aligned} R_{\infty} &= 10\ 973\ 731.568\ 51\ [1/m] = m * e^4 \,/\,(8\ h^3\ \epsilon^2\ c) \\ R_{He+} &= 10\ 972\ 227\ [1/m] \\ R_{H} &= 10\ 967\ 758.23\ [1/m] \end{aligned}$ 

To calculate the  $B_X$  value for a given atom X from the Rydberg constant  $R_X$ , one can calculate the reduced mass of the electron  $m_x$  from the formula (4) and substitute this mass into the formula (5) for the Rydberg constant  $R_X$  and then into the formula (6) for  $B_X$ :

 $m_x = m/(1+m/M)$ (4) m- electron mass  $m_x - reduced electron mass$ M- mass of a given nucleus

 $R_{X} = m_{x} * e^{4} / (8 h^{3} \epsilon^{2} c)$ (5)  $B_{X} = hcR_{X} Z^{2}$ (6)

Formula (6) is derived from Rydberg's formula for the emitted frequency:  $v = c R Z^2 (1/k^2 - 1/n^2)$  (n > k) because E = h v and for ionization  $(1/k^2 - 1/n^2) = 1$ .

If the nucleus was stationary (i.e. for an infinite mass nucleus) we get  $B_{\infty} = hcR_{\infty} = 13.605\ 693\ 01\ eV$ . (based on  $R_{\infty} = 10.973,731.568\ 51\ [1 / m]$ , Z = 1).

For <sup>4</sup>He+ we get  $B_{He+} = hcR_{He+} = 13.60384 \text{ eV}$ based on  $R_{He+} = 10\ 972\ 227\ [1/m]$ , Z = 1).

For <sup>1</sup>H we get  $B_H = hcR_H = 13.598433$  eV. (based on  $R_H = 10,967,758.23$  [1 / m], Z = 1).

 $B_{\infty} = 13.60569301 \text{ eV} \approx 13.6057 \text{ eV}$  is called the 1 Rydberg of energy. It is 1.0005344 of the ionization energy of hydrogen <sup>1</sup>H. This energy indirectly appears in all formulas of the BHM theory.

Applied values of the fundamental constants of physics [10] :

$m = 9.109 383 56 * 10^{-31} [kg]$
$e = 1.602 \ 176 \ 621 \ * \ 10^{-19} \ [C]$
$h = 6.626\ 070\ 040\ *\ 10^{-34}$ [kg * m * m/s]
c = 299 792 458 [m/s]
$\varepsilon = 8.854 \ 187 \ 817 * \ 10^{-12} \ [F/m]$

By the way,  $\epsilon \approx 17 * 17 * 11 * 7 * 5 / (4 \pi) * 10^{-15} = 8.8541874 * 10^{-12} [s*A/(V*m)]$ and because  $\mu = 4 \pi * 10^{-7} [V*s/(A*m)]$  then :  $\epsilon * \mu \approx 17 * 17 * 11 * 7 * 5 * 10^{-22} [s^2 / m^2].$ 

In turn, from Maxwell's theory we know that  $c^2 \epsilon \mu = 1$ , so our  $c \approx 299792465$  [m/s]. The last value is only 7 [m/s] higher than the one assumed as the constant c since 1980. The product of successive prime numbers presented here originates from the Theory of Hosons Interactions.

From the Hoson's Theory we also know that Newtonian constant of gravitation G is connected with h:

 $\begin{array}{l} G = (h' / (8 m))^2 * 1 / (j \pi) \\ j = 1 [kg * m] \\ h' = h / 2\pi = 1.054 571 800 \times 10^{-34} [(m / s) * (kg * m)] \\ G = 6.67408 \times 10^{-11} [(m^2 / s)^2 / (kg * m))] \end{array}$ 

### II. Calculation of the transition energy $n \Rightarrow k$ for He (+) or He II (Rydberg's atom).

From formula (1b), using the constant  $B_{He} = 13.60384 \text{ eV}$ , it is possible to calculate not only the helium ionization energy, but also the energies for individual transitions of the electron in singly ionized Helium He II or He (+) from the n orbit to the k orbit.

These transitions appear straightforwardly as spectral lines He II (Energy Levels of Singly-ionized Helium He II) !

Table 1 presents the results of such calculations of the energy of electrons transition from n orbit to k orbit for helium He (+), i.e. He II.

These results were compared with experimental data converted to [eV] from He II emission wavelengths given in [1] [J. E. Sansonetti and W. C. Martin 2005]. For He II multiplets (e.g. for He II heptet  $n = 3 \ k = 2$ ) the average energy value was assumed. In the case of the above-mentioned heptet (from 164.0332 nm to 164.0533 nm) it was 7.5580 eV. The results from formula (1b) are usually the same or lower only by about 0.0002 (to 0.0005 eV) than the averaged peak energy from work [1]. Only for k = 3 the differences amount to a maximum of 0.0014 eV.

The data in Table 1 are given in [eV].  $B_{He} = 13.60384 \text{ eV}$ , i.e.  $4 B_{He} = 54.41536 \text{ eV}$ . However, in order to obtain the best compliance with the experimental data, in the formula (1c) was adopted  $4 B_{He} \approx 54.41776 \text{ eV}$  that is the value equal to the ionization energy He(+) => He(++) according to [1] ionization energy He(+) = 54.417760 eV.

 $E = -B_{He} Z^2 (1/k^2 - 1/n^2)$  (n > k) (1 b)

In practice, the following formula has been used:

 $E = 54.41776 (1/k^2 - 1/n^2)$  (n > k) (1c)

	k=1	k=2	k=3	k=4	k=5	k=6
n=2	40.8131					
n=2	40.8133					
n=3	48.3713	7.5579				
n=3	48.3713	7.5580				
n=4	51.0167	10.2031	2.6460			
n=4	51.0166	10.2033	2.6453			
n=5	52.2411	11.4278	3.8707	1.2247		
n=5	52.2410	11.4277	3.8697	1.2244		
<b>n=6</b>	52.9062	12.0928	4.5361	1.8899	0.6653	
<b>n=6</b>	52.9062	12.0928	4.5348	1.8895	0.6651	
n=7	53.3072	12,4939	4.9372	2.2911	1.0664	0.4011
n=7	53.3072	12.4939	4.9359	2.2905	1.0661	0.4010
n=8	53.5675	12,7541	5.1976	2.5507		
n=8	53.5675	12.7542	5.1961	2.5508	1.3264	0.6613

Table 1. Experimental transition energies  $n \Rightarrow k$  for <sup>4</sup>He(+) and transition energies calculated from formula (1c).

k - number of the orbit onto which the electron falls

n - orbit number from which the electron drops (n > k)

Data written in blue (in the bottom line for a given n) are calculated from the expression (1c), while data written in red (in the top line) come from the conversion of data from paper [1].

It can also be seen that the value for k = 2 / n = 4 for He+ (10.2033 eV) corresponds to the value for k = 1 and n = 2 for hydrogen (10.2004 eV).

Value 12.0928 eV ( $n_{He} = 6$   $k_{He} = 2$ ) corresponds to 12.0894 eV ( $n_H = 3$   $k_H = 1$ ) etc.

Despite such spectacular successes (in Table 1 the error is below 0.001 eV !), opponents of the Bohr theory appeared. In the 1920s they argued that Bohr's Theory gave seemingly "inaccurate" results for two and more electron systems.

From around 1925, even the opinion was spread that due to various disturbances in the movement of electrons (especially difficult to calculate electron-electron interactions), Bohr Theory "could not" be used to calculate e.g. the helium spectrum.

According to this view, the Bohr theory was "not suitable" for calculating energy transitions in multi-electron atoms. At that time, the solution of the Schrödinger equations with an accuracy better than +/- 30% remained out of reach for a long time - without mathematical machines. Therefore, Heisenberg's uncertainty principle was soon to become some "key" to "understanding" and "development" of the further "probabilistic" science.

The late fruit of this science were works on pseudo-entanglement vide John Bell / Alain Aspect (1964/1968), the theories of which appeared shortly after, when Niels Henrik David Bohr died in November 1962.

After 2000, it becomes increasingly clear that nothing like the bilocation of matter or its visible blur have not been discovered.

On the contrary, most experiments, including the diffraction of electrons and even neutrons, confirm the existence of the de Broglie and David Bohm pilot wave. Electron energies are calculated for various crystals and semiconductors with accuracy of 0.001 eV and better. The paths of electrons in metals and metalloids are already known with accuracy to picometers - see, for example, the works on graphene authorized by Mohsin [4].

Therefore, semiconductor technologies are developing at a dizzying pace in some centers.

The so-called Bell's "teleportation" of quantum states turned out to be a logical and mathematical error. I demonstrated it in my HPT theory and pointed to the necessity of the existence of superluminal hosons in order to correctly explain, for example, the paradoxes of the path of light, the Fermat principle, tunneling phenomena, or the real cause of the appearance of time dilation, usually explained by the so-called Theory of Relativity. In turn, Malus's law can be explained by the Hoszowski phase angle for a single photon without "photon entanglement" and without quantum mechanics [12].

### III. Calculation of the nth ionization energies for various elements.

To meet the needs of quick estimation of electron energy in metals and semiconductors, I created a quick and simple BHM theory, which is part of the larger HECTHOR theory (Hot Electron Conductivity THeORy) since 2019 called HECTOR theory.

The Extended Bohr Theory is the Bohr theory enriched with a few simple factors.

The BHM theory was successfully used by me in 2017-2019 to explain 130 of the 139 strongest helium spectral lines contained in the paper [1]:

[Handbook of Basic Atomic Spectroscopic Data, J. E. Sansonetti and W. C. Martin published online 28 September 2005 © 2005 American Institute of Physics ].

One of the elements of BHM is the addition of the nucleus shielding constants by electron shells.

The screening constants in the BHM theory are analogous to the Moseley constants – known from the calculation of X-ray spectra.

Electron-electron interactions were also included in the BHM (in a non-exhaustive way in this article). It turned out that these few new constants greatly extend the applicability of Bohr's theory.

Using such modified BHM theory, in this work the ionization energies of atoms were recalculated. Obtained results - also for multi-electron ions! - in 90 percent of cases they do not differ by more than 0.05 eV from the table data. In a few cases the error is 0.06 eV but usually the error is less than 0.02 eV.

For example, Table 2 lists the third ionization energies for seven elements.

### Table 2.

Third ionization energies for seven elements - comparison of experimental data with BHM calculations.

Element	Z	III ionization energy experimentally determined Eion(III)xp	III ionization energy calculated from BHM Theory Eion(III)'	difference Eion(III)' - Eion(III)xp
		[eV]	[eV]	[eV]
Li	3	122.419	122.420	+0.0001
Be	4	153.85	153.842	-0.0080
В	5	37.926	37.9280	+0.0020
С	6	47.871	47.8712	+0.0002
Ν	7	47.435	47.4347	-0.0003
0	8	54.886	54.9031	+0.0171
F	9	62.646	62.6409	-0.0051

## The Bohr-Hoszowski-Moseley theory does not use the Schrödinger equation or the Heisenberg matrix anywhere.

In Bohr's theory, the basic expression for the energy of electron transition from n to k orbit was equation (7) analogous to (1b).

This equation contains the energy  $B_X$  for a given element X ( $B_X \approx 13.60 \text{ eV} \approx 1/2$  hartree) instead of the Rydberg constant:

$$E_{nk} = Z^2 B_X (1/k^2 - 1/n^2) (n > k)$$
 (7)

In BHM theory, expression (8) similar to (7) was used, except that instead of Z, 'Z effective' was used which is the charge of the nucleus less the shielding Mh, and the interaction energy detached Electron - Electrons EE has been added:

$$E_{nk} = (Z - Mh)^2 * B_X * (1/k^2 - 1/n^2) + EE$$
 (n > k) (8)

In the case of ionization, the  $1 / n^2$  component tends to zero, so the expression for the energy needed for ionization (the same for an ion or an atom!) simplifies to (9):

$$E_{ion} = (Z - Mh)^2 * B_X / k^2 + EE$$
 (9)

and:

### $E_{ion} = (Z - Mh)^2 * B_{efc} + EE$ (10)

# THIS IS HOSZOWSKI'S MODEL (10) FOR THE ENERGY OF IONIZATION OF ISOELECTRON SYSTEMS.

**Mh** is Henry Moseley's nucleus shielding constant, recalculated in 2021 year for the purposes of Hoszowski's theory. The Mh values are given in Table 3 below.

It turned out that:

### each isoelectron system has its own constant Mh value.

It should be emphasized that the value of Mh does not directly depend on the atomic number Z. It only depends on the number of electrons in the initial system subjected to ionization (regardless of whether it is a neutral atom or an ion!), i.e. it depends on the initial electron system (on the "cloud shape" in system). For the number of electrons u from 3 to 10, i.e. for the second shell k = 2, the following relations are approximately fulfilled:

$\mathbf{Mh} \approx 0.75 \ \mathbf{u} - 0.63$	(11 a)
Befc $\approx 3.42 + 0.01$ (u-3)	(11 b)

Equation (11 a) means that for the 2 electrons detached, the charge seen "outside" of the ion usually only increases by about 1.5  $q_e$ . However, since the electronicity of the system u decreases, the repulsion energy EE of the detached electron also decreases (in absolute value) and additionally **Befc** slightly increases. Consequently, the ionization energy generally increases more than 1.5 \* 1.5 = 2.25 times.

In total, for 2 electrons detached,  $E_{ion}$  increases not by 2.25, but by 3 to 4 times. However, in the BHM theory, the ionization energies were related to the electronicity of the u system. It resulted in much greater accuracy. The error between prediction and experiment became less than 0.05 eV.

For such accurate calculations of the E\_ion, the practical values of Mh and B\_effective (instead of  $B_X/k^2$ ) should be used from table 3. It's written in equation (10).

 $\mathbf{B}_{\mathbf{X}} / \mathbf{k}^2 \approx \mathbf{B}_{efc}$  or B\_effective - means the constant base of the ionization energy for a specific electron shell from which the electron is torn off. The number k is the number of the shell from which we detach the tested electron. As it is known, every successive shell can "fit" 2,8,8,18,18 electrons, so k depends only on the number of electrons in the system subjected to ionization. Thus, further rules follow this principle:

a) in the case of a 1 or 2 electron system  $B_{efc} \approx Rydberg \approx 13.6057$  eV because k = 1. BHM calculations show, that for u = 2 electron systems the value Befc = 13.6136 eV should be inserted, instead of  $B_{He}$  or  $B_{H}$ . b) in the case of a 3 to 10 electron system  $u = 3 \dots 10$ , i.e. k = 2

and then  $B_{efc} \approx 3.46 \text{ eV}$  (i.e. for k = 2  $B_{efc} \approx 13.6 / 2^2 + 0.06 \text{ eV}$ )

c) in the case of an 11 to 18 electron system  $u = 11 \dots 18$ , i.e. k = 3and then  $B_{efc} \approx 1.655 \text{ eV}$  (i.e. for k = 3  $B_{efc} \approx 13.6 / 3^2 + 0.144 \text{ eV}$ )

d) in the case of a system of more than 18 electrons, the relationships are similar, but less clear.

 $\mathbf{E}\mathbf{E}$  is the sum of the interaction of the detached electron with the remaining electrons along with the energy needed to rebuild the remaining u-electron system into the (u-1) electron system.

EE, as usually negative, reduces by a certain amount (usually by 1.097 eV for each electron of the system u) the energy needed to detach another electron from the u-electron system.

Table 3.

The practical Mh, Befc and EE values depending on u-electronicity system subjected to ionization.

system	Mh	<b>B_effective</b>	EE	EE as multiplicity of
u		Befc		-1.097 eV
electrons		[eV]	[eV]	(approx.)
1 <sup>1</sup> H	0	13.598433	0	0
1 other	0	13.603	0	0
2	0.6265	13.6136	-1.0918	1
3	1.6223	3.4222	-1.1140	1
4	2.1909	3.4311	-1.9108	2
5	3.1666	3.4541	-3.3247	3
6	3.8507	3.4652	-4.7571	4
7	4.5359	3.4713	-6.5356	6
8	5.4330	3.4933	-9.4180	9
9	6.0782	3.4622	-12.1640	11
10	6.8251	3.5070	-13.8040	13
11	8.500	1.6626	- 5.2683	5
12	9.096	1.6536	- 6.3309	6

Table 4 compares the ionization energies reported in the literature [1] [2] [3] with the calculated  $E_{ion from equation (10)}$  for the first 12 elements of the periodic table.

It can be seen that from the BHM theory it is possible to calculate with good accuracy not only the penultimate ionization energies, but also the previous energies before them and even singular spectral lines for many elements.

It turnes out that nothing prevents the calculation of all ionization energies for atoms with atomic numbers from Z = 1 to Z = 18.

The practical formula for calculating the ionization energy for a given u-electron system in the BHM theory takes the form (10), i.e. a form analogous to the formula from Bohr's theory. Therefore, this formula will be given here again: (10)

$$E_{ion} = (Z - Mh)^2 * B_{efc} + EE$$
 (10)

For a given system of electrons parameters Mh, B<sub>efc</sub> and EE should be read from Table 3.

* for calc. for $u = 1$ Rx = 13.603 eV was used instead of 13.598 eV for hydro E 1 E 2 E 3 E 4 E 5 E 6						
			EJ	E 4	Е 5	E 6
Z=1	13.598					
Z=1	13.598					
Z=2	24.587	54.418				
Z=2	24.592	54.412 *				
Z=3	5.392	75.640	122.419			
Z=3	5.382	75.603	122.427 *			
Z=4	9.323	18.211	153.850	217.657		
Z=4	9.318	18.230	153.842	217.648 *		
Z=5	8.298	25.155	37.926	259.298	340.127	
Z=5	8.287	25.164	37.928	259.307	340.075 *	
Z=6	11.260	24.383	47.871	64.476	391.986	489.84 [3]
Z=6	11.250	24.404	<b>47.871</b>	64.470	391.999	489.71 *
<b>Z=</b> 7	14.534	29.601	47.435	77.450	97.863	551.920
Z=7	14.541	29.612	47.435	77.441	97.855	551.920
Z=8	13.618	35.121	54.886	77.394	113.873	138.08
Z=8	13.600	35.120	54.903	77.374	113.873	138.08
Z=9	17.423	34.971	62.646	87.140	114.216	
Z=9	17.393	35.027	62.641	87.125	114.216	157.167
Z=10	21.565	41.070	63.500	97.020	126.290	
Z=10	21.545	41.087	63.442	97.104	126.277	157.969
<b>Z=11</b>	5.139	47.286	71.652	98.88	138.370	172.36
<b>Z=11</b>	5.135	47.321	71.702	98.843	138.511	172.36
Z=12	7.644	15.035	80.120	109.290	141.230	186.86
Z=12	7.619	15.095	80.110	109.250	141.230	186.86
				• 70		

Table 4. Ionization energies for elements from Z = 1 to Z = 12.

\* for calc for  $\mu = 1$  Rx = 13.603 eV was used instead of 13.598 eV for hydrogen

Data written in blue (in the bottom row for a given Z) are calculated from the expression (10), while data written in red come from work [1]. Data from paper [2] was written in black and data from paper [3] in purple.

### IV. EXAMPLES.

For example, to calculate the fourth ionization energy for carbon and the fifth ionization energy for nitrogen from the BHM formula (10), we first determine the number of electrons u in the system before ionization. The quantity u can be calculated from the expression:

u = P - nj + 1 ( P - number of protons, nj - number of ionization energy ). For the fourth ionization energy nj = 4, for carbon P = 6, so u = 3. For the fifth ionization energy nj = 5, for nitrogen P = 7, so also u = 3.

This means that in both cases we will ionize the (3 = 2 + 1) electron system.

To obtain a solution with an accuracy better than 0.02 eV, from Table 3 we read Mh = 1.6223 and Bef = 3.4222 for the (2 + 1) electron system. Notice that the value of 3.4222 is almost equal to  $13.6/2^2$ . The energy of repulsion of the 3rd electron (from the 2nd shell) by two electrons from the first shell is small and amounts to 1.114 eV, that is, the E\_ion value obtained from the Bohr-Moseley formula should be reduced by this amount.

The final BHM formula (10.3) for all 3-electron systems will then be:

$$E_{ion} = (Z - 1.6223)^2 * 3.4222 - 1.114$$
(10.3)

In the case of carbon Z = 6, we get  $E_4(C) = 64,470 \text{ eV}$  (64,476 eV from the experiment [1]). In the case of nitrogen Z = 7, we get  $E_5(N) = 97.855 \text{ eV}$  (97.863 eV from the experiment [1]). The lithium atom is also a u = 3 electron system, so equation (10.3) also provides the value of the first lithium ionization energy:

Z = 3 gives the result  $E_1(Li) = 5.382$  eV (5.392 eV from the experiment [1]).

For comparison: a quick approximate solution using the values from (11 a) and (11 b) without using the exact coefficients from table 3. After inserting the values from the expressions (11 a) and (11 b), hence Mh = 1.62; Befc = 3.42 and EE = 1.1 we will obtain approximate results with an accuracy of about 0.06 eV:

 $E_4(C)' = 64.51 \text{ eV}$   $E_5(N)' = 97.89 \text{ eV}$  $E_1(Li)' = 5.41 \text{ eV}$ 

while the values of Mh, Befc and EE from Table 3 give in equation (10.3) a deviation below 0.02 eV:

 $E_4(C) = 64.47 \text{ eV}$   $E_5(N) = 97.86 \text{ eV}$  $E_1(Li) = 5.38 \text{ eV}$ 

From the BHM theory one can calculate electroaffinities of atoms (after adding a new constant for anions), as well as energies of particular conduction electrons for semiconductors.

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