Examining the Electron Phase Transformation Theory in the Context of Atomic Structure

---

ABSTRACT

The shortcomings of the Rutherford atomic model can be eliminated by the suggested phase transformation of the electrons from point to non-revolving surface charge in the vicinity of the nucleus. The energy balance investigations of this atom model indicated that the stability of the surface charge valence electron shell is ensured by the one-dimensional Casimir effect. If this theoretical prediction is correct then the first ionization energies of the elements should correlate linearly to the inverse of atomic diameter. Classical physics approach, the electrostatic attraction of the nucleus and the repulsion of the surface charge electron shell result in an identical relationship. The problem with the classical physics approach is that it does not offer an adequate explanation for the photoelectric effect and the free electrons inside the metal. Therefore, classical electrostatics cannot be considered the right physical process responsible for the stability of the valence electron/s in neutral atoms.

The derived theoretical relationship, between atomic diameter and ionization energy, was tested up to 86 elements of the periodic table. The correlation coefficient is 0.9187. The correlation is stronger for individual periods. The empirical relationship between the ionization energy and atomic radii is well known, resulting in the same correlation coefficients. However, the correlation to the atomic radii does not reproduce the theoretically derived constant multiplier, contrarily to the atomic diameter relationship. Thus, the first ionization energy is the function of the atomic diameter.The uncertainties in the reported atomic sizes are relatively high. Therefore, the correlationbetween theory and experiments should be considered as excellent. The theoretically derived relationship between the first ionization energy and atomic diameter is the consequence of the proposed phase transformation of the electron. Thus the detected strong correlation between theory and experiments adds further support to the proposed atomic structure.

Keywords: Atom model; electronic structure; Casimir effect; electron stability; ionization energy.

1. INTRODUCTION

The reinterpretations of existing experiments indicate that the point charge electron transforms to a surface charge halo in the vicinity of the nucleus [1,2]. The schematic figure of the formed atom model is shown on Fig.1.

The word electron, in this text, refers to surface charge valence electrons in neutral atoms. Based on energy balance investigation of the electron it has been shown that the energy, which ensures the stability of the electron (E^{e-s}) is the one-dimensional Casimir effect (E^{e}_{C-1D}), which exerts pressure on the surface of the electron shell [2]. The Casimir energy on a spherical object (E_{Co}) is

$$E_{Co} \cong 3\alpha\hbar c\frac{1}{d}, \qquad (1)$$

where $\hbar$ is the reduced Planck constant, c is the speed of light in vacuum, d is the diameter of the sphere, and α is the fine structure constant defined as:

$$\alpha = \frac{1}{4\pi\varepsilon_o}\frac{e^2}{\hbar c}, \tag{2}$$

where ε_o is the permittivity of free space, and e is the elementary charge of the electron. The energy required for stabilizing the surface charge electron shell is then:

$$\mathrm{E}^{e-s} = \mathrm{E}^{e}_{\mathrm{C-1D}} = \frac{1}{3}\mathrm{E}^{e}_{\mathrm{Co}} \cong \alpha\hbar c\frac{1}{\mathrm{d_a}}, \tag{3}$$

where $\mathrm{d_a}$ is the diameter of the valence electron shell, which is the same as the atomic diameter.

Based on classical physics, the electron is stabilized by the energy of the electrostatic attraction of the nucleus ($\mathrm{E}^{e-s}_{\mathrm{attr}}$). The energy of the self-repulsion of the surface charge electron shell ($\mathrm{E}^{e-s}_{\mathrm{rep}}$) destabilizes the electron. The stabilizing energy of the electron is then the sum of these effects, which can be given as:

$$\mathrm{E}^{e-s} = \mathrm{E}^{e-s}_{\mathrm{attr}} - \mathrm{E}^{e-s}_{\mathrm{rep}} = \frac{e^2}{4\pi\varepsilon_o}\left(\frac{1}{r_a} - \frac{1}{d_a}\right) = \frac{e^2}{4\pi\varepsilon_o}\frac{1}{d_a} \tag{4}$$

where $\mathrm{r_a}$ is the radius of the surface charge valence electron shell. Substituting the fine structure constant (Eq. 2) into Equation 3, it can be shown that the derived relationships (Eqs. 3 and 4) are identical. Despite this identity, the physical processes ensuring the stability of the electron are different. Classical physics assumes that the stability of the electron shell is ensured by the electrostatic attraction of the nucleus, while quantum mechanics assumes that the stability results from the one-dimensional Casimir energy.

2. PHYSICAL PROCESS

In order to validate the physical process, which is responsible for the stability of the electrons, the stability of the electrons was investigated in metal [2]. The outcome of this investigation is summarized here. On the surface of a metal the Casimir effect is active on about half of the surface of the atom, since the neighbouring atoms shield the rest of the surface. If the Casimir effect is responsible for the stability of the valence electrons then, based on the reduced active surface of the Casimir effect, the electrons could be removed at lower energies. This prediction is consistent with the photoelectric effect since the work functions of the elements is about half of the ionization energy. Inside a metal where the entire surface of the atoms is shielded, the electrons should be unstable, which is consistent with the known "electron sea" or zero band energies of metals. Both of these experimental results indicate that the physical process of stabilizing the valence electrons in neutral atoms is the Casimir effect.

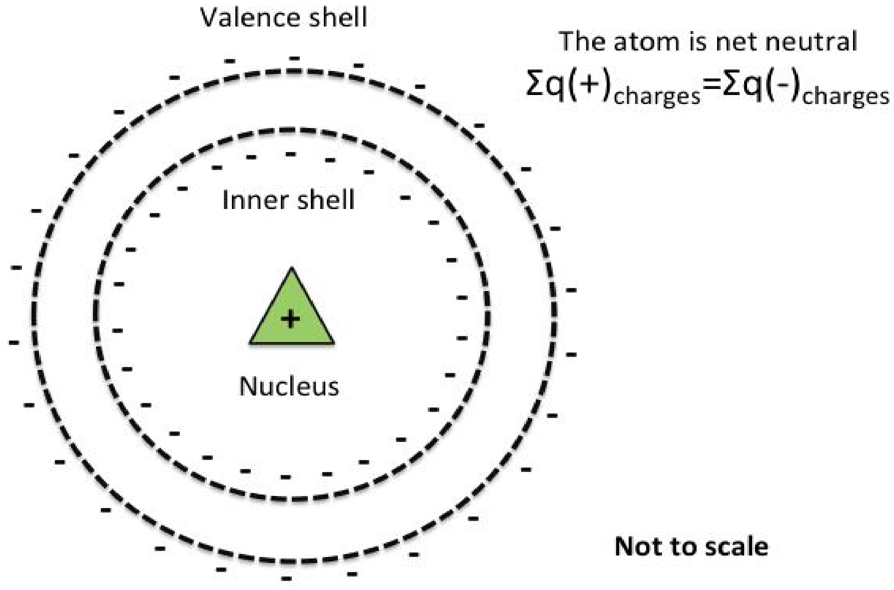

Fig. 1 Schematic figure of an atom is shown. The electrons do not revolve around the nucleus but rather form a static surface charge halo in the atom [2]. The formed electron halo contains all the electrons of the given period of the periodic system of the elements. In every period a new halo starts to form [3]. The nucleus is represented by an equilateral triangle, because the shape of the nucleus resembles a tetrahedron [3,4]

The first ionization energy (IE) is the energy, which requires removing a valence electron from a neutral atom. This energy should be equal with the stabilizing one-dimensional Casimir energy. Thus

$$\mathrm{IE} = \mathrm{E}^{\mathrm{e}}_{\mathrm{C-1D}} \tag{5}$$

Based on this assumption linear correlation between the first ionization energy and the inverse of the atomic diameter (Eq. 3) should exist as:

$$\mathrm{IE} = \mathrm{const}\,\frac{1}{d} \tag{6}$$

where the constant multiplier is

$$\mathrm{const} = \alpha\hbar c = \frac{\mathrm{e}^2}{4\pi\varepsilon_o}. \tag{7}$$

The derived theoretical relationship between the first ionization energies and the size of the atoms has been tested using the experimental data of the elements [5]. The distribution of the data is shown on Fig. 2.

The calculated correlation coefficient for all of the elements (1-86) is 0.9187. The correlation becomes stronger if only a certain period of the elements is investigated. Like, for the second period, elements 3-10, the correlation coefficient increases to 0.9631 (Fig. 3).

3. THEORETICAL EXPLANATION FOR THE RELATIONSHIP

The detected correlation is not new, since the empirical relationship between the atomic radii and the first ionization energies is well established [6-8]. The additional outcome of the current investigation is two folded. Theoretical explanation for the relationship is proposed, and the slope of the detected linear correlation within small uncertainty reproduces the theoretical value of $\alpha\hbar c$. For all the elements, the difference between $\alpha\hbar c$ and the slope of the best fit is 10%. This difference reduces to 3% when only the correlation of the second period is investigated. Based on previously reported empirical relationship [9], between the first ionization energy (E_n) and the electron orbit radius (r_o), the same constant had been derived and a new physical constant in atomic physics (Ω) had been proposed as:

$$E_n r_o = \Omega, \quad \text{where} \quad \Omega = 2.30 \times 10^{-28} \cong \alpha\hbar c. \tag{8}$$

In different publications of the same author[ex. 10] reveal that the author claims that the electron orbit radius of the hydrogen atom [r_o(H)] is $\mathbf{r_o(H) = 2 \times a_o}$, and the diameter of the Hydrogen atom is $\mathbf{d_o(H) = 4 \times a_o}$, where a_o is the Bohr`s radii. Thus, the proposed new empirical physical constant does not relate to the atomic radii but rather to the atomic diameter,which is consistent with the theoretically derived from (Eq. 7) in this study. If the radii of the elements are used in the relationship, then the multiplier is off by 52-55 percent.The reproduction of the theoretically predicted multiplier clearlyindicates that the inverse correlation betweenthe first ionization energy and diameter of the atom, derived from first principles, is the relevant one.

4. IONIZATION ENERGY

The experimental determination of the ionization energy is highly accurate, however the uncertainties in the reported atomic diameters are relatively high [11-13]. Taking into consideration the high uncertainty of the reported atomic sizes, the agreement between theory and experiments should be considered as excellent. The fitting parameters of the correlations are listed in Table 1.

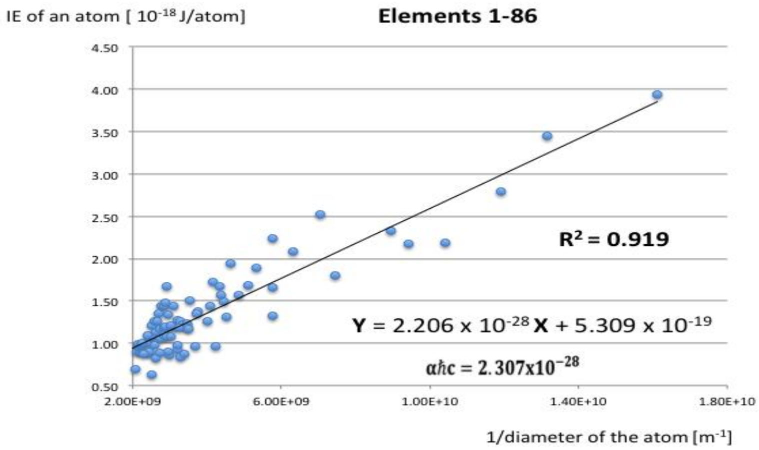

Fig.2. The first atomic ionization energy is plotted against the inverse size of the atom represented by its diameter for elements 1-86. The values are taken from ref. 5

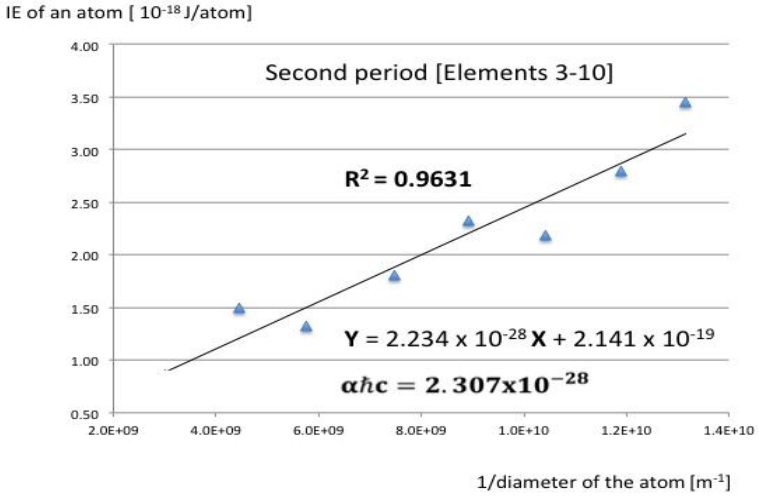

Fig. 3. The first atomic ionization energy is plotted against the inverse size of the atom represented by its diameter for the second period of the periodic table, for elements 3-10.

Table 1. Fitting parameters of the linear correlation are listed. The theoretically predicted slope of the relationship is reproduced with high accuracy

Elements Investigated	**Correlation Coefficient**	**Intersect ($x10^{-19}$ J/atom)**	**Slope ($x10^{-28}$ Nm^2/atom)**	**Theory ($x10^{-28}$ Nm^2/atom)**	**Difference %**
2^{nd} period (3-10)	0.9631	2.141	2.2336	$\alpha\hbar c$	3.3
Total (1-86)	0.9187	5.305	2.0611	2.3071	10.7

Table 2. Experimental data [5] of IE and r_{atom} are used to calculate the "Casimir "values based on the relationship of Eq. 6. The differences between the experimental and calculated values are given in percentage

Atomic Number	**Element**	**IE (kJ/mol)**	**r_{atom} (pm)**	**$IE_{Casimir}$ (kJ/mol)**	**$r_{Casimir}$ (pm)**	**Diff. %**
1	H	1312.75	53	1310.71	53	0
2	He	2372.32	31	2240.89	29	-6

Atomic Number	**Element**	**IE (kJ/mol)**	**r_{atom} (pm)**	**$IE_{Casimir}$ (kJ/mol)**	**$r_{Casimir}$ (pm)**	**Diff. %**
3	Li	520.22	167	415.97	134	-20
4	Be	899.50	112	620.25	77	-31
5	B	800.64	87	798.48	87	0
6	C	1086.45	67	1036.83	64	-5
7	N	1402.33	56	1240.50	50	-12
8	O	1313.95	48	1447.24	53	10
9	F	1681.04	42	1653.99	41	-2
10	Ne	2080.66	38	1828.10	33	-12
11	Na	495.85	190	365.62	140	-26
12	Mg	737.75	145	479.09	94	-35
13	Al	577.54	118	588.71	120	2
14	Si	786.52	111	625.84	88	-20
15	P	1011.81	98	708.85	69	-30
16	S	999.59	87	798.48	69	-20
17	Cl	1251.18	79	879.34	56	-30
18	Ar	1520.57	71	978.42	46	-36
19	K	418.81	243	285.88	166	-32
20	Ca	589.83	194	358.08	118	-39
21	Sc	633.09	184	377.54	110	-40
22	Ti	658.81	176	394.70	105	-40
23	V	650.91	171	406.24	107	-38
24	Cr	652.87	166	418.48	106	-36
25	Mn	717.27	161	431.48	97	-40
26	Fe	762.47	156	445.31	91	-42
27	Co	760.40	152	457.02	91	-40
28	Ni	737.14	149	466.23	94	-37
29	Cu	745.48	145	479.09	93	-36
30	Zn	906.40	142	489.21	77	-46
31	Ga	578.84	136	510.79	120	-12
32	Ge	762.18	125	555.74	91	-27
33	As	944.46	114	609.37	74	-35
34	Se	940.96	103	674.44	74	-28
35	Br	1139.86	94	739.02	61	-35
36	Kr	1350.76	87	798.48	51	-41
37	Rb	403.03	265	262.14	172	-35
38	Sr	549.47	219	317.20	126	-42
39	Y	599.88	212	327.68	116	-45
40	Zr	640.07	206	337.22	109	-47
41	Nb	652.13	198	350.85	107	-46
42	Mo	684.31	190	365.62	102	-47
43	Tc	702.41	183	379.61	99	-46
44	Ru	710.18	176	394.70	98	-44
45	Rh	719.67	173	401.55	97	-44
46	Pd	804.39	169	411.05	86	-49
47	Ag	730.99	165	421.02	95	-42
48	Cd	867.77	161	431.48	80	-50
49	In	558.30	156	445.31	124	-20
50	Sn	708.58	145	479.09	98	-32
51	Sb	830.58	133	522.31	84	-37
52	Te	869.29	123	564.78	80	-35
53	I	1008.40	115	604.07	69	-40
54	Xe	1170.35	108	643.22	59	-45
55	Cs	375.70	198	350.85	185	-7
56	Ba	502.85	153	454.04	138	-10
57	La	538.09	169	411.05	129	-24
58	Ce	534.40	183	379.61	130	-29

Atomic Number	**Element**	**IE (kJ/mol)**	**r_{atom} (pm)**	**$IE_{Casimir}$ (kJ/mol)**	**$r_{Casimir}$ (pm)**	**Diff. %**
59	Pr	528.06	147	472.57	132	-11
60	Nd	533.08	206	337.22	130	-37
61	Pm	538.58	205	338.87	129	-37
62	Sm	544.53	238	291.88	128	-46
63	Eu	547.11	231	300.73	127	-45
64	Gd	593.37	233	298.14	117	-50
65	Tb	565.77	225	308.75	123	-45
66	Dy	573.02	228	304.68	121	-47
67	Ho	580.99	226	307.38	120	-47
68	Er	589.30	226	307.38	118	-48
69	Tm	596.69	222	312.92	116	-48
70	Yb	603.44	222	312.92	115	-48
71	Lu	523.52	217	320.13	133	-39
72	Hf	658.52	208	333.98	105	-49
73	Ta	728.43	200	347.34	95	-52
74	W	758.76	193	359.94	92	-53
75	Re	755.82	188	369.51	92	-51
76	Os	814.16	185	375.50	85	-54
77	Ir	865.18	180	385.93	80	-55
78	Pt	864.39	177	392.47	80	-55
79	Au	890.13	174	399.24	78	-55
80	Hg	1007.07	171	406.24	69	-60
81	Tl	589.35	56	445.31	118	-24
82	Pb	715.60	154	451.09	97	-37
83	Bi	702.94	143	485.79	99	-31
84	Po	811.83	136	514.58	86	-37
85	At	-	127	546.99	-	
86	Rn	1037.07	120	578.90	67	-44

Using the derived theoretical relationship of equation 6, the atomic radii ($r_{Casimir}$) from the experimental data of the first ionization energies were calculated [14]. Conversely, the ionization energy ($IE_{Casimir}$) from the reported atomic size had also been calculated. These calculated values are listed in Table 2.

The ionization energies of the elements are measured with high accuracy contrarily to the atomic size. Thus, the calculated atomic radii ($r_{Casimir}$) from the experimental values of the ionization energies should have higher confidence. The calculated Casimir atomic sizes, with two exceptions, are lower than the reported values. The average difference, between the calculated and experimental values, is minus 34.6 percent. The standard deviation is 15.5 percent. The calculated smaller atomic sizes from the well-defined first ionization energies indicate that the sizes of the individual atoms in the gas phase might be smaller than in the crystal. This result seems to be consistent with the proposed atom model, since the Casimir pressure is effective on the entire surface of the atom in gas phase, contrarily to solid phase[15-16].

CONCLUSIONS

Based on energy balance investigation [2] the stability of the non-revolving surface charge electron shell in neutral atoms is ensured by the onedimensional Casimir energy. If this assumption is correct then the first ionization energy of the elements should correlate to the size of the atoms. Using the experimental data of the elements this correlation was tested with positive results. The correlation coefficient for elements 1-86 of the periodic table is 0.9187. The correlation is higher if individual periods are investigated. The detected correlations reproduce the value of the theoretical constant multiplier, drive from first principles, within 3 and 10 percent for the second period and the total data set respectively. The uncertainties in the reported atomic sizes are relatively high. Consequently, the correlation between theory and experiments should be considered as excellent. The strong correlation, which can be explained only by non revolving surface charge electron shells, additionally supports the phase transformation of the electron from point to surface charge and vice versa.

COMPETING INTERESTS

Author has declared that no competing interests exist.

REFERENCES

1. Garai J. The electronic structures of the atoms. Physics Essays. 2017;30(4):455-460.
2. Garai J. Atomic structure: validation of the electron phase transformation theory. Chem. Sci. Int. J. 2023;32(6):78-98.
3. Garai J. Nuclear lattice model and the electronic configuration of the chemical elements, mendeleev to oganesson. A Multidisciplinary Perspective on the Periodic Table, Ed. E. Scerri, and G. Restrepo, Oxford University Press; 2018.
4. Garai J. Mathematical formulas describing the sequences of the periodic table. Int. J. Quantum Chemistry. 2008;108:667-670.
5. Haynes WM. CRC handbook of chemistry and physics 95th edition. CRC Press Taylor and Francis Group, Boca Raton FL; 2014-2015.
6. Tamura S. An empirical correlation between the atomic radius and the first ionization energy for the elements, J. Mater. Sci. Lett. 1996;15:1678-1679.
7. Bohorquez HJ, Boyd RJ. Is the size of an atom determined by its ionization energy?, Chem. Phys. Lett. 2009;480(1-3):127-131.
8. DeKock RL, Strikwerda JR, Yu EX. Atomic size, ionization energy, polarizability, asymptotic behavior, and the Slater-Zener model, Chem. Phys. Lett. 2012;547:120-126.
9. Tursunbaev B. Atomic size: A new physical constant in atomic physics, European science Review, Volume 2., Section 14. Physics, Vienna. 2018;114-115.
10. Tursunbaev B. Deterministic electronic structure of an atom: the origins of the delusions of quantum mechanics and its resuscitation, LAP LAMBERT Academic Publishing. 2018;ISBN-13 : 978-6137323496
11. Rahm M, Hoffmann R, Ashcroft NW. Atomic and Ionic Radii of Elements 1–96, Chem. Eur. J. 2016;22:14625-14632.
12. Rahm M, Hoffmann R, Ashcroft NW. Atomic and ionic radii of elements 1–96, Chem. Eur. J., 2017;23(1)..
13. Yadav P, Tandon H, Malik B, Suhang V, Chakraborty T. A quest for the Universal Atomic Radii, Structural Chemistry. 2022;33:389-394.
14. Alio IA, Aboubacar A. Angular distribution of atomic photoelectrons as a function of photon field polarization: Case of Ns-type light atoms. Phys. Sci. Int. J. 2022;26(5):17-25.
    Accessed On:2024 May 19
    Available:https://journalpsij.com/index.php/PSIJ/article/view/743
15. Udema II. A mathematical relationship between hydrogenic periodic property and nuclear properties in furtherance of bohr's theory. Asian J. Res. Rev. Phys. 2022;6(3):1-6.
    Accessed On:2024 May 19
    Available:https://journalajr2p.com/index.php/AJR2P/article/view/117
16. Zatsepin DA, Boukhvalov DW, Zatsepin AF, Kuznetsova YA, Gogova D, Shur VY, Esin AA. Atomic structure, electronic states, and optical properties of epitaxially grown β-Ga2O3 layers. Superlattices and Microstructures. 2018;120:90-100.
