Estimation of the critical charge for atomic isoelectronic series

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Abstract

One-particle model with a spherically-symmetric screened Coulomb potential is proposed to describe a motion of a loosely bound electron in a multi-electron atom when charge of the atomic nucleus which is treated as a continuous parameter approaches the "critical" value. Parameters of the model are chosen to meet known binding energies of a neutral atom and the isoelectronic negative ion. This model correctly describes asymptotic behavior of the binding energy in the vicinity of the critical charge and gives accurate estimations of the critical charge.

I. INTRODUCTION

Stability of a given quantum system of charged particles is a question of fundamental importance in atomic, molecular, and nuclear physics. When charge of one of the particles changes, stability of the system can break. Consider, for example, the ground state of a helium isoelectronic ion as a function of the nuclear charge Z. Positive integer nuclear charges correspond to stable systems H^- ($Z = 1$), He ($Z = 2$), Li^+ ($Z = 3$) etc. When the charge is less than the critical charge $Z_c = 0.911$, the ground state cease to exist[1,2]. The critical charge is particularly important for the method of $1/Z$-expansion where it determines a radius of convergence of the series[2].

The critical charges are observed for a more general three-body Coulomb system of particles of variable mass[3,4], for a molecule[5], and for helium isoelectronic ions in space of variable dimensionality[6]. The latter study[6] points out resemblance of the behavior of binding energy near the critical charge to the critical-point behavior of the free energy. The analogy between breaking stability of quantum systems and phase transitions was elaborated further in series of papers[7–9]. Using the method of finite size scaling it was found that the critical charge for lithium isoelectronic series is almost two[9]. Recently, critical charges were determined for atomic isoelectronic series with number of electrons up to 19 by multireference configuration interaction computations[10].

Here, we use a simple one-particle model to predict critical charges of nuclei in N-electron atoms. A free parameter of the model is fitted to meet known binding energies of a neutral atom and an isoelectronic negative ion. The critical charges are found for atoms up to Rn ($N = 86$). For $N \leq 18$, our results agree with configuration interaction computations of[10].

II. ONE-PARTICLE MODEL

Superposition of the Coulomb and Yukawa potentials known as Hellmann potential[11] is widely used to represent interactions in atomic, molecular, and solid state physics, see[12,13]

and references therein. Here, the model potential

$$V(r) = -\frac{1}{r} + \frac{\gamma}{r}\left(1 - e^{-\delta r}\right) \tag{1}$$

is used to approximate an interaction between a loosely bound valent electron and a core in a multi-electron atom.

Let us consider N-electron atom with a nuclear charge Z. In atomic units, the potential of interaction between two electrons is $1/r_{ij}$ and the potential of interaction between an electron and the nucleus is $-Z/r_i$. The potential of interaction between a valent electron and an atomic core consisting of the nucleus and other $N-1$ electrons tends to $-Z/r$ at small r and tends to $(-Z+N-1)/r$ at large r. After the scaling transformation $r \to Zr$, the potential of interaction between two electrons is λ/r_{ij} with $\lambda = 1/Z$, and the potential of interaction between an electron and the nucleus is $-1/r_i$. In these scaled units (that will be used henceforth), the potential of interaction between a valent electron and a core tends to $-1/r$ at small r and tends to $(-1+\gamma)/r$ with $\gamma = (N-1)\lambda$ at large r. It is easy to see that the model (1) correctly reproduces such an effective potential both at small r and at large r. The transition region between $-1/r$-behavior and $(-1+\gamma)/r$-behavior has the size of the core that is about $1/\delta$.

Eigenvalues in the potential (1) were found by two independent methods. The first method is numerical solving of Sturm - Liouville eigenvalue problem by integration of the differential equation. The energies can be easily calculated for any quantum numbers n, l and any parameter γ, δ as long as the state is bound. The second method is perturbation theory for small δ. The potential (1) is expanded into power series

$$V(r) = -\frac{1}{r} + \gamma\delta - \frac{1}{2}\gamma r\delta^2 + \frac{1}{6}\gamma r^2\delta^3 - \frac{1}{24}\gamma r^3\delta^4 + ... \tag{2}$$

where the zero-order term is the Coulomb potential. The zero-order energy is given by Rydberg formula $E_0 = -1/2n^2$. To find corrections to the zero-order energy, we use Rayleigh - Schrödinger perturbation theory for screened Coulomb potentials. The result is a power series in δ

$$E = -\frac{1}{2n^2} + \sum_{i=1}^{\infty} E_i \delta^i \tag{3}$$

where the coefficients E_i were found up to high orders $i \sim 100$ by method used in[14]:

$$E_1 = \gamma, \quad E_2 = \left[-\frac{3}{4}n^2 + \frac{1}{4}l(l+1)\right]\gamma, \quad E_3 = n\left[n^2 - \frac{1}{2}l(l+1) - \frac{1}{2}\right]\gamma, \quad ... \tag{4}$$

The series (3) is summed using quadratic Padé approximants that considerably accelerate the convergence and allow to find even complex energies of resonances when the perturbation parameter is sufficiently large[15]. For bound states, the results of summation appear the same as the results of numerical integration (the first method) except in the vicinity of the threshold, see discussion below.

Results for the ground state and for 2p state are shown on Fig. 1 and 2 respectively. At $\gamma = 1$, the potential turns into the short-range Yukawa potential. Fig. 1 and 2 demonstrate that behavior of the function $E(\gamma)$ crucially depends on an existence of a bound state at $\gamma = 1$, i.e. weather or not $\delta < \delta_c^{\rm Y}$ where $\delta_c^{\rm Y}$ is a critical screening parameter for Yukawa potential tabulated in[16] (1.1906 for the ground state and 0.2202 for 2p state). If $\delta < \delta_c^{\rm Y}$ then the energy crosses the border of continuum spectrum at $\gamma > 1$ with positive derivative, otherwise it tends to Coulomb energy $-(1-\gamma)^2/2n^2$ (fat lines on Fig. 1 and 2, corresponding to $\delta \to \infty$) and touches the border of continuum spectrum at $\gamma \to 1$. In the latter case, the wave function becomes more and more diffuse as $\gamma \to 1$, and at the limit $\gamma = 1$ it is no more square-integrable [17]. We found that the results of summation of the perturbation series diverge in this region for S-states ($l = 0$). Perturbation theory fails because of considerable diffusion of the wave function that becomes essentially different from the zero-order Coulomb wave function. However for $l \neq 0$ states, quadratic Padé approximants converge when $\gamma \gtrapprox 0.9$, but to complex-valued energy, see Fig. 2. There, an effective potential (including the centrifugal term $-1/2r^2$) has a secondary minimum at relatively small r that gives rise of a quasistationary state, see Fig. 3. Note that the bound state is centered around another shallow minimum which is far from the origin. When $\gamma \geq 1$, the quasistationary state continues to exist while the diffuse bound state merges to continuum spectrum.

Fig. 4 shows the derivative of the energy for the ground state. It demonstrates that the derivative at the threshold may be nonzero or zero for $\delta < \delta_c^{\rm Y}$ or $\delta > \delta_c^{\rm Y}$ respectively.

The critical parameter $\gamma = \gamma_c$ where the level enters continuum spectrum $E = 0$ is of particular interest. For small δ, it can be found in the form of an expansion

$$\gamma_c(\delta) = \delta^{-1} \sum_{i=1}^{\infty} \gamma_i \delta^i \tag{5}$$

Coefficients γ_i are found from the equation $E = 0$ where E is represented by the series (3), coefficients E_i are given by formulas (4) with substitution $\gamma \to \gamma_c$. It is important that all coefficients E_i are polynomials in γ of degree $[i/2]$, except $i = 1$ when the degree is 1 (this fact was supported by computations up to $i \sim 100$). By elementary algebraic manipulations, we found that

$$\gamma_0 = \frac{1}{2n^2}, \quad \gamma_1 = \frac{1}{2n^2}\left[\frac{3}{4}n^2 - \frac{1}{4}l(l+1)\right], \quad \ldots \tag{6}$$

The series (6) is summed by quadratic Padé approximants. We found that the function $\gamma_c(\delta)$ exhibits the critical behavior at $\gamma = 1$ similar to the behavior of the energy $E(\delta)$ at $E = 0$ for Yukawa potential, see Fig. 5. If $l = 0$, then $\gamma_c(\delta)$ approaches $\gamma = 1$ at $\delta = \delta_c^{\rm Y}$ with zero derivative and a virtual state appears when $\delta > \delta_c^{\rm Y}$. If $l \neq 0$, then $\gamma_c(\delta)$ crosses the line $\gamma = 1$ with non-zero derivative and a resonant state appears when $\delta > \delta_c^{\rm Y}$. Dependence of $1 - \gamma_c$ on δ is shown on Fig. 5. Note that $1 - \gamma_c$ is an eigenvalue of the generalized Schrödinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{e^{-\delta r}}{r}\right) P(r) = (1 - \gamma_c)\frac{1 - e^{-\delta r}}{r} P(r) \tag{7}$$

Eq. (7) has a form of the Schrödinger equation for Yukawa potential,

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{e^{-\delta r}}{r}\right) P(r) = E^Y P(r) \tag{8}$$

with an additional weight operator $[1 - \exp(-\delta r)]/r$ in the r. h. s. Moreover, we found that eigenvalues of Eq. (7) are similar to eigenenergies in Yukawa potential, compare upper and lower panels of Fig. 5. Complex eigenenergies assume resonant states (the real part is

the position of a resonance, and the imaginary part is the half-width). Meaning of complex critical parameters is unclear for us.

Another simple one-dimensional potential of a square well with barrier was proposed to describe mechanism of pushing of a bound state into continuum[18]. It was found that the bound state turns to a resonance via a virtual state. There are no virtual states in our model potential (1) because it has Coulomb barrier when $\lambda > 1$, cf. Fig. 2 from[18] with Fig. 1 from the present paper.

III. MAPPING OF A MULTI-ELECTRON ATOM TO THE ONE-PARTICLE MODEL

Analysis of electron-electron correlations in a negative atomic ion shows that one of the electrons is held much farther from the nucleus than the others[19]. It suggests one-particle model of this electron regarded as weakly bound in a short-range attractive potential. Even a simple zero-range model potential gives very good description of photoabsorption processes in H^-, see references in[19].

The present study is not restricted to negative ions only. Our model potential (1) approximates both short-range potential of a negative ion ($Z = N-1$) and a partially screened long-range Coulomb potential ($Z \neq N-1$). The free parameter δ is chosen to make the binding energy $-E$ in the potential (1) be equal to the ionization energy of an atom (or an ion) which is known from theory[20,22] or experiments[21,23]. Results of fitting the parameter δ for elements with $5 \leq N \leq 10$ having 2p-electron on an external shell are shown on Fig. 6. It is clear that δ depends on γ almost linearly. We found that it is also the case for another light atoms with $2 \leq N \leq 18$ for which energies of the isoelectronic series are available in literature[20]. Behavior of the function $\delta(\gamma)$ near $\gamma = 1$ that corresponds to $Z = N-1$ can be fairly well approximated by linear dependence

$$\delta = \frac{\delta_0(\gamma - \gamma_1) - \delta_1(\gamma - \gamma_0)}{\gamma_0 - \gamma_1} \tag{9}$$

where (γ_0, δ_0) are parameters corresponding to the neutral atom and (γ_1, δ_1) are parameters corresponding to the isoelectronic negative ion (if the negative ion does not exist, we use parameters corresponding to the positive ion). Ionization energy $E_{\rm I}$ is calculated by solving the Schrödinger equation with the potential (1) at $\gamma = (N-1)\lambda$ and δ determined by Eq. (9). In essence, our method consists of extrapolation of the binding energy from two data points $\gamma = \gamma_0 = (N-1)/N$ (neutral atom) and $\gamma = \gamma_1 = 1$ to the region of $\gamma \sim 1$.

Let us consider the ground and an excited 1s 2s ^{3}S states of helium isoelectronic ions (Fig. 7). For the ground state, dependence of ionization energy on γ is typical for multi-electron atoms having stable negative ions[10]. We reproduce the ionization energy curve using only the energies of He and H^- as it was described above within an accuracy of $5 \cdot 10^{-4}$. Since 1s 2s ^{3}S state is unstable for $Z = 1$, we used ionization energies of Li^+ (instead of H^-) and He to perform the extrapolation. An accuracy of extrapolation for 1s 2s ^{3}S state is better than 10^{-5}. It is evident that direct extrapolation of the binding energy by a linear fit is inaccurate because of strong non-linearity in the vicinity of the critical point, see Fig. 7 and similar Fig. 2, 3 of the paper[22]. In addition, the energy has a singularity at the critical point which deteriorates further an accuracy of linear extrapolation. Our method takes advantage of the fact that an atomic core depends much weakly on λ in the vicinity of λ_c than an orbit of the outer electron that is about to dissociate. Numerical evidence is that reciprocal of the core radius can be extrapolated fairly well by a linear function (9).

The critical charge is found from an equation

$$E_{\rm I}(\lambda_{\rm c}) = 0, \qquad Z_{\rm c} = 1/\lambda_{\rm c} \tag{10}$$

where $E_{\rm I}$ is the extrapolated ionization energy. Results are given in table 1. They agree (mostly within an accuracy of 0.01) both with results of sophisticated ab initio calculations of Hogreve[10] and with critical charges extracted by us from Fig. 2, 3 of[22] (shown in the last two columns of table 1). Table 1 lists also quantum numbers of an outer-shell electron and parameters δ_0 and δ_1 for neutral atoms and isoelectronic negative ions. Note that if a negative ion does not exist, then $Z_c = N - 1$[10].

Our computations of critical charges were extended to another elements with $N > 18$ with stable negative ions. Here, we used experimental ionization energies from atomic data tables[23]. For many atoms with $N > 18$, the ionization energy is not a continuous function of Z because ground-state electronic configurations of N-electron atom and $N-1$-electron positive ion may be different from that of N-electron negative ion and $N-1$-electron atom. For example, ionization of a neutral atom of scandium ($N = 21$) consists of transition from the term 3d $4s^2$ $^2D_{3/2}$ (Sc) to 3d 4s $^3D_1$ (Sc^+), while ionization of an isoelectronic negative ion consists of transition from $4s^2$ 4p $^2P_{1/2}$ (Ca^-) to $4s^2$ $^1S_0$ (Ca). We conjecture here that the critical charge configurations are the same as that for the negative ion. To make ionization energy a continuous function of Z, we fixed configurations to that of the negative ion and $N-1$-electron atom (ionized state). For example, for a neutral atom of scandium ($N = 21$) we considered a difference between energies of terms $4s^2$ 4p $^2P_{1/2}$ (Sc^*) and $4s^2$ $^1S_0$ (Sc^{+*}) as a "modified" ionization energy which is a continuous function of charge to be extrapolated to the region of $\gamma > 1$. Results for critical charges are given in table 2.

Experimental results for negative ions of lantanides remain unreliable[24,25]. We did not calculate critical charges for lantanides. Since electron affinities of lantanides are relatively small ≤ 0.5 eV[21], we expect that surcharges are small also (grey areas on Fig. 8).

For $N = 56$ (Ba), Eq. (10) has no roots and our method fails (possibly because of errors in available experimental data).

To our knowledge, results for $N > 18$ are new. We found that "surcharge" $S_e(N) = N - Z_c$ is correlated with electron affinity $\mathrm{EA}(N-1)$, see Fig. 8. Surcharges and affinities reach maxima for N corresponding to noble gases (and $N-1$ corresponding to halogens). We found that surcharge never exceeds two, i. e. we confirmed non-existence of doubly negative ions[10]. Note that surcharge of noble gases increases with N despite electron affinity of corresponding halogens slightly decreases.

IV. DEPENDENCE OF THE CRITICAL CHARGES ON A MAGNETIC FIELD

Within the one-particle model, an interaction with a magnetic field directed along z-axis is described by a diamagnetic term

$$V_I(r) = \frac{B^2\rho^2}{8Z^4}; \quad \rho^2 = x^2 + y^2 \tag{11}$$

where the magnetic field strength B is given in atomic units (1 a.u =2.3505 10^9 G). By solving the Schrödinger equation with the model potential (1) plus the interaction term (11) at zero energy, we found critical parameters γ_c as a function of the scaled magnetic field $B' = B/Z_c^2$. By varying B', we determined dependence of $Z_c = (N-1)/\gamma_c$ on $B = B'Z_c^2$ parametrically.

The parameter δ was set to δ_c of a free atom (at zero field). We found that increase of a magnetic field generally leads to decrease of the critical charge. Although weakening interaction with the atomic nucleous makes the atomic core less compact and decreases the parameter δ, increase of diamagnetic interaction produces an opposite effect (tightens the atomic core). We conjecture here, that both effects almost compensate one another making the assumption δ =const a good approximation.

Weak field interacts mostly with a loosly bound electron and does not change an atomic core (the nucleus plus $N-1$ electrons). However, strong magnetic field can significantly change the shape and the radius of an atomic core breaking the model.

Accuracy of our model was tested for helium isoelectronic series. Critical charges were found independently (without any additional simplifications) by direct variational calculations (details will be published elsewhere). Results of comparison with the one-particle model are shown on Fig. 9. For weak fields $B < 0.2$, there is a good agreement between the one-particle model and more accurate variational calculations. For strong fields, our model significantly underestimates the critical charge because it does not take into account squeezing of the atomic core.

Results of surcharge, S_e, for closed-shells noble gases are shown in Fig. 10. Results for the critical magnetic field B_c, the minimum field necessary to obtain the surcharge $S_e = 2$,

for selected atoms are listed in Table 3. We have found that dianions with closed shell configurations such as O^{-2}, S^{-2}, Se^{-2}, Te^{-2}, and Po^{-2} became stable at about 1 to 2 a.u. However, dianions with an external s-electron such as Ne^{-2}, Ar^{-2} and Kr^{-2} do not exist at any magnetic field strength, B. This can be attributed to the fact that because of the different symmetry between s and p orbitals, the average $< \rho^2 >$ for p-electron will be smaller than that for s-electron and as a result the shift in the ionization energy will be larger in the presence of a magnetic field for an atom with a weakly bound p-electron. Although it is not feasible to obtain such dianions in the laboratory, because of the strong magnetic field, they might be of considerable interest to models of magnetic white dwarf stellar atmospheres.

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TABLES

TABLE I. Critical charges for atoms with $N \leq 18$

N	nl	δ_0	δ_1	Z_c	[10]	[22]
2 He	1s	1.066	0.881	0.912	0.91	0.92
4 Be	2s	0.339	0.258	2.864	2.85	2.86
6 C	2p	0.255	0.218	4.961	4.95	
7 N	2p	0.242	0.213	5.862	5.85	5.85
9 F	2p	0.239	0.215	7.876	7.87	7.87
10 Ne	2p	0.232	0.211	8.752	8.74	8.74
12 Mg	3s	0.162	0.130	10.880	10.86	
14 Si	3p	0.128	0.112	12.925	12.93	12.90
15 P	3p	0.123	0.110	13.796	13.78	13.79
16 S	3p	0.124	0.111	14.900	14.89	14.90
17 Cl	3p	0.120	0.109	15.758	15.74	15.75
18 Ar	3p	0.117	0.108	16.629	16.60	16.61

TABLE II. Critical charges for atoms with $N > 18$

N	nl	δ_0	δ_1	Z_c
20 Ca	4s	0.0897	0.0748	18.867
21 Sc	4p	0.0776	0.0678	19.989
22 Ti	4p	0.0764	0.0675	20.958
23 V	3d	0.0970	0.0913	21.992
24 Cr	3d	0.0966	0.0912	22.946
25 Mn	4s	0.0871	0.0751	23.863
27 Co	3d	0.0962	0.0913	25.985
28 Ni	3d	0.0959	0.0912	26.941
29 Cu	3d	0.0956	0.0911	27.900
30 Zn	4s	0.0839	0.0748	28.817
32 Ge	4p	0.0745	0.0676	30.946
33 As	4p	0.0727	0.0670	31.814
34 Se	4p	0.0728	0.0673	32.887
35 Br	4p	0.0715	0.0667	33.747
36 Kr	4p	0.0704	0.0661	34.614
38 Sr	5s	0.0573	0.0489	36.830
39 Y	5p	0.0505	0.0451	37.986
40 Zr	5p	0.0487	0.0450	38.942
41 Nb	4d	0.0614	0.0580	39.912
42 Mo	5s	0.0544	0.0485	40.802
43 Tc	5s	0.0544	0.0488	41.849
44 Ru	4d	0.0607	0.0580	42.937
45 Rh	5s	0.0537	0.0485	43.801
46 Pd	5s	0.0533	0.0485	44.797
47 Ag	5s	0.0545	0.0491	45.897

48 Cd	5s	0.0528	0.0484	46.789
50 Sn	5p	0.0486	0.0450	48.945
51 Sb	5p	0.0479	0.0447	49.807
52 Te	5p	0.0478	0.0447	50.833
53 I	5p	0.0472	0.0445	51.715
54 Xe	5p	0.0466	0.0442	52.590
57 La	6p	0.0349	0.0321	55.954
58 Ce	5d	0.0419	0.0400	56.905
60 Nd	5d	0.0423	0.0400	58.948
70 Yb	6p	0.0353	0.0322	68.985
74 W	5d	0.0415	0.0400	72.955
75 Re	5d	0.0415	0.0400	73.884
78 Pt	5d	0.0412	0.0399	76.822
79 Au	6s	0.0360	0.0338	77.656
80 Hg	6s	0.0359	0.0338	78.650
82 Pb	6p	0.0340	0.0321	80.946
83 Tl	6p	0.0341	0.0321	81.929
84 Po	6p	0.0338	0.0320	82.837
86 Rn	6p	0.0333	0.0317	84.518
89 Ac	7p	0.0256	0.0240	87.958

TABLE III. Critical magnetic fields for N-electron atoms

Atom	N	B_c
He	2	No
Be	4	No
C	6	1.89
N	7	1.63
F	9	1.98
Ne	10	1.70
Mg	12	No
Si	14	3.36
P	15	1.90
S	16	2.65
Cl	17	1.71
Ar	18	1.26
Kr	36	1.32
Xe	54	1.21
Hg	80	No
Rn	86	1.06

Figure captions

Fig. 1. Ground-state energy in the screened Coulomb potential (1), in atomic units. Dashed lines are imaginary parts, or half-widths of a quasistationary level.

Fig. 2. The same as Fig. 1 but for an excited 2p-state.

Fig. 3. Shape of an effective potential for $l = 1$, $\delta = 0.25$, and $\gamma = 0.97$. E is energy of the bound state localized around the shallow minimum at $r \sim 60$. E_1 is real part of energy of the quasistationary state associated with a deep minimum at relatively small r.

Fig. 4. Derivative of the ground-state energy in the screened Coulomb potential (1). Dashed lines are imaginary parts the derivative (for quasistationary levels).

Fig. 5. Critical parameter γ_c, Eq. (7), and energy levels in Yukawa potential, Eq. (8), as a function of the screening parameter δ found by summation of the corresponding perturbation series. Dashed lines are imaginary parts.

Fig. 6. The parameter δ of the one-particle model for different isoelectronic series. Here, N is the number of electrons ($N \leq 18$) and $\gamma = (N-1)/Z$.

Fig. 7. Binding energy (found by summation of $1/Z$-expansion) for the groung and an excited 1s 2s ^{3}S states of two-electron isoelectronic series. Dashed curves are errors of our extrapolations, see the text.

Fig. 8. Electron affinities and surcharges as functions of the number of electrons.

Fig. 9. Critical charge for helium isoelectronic series in a magnetic field. Solid line - exact variational calculation, dashed line - one-particle model.

Fig. 10. Surcharge, S_e, as a function of the magnetic field strength, B, for noble gas atoms.

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