Heliumlike and lithiumlike ionic sequences: Critical charges

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In nonrelativistic quantum mechanics we study the Coulomb systems of infinitely massive center of charge Z and two-three electrons: (Z,e,e) and (Z,e,e,e). It is shown that in both cases the total energy curve in Z is smooth, without any visible irregularities. Thus, for both systems the physical integer charges $Z = 1, 2, \ldots$ do not play a distinguished role as would be associated with charge quantization. By definition, a critical charge $Z_{\rm cr}$ is a charge which separates a domain of the existence of bound states from a domain of unbound ones (continuum). For both systems the critical charges are found, $Z_{{\rm cr},2e} = 0.910850$ and $Z_{{\rm cr},3e} = 2.0090$, respectively. Based on numerical analysis, the Puiseux expansion in fractional powers of $(Z - Z_{\rm cr})$ is constructed for both systems. Our results indicate the existence of a square-root branch point singularity at $Z_{\rm cr}$ with exponent $3/2$. A connection between the critical charge and the radius of convergence of $1/Z$ expansion is briefly discussed.

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Let us consider the Hamiltonian which describes the charged center Z and k electrons

$$\mathcal{H} = -\frac{1}{2}\sum_{a=1}^{k}\Delta_a - \sum_{a=1}^{k}\frac{Z}{r_a} + \sum_{a<b}^{k}\frac{1}{r_{ab}}. \qquad (1)$$

The case $Z = k$ corresponds to a neutral atom and $Z = k+1, 2, \ldots$ describes positive ions. Sometimes there exist negative ions $Z < k$, for example, at $Z = 1$, $k = 2$. Critical charge $Z_{\rm cr}$ is a value of Z which separates the domains "existence and nonexistence" of square-integrable solution(s) of the Schrödinger equation $\mathcal{H}\Psi = E(Z)\Psi$. In other words, it separates the domain of charge Z of the Hamiltonian where the bound state(s) exists from the domain where it does not. Constructively, $Z_{\rm cr}$ is determined by the condition that the ionization energy vanishes. The goal of this Brief Report is to find the critical charge $Z_{\rm cr}$ for two-electron (heliumlike) and for three-electron (lithiumlike) sequence. It was claimed long ago that the question about critical charge is closely related to one of the first theoretical questions of newly born atomic physics about the radius of convergence Z_* in the $1/Z$ expansion (see Ref. [1] where extensive discussion with extended bibliography together with historical account is presented). Making change of variables in Eq. (1), $\vec{r} \to \vec{r}/Z$, we arrive at

$$\mathcal{H}_t = -\frac{1}{2}\sum_{a=1}^{k}\Delta_a - \sum_{a=1}^{k}\frac{1}{r_a} + \frac{1}{Z}\sum_{a<b}^{k}\frac{1}{r_{ab}}, \qquad (2)$$

where the new energy $\tilde{E}(\xi = \frac{1}{Z}) = \frac{E(Z)}{Z^2}$. In general, for all studied cases of integer Z the ground-state energy $\tilde{E}(\xi)$ is a smooth, slow-changing real function in $\xi \in [0,\xi_{\rm cr}]$. In particular, for two-electron case $k = 2$ the radius of convergence ξ_* for the expansion of $\tilde{E}$,

$$\tilde{E} = \sum_{n=0}^{\infty} e_n \xi^n \qquad (3)$$

should be given by $\xi_* = 1/Z_{\rm cr}$ (see Ref. [1] and references therein). Furthermore, it was claimed that the nearest singularity to $\xi = 0$, which defines the radius of convergence, is situated at a real ξ axis and even at $\xi = \xi_* = \xi_{\rm cr} \equiv 1/Z_{\rm cr}$ (see Ref. [1] and references therein). Based on the analysis of a large number of computed coefficients of $1/Z$ expansion ($\sim$401) it was found that the critical charge for the two-electron sequence is

$$Z^{[1]}_{{\rm cr},2e} = 0.91103\ldots, \qquad (4)$$

and the singularity associated with it is an essential singularity of a quite complicated nature [1]. Although this value of the critical charge is actually quite close to the first estimate of the critical charge given by Stillinger and Stillinger [2]

$$Z^{[2]}_{{\rm cr},2e} = 0.8941\ldots, \qquad (5)$$

it is in contradiction with the nature of the singularity. It is claimed in Ref. [2] [see Eq. (2.17)] that it is a branch point with exponent $3/2$. Recently, the result (4) was challenged in Ref. [3] by using the accurate numerical analysis of a different set of coefficients in $1/Z$ expansion than the one used in Ref. [1]. It is stated in Ref. [3] that

$$Z^{[3]}_{{\rm cr},2e} = 0.90223\ldots. \qquad (6)$$

This result agrees with [2] on the nature of the singularity as a branch point with exponent $3/2$. Our analysis, which does not rely on perturbation theory, excludes the results (5) and (6) concerning the value of the critical charge, as well as the position of the singularity defining the radius of convergence of (3). Our critical charge is close to $Z^{[1]}_{\rm cr}$ (see below). However, we confirm the observation by [2] and [3] that the singularity at the critical charge is a branch point with exponent $3/2$. We

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are not certain about a nature of singularity(ies) which define the radius of convergence of the $1/Z$ expansion (3).

Our approach is not related to an analysis of $1/Z$ expansion being instead based on accurate calculation of the total energy as a function of the charge Z in vicinity of the critical point with further extrapolation to the critical point. The extrapolating function is assumed to be in a form of the Puiseux expansion for $Z > Z_{\rm cr}$,

$$E(Z) = \sum_{n=0}^{\infty} B_n (Z - Z_{\rm cr})^{\alpha_n}, \tag{7}$$

with the condition that exponents α_n grow with increasing n according to $\alpha_n < \alpha_{n+1}$. Both cases of two- and three-electron systems are considered.

Heliumlike sequence. In order to find the total energy of the $1\,^1S$ state (the ground state) as the function of Z, we used as a trial function a linear superposition of the exponential, explicitly correlated functions (see, e.g., Ref. [4])

$$\Psi_{\rm trial} = \sum_{i=0}^{N} A_i [\exp(-\beta_i r_1 - \gamma_i r_2) + (1 \leftrightarrow 2)] \exp(-a_i r_{12}), \tag{8}$$

where $\{A_i\}$ and $\{\beta_i, \gamma_i, a_i\}$ are linear and nonlinear parameters, respectively. It was shown that this basis provides at present the fastest convergence in ground-state energy for helium ($Z = 2$) and H^- ($Z = 1$) among known bases. Namely, using this basis the ground-state energy for $Z = 1, 2$ was found with 24 s.d. (significant digits) [4].

Using the computer code kindly provided by Pachucki [5], following the work of [4], we see that the fast convergence in energy is also obtained for Z for other than 1 and 2. We calculated the ground-state energies for different Z varying from 0.95 up to 2.00 with an interval 0.05 with 12 significant digits (see Table I for some examples). It is worth noting that for $Z < 0.95$ the rate of convergence starts to deteriorate dramatically with a decrease of Z, it requires many more terms in Eq. (8) to be included to reach desired accuracy unlike for $Z > 0.95$. We exclude the domain $Z < 0.95$ from the calculation of energies based on (8).

Calculations of the ground-state energy for different values of ξ (in 30 points) demonstrate that the energy $\tilde{E}_{2e}(\xi)$ is a smooth, slow-changing function without any visible irregularities in domain $[0, 1/Z_{\rm cr,2e}]$. It does not exhibit any distinguished role of points $1/M$, $M = 1, 2, \ldots$, which would indicate the appearance of the charge quantization. The existence of such a quantization is a fundamental experimental fact.

TABLE I. Ground-state energy E_{2e} for a two-electron sequence for selected values of Z found using (8) where all displayed digits are assumed to be correct and $E_{2e}^{\rm (fit)}$ from the fit (10).

Z	E_{2e}	$E_{2e}^{\rm (fit)}$
1.3	−1.029896662309	−1.0298967
1.25	−0.933575272295	−0.9335753
1.15	−0.756014315641	−0.7560143
0.95	−0.462124684391	−0.4621247

We fit the data in Table I with an expansion of the form (7), but truncated at the value $n = 3$, and then subsequently increased it up to $n = 7$. Taking the ground-state energy at a large number of points in the interval $Z \in [0.95, 1.5]$ and making fit, it is obtained in a stable way with sufficiently high accuracy that α_n takes either integer or half-integer values,

$$\alpha_0 = 0, \quad \alpha_2 = 1, \quad \alpha_3 = 3/2, \quad \alpha_4 = 2, \quad \alpha_5 = 5/2, \quad \alpha_6 = 3, \quad \alpha_7 = 7/2. \tag{9}$$

It confirms, in particular, the rigorous result by Simon [6] about the absence of the square-root term $\alpha = 1/2$ and the presence of the linear term $\alpha = 1$ in this expansion. It contradicts a statement from [7] that the term $\alpha = 3/2$ is absent. In general, such an expansion is in agreement with one proposed in Refs. [2,3]. Eventually, assuming the exponents (9) and taking a data set for energy E_{2e} at nine points $Z \in [0.95, 1, 1.05, 1.1, 1.15, 1.2, 1.25, 1.3, 1.35]$, a careful interpolation leads to the expansion [see Eq. (7)]

$$\begin{aligned} E_{2e}^{\rm (fit)}(Z) = &-\frac{Z_{\rm cr}^2}{2} - 1.142552(Z - Z_{\rm cr}) \\ &- 0.174110(Z - Z_{\rm cr})^{3/2} - 0.770010(Z - Z_{\rm cr})^2 \\ &- 0.139923(Z - Z_{\rm cr})^{5/2} + 0.022469(Z - Z_{\rm cr})^3 \\ &+ 0.008730(Z - Z_{\rm cr})^{7/2}, \end{aligned} \tag{10}$$

with the critical charge

$$Z_{\rm cr,2e} = 0.910850\,. \tag{11}$$

The expression (10) reproduces 7 s.d. in energies at nine points in Z mentioned above, for an illustration see Table I. As for an analysis of the uncertainty in coefficients, we state that the addition of one more digit to any coefficient in (10) or to $Z_{\rm cr,2e}$ (11) does not change 7 s.d. in energies giving a contribution to the eighth digit. Estimating the remainder we find that the next term in the expansion (7) $a_8(Z - Z_{\rm cr})^4$ [cf. Eq. (10)] should have the coefficient $|a_8| < 10^{-6}$ in order to have 7 s.d. in energies unchanged (see Table I).

The explicit knowledge of the first terms of the Puiseux expansion (10) allows us to check whether the singularity at the critical charge defines the radius of convergence of the expansion (3). In order to do it we construct the Puiseux expansion of the function $\tilde{E}_{2e}(\xi)$ near the critical $\xi_{\rm cr} = 1/Z_{\rm cr}$,

$$\begin{aligned} \tilde{E}_{2e}(\xi) = &-\frac{1}{2} + \tilde{B}_1(\xi_{\rm cr} - \xi) + \frac{B_3}{\xi_{\rm cr}}(\xi_{\rm cr} - \xi)^{3/2} \\ &+ \tilde{B}_4(\xi_{\rm cr} - \xi)^2 + \frac{1}{\xi_{\rm cr}^3}\left(B_5 - \xi_{\rm cr}\frac{B_3}{2}\right)(\xi_{\rm cr} - \xi)^{5/2} \\ &+ \frac{B_6}{\xi_c^4}(\xi_{\rm cr} - \xi)^3 + \frac{1}{\xi_{\rm cr}^5}\left(B_7 + \xi_{\rm cr}\frac{B_5}{2}\right. \\ &\left. - \xi_{\rm cr}^2\frac{B_3}{8}\right)(\xi_{\rm cr} - \xi)^{7/2} + \cdots, \end{aligned} \tag{12}$$

where $\tilde{B}_{1,4}$ are related to coefficients in the expansions (7) and (10). It leads to the following form of the coefficient e_n in

TABLE II. Comparison the α_n coefficients in the expansion (3) calculated in Ref. [1] (rounded to 3–5 s.d.), obtained in Ref. [3] and found by using the formula (13). The number in square brackets represents the power of 10.

n	[1]	[3]	(13)
20	−0.76862[−5]	−0.76862[−5]	−0.71475[−5]
100	−0.398[−10]	–	−0.689[−10]
200	−0.301[−15]	−0.222[−15]	−1.065[−15]
300	−0.522[−20]	–	−3.394[−20]

Eq. (3) at large n:

$$e_n = (-)^n \frac{\Gamma\left(\frac{5}{2}\right)}{\Gamma(n+1)\Gamma\left(\frac{5}{2}-n\right)} \frac{1}{\xi_{cr}^{n-\frac{1}{2}}}\left[B_3 + \left(B_5 - \xi_{\rm cr}\frac{B_3}{2}\right) \times \frac{5}{5-2n}\xi_{\rm cr}^{-1} + \left(B_7 + \xi_{\rm cr}\frac{B_5}{2} - \xi_{\rm cr}^2\frac{B_3}{8}\right) \times \frac{35}{(5-2n)(7-2n)}\xi_{\rm cr}^{-2} + \cdots\right], \quad (13)$$

which is a type of $1/n$ expansion for e_n. Now we can make a comparison of these coefficients with ones calculated in Ref. [1], see Table II. One can see that for $n > 20$ the coefficients are becoming sufficiently close. However, a relative deviation in coefficients is growing with an increase of n. For $n = 300$, where $1/n$ corrections to the asymptotic behavior of e_n at n tending to infinity presumably can be neglected, the deviation reaches ∼6 times when the coefficients are more or less of the same order of magnitude 10^{-20}. If, for a moment, we exclude a possibility that the large-order coefficients in Ref. [1] might be calculated incorrectly (see, e.g., Ref. [3]) we arrive at the immediate conclusion that the singularity related with the critical charge (11) defined by the Puiseux expansion (12) cannot explain the large-n behavior of the e_n coefficients. Hence, there must exist other singularity(ies) on the circle of convergence which define the asymptotic behavior of e_n in Eq. (3) at large n.

Indeed, such singularities might naturally exist. Certainly there exist the square-root branch points, which appear in Landau-Zener theory of level quasicrossings (see, e.g., Ref. [8]) due to the level crossing (for discussion see, e.g., the case of quartic anharmonic oscillator [9,10]). The most natural candidate for such a quasicrossing might be a pair of two complex-conjugated square-root branch points due to the crossing of spin-singlet $1\,^1S$ and $2\,^1S$ states, which have the closest energies at real Z when both states coexist. Following this idea we assume that the behavior of the energy is

$$\tilde{E}_{2e}(\xi) = \sqrt{(\xi+a)^2+b^2}\{A_1 + A_2[(\xi+a)^2+b^2] + \cdots\}$$

near square-root branch points at $a \pm \imath b$. However, we were unable to find a, b, A_1, A_2 with $r = (a^2+b^2)^{1/2} < \frac{1}{Z_{\rm cr,2e}}$, which would reproduce the behavior of e_n coefficients at $n > 100$ found in Ref. [1]. It seems that the only possibility which is left is to assume the existence of three (or more) singularities on the circle of convergence: one of them is of the critical charge and the others are pair(s) due to level crossing(s). This possibility looks quite exotic and thus unlikely. Before going to explore it we think that the independent calculation of the large-order coefficients e_n in Eq. (3) is highly needed (see below *Note Added*).

Lithiumlike sequence. In order to find the ground-state energy of the $(Z,3e)$ system as the function of Z, we use the variational methods with Hylleraas basis set as a trial function [11,12]. The ground-state wave function Ψ is expressed as a linear combination of ψ, the antisymmetrized product of ϕ and the spin function χ,

$$\begin{aligned} \psi &= \mathcal{A}[\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3)\chi], \\ \phi_{\rm trial} &= \left[r_1^{n_1} r_2^{n_2} r_3^{n_3} r_{12}^{n_4} r_{13}^{n_5} r_{23}^{n_6} \exp(-a_i r_1 - b_i r_2 - c_i r_3)\right], \\ \chi &= \alpha(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\alpha(3), \end{aligned} \quad (14)$$

where $\{a_i,b_i,c_i\}$ are positive real parameters and $n_{1\text{–}6}$ are nonnegative integers.[1] Using this basis set with 15 variational (nonlinear) parameters plus an analytic evaluation of some Hylleraas integrals as well as recursion relations, Puchalski *et al.* [12] have reached the impressive accuracy 10^{-14} in the ground-state energy for both $Z = 3$ (Li atom) and $Z = 4$ (the Be^+ ion).[2] The results of these authors also indicate that the accuracy of the previous calculation [11] is overestimated and is limited to 10 s.d. Making use of the computer code employed in Ref. [12], and kindly provided by Pachucki [5] and modified by adding MINUIT minimization routine from CERN-LIB, we are able to see that the fast convergence in energy is also obtained for Z other than for 3 and 4.

Calculations of the ground-state energy for different values of ξ confirm that the function $\tilde{E}_{3e}(\xi)$ is a smooth, slow-changing function without any visible irregularities in domain $[0,1/Z_{\rm cr,3e}]$ (see below). It does not indicate any distinguished role of points $1/M$, $M = 3,4,\ldots$, whose would be associated with the appearance of charge quantization.

We calculated the total energies for different Z varying from 2.02 up to 3.00 and reached 7 s.d., the total basis length was equal to 502.[3] To make fit we assume the same exponents (9) in the Puiseux expansion. The data set which was used for interpolation contains seven points $Z \in [2.02, 2.03, 2.07, 2.08, 2.10, 2.12, 2.16]$ (see Table III). We arrive at the interpolation in a form of the expansion (7),

$$\begin{aligned} E_{3e}^{\rm (fit)}(Z) = &-2.934278 - 3.390491(Z - Z_{\rm cr,3e}) \\ &- 0.114813(Z - Z_{\rm cr,3e})^{3/2} \\ &- 1.102097(Z - Z_{\rm cr,3e})^2 \end{aligned} \quad (15)$$

[cf. Eq. (10)], where the critical charge

$$Z_{\rm cr,3e} = 2.0090. \quad (16)$$

In order to check consistency we found that (15) at the critical point $Z = Z_{\rm cr,3e}$ reproduces the ground-state energy of the $2e$

[1]The second spin function is not taken into account in this calculation, for discussion see, e.g., Ref. [14].

[2]Recently, a new calculation of the lowest states of lithium atom carried out along the lines of [11] was published [13]. It confirmed 14 s.d. in the ground-state energy obtained in Ref. [12] and states that "the overall accuracy achieved is 7 parts in 10^{14} for the $2\,^2P$ state and about 5 parts in 10^{16} for the $2\,^2S$ and $3\,^2S$ states" .

[3]Stability of these 7 s.d. was checked directly making a control calculation with the (optimized) basis of length 918. We observe that the accuracy starts to deteriorate dramatically for $Z < 2.02$. We never used data from this domain for analysis.

TABLE III. Ground-state energy E_{3e} for three-electron sequence for selected values of Z found using (14) where all displayed digits assumed to be correct and $E_{3e}^{(\mathrm{fit})}$ from the fit (15).

Z	E_{3e}	$E_{3e}^{(\mathrm{fit})}$
2.16	−3.47810826	−3.478108
2.10	−3.25509127	−3.255091
2.075	−3.16479824	−3.164798
2.02	−2.971839	−2.971839

system E_{2e} in 6 s.d. In general, the expression (15) reproduces 6 s.d. in all seven calculated ground-state energies mentioned above, for an illustration see Table III. As for an analysis of the uncertainty in coefficients, we state that the addition of one more digit to any coefficient in Eq. (15) or to $Z_{\mathrm{cr},3e}$ (16) does not change 6 s.d. in energies giving a contribution to the seventh digit. Estimating the remainder in Eq. (15) we find that the next term in the expansion (7), $a_5(Z - Z_{\mathrm{cr}})^{5/2}$ [cf. Eq. (15)] should have the coefficient $|a_5| < 10^{-4}$ in order to keep unchanged 6 s.d. in the fit of all seven calculated ground-state energies mentioned above.

It is worth noting that the critical charge (16) is inside the intervals for critical charges proposed in Ref. [15]. It seems the method of analysis used in Ref. [15] is quite rough, leading to not very precise results, a direct calculation of the ionization energy $\propto[E_{3e}(Z) - E_{2e}(Z)]$ immediately exclude essential parts of those intervals for critical charge presented in this work.

As a conclusion, we state that based on extrapolation of highly accurate results for the ground-state energy for $(Z,2e)$ and $(Z,3e)$ to the critical charge, the square-root branch point occurs with the exponent $3/2$. This is in agreement with a statement made in Refs. [2,3] for $(Z,2e)$. Furthermore, it is in agreement with recent results for one-two electron molecular systems $(2Z,e)$,$(3Z,e)$,$(4Z,e)$ and $(2Z,2e)$,$(3Z,2e)$ [16]. All these results seem to indicate a universal nature of singularity at a critical charge for Coulomb systems. So far, present authors are unable to give a physics explanation of this phenomenon. For all studied systems we did not see any indication of a charge quantization.

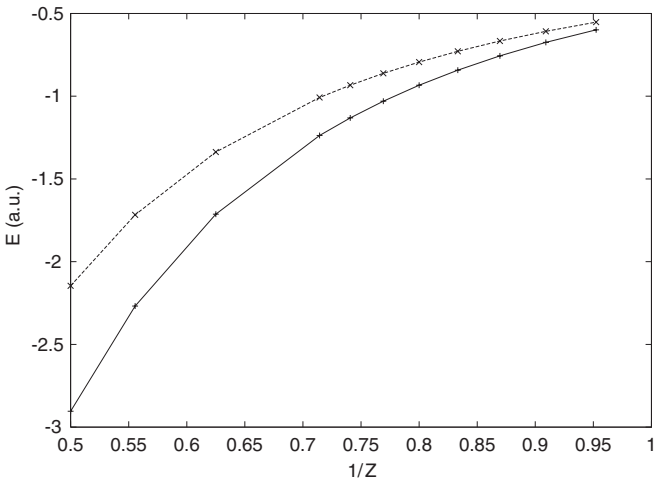

FIG. 1. Energy curves vs Z for the (Z,e,e) system for the spin-singlet $1\,^1S$ (solid line) and $2\,^1S$ (dashed line) states.

Note Added. Recently, we made a preliminary numerical study of energy behavior vs Z of the $2\,^1S$ and $3\,^1S$ states of a two-electron system in domain $Z \in [1, 2]$. These calculations were carried out using a computer code provided by Pachucki [5]. We found a value of the critical charge $Z_{\mathrm{cr},2e}^{(2\,^1S)} = 1.02$ [cf. (6)]. Energy curves in ξ did not display in a clear way a behavior indicating quasicrossings, see Fig. 1. It might be considered as a signal that their square-root branch points are situated far away from the real ξ axis. A localization of these branch points requires a separate study which might be done elsewhere. A general situation with analytic structure of $E(\xi)$ remains unclear.

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