

Approach towards the critical charge of some excited states of the Be isoelectronic series

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A definitive determination of the nature of the approach to the critical charge is illustrated for the $(1s^2 2s 3s)^{1,3}S$ and the $(1s^2 2s 3p)^{1,3}P$ states of the Be isoelectronic series. The features that conclusively indicate that the outermost orbital becomes an infinitely diffuse hydrogenlike orbital upon approaching the critical charge $Z_c = 3$ are the asymptotic proportionality of the ionization energy to $(Z - 3)^2$ and the approach of the corresponding quantum defect to an integer which is equal to the number of orbitals of the same symmetry in the atomic core.

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I. INTRODUCTION

An atomic isoelectronic series has two obvious limiting cases. On the one hand, there is the high nuclear charge limit, where (if one ignores relativistic effects) the system becomes asymptotically hydrogenic, the interelectronic repulsions diminishing in significance. This limit is routinely considered within $\frac{1}{Z}$ -perturbation theory, where the leading term in the energy expansion is the sum of the hydrogenlike energies of the electrons, and the first order term is given by the expectation value of the interelectronic repulsion with respect to the zero-order wave function. The latter is an antisymmetrized and symmetry-adapted product of hydrogenic wave functions, unless, even after symmetry adaptation, zero order degeneracy remains, in which case the appropriate modification is required [1].

The other limit is the “critical charge”, i.e., the nuclear charge below which the outermost electron is not bound. This charge has been of interest for quite some time. Early considerations of the critical charge in the He isoelectronic series are due to Stillinger [2], and to Brändas and Goscinski [3]. Since H^- has a bound ground state (but no bound singly excited states) [4,5], the ground state critical charge of the He isoelectronic series satisfies $Z_c < 1$ {in fact, $Z_c = 0.911\,028\,224\,077\,255\,73(4)$ [6], the leading six digits in agreement with [7]} but it is equal to unity for all the singly excited states. The doubly excited state of H^- , $(2p)^2\ ^3P$ has been shown to be (nonrelativistically) bound as well [8–10]. A rigorously established significant distinction between the 1S ground state and the lowest 3S singly excited state has to do with the fact that in the former the wave function remains

bound (square integrable) at the critical charge [11] whereas in the latter it does not [12]. This 3S state, as well as the $(1s2p)^{1,3}P$ states, were studied by Ivanov *et al.* [13,14], who confirmed that the critical charge is equal to 1 for all three isoelectronic series. Expressing the binding energy of the outermost electron in terms of the Rydberg-Bohr-like formula $-\frac{(Z-Z_c)^2}{2(n-\delta)^2}$, where n is the principal quantum number, Ivanov noted that the quantum defect δ is asymptotically equal to unity for the 3S state and to zero for the two P states, at the critical charge. The asymptotic quantum defect, at the critical charge, was found to approach unity for the $(1s\ 2s)^1S$ isoelectronic series as well [15]. Hence, the $2s$ orbital becomes, at the critical charge, $1s$ -like, although this state is not the lowest of the 1S symmetry. This observation will be further discussed below.

Critical charges for the ground states of the first 19 atoms were determined by Hogreve [16], and estimated for atoms up to Ac ($Z = 89$) by Sergeev and Kais [17]. A study of the ten-electron (Ne) isoelectronic series by Hogreve [18] established a complete analogy with the He isoelectronic series: the ground state has a critical charge $Z_c \approx 8.74$, the ionization energy approaching the critical charge linearly in $Z - Z_c$, whereas the lowest (3P) excited state has $Z_c = 9$, the ionization energy approaching it quadratically in $Z - Z_c$.

The present understanding consists of the mathematical theorem according to which as long as the nuclear charge is (even infinitesimally) larger than $N - 1$, where N is the number of electrons, the system has an infinite number of bound states below the lowest ionization limit [19]. For $Z < N - 1$ there is at most a finite number of bound states. Obviously, the critical charge may be different for different states of any given isoelectronic series. If the critical charge is equal to $N - 1$ then, upon approaching this critical charge, the outermost electron becomes infinitely diffuse, a behavior referred to as “expanding”. However, for N -electron states that are bound at $Z = N - 1$ [i.e., the neutral $(N - 1)$ -electron atom has a positive electron affinity] the critical charge is, of course, less than $N - 1$, and at the critical charge the N -electron wave function is square integrable (bound) although the binding energy vanishes [20]. This kind of

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confinement behavior at the critical charge has been referred to as “absorbing.” As pointed out above, the ground state of the He isoelectronic series is of the latter type, whereas all singly excited states of this isoelectronic series are of the expanding type, the outermost electron becoming infinitely diffuse (with an effective charge that asymptotically approaches $Z - 1$), as $Z \rightarrow 1$. The same is true for the Li isoelectronic series, both for the ground state and for all states involving excitation of the outermost electron.

This dichotomy raises several questions that we do not deal with in the present paper:

(i) Is the presence of two (or more) electrons in a common outermost shell sufficient to yield an absorbing scenario? Indeed, systems with such configurations remain bound as singly negative ions.

(ii) Can a two-electron open shell with the two electrons in distinct subshells, e.g., $1s^2 2s 2p^1 \ ^3P$, be absorbing?

(iii) In an open shell, such as the $1s^2 2s^2 2p^2 \ ^3P, ^1D, ^1S$ states of the C isoelectronic series, will different multiplets have distinct critical charges? Can some be absorbing while the others are expanding? In other words, is it possible for some of these states, but not all of them, to be bound for the singly negative ion? Indeed, in the isoelectronic series mentioned above, the negative ion B^- has a bound 3P state (with binding energy 280 meV) but the corresponding 1D and 1S are resonances [21].

(iv) Can a doubly excited state, e.g., $1s^2 2p^2$, be absorbing? Indeed, the $(2p)^2 \ ^3P$ state of the H^- ion is (nonrelativistically) bound, as pointed out above.

In the present paper we examine the approach to the critical charge of several singly excited states of the Be isoelectronic series. The results confirm the remarks made above, based on earlier observations, concerning the values of the asymptotic quantum defects for expanding series, including the irrelevance of the existence of a lower energy absorbing series of common symmetry. The nature of the approach to the critical charge, which is much more abrupt for an outermost p orbital than for an outermost s orbital, is also confirmed.

We used the relativistic multiconfiguration Dirac-Fock (MCDF) approach to obtain the bound-state wave functions and energies. Details of the method and its implementation are briefly described in Sec. II.

II. THEORETICAL CALCULATIONS

The calculations of the binding energy values were carried out within the MCDF approach using the general relativistic MCDF code (MDFGME) developed by Desclaux *et al.* [22–24]. In that approach, the electrons are treated in the independent-particle model, and their wave functions and energies are evaluated in the Coulomb field of the nucleus and the spherically averaged electronic field. To improve the accuracy of this approach we went beyond the Coulomb approximation for the two-electron interaction by including in the calculation the Breit interaction, that accounts for magnetic interactions and retardation effects. The code description and the formulas implemented can be obtained in Ref. [25].

All calculations were done for a finite nucleus using a uniformly charged sphere. The atomic masses and the nuclear

radii were taken from the tables by Audi *et al.* [26] and Angeli [27], respectively. Quantum electrodynamics (QED) radiative corrections to the electron-nucleus interaction, namely the self-energy and vacuum polarization, were also included. The one-electron self-energy was evaluated using the one-electron values of Mohr and co-workers [28–30] and corrected for finite nuclear size [31]. The self-energy screening and vacuum polarization were included using the methods developed by Indelicato and co-workers [23,24,32,33].

III. CONSIDERATIONS ON THE ASYMPTOTIC BEHAVIOR AT THE CRITICAL CHARGE

Since the characterizing feature of the critical charge is the vanishing of the ionization energy ϵ , it is plausible to expect a behavior of the form $\epsilon = \alpha(Z - Z_c)^\zeta$, where $\zeta > 0$ and α is a constant, upon approach of the critical charge. The value of ζ is fixed by the nature of the scenario, as discussed below.

A. Absorbing isoelectronic series

For the absorbing case, $Z_c < N - 1$, the wave function remains localized (square integrable) at the critical charge. Since at the critical charge the ionization energy vanishes, the virial theorem implies that the contribution of the kinetic energy to the ionization energy (i.e., the difference between the kinetic energy of the N -electron system and the $(N - 1)$ -electron system) vanishes as well. Considering the paradigmatic absorbing isoelectronic series, i.e., the ground state of the two-electron atom, we note that the contribution of the interelectronic repulsion to the ionization energy is equal to the total interelectronic repulsion in this system, since there is no interelectronic repulsion in the ionized (one-electron) system. Obviously, for a localized two-electron wave function the expectation value of the inverse of the interelectronic distance $\frac{1}{r_{12}}$, that we shall denote by C , is larger than zero. The Hellmann-Feynman theorem implies that, at the critical charge, $C = -Z_c \frac{d\epsilon}{dZ} |_{Z=Z_c}$, which is only larger than zero if $\zeta = 1$ [7]. In order to extend this claim to absorbing systems with more than two electrons we note that for $Z \rightarrow Z_c$, if $\zeta > 1$ then not only the ionization energy but also each of its components (nuclear attraction and interelectronic repulsion, the kinetic energy contribution vanishing by the virial theorem) would have to vanish simultaneously, which is highly unlikely for an absorbing scenario (with a bound wave function at the critical charge). Of course, ζ cannot be less than unity because that would imply a singular behavior of the contribution of the interelectronic repulsion (as well as that of the nuclear attraction) at the critical charge.

As an illustration of the kind of accuracy that a naive treatment of the spectroscopic binding energies allows, we examine the ground state of the two-electron isoelectronic series. Fitting the NIST [34] ionization energies for $2 < Z < 6$ we obtain (setting $Z_c = 0.911$) the two-term expression $\epsilon \approx 0.285(Z - Z_c) + 0.500(Z - Z_c)^2$ (in a.u.), that yields $C \approx 0.26, 0.316, \text{ and } 0.942$ a.u. at $Z = Z_c, 1, 2$, respectively. The (crude) value at the critical charge is in agreement with a recent 10-digit expectation value of the interelectronic repulsion [0.245 1890 639(1)] [6]. The values at $Z = 1, 2$ compare reasonably well with the highly accurate computed

values, 0.3110 and 0.9458, respectively (cf. [35], where more digits are presented). We note that the energy of the ground state of the helium isoelectronic sequence has an essential singularity at $Z = Z_c$ [7], so it is not surprising that taking just the first two terms in a series expansion yields rather crude results.

B. Expanding isoelectronic series

In the expanding case the outermost electronic orbital becomes infinitely diffuse upon approaching the critical charge. Hence, the core, consisting of the nucleus and the inner electrons, appears more and more pointlike. As a consequence, the outermost electron's wave function approaches a hydrogenlike shape, i.e., the quantum defect approaches an integer. Therefore, the asymptotic behavior of the ionization energy, upon approaching the critical charge, is expected to be quadratic, the leading term being $\epsilon \approx \frac{(Z-Z_c)^2}{2(n-\delta)^2}$, in a.u. This heuristic argument was invoked to offer the conjecture that the limiting quantum defect for a given orbital is equal to the number of occupied shells of the same symmetry (orbital angular momentum) in the core [15]. It was verified for several isoelectronic series by extrapolating the quantum defects evaluated from the NIST [34] data (or other sources) for integer valued nuclear charges. However, in examining such data for the B isoelectronic series it turned out that the monotonically decreasing trend of the $2p$ quantum defects for $Z = 5, 6, 7, \dots$ does not allow extrapolation to the value $\delta_{2p} = 0$ expected at $Z_c = 4$. Hence, a series of computations for nonintegral values of the nuclear charge, in the range $4 < Z \leq 5$ was undertaken [36], indicating that $\lim_{Z \rightarrow 4} \delta_{2p} = 0$, but that δ_{2p} obtains a maximum at $Z \approx 4.25$, only below which it decreases to its (expected) critical value.

IV. RESULTS

A preliminary examination of several states of the Be isoelectronic series, using the NIST [34] data for $Z = 4, 5, 6, \dots$, allows a crude graphical estimate of the corresponding critical charges with error bars of at least ± 0.1 atomic charge units. The ground state, $(1s^2 2s^2) ^1S$, is absorbing, which is consistent with the positive electron affinity of the Li atom [21]. The critical charges estimated for the $(1s^2 2s 3s) ^{1,3}S$ as well as for the $(1s^2 2s 3p) ^{1,3}P$ states appear to be consistent with an expanding scenario.

Following the extrapolation of the binding energy to find the nuclear charge at which it vanishes, it is useful to confirm the expanding scenario by evaluating the quantum defect of the outermost electronic orbital, $\delta = n - \frac{Z-3}{(2\epsilon)^{1/2}}$, where n is its principal quantum number and ϵ is its binding energy, and extrapolate it to $Z \rightarrow Z_c = N - 1 = 3$. Using the data referred to above, the asymptotic quantum defects can crudely be estimated for the $(1s^2 2s 3s) ^{1,3}S$ states, in which they are consistent with $\lim_{Z \rightarrow 3} \delta_{3s} = 2$. However, just like the ground state of the B series, the excited P states of the Be series do not allow a credible estimate of the asymptotic quantum defect on the basis of such integral Z data.

To overcome these difficulties, computations of the binding energy were undertaken for fractional nuclear charges within

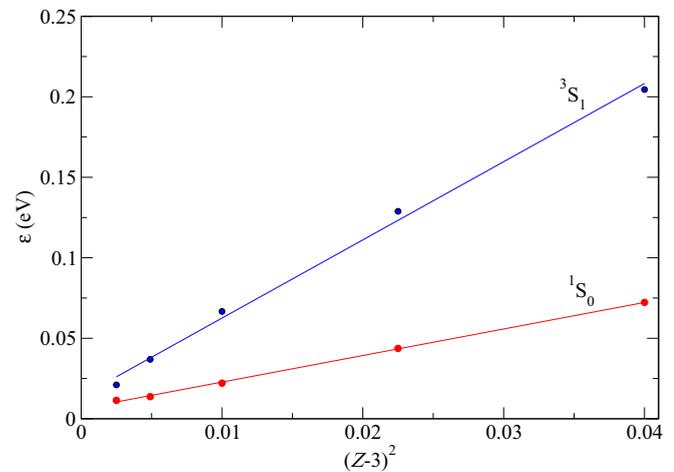


FIG. 1. (Color online) Binding energy of the $1s^2 2s 3s$ 3S_1 and $1s^2 2s 3s$ 1S_0 levels as a function of $(Z - 3)^2$.

the range $3 < Z \leq 4$. The results are described below for each state considered.

A. Be $1s^2 2s 3s$ 3S isoelectronic series

A plot of the binding energy, relative to the three-electron ground state $1s^2 2s^2$ 2S , vs $(Z - 3)^2$, over the range $3 < Z \leq 4$, extrapolates to zero within the range $2.98 \leq Z_c \leq 3.01$ (see Fig. 1). The plot of the quantum defect, $\delta_{3s} = 3 - \frac{Z-3}{(2\epsilon)^{1/2}}$, vs Z , where ϵ is the first ionization energy (given in a.u.), Fig. 2, suggests rather convincingly that $\lim_{Z \rightarrow 3} \delta_{3s} = 2$.

We interpret this combination of data as strong evidence for the (expected) expanding scenario, since there is no reason for the asymptotic quantum defect to be even close to 2 for an absorbing scenario.

B. Be $1s^2 2s 3s$ 1S isoelectronic series

Extrapolating the binding energies as above, the critical charge is estimated to be within $2.98 < Z_c < 3.01$ (see Fig. 1).

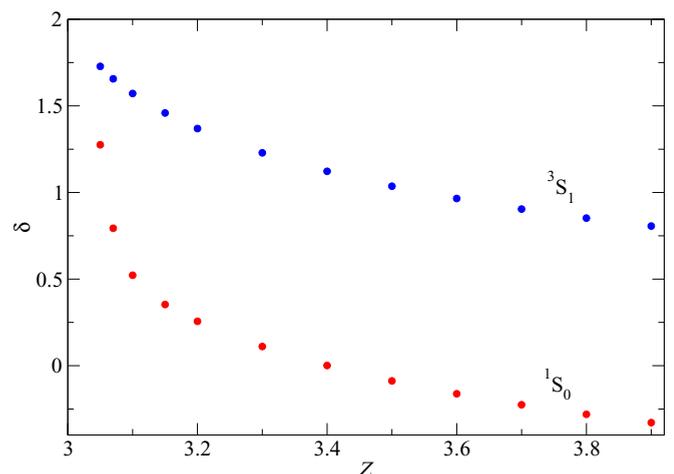


FIG. 2. (Color online) Quantum defect of the $1s^2 2s 3s$ 3S_1 and $1s^2 2s 3s$ 1S_0 levels as a function of Z .

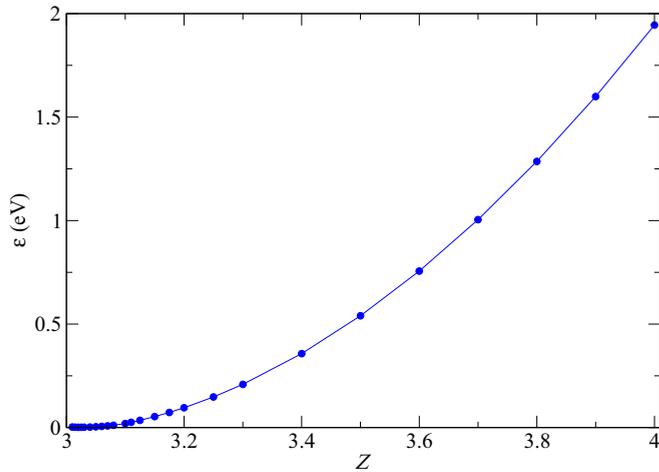


FIG. 3. (Color online) $1s^2 2s 3p \ ^3P_0$ level binding energy as a function of Z .

The quantum defects for $Z < 3.2$, as illustrated in Fig. 2, appear to be too large (consistent with the binding energies being too low). This is probably due to the computation failing to converge at such low nuclear charges. Ignoring these low Z results the quantum defects are consistent with $\lim_{Z \rightarrow 3} \delta_{3s} = 2$, just like those for the triplet.

The $1s^2 2s 3s \ ^1S$ state is not the lowest state of its symmetry type. However, the lower state of the same symmetry, $(1s^2 2s^2)^1S$, is absorbing. Therefore, the requirement of orthogonality to this state cannot be translated into orthogonality of the corresponding outermost orbitals, not even at the critical charge. Just like the $(1s 2s)^1S$ state of the He series, in which the $2s$ orbital becomes $1s$ -like upon approaching the critical charge, the $3s$ orbital here becomes $1s$ -like (everywhere except within a tiny volume consisting of the core orbitals, where a nodal structure required by the demands of orthogonality must show up) in the same limit.

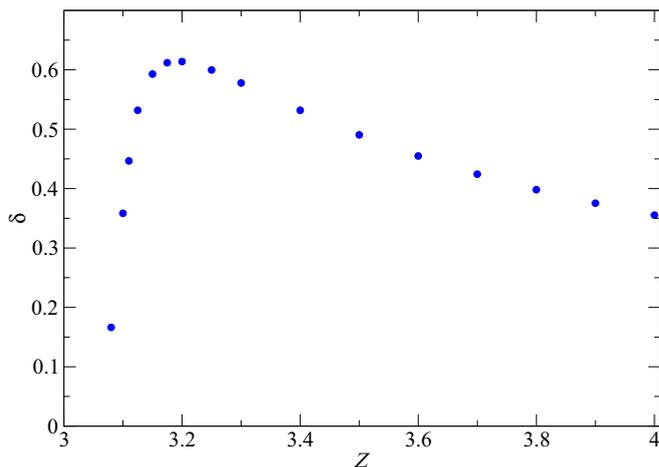


FIG. 4. (Color online) Quantum defect of the outermost electron for the $1s^2 2s 3p \ ^3P_0$ level.

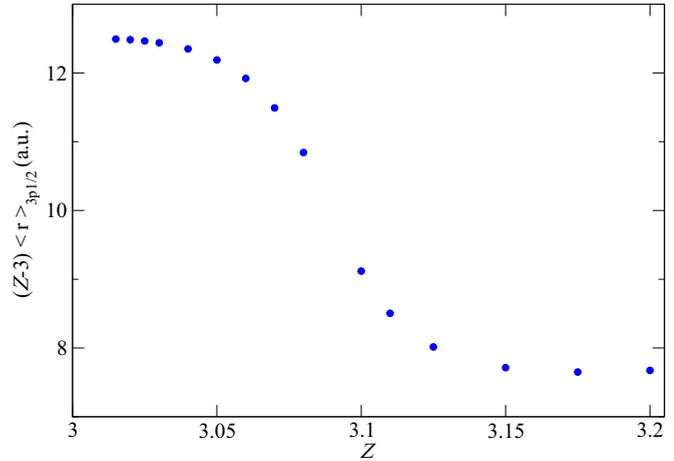


FIG. 5. (Color online) Plot of the average radius of the $3p_{1/2}$ electron for the $1s^2 2s 3p \ ^3P_0$ level multiplied by $(Z - 3)$ as a function of Z .

C. Be $1s^2 2s 3p \ ^3P_0$ isoelectronic series

The energies evaluated for $3 < Z \leq 4$ allow an extrapolation that fixes the critical charge within the range $2.98 < Z \leq 3.00$ (Fig. 3). The $3p$ quantum defect (Fig. 4) vanishes, asymptotically, at large Z , rising upon lowering the nuclear charge, reaching a maximum ($\delta_{2p} \approx 0.61$) at $Z \approx 3.2$. It then decreases rapidly, vanishing, with a vanishing slope, as $Z \rightarrow \sim 3$. An expanding behavior at $Z = 3$ is expected, the $3p$ orbital being definitely the outermost occupied orbital, and the clear vanishing of the quantum defect does signal this behavior. A further confirmation of the expanding behavior is obtained by evaluating $(Z - 3)\langle 3p|r|3p \rangle$, that approaches the hydrogenic value 12.5 as $Z \rightarrow 3$ (Fig. 5).

The 3P_1 and 3P_2 isoelectronic series exhibit essentially identical behavior upon approaching $Z = 3$.

D. Be $1s^2 2s 3p \ ^1P_1$ isoelectronic series

The behavior of the ionization energy (Fig. 6) and the limiting value of the $3p$ quantum defect (Fig. 7), upon

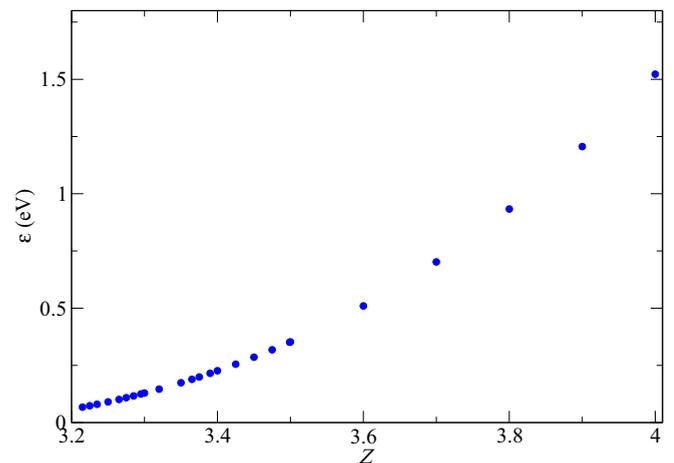


FIG. 6. (Color online) $1s^2 2s 3p \ ^1P_1$ level binding energy as a function of Z .

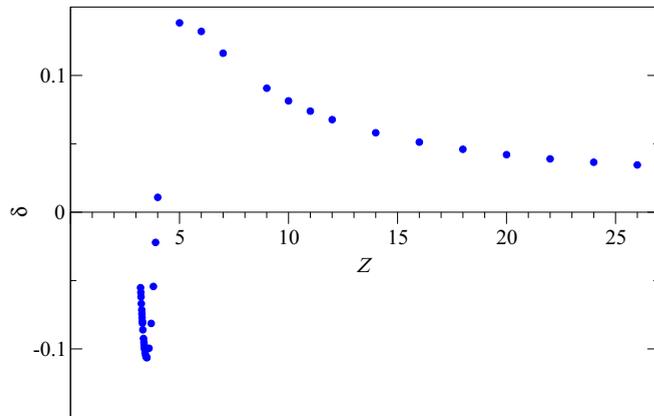


FIG. 7. (Color online) Quantum defect of the outermost electron for the $1s^2 2s 3p \ ^1P_1$ level.

approaching $Z \approx 3$, are very similar to those in the 3P state. However, the quantum defect exhibits a more complicated behavior. It vanishes asymptotically at large Z and rises to a maximum ($\delta_{3p} \approx 0.14$) at $Z \approx 5$, becomes negative at $Z \approx 3.97$, reaching a minimum ($\delta_{2p} \approx -0.107$) at $Z \approx 3.5$, from which it rises towards zero at $Z \approx 3$.

V. CONCLUSIONS

The four states $(1s^2 2s 3s)^{1,3}S$ and $(1s^2 2s 3p)^{1,3}P$ of the Be isoelectronic series have been established to exhibit an expanding behavior, the outermost orbital becoming an infinitely

diffuse hydrogenlike orbital upon approaching the critical charge, $Z_c = 3$. The mere extrapolation of the ionization energies allows a (narrow) range of indefiniteness of the value of the critical charge. However, two features allow a conclusive establishment of the expanding nature of the approach to the critical charge: (1) the ionization energy vanishes linearly in $(Z - Z_c)^2$; (2) the quantum defect corresponding to the outermost orbital approaches an integer that is equal to the number of occupied (or partially occupied) subshells of the same symmetry in the atomic core.

We propose to study the influence of relativistic and QED effects on the critical charge in some heavy and super-heavy elements, where these effects should be important. For instance, Eliav *et al.* [37] found that the rare gas element 118 is the first rare gas with an electron affinity. It follows that the “alkali metal” $Z = 119$ is absorbing, although all lighter alkali metals are expanding.

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