Complex scaled relativistic configuration-interaction study of the

LL resonances in helium-like ions: from Boron to Argon

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Abstract

Energies and Auger widths of the LL resonances in He-like ions from boron to argon are evaluated by means of a complex scaled configuration-interaction approach within the framework of the Dirac-Coulomb-Breit Hamiltonian. The nuclear recoil and QED corrections are also taken into account. The obtained results are compared with other calculations based on the complex scaling method as well as with the related results evaluated using the stabilization and basis balancing methods.
I. INTRODUCTION

Autoionizing states of atomic or ionic systems are the excited states which can decay due to the electron-electron interactions via emission of one (or more) electrons. A special place among such states is held by the levels of the $LL$ resonance groups of He-like systems. The simplicity of these systems makes them attractive for both theoretical and experimental investigations. The investigations aimed at determining of the energies of these levels are of particular interest for plasma diagnostics [1–4], cosmological [5] and fusion research (see, e.g., the review [6]). A new interest in studying the characteristics of the $LL$ resonances was caused by the recent experiment [7]. In this experiment, a new level of accuracy for the energy of the autoionizing states of the He-like carbon ion was reached. Experimental data of such accuracy being complemented by the theoretical predictions of the same precision allow one to set these states as energy-reference standards at synchrotron radiation facilities. The precise theoretical predictions for the energies of the $LL$ resonances are, therefore, highly demanded.

For the accurate evaluation of the energies of autoionizing states, which are strongly affected by electron correlations, the high-precision many-electron methods such as coupled-cluster and configuration-interaction are required. These methods, being successfully applied for the calculations of bound-level energies, however, fail when naively applied for the description of resonances. The energies of such resonances show a strong dependence on the parameters of the basis set, e.g., the convergence of the resonance energy with respect to the number of basis functions, which is one of the basis-set parameters, is very weak or even absent. This is explained by the fact that the autoionizing states are embedded into the positive-energy continuum. As a result, they can not be described by square-integrable functions which form the basis set of the coupled-cluster and configuration-interaction methods. This problem can be naturally solved with the usage of the complex scaling approach which is based on the analytical properties of the spectrum of a Hamiltonian being dilated into the complex plane. The first mathematical analysis of these properties was performed in Refs. [8, 9] for the nonrelativistic Hamiltonian and in Refs. [10–12] for the relativistic one. In these works, it was shown that in the spectra of the dilated Hamiltonian the autoionizing states are separated from the continuum. The wave functions of these states, therefore, become square-integrable and can be investigated with conventional many-electron methods. That makes the complex scaling approach a powerful tool for studying for studying properties of resonances appearing in various systems and processes. As examples, the resonances
of nuclei [13–16], few-electron systems [17–23], and molecules [24, 25] were investigated with the usage of this method. More applications, as well as the details of the complex scaling approach, can be found in the reviews [26–31]. It is also worth noting that the dilated Hamiltonian is not hermitian but symmetric operator with complex eigenvalues. The real and imaginary parts of the eigenvalues corresponding to the autoionizing states give the energies and Auger widths of the states, respectively.

Apart from the complex scaling approach, one can apply the stabilization or basis balancing methods. The stabilization method (SM) was pioneered by Hoiløien and Midtal [32] and was utilized in numerous investigations [33–37]. The basis balancing method (BBM) was worked out by Yerokhin with co-authors just recently [38] and was applied for the calculation of the energies of the autoionizing levels of Li-like ions in a wide range of the nucleus charge number [39]. Both methods are applied to the conventional hermitian Hamiltonian and, as a result, only the real arithmetic is involved that provides a considerable computational advantage. However, the energy of the autoionizing state obtained within SM or BBM can differ from the exact one by a shift arising due to the inappropriate treatment of the interaction with the continuum. The advantages of these methods over the complex scaling approach, thus, can be completely lost in some cases. In view of the considerable progress in experimental accuracy for the energies of the autoionizing states [7], the revision of the applicability of the SM and BBM is required.

In the present paper, we apply the configuration interaction (CI) coupled with the complex scaling (CS) approach to solve the Dirac-Coulomb-Breit (DCB) equation for $LL$ resonances of He-like ions in the range from boron to argon. The configuration space is spanned on the one-electron Dirac orbitals being constructed from the B-splines. The DCB energies are supplemented with the quantum electrodynamics (QED), nuclear recoil, and frequency-dependent Breit corrections. We also estimate the difference of the energies obtained within the SM and BBM with ones calculated employing the complex scaling approach. In case of the $2s^2$ level of the He-like carbon ion, it is found that the energy difference between these three methods exceeds the uncertainty reached in the recent experiment [7].

Units $m_e = h = 1$ and the Heaviside charge unit ($e^2 = 4\pi\alpha$) are used in the paper.
II. BASIC FORMALISM

We start with the formulation of the basic principles of the configuration-interaction with complex scaling approach for the solution of the few-electron DCB equation (for the detailed description see, e.g., the review [31]). Here we consider the simplest variant of the CS, namely, the uniform complex rotation. In this case, the radial variable \( r \) is transformed as

\[
   r 
   \rightarrow 
   re^{i\theta},
\]

with \( \theta \) being a constant rotation angle. This transformation leads to the following complex rotated DCB Hamiltonian

\[
   H_{\text{DCB}}^{(\theta)} = \sum_{j} h_{D}^{(\theta)}(j) + e^{-i\theta} \sum_{j<k} [V_{C}(j,k) + V_{B}(j,k)], \quad j, k = 1, \ldots, N.
\]

Here \( N \) stands for the total number of the electrons and \( h_{D}^{(\theta)} \) is the scaled one-electron Dirac Hamiltonian given by

\[
   h_{D}^{(\theta)}(j) = e^{-i\theta} c \alpha_{j} \cdot p_{j} + (\beta - 1) m_{e} c^{2} + V_{\text{nuc}}(r_{j}e^{i\theta}),
\]

with \( \alpha \) and \( \beta \) being the Dirac matrices, \( p \) is the momentum operator, and \( V_{\text{nuc}} \) is the nucleus potential. In the present paper, we use the spherical model of the nucleus which is transformed in accordance with the rule \( (1) \).

\[
   V_{\text{nuc}}(re^{i\theta}) = \begin{cases} 
   -\frac{\alpha Zc}{2R_{\text{nuc}}} \left( 3 - e^{2i\theta} \frac{r^{2}}{R_{\text{nuc}}^{2}} \right), & r < R_{\text{nuc}} \\
   -e^{-i\theta} \frac{\alpha Zc}{r}, & r > R_{\text{nuc}} 
   \end{cases}
\]

In accordance with Eq. (2) the Coulomb and Breit interelectronic-interaction operators are given by

\[
   V_{C}(j,k) = \frac{\alpha c}{r_{jk}},
\]

\[
   V_{B}(j,k) = \frac{\alpha c}{2r_{jk}^{2}} \left[ h_{D}^{(\theta)}(j), h_{D}^{(\theta)}(k), r_{jk} \right] - \frac{\alpha_{j} \cdot \alpha_{k}}{r_{jk}} \right],
\]

\[
   = -\frac{\alpha c}{2r_{jk}^{2}} \left[ \alpha_{j} \cdot \alpha_{k} + (\alpha_{j} \cdot \hat{r}_{jk}) (\alpha_{k} \cdot \hat{r}_{jk}) \right],
\]

respectively. In Eqs. (5) and (7), \( \hat{r}_{jk} = r_{jk}/r_{jk} \) with \( r_{jk} = r_{j} - r_{k} \) and \( r_{jk} = |r_{jk}| \). Having performed the complex rotation of the DCB Hamiltonian (2) we now proceed to the construction
of its eigenfunctions.

As in the conventional CI method [40, 51], the \(N\)-electron eigenfunction \(\Psi(PJM)\) with the parity \(P\), total angular momentum \(J\), and its projection \(M\) is expressed as a linear superposition of the configuration-state functions (CSFs) \(\Phi(\gamma_rPJM)\)

\[
\Psi(PJM) = \sum_{r=1}^{N_{CSF}} c_r \Phi(\gamma_rPJM),
\]

where \(\gamma_r\) stands for all additional quantum numbers which determine uniquely the CSF. The CSFs are eigenstates of the total angular momentum operators \(J^2\) and \(J_z\), constructed from antisymmetrized products of one-electron Dirac orbitals. Here these orbitals are chosen to be the solutions of the scaled one-electron Dirac Hamiltonian (3) of the form

\[
\psi^{(\theta)}_{\kappa m}(\mathbf{r}) = \frac{e^{-i\theta}}{r} \begin{pmatrix} G^{(\theta)}_{\kappa}(r) \Omega_{\kappa m}(\mathbf{r}) \\ iF^{(\theta)}_{\kappa}(r) \Omega_{-\kappa m}(\mathbf{r}) \end{pmatrix},
\]

where \(\kappa = (-1)^{l+j+1/2}(j + 1/2)\) is the Dirac quantum number determined by the angular momentum \(j\) and the parity \(l\) and \(\Omega_{\kappa m}\) is the spinor spherical harmonic [41]. As usual in accordance with the basic principles of the relativistic theory with the DCB approximation, the CSF are constructed only from positive-energy one-electron Dirac orbitals.

As already mentioned, autoionizing levels after the complex scaling are described by the square-integrable and localized wave functions. To good accuracy these wave functions can be represented by the corresponding solutions of the scaled DCB equation in a spherical cavity of a finite radius. In the present paper, this equation is solved using the dual-kinetic-balance finite basis set method [42] with the basis functions constructed from B-splines [43, 44],

\[
\begin{pmatrix} G^{(\theta)}_{\kappa}(r) \\ F^{(\theta)}_{\kappa}(r) \end{pmatrix} = \sum_{i=1}^{N} C^{(\theta)}_{\kappa,i} \begin{pmatrix} B_i(r) \\ \frac{e^{-i\theta}}{2M_e} \left[ \frac{d}{dr} + \kappa \frac{1}{r} \right] B_i(r) \end{pmatrix} + \sum_{i=N+1}^{2N} C^{(\theta)}_{\kappa,i} \begin{pmatrix} \frac{e^{-i\theta}}{2M_e} \left[ \frac{d}{dr} - \kappa \frac{1}{r} \right] B_{i-N}(r) \\ B_{i-N}(r) \end{pmatrix}.
\]

III. RESULTS AND DISCUSSIONS

A. Comparison of the stabilization and basis balancing methods with the complex scaling approach

Let us start with a brief description of the principles of the stabilization and basis balancing methods, which are applied to the conventional (hermitian) Hamiltonian. In the SM [32], the
basis-set parameters are chosen in such a way to provide a minimal value for the rate of change of the energy with respect to a variation of these parameters. In the framework of the BBM \[38\], one needs to manipulate the basis to place the resonance just in the middle between the closest quasi-continuum states in the energy scale. Both these methods utilize the advantages of the finite basis set constructed from the square-integrable functions. As already was mentioned, such basis set functions cannot properly describe the contribution of the continuum to the autoionizing states. That is expressed in the energy shift of the state from the exact value. The size of this shift is, however, strongly resonance-dependent and may be negligible in some cases. Here we estimate the difference between the results of the complex scaling approach with ones from the stabilization and basis balancing methods considering the state which is known to be significantly coupled with the continuum, namely, \(2s^2\) autoionizing state of the He-like carbon ion \((Z = 6)\). For this purpose, we choose the radial grid, which uniquely defines the basis functions constructed from the B-splines, as in Ref. \[38\]:

\[ t_i = t_0 e^{A(i/N)\gamma}, \]  

(9)

where \(A = \ln(t_{\text{max}}/t_0)\), \(t_{\text{max}}\) is the radial size of the spherical cavity, \(t_0\) is the radius of the nucleus, and \(\gamma\) is the basis set parameter. The energies of the autoionizing and quasi-continuum states depend strongly on the parameter \(\gamma\) and form \(\gamma\)-parametric trajectories, which are analyzed in accordance with the SM and BBM. For the sake of simplicity, we include only the CSFs being constructed from one-electron \(s\) and \(p\) Dirac orbitals. Fig. 1 presents the \(\gamma\)-parametric energy trajectories for the \(2s^2\) state of the He-like carbon \((Z = 6)\) ion obtained in the basis of 30 B-splines. This figure also presents the energies obtained with the usage of the SM and BBM for each \(\gamma\)-parametric trajectory. From Fig. 1 it is seen that at \(\gamma\) smaller than 0.5 the results of the SM and BBM are very close to each other. Before we proceed to the investigation of the convergence with respect to the number of B-splines, let us explore the dependence of the results obtained within the CS approach on the \(\gamma\) parameter.

As was discussed in the preceding section, in the uniform complex rotation approach, the Hamiltonian depends on the \(\theta\) parameter. Energies of the bound and quasi-bound states in this method are, however, \(\theta\)-independent for \(\theta_c \leq \theta < \pi/2\) where \(\theta_c\) is the critical angle given by \[8, 45\]

\[ \theta_c = \arctan \left[ \frac{\Gamma}{(2(E - E_t))} \right]. \]  

(10)

Here \(\Gamma\) and \(E\) are the Auger width and energy of the level of interest, respectively, and \(E_t\) is the autoionization threshold energy, which for the \(2s^2\) state is provided by the ground state of the
FIG. 1. Energy of the 2s² state of the He-like carbon (Z = 6) ion as a function of the parameter γ (see Eq. (9)). The CSFs are constructed from one-electron s and p Dirac orbitals obtained in the basis of 30 B-splines. The size of the spherical box was chosen to be 15 a.u. Blue circles and red squares correspond to the γ parameters chosen in accordance with the stabilization and basis balancing methods, respectively.

It should be noted that the energies do not depend on θ only if the complete or large basis set is utilized. In practice, however, one has to deal with an incomplete basis set that requires a search of an optimal angle for the uniform complex rotation. This angle corresponds to the stationary point of the θ-parametric energy curve in the complex plane. In our case, one needs to find the stationary point of the (γ,θ)-parametric energy surface in the complex plane. That is equivalent to the search for the minimum of the function

$$s(γ,θ) \equiv \sqrt{\left(\frac{dE}{dθ}\right)^2 + \left(\frac{dE}{dγ}\right)^2}.$$ (11)

Fig. 2 presents the s function (11) for the 2s² state of the He-like carbon (Z = 6) ion obtained in the basis of 30 B-splines. From this figure it is seen that the s(γ,θ) function takes minimal values at γ from 0.3 to 0.5 and θ from 20° to 30°. For γ and θ changing within this area, the energy of the 2s² state exhibits very stable behavior.
FIG. 2. Dependence of the $s$ function (in a.u.) given by Eq. [11] on the $\theta$ and $\gamma$ parameters for the $2s^2$ state of the He-like carbon ($Z = 6$) ion. The CSFs are constructed from one-electron $s$ and $p$ Dirac orbitals obtained in the basis of 30 B-splines. The size of the spherical box was chosen to be 15 a.u.

We now turn to the investigation of the convergence of the results obtained within the SM, BBM, and CS methods with respect to the number of basis functions. Table I presents the energy of the $2s^2$ state of the He-like C ($Z = 6$) ion for different numbers of the B-splines.

TABLE I. Energy (in a.u.) of the $2s^2$ state of the He-like C ($Z = 6$) ion obtained within the stabilization method (SM), the basis balancing method (BBM), and the complex scaling (CS) approach. The CSFs are constructed from one-electron $s$ and $p$ Dirac orbitals obtained in the basis of $N$ functions. The size of the spherical box was chosen to be 15 a.u. Parameter $\gamma$ is varied in the range between 0.3 and 0.5. The calculations within the CS approach are performed for $\theta$ varying from $20^\circ$ to $25^\circ$.

| $N$ | SM | BBM | CS |
|-----|----|-----|----|
|     | Re ($E$) | Im ($E \times 10^3$) |
| 30  | -8.29130(3) | -8.2924(2) | -8.291450(4) | -3.529(4) |
| 40  | -8.29134(4) | -8.2921(1) | -8.2914499(2) | -3.5290(3) |
| 50  | -8.29137(3) | -8.29197(3) | -8.29144998(9) | -3.52906(15) |
| 60  | -8.29140(2) | -8.2919(1) | -8.29144998(9) | -3.52907(13) |
The calculations within the stabilization and basis balancing methods are performed for the \( \gamma \) parameter varying from 0.3 to 0.5. In Table I, we present the average values of the energies originating from different energetic curves corresponding to this \( \gamma \) interval (see Fig. 1). The uncertainty reflects the dependence of the results on the choice of the curve. From Table I, it is seen that the BBM results stronger depend on the energetic curve than the SM ones. It can be due to the fact that in the BBM the resonance position is balanced with respect to the closest quasi-continuum states whereas in the SM the whole spectra is effectively taken into account. For both methods, the dependence on the energetic curve strongly masks the convergence with respect to the number of basis functions and gives the main source of the uncertainty. The calculations within the CS approach are performed for \( \gamma \) varying from 0.3 to 0.5 and \( \theta \) varying in the range between 20° and 25°. The dependence of the energy on the \( \gamma \) and \( \theta \) parameters forms the uncertainty indicated in Table I. It is seen that the energy obtained within the CS approach exhibits extremely fast convergence with respect to the number of basis functions. It is also seen that the energies obtained within the SM and BBM differ from the one calculated using the complex scaling approach by more than 1 meV and 10 meV, respectively, the values which actually define accuracy limits of the SM and BBM. We note also that, working with SM and BBM, one needs to re-select the basis set parameters each time when the number of the basis functions is enlarged. The necessity of this procedure drastically increase the number of required computation time and, thus, strongly reduces the advantage of the real arithmetic.

**B. Energies and Auger widths of the \( LL \) resonances**

We now apply the configuration-interaction complex-scaling method for the calculation of the energies and Auger width of \( LL \) resonances of the He-like ions from boron (\( Z = 5 \)) to argon (\( Z = 18 \)). The simplicity of the system studied allows performing the full CI calculations, i.e. the configuration space is formed from all possible combinations of the one-electron Dirac orbitals appearing for a given number of the B-splines. In the present paper, the B-splines of order 11 are utilized. Such a high order of the B-splines is chosen to guarantee the correct behavior of the one-electron Dirac orbitals with orbital angular momenta up to \( L = 8 \) at the origin. The one-electron orbitals with proper behavior at the origin appear to be less dependent on the choice of the complex rotation angle \( \theta \) and, thus, provide more accurate results. The accuracy of the
DCB eigenvalues apart from the choice of the $\theta$ and $\gamma$ parameters depends on the number of B-splines and the number of the orbital angular momenta $L$ included. In order to estimate the uncertainty arising from the number of orbital angular momenta we carry out the CI calculations for $L \leq 8$ and estimate the tail contributions via polynomial least square fitting of the increments in powers of $1/L$ as in Refs. [38, 46, 47]. An example of such uncertainty analysis is presented in Table II for the $2s^2$ state of the carbon ($Z = 6$) ion.

**TABLE II.** Energy $E$ and Auger width $\Gamma_{\text{Aug}}$ of the $2s^2$ state of the He-like carbon ($Z = 6$) ion obtained within the configuration-interaction complex-scaling method. The CSFs are constructed from one-electron Dirac orbitals with orbital angular momenta up to $L_{\text{max}}$ being obtained in the basis of $N$ B-splines. The size of the spherical box was chosen to be 15 a.u., $\gamma = 0.3$, and $\theta = 20^\circ$. The values listed after the second row are the increments obtained on successively adding configurations while increasing $L_{\text{max}}$.

| $L_{\text{max}}$ | $E$ [a.u.] | $\Gamma_{\text{Aug}} \times 10^3$ [a.u.] |
|------------------|-----------|-----------------|
|                  | $N = 30$  | $N = 40$  | $N = 50$    | $N = 30$  | $N = 40$  | $N = 50$    |
| 1                | -8.291 450.6 | -8.291 450.0 | -8.291 449.9 | 7.056 59  | 7.058 01  | 7.058 00    |
| 2                | -0.000 796 1 | -0.000 796 0 | -0.000 796 0 | -0.081 75 | -0.081 55 | -0.081 52   |
| 3                | -0.000 118 0 | -0.000 118 3 | -0.000 118 3 | -0.018 88 | -0.018 72 | -0.018 70   |
| 4                | -0.000 037 5 | -0.000 037 8 | -0.000 037 8 | -0.006 72 | -0.006 58 | -0.006 56   |
| 5                | -0.000 015 9 | -0.000 016 1 | -0.000 016 2 | -0.003 02 | -0.002 91 | -0.002 89   |
| 6                | -0.000 007 8 | -0.000 008 1 | -0.000 008 1 | -0.001 57 | -0.001 49 | -0.001 48   |
| 7                | -0.000 004 3 | -0.000 004 5 | -0.000 004 5 | -0.000 91 | -0.000 85 | -0.000 83   |
| 8                | -0.000 002 5 | -0.000 002 7 | -0.000 002 7 | -0.000 57 | -0.000 52 | -0.000 51   |
| 9-$\infty$      | -0.000 005 7 | -0.000 006 8 | -0.000 007 1 | -0.001 76 | -0.001 49 | -0.001 42   |
| **Total**        | -8.292 438 3 | -8.292 440 2 | -8.292 440 7 | 6.941 41  | 6.943 91  | 6.944 07    |

From this table, it is seen that for the basis of more than 40 B-splines the dominant contribution to the uncertainty of the DCB eigenvalues is provided by the configuration states with orbital angular momenta $L \geq 9$, whose contributions are taken into account by extrapolation. Therefore, in what follows we solve the complex rotated DCB equation in the configuration space formed from all possible combinations of the one-electron Dirac orbitals constructed out of 40 or 50
B-splines.

In order to obtain the energies of the $LL$ resonances with an accuracy at a few meV level, we supplement the solutions of the complex rotated DCB equation with the nuclear recoil and QED corrections. Both corrections are obtained with the usage of the conventional (hermitian) DCB Hamiltonian. The nuclear recoil effect arising due to the finite nuclear mass $M$ admits fully relativistic treatment only within the framework of QED [48, 49]. Here we account for this effect in the lowest-order relativistic approximation and to first order in $m/M$ via the inclusion of the mass shift operator [48, 50]

$$H_{MS} = \frac{1}{2M} \sum_{ij} \left\{ \mathbf{p}_i \cdot \mathbf{p}_j - \frac{\alpha Z}{r_i} \left[ \alpha_i + \frac{(\alpha_i \cdot \mathbf{r}_i) \mathbf{r}_i}{r_i^2} \right] \cdot \mathbf{p}_j \right\}, \quad (12)$$

into the DCB Hamiltonian. The nuclear recoil correction to the energy of the particular $LL$ resonance is given by the first-order perturbation theory with respect to this additional term [51].

As already mentioned, in addition to the nuclear recoil corrections we supplement the complex rotated DCB energies with the QED corrections. The ab initio evaluation of these corrections still remains a challenging task even for He-like systems for which the methods of the QED calculations are currently well established (see, e.g., [52–54] and references therein). It is also worth to mention that to the best of our knowledge no attempt was made to compute the two-electron QED effects on the energies of the autoionizing states. In the present paper, we evaluate the QED corrections utilizing the model QED operator [55], constructed with the usage of the QEDMOD package [56]. We evaluate the QED correction as the difference between the CI results obtained with and without the model QED operator included into the DCB Hamiltonian. This approach has shown its efficiency in numerous investigations [38, 39, 47, 57]. However, in the QED model operator method, the screened QED corrections are taken into account only approximately. These corrections as well as the QED part of the two-photon-exchange contributions give rise to another source of uncertainty. We also note that the frequency-dependent Breit correction was found to be of minor importance for systems under investigation and, therefore, its contribution can be omitted.

Table III presents the energies and Auger widths of the $LL$ resonances of the He-like ions from boron ($Z = 5$) to argon ($Z = 18$). In this table, the complex rotated DCB energy, the QED correction, and the nuclear recoil correction are explicitly shown. The presented Auger widths $\Gamma_{Aug}$ were calculated only by means of the CS DCB Hamiltonian. The smallness of the Auger
widths of the $2p_{1/2}^2 (J = 0)$, $2p_{3/2}^2 (J = 2)$, and $2p_1p_3/2 (J = 1)$ resonances is explained by the fact that the Auger decay of the $^3P_0$, $^3P_2$, and $^3P_1$ states corresponding to these resonances in the LS-coupling scheme, respectively, is strictly forbidden in the nonrelativistic limit. Energies $E_{\text{tot}}$ are supplemented with the total uncertainties from all calculated contributions as well as from uncalculated high-order QED corrections. The uncertainty due to the uncalculated QED corrections was estimated by analysis of the related contributions for the ground and single-excited states in He-like ions \cite{52}. In most cases, the accuracy of the present calculations is limited by the uncertainties from the QED contributions. Using the presented results with the available high-precision data for the energies of the ground and lowest excited states (see Refs. \cite{52, 54}), one can easily find the corresponding transition energies.

TABLE III: Energies $E_{\text{tot}}$ and Auger widths $\Gamma_{\text{Aug}}$ of the $LL$ resonances of the He-like ions from boron ($Z = 5$) to argon ($Z = 18$), in a.u. The CS DCB energy, the QED correction, and the nuclear recoil correction are explicitly shown. Energies $E_{\text{tot}}$ are supplemented with the total uncertainties from all calculated and uncalculated contributions. The nuclear charge radii are taken from Ref. \cite{58}.

| Ion  | Resonance $J$ | DCB       | Recoil     | QED        | $E_{\text{tot}}$       | $\Gamma_{\text{Aug}}$ |
|------|---------------|-----------|------------|------------|-----------------------|---------------------|
| $^{11}\text{B}^{3+}$ | $2s_{1/2}^2$ 0 | $-5.6628771$ | $0.0002821$ | $0.0000856$ | $-5.662509(24)$ | $6.674(1)\times10^{-3}$ |
|      | $2p_{1/2}^2$ 0 | $-5.4702350$ | $0.0002805$ | $-0.0000007$ | $-5.4699552(88)$ | $<10^{-6}$ |
|      | $2p_{3/2}^2$ 0 | $-5.1457619$ | $0.0002760$ | $0.0000203$ | $-5.145466(42)$ | $3.0(2)\times10^{-4}$ |
|      | 2             | $-5.4694360$ | $0.0002804$ | $0.0000013$ | $-5.4691543(48)$ | $<2\times10^{-6}$ |
|      | $2s_{1/2}^2p_{1/2}$ 0 | $-5.6151794$ | $0.0002811$ | $0.0000541$ | $-5.614844(13)$ | $3.314(7)\times10^{-4}$ |
|      | 1             | $-5.6149173$ | $0.0002811$ | $0.0000548$ | $-5.614582(13)$ | $3.277(7)\times10^{-4}$ |
|      | $2s_{1/2}^2p_{3/2}$ 1 | $-5.3817344$ | $0.0002710$ | $0.0000465$ | $-5.381417(54)$ | $3.09(4)\times10^{-3}$ |
|      | 2             | $-5.6143278$ | $0.0002810$ | $0.0000562$ | $-5.613991(13)$ | $3.241(5)\times10^{-4}$ |
|      | $2p_{1/2}^2p_{3/2}$ 1 | $-5.4699408$ | $0.0002805$ | 0.0         | $-5.4696604(36)$ | $<10^{-6}$ |
|      | 2             | $-5.4044733$ | $0.0002711$ | $0.0000018$ | $-5.404200(30)$ | $5.52(1)\times10^{-3}$ |
| $^{12}\text{C}^{4+}$ | $2s_{1/2}^2$ 0 | $-8.2924407$ | $0.0003786$ | $0.0001679$ | $-8.291894(41)$ | $6.944(1)\times10^{-3}$ |
|      | $2p_{1/2}^2$ 0 | $-8.0579693$ | $0.0003770$ | $-0.000015$ | $-8.057594(13)$ | $<2\times10^{-7}$ |
|      | $2p_{3/2}^2$ 0 | $-7.6535338$ | $0.0003724$ | $0.0000413$ | $-7.653120(54)$ | $3.1(1)\times10^{-4}$ |
|      | 2             | $-8.0562426$ | $0.0003770$ | $0.0000028$ | $-8.0558628(66)$ | $6.9(9)\times10^{-7}$ |
|      | $2s_{1/2}^2p_{1/2}$ 0 | $-8.2349686$ | $0.0003777$ | $0.0001058$ | $-8.234485(22)$ | $3.377(6)\times10^{-4}$ |
| Ion  | Resonance J   | DCB    | Recoil  | QED    | $E_{\text{tot}}$  | $\Gamma_{\text{Aug}}$ |
|------|---------------|--------|---------|--------|-------------------|---------------------|
|      |               |        |         |        |                   |                     |
| 1    | $-8.233 \, 399\, 8$ | 0.000 \, 377\, 6 | 0.000 \, 107\, 2 | $-8.233 \, 915(22)$ | 3.32(1)$\times 10^{-4}$ |
| 2$s_{1/2}2p_{3/2}$ | 1   | $-7.943 \, 567\, 5$ | 0.000 \, 366\, 1 | 0.000 \, 094\, 0 | $-7.943 \, 107(71)$ | 3.35(4)$\times 10^{-3}$ |
|      | 2   | $-8.233 \, 140\, 3$ | 0.000 \, 377\, 6 | 0.000 \, 110\, 2 | $-8.232 \, 653(22)$ | 3.27(1)$\times 10^{-4}$ |
| 2$p_{1/2}2p_{3/2}$ | 1   | $-8.057 \, 340\, 5$ | 0.000 \, 377\, 0 | 0.0 | $-8.056 \, 963.5(38) < 10^{-6}$ |                     |
|      | 2   | $-7.971 \, 252\, 5$ | 0.000 \, 366\, 7 | 0.000 \, 031\, 1 | $-7.970 \, 883(40)$ | 6.017(9)$\times 10^{-3}$ |
| $^{14}$N$^{5+}$ | 2$s_{1/2}^2$ | 0   | $-11.423 \, 448\, 0$ | 0.000 \, 447\, 0 | 0.000 \, 295\, 3 | $-11.422 \, 706(64)$ | 7.146(1)$\times 10^{-3}$ |
|      | 2$p_{1/2}^2$ | 0   | $-11.146 \, 890\, 5$ | 0.000 \, 445\, 6 | $-0.000 \, 027$ | $-11.146 \, 448(19)$ | 1.1(6)$\times 10^{-7}$ |
|      | 2$p_{3/2}^2$ | 0   | $-10.662 \, 027\, 6$ | 0.000 \, 441\, 2 | 0.000 \, 074\, 5 | $-10.661 \, 512(64)$ | 3.3(2)$\times 10^{-4}$ |
|      | 2   | $-11.143 \, 596\, 4$ | 0.000 \, 445\, 5 | 0.000 \, 005\, 4 | $-11.143 \, 145\, 5(93)$ | 1.8(6)$\times 10^{-4}$ |
| 2$s_{1/2}2p_{1/2}$ | 1   | $-11.356 \, 413\, 0$ | 0.000 \, 446\, 2 | 0.000 \, 185\, 6 | $-11.355 \, 781(34)$ | 3.444(2)$\times 10^{-4}$ |
|      | 1   | $-11.355 \, 325\, 6$ | 0.000 \, 446\, 2 | 0.000 \, 188\, 3 | $-11.354 \, 691(34)$ | 3.363(6)$\times 10^{-4}$ |
| 2$s_{1/2}2p_{3/2}$ | 1   | $-11.006 \, 211\, 3$ | 0.000 \, 434\, 3 | 0.000 \, 168\, 9 | $-11.005 \, 608(88)$ | 3.54(4)$\times 10^{-3}$ |
|      | 2   | $-11.352 \, 940\, 9$ | 0.000 \, 446\, 1 | 0.000 \, 193\, 9 | $-11.352 \, 301(34)$ | 3.289(5)$\times 10^{-4}$ |
| 2$p_{1/2}2p_{3/2}$ | 1   | $-11.145 \, 698\, 1$ | 0.000 \, 445\, 6 | 0.0 | $-11.145 \, 252\, 5(40) < 10^{-6}$ |                     |
|      | 2   | $-11.038 \, 563\, 4$ | 0.000 \, 435\, 2 | 0.000 \, 051\, 1 | $-11.038 \, 123\, 4(40)$ | 6.39(2)$\times 10^{-3}$ |
| $^{16}$O$^{6+}$ | 2$s_{1/2}^2$ | 0   | $-15.056 \, 486\, 6$ | 0.000 \, 515\, 5 | 0.000 \, 480\, 2 | $-15.055 \, 491(96)$ | 7.304(1)$\times 10^{-3}$ |
|      | 2$p_{1/2}^2$ | 0   | $-14.737 \, 464\, 3$ | 0.000 \, 514\, 2 | $-0.000 \, 045$ | $-14.736 \, 955(27)$ | 2.3(7)$\times 10^{-7}$ |
|      | 2$p_{3/2}^2$ | 0   | $-14.171 \, 660\, 3$ | 0.000 \, 509\, 9 | 0.000 \, 123\, 3 | $-14.171 \, 027(76)$ | 3.4(2)$\times 10^{-4}$ |
|      | 2   | $-14.731 \, 723\, 8$ | 0.000 \, 514\, 0 | 0.000 \, 094\, 9 | $-14.731 \, 200(14)$ | 3.9(3)$\times 10^{-6}$ |
| 2$s_{1/2}2p_{1/2}$ | 0   | $-14.980 \, 155\, 6$ | 0.000 \, 514\, 8 | 0.000 \, 300\, 9 | $-14.979 \, 340(50)$ | 3.516(5)$\times 10^{-4}$ |
|      | 1   | $-14.978 \, 259\, 4$ | 0.000 \, 514\, 8 | 0.000 \, 305\, 6 | $-14.977 \, 439(50)$ | 3.409(6)$\times 10^{-4}$ |
| 2$s_{1/2}2p_{3/2}$ | 1   | $-14.570 \, 258\, 8$ | 0.000 \, 502\, 7 | 0.000 \, 279\, 0 | $-14.569 \, 48(11)$ | 3.69(5)$\times 10^{-3}$ |
|      | 2   | $-14.974 \, 120\, 9$ | 0.000 \, 514\, 6 | 0.000 \, 315\, 2 | $-14.973 \, 291(50)$ | 3.304(5)$\times 10^{-4}$ |
| 2$p_{1/2}2p_{3/2}$ | 1   | $-14.735 \, 390\, 8$ | 0.000 \, 514\, 1 | 0.000 \, 000\, 3 | $-14.734 \, 876\, 4(44) < 10^{-6}$ |                     |
|      | 2   | $-14.606 \, 769\, 5$ | 0.000 \, 503\, 7 | 0.000 \, 008\, 0 | $-14.606 \, 258(44)$ | 6.67(3)$\times 10^{-3}$ |
| $^{19}$F$^{7+}$ | 2$s_{1/2}^2$ | 0   | $-19.192 \, 230\, 3$ | 0.000 \, 553\, 3 | 0.000 \, 735\, 5 | $-19.190 \, 94(14)$ | 7.43(3)$\times 10^{-3}$ |
|      | 2$p_{1/2}^2$ | 0   | $-18.830 \, 232\, 1$ | 0.000 \, 552\, 2 | $-0.000 \, 069$ | $-18.829 \, 687(37)$ | 4.8(6)$\times 10^{-7}$ |
Table III (Continued.)

| Ion       | Resonance   | $J$ | DCB        | Recoil       | QED          | $E_{\text{tot}}$ | $\Gamma_{\text{Aug}}$ |
|-----------|-------------|-----|------------|--------------|--------------|-----------------|----------------------|
| $2p_{3/2}$ | 0           | −18.182 869.3 | 0.000 548 2 | 0.000 191.0  | −18.182 130(88) | 3.5(3)×10$^{-4}$    |
|           | 2           | −18.820 891.7 | 0.000 551.9 | 0.000 015.3  | −18.820 324(19) | 8(1)×10$^{-6}$      |
| $2s_{1/2}2p_{1/2}$ | 0   | −19.106 935.9 | 0.000 552.8 | 0.000 459.7  | −19.105 923(70) | 3.600(7)×10$^{-4}$  |
|           | 1           | −19.103 851.9 | 0.000 552.7 | 0.000 467.2  | −19.102 832(70) | 3.463(7)×10$^{-4}$  |
| $2s_{1/2}2p_{3/2}$ | 1   | −18.636 316.1 | 0.000 541.1 | 0.000 432.5  | −18.635 34(13)  | 3.81(4)×10$^{-3}$   |
|           | 2           | −19.097 127.7 | 0.000 552.5 | 0.000 482.8  | −19.096 092(70) | 3.326(8)×10$^{-4}$  |
| $2p_{1/2}2p_{3/2}$ | 1   | −18.826 854.3 | 0.000 552.1 | 0.000 000.7  | −18.826 3015(50) | < 2 × 10$^{-6}$     |
|           | 2           | −18.676 234.3 | 0.000 542.2 | 0.000 012.3  | −18.675 680(50) | 6.90(4)×10$^{-3}$   |
| $^{20}\text{Ne}^{8+}$ | $2s_{1/2}$ | −23.831 447.0 | 0.000 652.7 | 0.001 075.2  | −23.829 72(19)  | 7.542(1)×10$^{-3}$  |
|           | $2p_{1/2}$ | −23.425 814.7 | 0.000 651.6 | 0.000 010.0  | −23.425 173(50) | 9.5(4)×10$^{-7}$    |
|           | $2p_{3/2}$ | −22.696 122.6 | 0.000 647.4 | 0.000 281.1  | −22.695 19(10)  | 3.6(2)×10$^{-4}$    |
|           | 2           | −23.411 414.9 | 0.000 651.2 | 0.000 023.5  | −23.410 740(28) | 1.47(5)×10$^{-5}$   |
| $2s_{1/2}2p_{1/2}$ | 0   | −23.737 593.9 | 0.000 652.2 | 0.000 670.1  | −23.736 272(96) | 3.690(4)×10$^{-4}$  |
|           | 1           | −23.732 844.2 | 0.000 652.1 | 0.000 681.5  | −23.731 511(96) | 3.518(3)×10$^{-4}$  |
| $2s_{1/2}2p_{3/2}$ | 1   | −23.205 029.4 | 0.000 639.7 | 0.000 638.1  | −23.203 75(16)  | 3.91(4)×10$^{-3}$   |
|           | 2           | −23.722 467.3 | 0.000 651.8 | 0.000 705.6  | −23.721 110(96) | 3.346(7)×10$^{-4}$  |
| $2p_{1/2}2p_{3/2}$ | 1   | −23.420 584.6 | 0.000 651.4 | 0.000 001.6  | −23.419 9316(61) | < 2 × 10$^{-6}$    |
|           | 2           | −23.247 336.3 | 0.000 640.9 | 0.000 018.6  | −23.246 677(59) | 7.08(4)×10$^{-3}$   |
| $^{13}\text{Na}^{9+}$ | $2s_{1/2}$ | −28.975 002  | 0.000 690  | 0.001 514  | −28.972 80(25) | 7.635(1)×10$^{-3}$  |
|           | $2p_{1/2}$ | −28.524 916  | 0.000 689  | 0.000 013  | −28.524 240(66) | 1.72(8)×10$^{-6}$  |
|           | $2p_{3/2}$ | −27.711 922  | 0.000 685  | 0.000 397  | −27.710 84(12) | 3.7(2)×10$^{-4}$  |
|           | 2           | −28.503 662  | 0.000 688  | 0.000 035  | −28.502 939(39) | 2.7(1)×10$^{-5}$  |
| $2s_{1/2}2p_{1/2}$ | 0   | −28.873 071  | 0.000 690  | 0.000 941  | −28.871 44(13) | 3.790(5)×10$^{-4}$ |
|           | 1           | −28.866 072  | 0.000 690  | 0.000 957  | −28.864 43(13) | 3.581(2)×10$^{-4}$ |
| $2s_{1/2}2p_{3/2}$ | 1   | −28.277 097  | 0.000 677  | 0.000 905  | −28.275 51(20) | 3.99(4)×10$^{-3}$  |
|           | 2           | −28.850 706  | 0.000 689  | 0.000 993  | −28.849 02(13) | 3.367(3)×10$^{-4}$ |
| $2p_{1/2}2p_{3/2}$ | 1   | −28.517 138  | 0.000 689  | 0.000 003  | −28.516 446.6(78) | < 2 × 10$^{-6}$  |
Table III (Continued.)

| Ion   | Resonance | J   | DCB     | Recoil | QED     | $E_{\text{tot}}$ | $\Gamma_{\text{Aug}}$ |
|-------|-----------|-----|---------|--------|---------|------------------|---------------------|
| $^{24}\text{Mg}^{10+}$ | $2s_{1/2}$ | 0   | -34.623863 | 0.000790 | 0.002068 | -34.62101(33) | 7.16(1)×10^{-3} |
|       | $2p_{1/2}$ | 0   | -34.128362 | 0.000789 | -0.00017 | -34.12755(85) | 2.91(7)×10^{-6} |
|       | $2p_{3/2}$ | 0   | -33.230758 | 0.000755 | 0.000542 | -33.22247(14) | 3.9(2)×10^{-4}  |
|       | 2         |     | -34.098066 | 0.000788 | 0.000499 | -34.09722(54) | 4.49(6)×10^{-5} |
| $^{2s_{1/2}2p_{1/2}}$ | 0   |     | -34.514412 | 0.000790 | 0.001281 | -34.51234(17) | 3.90(4)×10^{-4} |
|       | 1         |     | -34.504470 | 0.000790 | 0.001304 | -34.50238(17) | 3.65(5)×10^{-4} |
| $^{2s_{1/2}2p_{3/2}}$ | 1   |     | -33.853273 | 0.000777 | 0.001263 | -33.85125(24) | 4.06(4)×10^{-3} |
|       | 2         |     | -34.482472 | 0.000789 | 0.001355 | -34.48033(17) | 3.38(7)×10^{-4} |
| $^{2p_{1/2}2p_{3/2}}$ | 1   |     | -34.117134 | 0.000789 | 0.000805 | -34.11634(10) | <2×10^{-6} |
|       | 2         |     | -33.896040 | 0.000788 | 0.000400 | -33.89522(86) | 7.34(4)×10^{-3} |
| $^{27}\text{Al}^{11+}$ | $2s_{1/2}$ | 0   | -40.779109 | 0.000827 | 0.002752 | -40.77553(42) | 7.88(1)×10^{-3} |
|       | $2p_{1/2}$ | 0   | -40.236929 | 0.000826 | -0.000204 | -40.23612(11) | 4.66(6)×10^{-6} |
|       | $2p_{3/2}$ | 0   | -39.253305 | 0.000822 | 0.000718 | -39.25177(17) | 4.0(2)×10^{-4}  |
|       | 2         |     | -40.195135 | 0.000825 | 0.000607 | -40.19424(72) | 7.4(1)×10^{-5}  |
| $^{2s_{1/2}2p_{1/2}}$ | 0   |     | -40.662765 | 0.000827 | 0.001699 | -40.66024(21) | 4.02(5)×10^{-5} |
|       | 1         |     | -40.649071 | 0.000827 | 0.001730 | -40.64651(21) | 3.73(6)×10^{-4} |
| $^{2s_{1/2}2p_{3/2}}$ | 1   |     | -39.934371 | 0.000814 | 0.001661 | -39.93190(29) | 4.12(5)×10^{-3} |
|       | 2         |     | -40.618454 | 0.000826 | 0.001801 | -40.61583(21) | 3.41(7)×10^{-4} |
| $^{2p_{1/2}2p_{3/2}}$ | 1   |     | -40.221253 | 0.000826 | 0.000009 | -40.22041(14) | <2×10^{-6} |
|       | 2         |     | -39.974458 | 0.000816 | 0.000058 | -39.97358(10) | 7.42(4)×10^{-3} |
| $^{28}\text{Si}^{12+}$ | $2s_{1/2}$ | 0   | -47.441930 | 0.000928 | 0.003583 | -47.43742(52) | 7.85(2)×10^{-3} |
|       | $2p_{1/2}$ | 0   | -46.851709 | 0.000927 | -0.000021 | -46.85080(13) | 7.1(1)×10^{-6} |
|       | $2p_{3/2}$ | 0   | -45.780017 | 0.000923 | 0.000928 | -45.77717(19) | 4.1(2)×10^{-4} |
|       | 2         |     | -46.795465 | 0.000926 | 0.000899 | -46.79445(95) | 1.16(1)×10^{-4} |
| $^{2s_{1/2}2p_{1/2}}$ | 0   |     | -47.319385 | 0.000928 | 0.002206 | -47.31625(26) | 4.15(2)×10^{-4} |
|       | 1         |     | -47.301016 | 0.000928 | 0.002247 | -47.29784(26) | 3.84(1)×10^{-4} |
Table III (Continued.)

| Ion       | Resonance J | DCB      | Recoil   | QED       | $E_{\text{tot}}$ | $\Gamma_{\text{Aug}}$ |
|-----------|-------------|----------|----------|-----------|-----------------|------------------------|
| $2s_{1/2}2p_{3/2}$ | 1           | −46.521 263 | 0.000 914 | 0.002 171 | −46.518 18(34) | 4.17(5)$\times 10^{-3}$ |
|           | 2           | −47.259 405 | 0.000 927 | 0.002 343 | −47.256 14(26) | 3.437(9)$\times 10^{-4}$ |
| $2p_{1/2}2p_{3/2}$ | 1           | −46.830 238 | 0.000 926 | 0.000 014 | −46.829 298(20) | 6(3)$\times 10^{-7}$ |
|           | 2           | −46.556 124 | 0.000 916 | 0.000 082 | −46.555 13(13) | 7.48(4)$\times 10^{-3}$ |
| $^{31}\text{P}^{13+}$ | $2s_{1/2}$ | 0         | −54.613 632 | 0.000 965 | 0.004 579 | −54.608 09(64) | 7.911(1)$\times 10^{-3}$ |
|           | $2p_{1/2}$ | 0         | −53.973 757 | 0.000 964 | −0.000 017 | −53.972 81(16) | 1.05(2)$\times 10^{-5}$ |
|           | $2p_{3/2}$ | 0         | −52.811 508 | 0.000 959 | 0.001 175 | −52.809 37(22) | 4.3(2)$\times 10^{-4}$ |
|           | 2           | −53.899 759 | 0.000 962 | 0.000 115 | −53.898 68(12) | 1.77(2)$\times 10^{-4}$ |
| $2s_{1/2}2p_{1/2}$ | 0           | −54.485 633 | 0.000 965 | 0.002 810 | −54.481 86(32) | 4.305(1)$\times 10^{-4}$ |
|           | 1           | −54.461 556 | 0.000 964 | 0.002 862 | −54.457 73(32) | 3.946(7)$\times 10^{-4}$ |
| $2s_{1/2}2p_{3/2}$ | 1           | −53.614 881 | 0.000 952 | 0.002 783 | −53.611 15(40) | 4.21(5)$\times 10^{-3}$ |
|           | 2           | −54.406 141 | 0.000 963 | 0.002 991 | −54.402 19(32) | 3.47(2)$\times 10^{-4}$ |
| $2p_{1/2}2p_{3/2}$ | 1           | −53.944 897 | 0.000 963 | 0.000 21 | −53.943 91(28) | 8(4)$\times 10^{-7}$ |
|           | 2           | −53.641 418 | 0.000 953 | 0.000 114 | −53.640 35(17) | 7.50(5)$\times 10^{-3}$ |
| $^{32}\text{S}^{14+}$ | $2s_{1/2}$ | 0         | −62.295 647 | 0.001 066 | 0.005 757 | −62.288 82(78) | 7.963(1)$\times 10^{-3}$ |
|           | $2p_{1/2}$ | 0         | −61.604 283 | 0.001 065 | −0.000 066 | −61.603 22(20) | 1.48(2)$\times 10^{-5}$ |
|           | $2p_{3/2}$ | 0         | −60.348 353 | 0.001 060 | 0.001 458 | −60.345 83(26) | 4.5(2)$\times 10^{-4}$ |
|           | 2           | −61.230 680 | 0.001 063 | 0.000 144 | −61.229 47(21) | 7.48(5)$\times 10^{-4}$ |
| $2s_{1/2}2p_{1/2}$ | 0           | −62.162 977 | 0.001 066 | 0.003 522 | −62.158 39(39) | 4.468(1)$\times 10^{-4}$ |
|           | 1           | −62.132 053 | 0.001 066 | 0.003 588 | −62.127 40(39) | 4.078(6)$\times 10^{-4}$ |
| $2s_{1/2}2p_{3/2}$ | 1           | −61.216 210 | 0.001 052 | 0.003 508 | −61.211 65(48) | 4.24(5)$\times 10^{-3}$ |
|           | 2           | −62.059 542 | 0.001 064 | 0.003 756 | −62.054 72(39) | 3.50(2)$\times 10^{-4}$ |
| $2p_{1/2}2p_{3/2}$ | 1           | −61.566 101 | 0.001 064 | 0.000 031 | −61.565 007(38) | 1.0(3)$\times 10^{-6}$ |
|           | 2           | −61.508 840 | 0.001 053 | 0.000 157 | −61.507 63(17) | 2.63(3)$\times 10^{-4}$ |
| $^{35}\text{Cl}^{15+}$ | $2s_{1/2}$ | 0         | −70.489 528 | 0.001 103 | 0.007 135 | −70.481 29(94) | 8.012(1)$\times 10^{-3}$ |
|           | $2p_{1/2}$ | 0         | −69.744 626 | 0.001 101 | 0.000 017 | −69.743 51(24) | 2.01(2)$\times 10^{-5}$ |
|           | $2p_{3/2}$ | 0         | −68.391 105 | 0.001 097 | 0.001 778 | −68.388 23(30) | 4.7(2)$\times 10^{-4}$ |
Since the nonrelativistic method cannot resolve the fine structure of the $2s$ resonance in combination with Hylleraas-type functions without taking into account the QED corrections. In Ref. [59], the calculations were performed using the complex scaling technique in combination with Hylleraas-type functions without taking into account the QED corrections. Since the nonrelativistic method cannot resolve the fine structure of the $2s2p$ resonance, for our three values for the $2s_1/22p_{1/2}(J = 0, 1)$ and $2s_1/22p_{3/2}(J = 2)$ states there is only one corresponding value of Ref. [59]. As one can see from the table, our results are in reasonable agreement with the nonrelativistic ones. We also compared the values obtained for the carbon ion ($Z = 6$) with the recent relativistic calculations of Ref. [7]. These calculations were performed employing the many-body perturbation theory in an all-order formulation with the complex

| Ion       | Resonance | $J$ | DCB        | Recoil | QED     | $E_{\text{tot}}$ | $\Gamma_{\text{Aug}}$ |
|-----------|-----------|----|------------|--------|---------|-----------------|-----------------------|
| $2s_{1/2}$ | 2         |    | -69.324198 | 0.001 099 | 0.000 178 | -69.32292(25)  | 7.43(4)×10^{-3}       |
|           | 0         |    | -70.352997 | 0.001 103 | 0.004 351 | -70.34754(47)  | 4.64(1)×10^{-4}       |
|           | 1         |    | -70.313991 | 0.001 102 | 0.004 433 | -70.30846(47)  | 4.22(5)×10^{-4}       |
| $2p_{1/2}$ | 1         |    | -69.326288 | 0.001 089 | 0.004 357 | -69.32084(56)  | 4.27(6)×10^{-3}       |
|           | 2         |    | -70.220551 | 0.001 101 | 0.004 650 | -70.21480(47)  | 3.53(2)×10^{-4}       |
| $2p_{3/2}$ | 1         |    | -69.694787 | 0.001 101 | 0.000 444 | -69.69364(52)  | 1.3(8)×10^{-6}        |
|           | 2         |    | -69.623669 | 0.001 090 | 0.000 214 | -69.62236(23)  | 3.79(3)×10^{-4}       |
| $40\text{Ar}^{16+}$ | $2s_{1/2}$ | 0   | -79.196961 | 0.001 084 | 0.008 730 | -79.18711(11)  | 8.05(6)×10^{-3}       |
|           | $2p_{1/2}$ | 0   | -78.396270 | 0.001 083 | 0.000 660 | -78.39513(28)  | 2.66(3)×10^{-5}       |
|           | $2p_{3/2}$ | 0   | -76.940290 | 0.001 078 | 0.002 134 | -76.93708(34)  | 4.9(3)×10^{-4}        |
|           | 2         |    | -77.922194 | 0.001 080 | 0.000 215 | -77.92090(29)  | 7.33(4)×10^{-4}       |
| $2s_{1/2}$ | 0         |    | -79.057381 | 0.001 084 | 0.005 310 | -79.05099(56)  | 4.83(3)×10^{-4}       |
|           | 1         |    | -79.008977 | 0.001 084 | 0.005 408 | -79.00249(56)  | 4.40(6)×10^{-4}       |
| $2s_{1/2}$ | 1         |    | -77.946209 | 0.001 071 | 0.005 344 | -77.93979(64)  | 4.30(6)×10^{-3}       |
|           | 2         |    | -78.890181 | 0.001 082 | 0.005 685 | -78.88341(56)  | 3.57(2)×10^{-4}       |
| $2p_{1/2}$ | 1         |    | -78.331956 | 0.001 082 | 0.000 661 | -78.33013(70)  | 1.7(7)×10^{-6}        |
|           | 2         |    | -78.245356 | 0.001 072 | 0.000 288 | -78.24400(31)  | 5.31(4)×10^{-4}       |

In Table IV, we compare some of our results with other nonrelativistic [59] and relativistic calculations [7]. In Ref. [59], the calculations were performed using the complex scaling technique in combination with Hylleraas-type functions without taking into account the QED corrections. Since the nonrelativistic method cannot resolve the fine structure of the $2s2p$ resonance, for our three values for the $2s_1/22p_{1/2}(J = 0, 1)$ and $2s_1/22p_{3/2}(J = 2)$ states there is only one corresponding value of Ref. [59]. As one can see from the table, our results are in reasonable agreement with the nonrelativistic ones. We also compared the values obtained for the carbon ion ($Z = 6$) with the recent relativistic calculations of Ref. [7]. These calculations were performed employing the many-body perturbation theory in an all-order formulation with the complex
scaling technique (see Ref. [31] and references therein). The QED corrections were taken into account using the Welton method which is different from the QED model operator approach. However, the results of Ref. [7] are in excellent agreement with our values.

TABLE IV: The comparison of the calculated energies $E$ and Auger widths $\Gamma_{\text{Aug}}$ of the $LL$ resonances of the He-like ions with other nonrelativistic [59] and relativistic results [7].

| $Z$ | Resonance $J$ | $E$ [a] | $\Gamma_{\text{Aug}}$ [a] | This work | $E$ [b] | $\Gamma_{\text{Aug}}$ [b] |
|-----|----------------|---------|----------------|----------|---------|----------------|
| 5   | $2s_{1/2}^2$   | $0$     | $-5.662502(24)$ | $6.674(1) \times 10^{-3}$ | $-5.66088$ | $6.650 \times 10^{-3}$ |
|     | $2p_{3/2}^2$   | $0$     | $-5.145465(42)$ | $3.0(2) \times 10^{-4}$ | $-5.14464$ | $3.010 \times 10^{-4}$ |
|     | $2s_{1/2}^2p_{1/2}$ | $0$ | $-5.614844(13)$ | $3.314(7) \times 10^{-4}$ | $-5.61299$ | $3.208 \times 10^{-4}$ |
| 1   |               | $1$     | $-5.614581(13)$ | $3.277(7) \times 10^{-4}$ |         |                      |
|     | $2s_{1/2}^2p_{3/2}$ | $2$ | $-5.613991(13)$ | $3.241(5) \times 10^{-4}$ |         |                      |
| 6   | $2s_{1/2}^2$   | $0$     | $-8.291878(40)$ | $6.944(1) \times 10^{-3}$ | $-8.28821$ | $6.910 \times 10^{-3}$ |
|     | $2p_{3/2}^2$   | $0$     | $-7.653119(54)$ | $3.1(1) \times 10^{-4}$ | $-7.65106$ | $3.210 \times 10^{-4}$ |
|     | $2s_{1/2}^2p_{1/2}$ | $0$ | $-8.234485(22)$ | $3.377(6) \times 10^{-4}$ | $-8.23029$ | $3.220 \times 10^{-4}$ |
| 1   |               | $1$     | $-8.233915(22)$ | $3.32(1) \times 10^{-4}$ | $-8.233914$ | $3.327 \times 10^{-4}$ |
|     | $2s_{1/2}^2p_{3/2}$ | $2$ | $-8.232652(22)$ | $3.27(1) \times 10^{-4}$ | $-8.232654$ | $3.269 \times 10^{-4}$ |
| 7   | $2s_{1/2}^2$   | $0$     | $-11.422672(64)$ | $7.146(1) \times 10^{-3}$ | $-11.41546$ | $7.100 \times 10^{-3}$ |
|     | $2p_{3/2}^2$   | $0$     | $-10.661511(64)$ | $3.3(2) \times 10^{-4}$ | $-10.65732$ | $3.340 \times 10^{-4}$ |
|     | $2s_{1/2}^2p_{1/2}$ | $0$ | $-11.355781(34)$ | $3.444(2) \times 10^{-4}$ | $-11.34755$ | $3.230 \times 10^{-4}$ |
| 1   |               | $1$     | $-11.354691(34)$ | $3.363(6) \times 10^{-4}$ |         |                      |
|     | $2s_{1/2}^2p_{3/2}$ | $2$ | $-11.352301(34)$ | $3.289(5) \times 10^{-4}$ |         |                      |
| 8   | $2s_{1/2}^2$   | $0$     | $-15.055424(96)$ | $7.304(1) \times 10^{-3}$ | $-15.04266$ | $7.250 \times 10^{-3}$ |
|     | $2p_{3/2}^2$   | $0$     | $-14.171026(76)$ | $3.4(2) \times 10^{-4}$ | $-14.16345$ | $3.440 \times 10^{-4}$ |
|     | $2s_{1/2}^2p_{1/2}$ | $0$ | $-14.979340(50)$ | $3.516(5) \times 10^{-4}$ | $-14.96481$ | $3.235 \times 10^{-4}$ |
|     | $1$           |         | $-14.977439(49)$ | $3.409(6) \times 10^{-4}$ |         |                      |
|     | $2s_{1/2}^2p_{3/2}$ | $2$ | $-14.973291(50)$ | $3.304(5) \times 10^{-4}$ |         |                      |
### IV. CONCLUSION

The energies and Auger widths of the $LL$ resonances of the He-like ions from boron ($Z = 5$) to argon ($Z = 18$) have been evaluated by means of the complex scaled configuration-interaction method. The systematic analysis of the uncertainty arising from the limited size of the configuration space was performed. The obtained energies have been compared with the ones calculated using the stabilization and basic balancing methods. It was found that the energies obtained with these methods differ from the complex scaling results by a shift that varies from about 1 meV to 10 meV.

The nuclear recoil and QED corrections were evaluated separately and added to the complex rotated Dirac-Coulomb-Breit energies. As the result, the most accurate theoretical predictions for the energies of the $LL$ resonances are obtained. In most cases, the accuracy of the total results is limited by the uncertainties from the higher-order QED corrections.
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