

Complex-scaled *ab initio* QED approach to autoionizing statesV. A. Zaytsev , A. V. Malyshev , and V. M. Shabaev *Department of Physics, St. Petersburg State University, Universitetskaya 7/9, 199034 St. Petersburg, Russia*

(Received 5 October 2022; accepted 15 February 2023; published 2 March 2023)

An *ab initio* method based on a complex-scaling approach and aimed at a rigorous QED description of autoionizing states is worked out. The autoionizing-state binding energies are treated nonperturbatively in αZ and include all the many-electron QED contributions up to the second order. The higher-order electron correlation, nuclear recoil, and nuclear polarization effects are taken into account as well. The developed formalism is demonstrated on the *LL* resonances in helium-like argon and uranium. The most accurate theoretical predictions for the binding energies are obtained.

DOI: [10.1103/PhysRevA.107.032801](https://doi.org/10.1103/PhysRevA.107.032801)

Autoionizing states of atomic or ionic systems are the excited states which can decay by virtue of the electron-electron interaction via the emission of one or more electrons. The high-precision energies of such states are in demand for plasma diagnostics [1–4], e.g., in fusion facilities [5] and astrophysical searches [6]. Furthermore, the possibility of using the autoionizing states as the energy-reference standards at synchrotron-radiation facilities is currently investigated [7–10].

To obtain the energies of the autoionizing states with the precision necessary for all these and many other applications, accurate calculations of the electron-electron correlations and quantum-electrodynamics (QED) corrections are required. State-of-the-art QED calculations constitute an extremely difficult task, and previously they were performed only for the ground and singly excited states, see Refs. [11–16] for review. These calculations usually employ finite-basis-set approaches, which fail when being applied to the computation of autoionizing-state energies. The failure originates from the fact that the autoionizing states are embedded into the positive-energy continuum, which is discretized in the finite-basis-set approaches. Discretization leads to the problem of small denominators in certain many-electron QED corrections as well as in correlation contributions treated perturbatively. As a result, the convergence of the correlation and QED corrections with respect to the size of the basis set is weak or even absent that strongly limits the accuracy. Moreover, the bases are often constructed from the square-integrable functions that do not properly describe the nonlocalized autoionizing states. This, in turn, limits the accuracy of the nonperturbative many-electron methods such as, e.g., configuration-interaction (CI) and coupled-cluster (CC) ones.

The problems associated with the embedding of the autoionizing states into the continuum can be naturally solved by the complex-scaling (CS) approach in which the Hamiltonian is dilated into the complex plane. The autoionizing states corresponding to the dilated Hamiltonian detach from the continuum and admit description by square-integrable functions. As a result, the CS provides an opportunity to utilize the standard well-established techniques with minor modifications. A

detailed description of the CS approach as well as its various applications can be found in Refs. [17–20]. We note that, even though the analysis of the spectral properties of the Dirac Hamiltonian was studied almost five decades ago [21–23], much less attention was paid to the application of the CS approach to relativistic problems [24–31].

The CS approach combined with the perturbation theory [10,32,33], Hylleraas [34], Hylleraas-CI [35–37], CI [38–44], CC [45,46], and multiconfigurational self-consistent field [47–49] methods has been successfully applied to the evaluation of the autoionizing-state energies. In all these calculations, the QED corrections were at best only estimated or not even taken into account that strongly limited the accuracy of the results. As far as we know, *ab initio* QED description of the states being in resonance with the continuum has not been undertaken. Here we combine the rigorous QED treatment with the CS approach and calculate the complete set of many-electron QED corrections to the energies of autoionizing states. We also account for the one- and two-loop QED contributions, nuclear recoil effect, and higher-order correlation and QED corrections. The developed approach is applied to the lowest nonmixing autoionizing states of several helium-like ions, namely, to the $(2s2p_{1/2})_0$, $(2p_{1/2}2p_{3/2})_1$, and $(2s2p_{3/2})_2$ levels in Ar^{16+} and U^{90+} .

We use the Dirac equation as a zeroth-order approximation and utilize the Furry picture in which the electron-nucleus interaction is treated nonperturbatively. The electron-electron correlation and QED contributions are accounted for by perturbation series. We consider all the contributions to the binding energies up to the second order that, to date, correspond to the most advanced bound-state QED calculations. Below we present the details of the method.

Let us start with the two-photon exchange contribution whose evaluation causes the main difficulties for autoionizing states (the calculations for nonresonant states were performed, e.g., in Refs. [50–60]). For two-electron system, this correction is given by the Feynman diagrams shown in Fig. 1.

The ladder contribution is naturally divided into the irreducible and reducible parts [61,62]. For nonmixing states, the

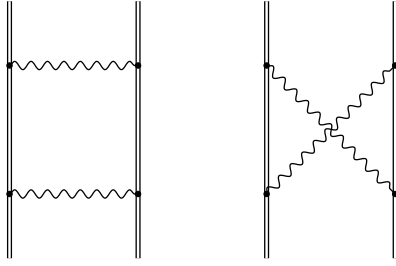


FIG. 1. Two-photon exchange diagrams: the ladder (left) and crossed (right) contributions. The double line represents the electron propagator in the nucleus field and the wavy line designates the photon propagator.

irreducible part reads as (relativistic units, $\hbar = c = m_e = 1$ where m_e is the electron mass, are employed)

$$E_{\text{irr}}^{\text{lad}} = \sum_P (-1)^P \sum'_{n_1 n_2} \frac{i}{2\pi} \times \int d\omega \frac{\langle PaPb | I(\Delta - \omega) | n_1 n_2 \rangle \langle n_1 n_2 | I(\omega) | ab \rangle}{[\varepsilon_a + \omega - \varepsilon_{n_1}(1 - i0)][\varepsilon_b - \omega - \varepsilon_{n_2}(1 - i0)]}, \quad (1)$$

where P is the permutation operator, $(-1)^P$ is its parity, I is the interelectronic-interaction operator, ε_n is the Dirac energy of the one-electron orbital $|n\rangle$, and $\Delta = \varepsilon_{Pa} - \varepsilon_a$. The summation over n_1 and n_2 is restricted by the condition $\varepsilon_{n_1} + \varepsilon_{n_2} \neq \varepsilon_a + \varepsilon_b$. For autoionizing states, $\varepsilon_a + \varepsilon_b > \varepsilon_{1s} + 1$, and this condition is fulfilled when one of the n_1 and n_2 states equals $1s$ and the other lies in the continuum. Nevertheless, such intermediate states should be attributed to the summation in Eq. (1). For the sake of simplicity, Eq. (1) is given for a one-determinant state. The transition to the general case of a many-determinant wave function is straightforward and does not pose additional issues.

Let us discuss in detail the computational difficulties occurring for the irreducible ladder contribution. In Fig. 2(a), we present the pole structure for its direct part given by the term $(PaPb) = (ab)$ in Eq. (1). Upon the Wick's rotation, convenient from the practical point of view, the poles of the electron Green's function are picked up as residues. For autoionizing states, the residues embedded into the continuum arise, see Fig. 2(a), that causes the failure of the conventional finite-basis-set techniques. Indeed, in these approaches, the

continuum is discretized by the quasicontinuum states with energies depending on the parameters of the basis set. As a result, the energy difference $\varepsilon_a + \varepsilon_b - \varepsilon_{1s} - \varepsilon_n$ appearing, e.g., in the denominator of the residue for the LL resonances may become arbitrarily small, thus leading to large numerical instabilities. The same difficulty takes place for the exchange part as well. We note that the issue of arbitrarily small denominators can be avoided in the approaches based on the exact Dirac Green's function. These approaches, however, are much more complicated in implementation and are not usually utilized for the evaluation of the two-photon exchange diagrams.

We apply the CS approach to detach the poles from the continuum and overcome the stated difficulties. We utilize the simplest variant of the CS, namely, the uniform one, in which the radial variable r is transformed according to

$$r \rightarrow r e^{i\theta_{\text{CS}}}, \quad (2)$$

where θ_{CS} is the CS angle. This transformation allows us to construct the analytic continuation of the Dirac Hamiltonian into the complex plane. The discrete spectrum of the dilated Hamiltonian does not change, whereas the continuum spectrum “rotates.” As a result, the pole structure of the integrand in Eq. (1) changes, as schematically depicted in Fig. 2(b). The CS separates the problematic poles from the continuum and, therefore, eliminates the issue of small denominators making the calculations numerically stable.

In fact, the CS is required only for terms in Eq. (1) with Dirac quantum numbers κ_{n_1} and κ_{n_2} that can form an intermediate state into which the Auger decay is allowed. For instance, the Auger-decay channel of the $(2s2p_{1/2})_0$ state is $(2s2p_{1/2})_0 \rightarrow 1s + \varepsilon p_{1/2}$ that corresponds to $(\kappa_{n_1}, \kappa_{n_2}) = (-1, 1)$ and $(\kappa_{n_1}, \kappa_{n_2}) = (1, -1)$. Hereafter, we refer to such terms as the resonant ones. When applying the CS, one needs to take the CS angle from the range $\theta_{\text{cr}} < \theta_{\text{CS}} < \pi/2$, where θ_{cr} is the critical angle defined by the parameters of the Auger-decay channel [63–65]. For the complete basis set, the value of θ_{CS} within this interval does not affect the computation results. In practice, however, incomplete basis sets are used, and one has to find an optimal θ_{CS} that minimizes the result-variation rate [43,44].

We use the finite basis with the basis functions constructed from the B splines [66,67] within the dual-kinetic-balance approach [68]. To investigate the dependence of the irreducible

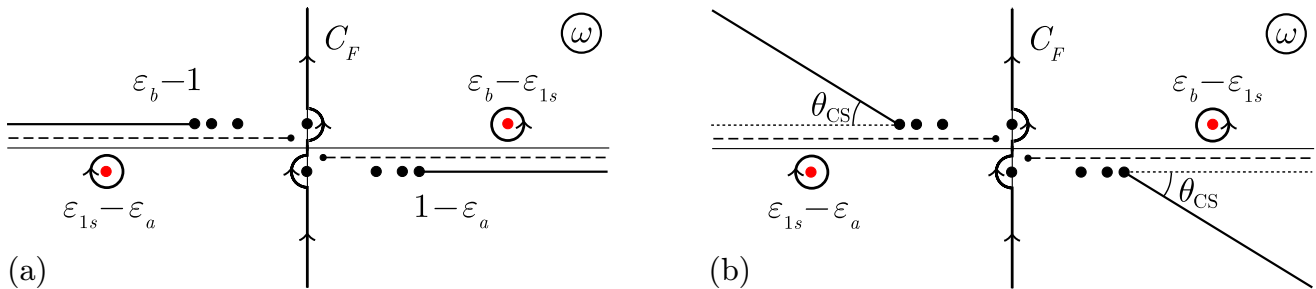


FIG. 2. Poles and branch cuts of the integrand and the integration contour for the direct part of the irreducible ladder contribution for $\varepsilon_{1s} < \varepsilon_a \leq \varepsilon_b$. The solid line representing the continuum turns into a set of poles for the finite basis. The dashed lines denote the cuts due to the photon propagators.

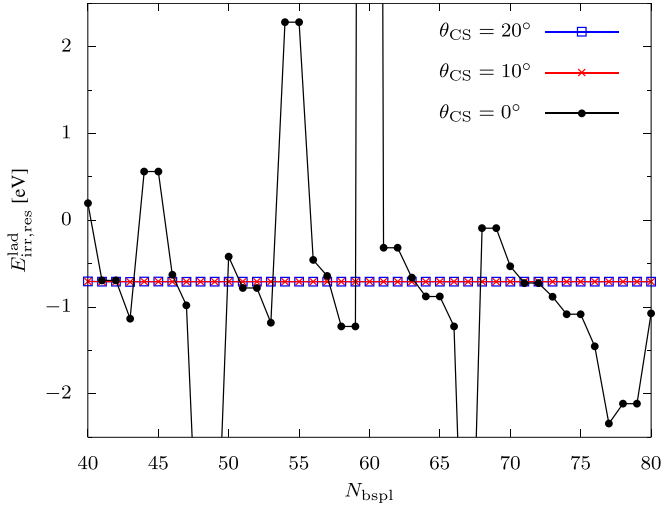


FIG. 3. The total resonant contribution, $(\kappa_{n_1}, \kappa_{n_2}) = (-1, 1)$ and $(\kappa_{n_1}, \kappa_{n_2}) = (1, -1)$, for the state $(2s2p_{1/2})_0$ in uranium as a function of N_{bspl} being the number of the B splines.

ladder contribution on the parameters of the basis set with and without the CS, in Fig. 3 we present the resonant terms for the $(2s2p_{1/2})_0$ state as a function of the B -spline number N_{bspl} for various values of θ_{CS} .

It is seen that the direct approach with $\theta_{\text{CS}} = 0^\circ$ fails. The CS approach, meanwhile, allows us to obtain the results which are free from the irregular dependence on N_{bspl} . We note also that inaccuracy in the choice of θ_{CS} can be easily compensated by extending the basis set and does not influence strongly the accuracy of the results. Finally, we point out that the reducible part of the ladder contribution, the crossed diagram, and other second-order many-electron QED corrections do not contain additional difficulties for autoionizing states and can be evaluated directly. The relevant formulas can be found in, e.g., Refs. [61,69–72]. The developed formalism can be

readily adapted for ions with more electrons as well as for the mixing states.

In Table I we present the energies of the autoionizing $(2s2p_{1/2})_0$, $(2p_{1/2}2p_{3/2})_1$, and $(2s2p_{3/2})_2$ states in helium-like argon and uranium. The nuclear-charge distribution is described by the Fermi model. The values of the fundamental constants are taken from Ref. [74], in particular, the inverse fine-structure constant $\alpha^{-1} = 137.035999084(21)$ and $m_e c^2 = 0.51099895000(15)$. The interelectronic-interaction and QED corrections are treated in the Furry picture. To zeroth order, the energy equals the sum of the one-electron Dirac energies. The contribution of the first order is provided by the one-photon exchange and one-loop QED diagrams. We also account for the complete set of the second-order corrections. The two-photon exchange contribution is evaluated within the *ab initio* QED approach combined with the CS as described above. We divide it into the Breit and QED contributions, see, e.g., Ref. [75]. The two-electron self-energy and vacuum-polarization corrections (the row “ScrQED”) are calculated using the approaches described in Ref. [72]. The one- and two-loop one-electron QED contributions are taken from Ref. [76]. The contribution arising from the exchange by three and more photons are accounted for within the Breit approximation. To this end, we utilize the CS version of the Dirac-Coulomb-Breit (CS-DCB) Hamiltonian and calculate the total energies by means of the CI approach, see Ref. [43]. The desired higher-order contribution is extracted following the procedure from Refs. [72,77,78]. The nuclear recoil contribution is also divided into the Breit and QED parts. Within the Breit approximation, it is treated by employing the mass-shift operator [79–82] included into the CS-DCB Hamiltonian. We dilate the mass-shift operator into the complex plane, which differs the present approach from the one utilized in Ref. [43], where the conventional (Hermitian) operator was used. This allows us to obtain considerably more stable numerical results. The QED nuclear recoil contribution is calculated to zeroth order in $1/Z$, see, e.g.,

TABLE I. Individual contributions to the energies in eV of the autoionizing $(2s2p_{1/2})_0$, $(2p_{1/2}2p_{3/2})_1$, and $(2s2p_{3/2})_2$ states in helium-like argon ($Z = 18$) and uranium ($Z = 92$) ions. See the text for the details.

	$Z = 18$			$Z = 92$		
	$(2s2p_{1/2})_0$	$(2p_{1/2}2p_{3/2})_1$	$(2s2p_{3/2})_2$	$(2s2p_{1/2})_0$	$(2p_{1/2}2p_{3/2})_1$	$(2s2p_{3/2})_2$
Dirac	-2216.113946	-2211.309654	-2211.308511	-68388.842	-63860.911	-63827.605
1 ph	65.614133	80.880215	65.354183	440.134	492.711	379.773
1 loop	0.148270	0.001855	0.158836	56.630	15.639	58.568
2 ph (Br.)	-0.766652	-1.095086	-0.762486	-1.318	-1.853	-0.974
2 ph (QED)	0.000033	0.000064	-0.000006	0.087	0.051	0.020
ScrQED	-0.003329	-0.000044	-0.003828	-0.442	-0.215	-0.343
2 loop	-0.000086	0.000009	-0.000103	-0.248	-0.018	-0.258
≥ 3 ph (Br.)	0.005489	0.003367	0.005577	-0.000	0.006	0.002
Recoil (Br.)	0.029503	0.029469	0.029440	0.146	0.141	0.135
Recoil (QED)	0.000044	-0.000004	0.000044	0.058	0.012	0.050
Nuc. Pol.	-0.000025	0.000000	-0.000025	-0.044	-0.004	-0.039
ScrScrQED	-0.000017	-0.000013	-0.000001	0.012	0.002	0.000
Total	-2151.086583(82)	-2131.489821(16)	-2146.526880(97)	-67893.833(97)	-63354.439(19)	-63390.654(95)
Reference [43]	-2151.087(15)	-2131.4900(19)	-2146.527(15)			
Reference [73]				-67892.71(30)	-63353.44(25)	-63389.68(30)

Refs. [79,80,82–87]. Finally, we account for the nuclear polarization [76,88–90] and deformation [77] effects. To estimate the higher-order QED corrections (the row “ScrScrQED”), we use the model-QED operator [91] realized in the QEDMOD package [92] and follow the procedure from Ref. [93]. For argon, the dominant uncertainties arise from the uncalculated higher-order QED corrections. In the case of uranium, the largest uncertainty comes from the nuclear size effect and two-loop QED correction [76].

In Table I, we also compare our results with the previous calculations. For argon, an excellent agreement is observed with the previous most-accurate results [43], but the present ones are much more precise. For uranium, in contrast, the obtained energies differ from the ones given in Ref. [73] by 3 to 4 standard deviations depending on the state. In Ref. [73], the conventional CI approach with the basis constructed from the B splines and supplemented with the continuum wave functions was applied. The uncertainties in Ref. [73] were determined from the dependence of the energies on the basis-set parameters. As was shown in Ref. [43], this approach can converge to an incorrect value due to improper accounting of

the interaction with the continuum, which, in turn, leads to an incorrect estimation of the uncertainty.

To summarize, we worked out an effective and reliable method based on the complex-scaling approach and aimed at describing the autoionizing states within the *ab initio* QED formalism. To demonstrate the developed approach, we evaluated the energies of the autoionizing $(2s2p_{1/2})_0$, $(2p_{1/2}2p_{3/2})_1$, and $(2s2p_{3/2})_2$ states in helium-like argon and uranium rigorously accounting for all the QED contributions up to the second order of the perturbation theory. The obtained energies are several orders of magnitude more precise than the previous most-accurate values. Theoretical predictions of this level of accuracy being supplemented with the experimental data provide an alternative kind of opportunity to test bound-state QED effects. Moreover, we believe that the combination of the complex scaling with the rigorous QED theory can be utilized for the evaluation of the QED effects in the external and even supercritical electromagnetic fields.

This study was supported by the Russian Science Foundation (Grant No. 22-22-00370).

-
- [1] P. Beiersdorfer, T. Phillips, V. L. Jacobs, K. W. Hill, M. Bitter, S. von Goeler, and S. M. Kahn, *Astrophys. J.* **409**, 846 (1993).
- [2] K. Widmann, P. Beiersdorfer, V. Decaux, S. R. Elliott, D. Knapp, A. Osterheld, M. Bitter, and A. Smith, *Rev. Sci. Instrum.* **66**, 761 (1995).
- [3] H.-J. Kunze, *Introduction to Plasma Spectroscopy* (Springer, Berlin, 2009).
- [4] G. J. Tallents, *An Introduction to the Atomic and Radiation Physics of Plasmas* (Cambridge University Press, Cambridge, England, 2018).
- [5] A. C. Fabian and I. M. George, in *Iron Line Diagnostics in X-Ray Sources*, edited by A. Treves, G. C. Perola, and L. Stella, Lecture Notes in Physics (Springer, Berlin, 1991), pp. 167–176.
- [6] D. Porquet, J. Dubau, and N. Grosso, *Space Sci. Rev.* **157**, 103 (2010).
- [7] M. C. Simon, J. R. Crespo López-Urrutia, C. Beilmann, M. Schwarz, Z. Harman, S. W. Epp, B. L. Schmitt, T. M. Baumann, E. Behar, S. Bernitt, R. Follath, R. Ginzler, C. H. Keitel, R. Klawitter, K. Kubiček, V. Mäkel, P. H. Mokler, G. Reichardt, O. Schwarzkopf, and J. Ullrich, *Phys. Rev. Lett.* **105**, 183001 (2010).
- [8] A. Müller, *Phys. Scr.* **90**, 054004 (2015).
- [9] S. Schippers, A. L. D. Kilcoyne, R. A. Phaneuf, and A. Müller, *Contemp. Phys.* **57**, 215 (2016).
- [10] A. Müller, E. Lindroth, S. Bari, A. Borovik, P.-M. Hillenbrand, K. Holste, P. Indelicato, A. L. D. Kilcoyne, S. Klumpp, M. Martins, J. Viehhaus, P. Wilhelm, and S. Schippers, *Phys. Rev. A* **98**, 033416 (2018).
- [11] J. Sapirstein and K. T. Cheng, *Can. J. Phys.* **86**, 25 (2008).
- [12] V. M. Shabaev, *Phys. Usp.* **51**, 1175 (2008).
- [13] D. A. Glazov, Y. S. Kozhedub, A. V. Maiorova, V. M. Shabaev, I. I. Tupitsyn, A. V. Volotka, C. Kozhuharov, G. Plunien, and Th. Stöhlker, *Hyp. Interact.* **199**, 71 (2011).
- [14] A. V. Volotka, D. A. Glazov, G. Plunien, and V. M. Shabaev, *Ann. Phys. (Berlin)* **525**, 636 (2013).
- [15] V. M. Shabaev, A. I. Bondarev, D. A. Glazov, M. Y. Kaygorodov, Y. S. Kozhedub, I. A. Maltsev, A. V. Malyshev, R. V. Popov, I. I. Tupitsyn, and N. A. Zubova, *Hyp. Interact.* **239**, 60 (2018).
- [16] P. Indelicato, *J. Phys. B: At. Mol. Opt. Phys.* **52**, 232001 (2019).
- [17] Y. K. Ho, *Phys. Rep.* **99**, 1 (1983).
- [18] N. Moiseyev, *Phys. Rep.* **302**, 212 (1998).
- [19] N. Moiseyev, *Non-Hermitian Quantum Mechanics* (Cambridge University Press, Cambridge, England, 2011).
- [20] E. Lindroth and L. Argenti, *Adv. Quantum Chem.* **63**, 247 (2012).
- [21] R. A. Weder, *J. Math. Phys.* **15**, 20 (1974).
- [22] R. A. Weder, *J. Funct. Anal.* **20**, 319 (1975).
- [23] P. Šeba, *Lett. Math. Phys.* **16**, 51 (1988).
- [24] I. A. Ivanov and Y. K. Ho, *Phys. Rev. A* **69**, 023407 (2004).
- [25] A. D. Alhaidari, *Phys. Rev. A* **75**, 042707 (2007).
- [26] J.-Y. Guo, X.-Zh. Fang, P. Jiao, J. Wang, and B.-M. Yao, *Phys. Rev. C* **82**, 034318 (2010).
- [27] J.-Y. Guo, M. Yu, J. Wang, B.-M. Yao, and P. Jiao, *Comput. Phys. Commun.* **181**, 550 (2010).
- [28] E. Ackad and M. Horbatsch, *Phys. Rev. A* **75**, 022508 (2007).
- [29] E. Ackad and M. Horbatsch, *Phys. Rev. A* **76**, 022503 (2007).
- [30] I. A. Maltsev, V. M. Shabaev, V. A. Zaytsev, R. V. Popov, Y. S. Kozhedub, and D. A. Tumakov, *Opt. Spectrosc.* **128**, 1100 (2020).
- [31] R. V. Popov, V. M. Shabaev, D. A. Telnov, I. I. Tupitsyn, I. A. Maltsev, Y. S. Kozhedub, A. I. Bondarev, N. V. Kozin, X. Ma, G. Plunien, T. Stöhlker, D. A. Tumakov, and V. A. Zaytsev, *Phys. Rev. D* **102**, 076005 (2020).
- [32] E. Lindroth, *Phys. Rev. A* **49**, 4473 (1994).
- [33] E. Lindroth, *Phys. Rev. A* **52**, 2737 (1995).
- [34] Y. K. Ho, *Phys. Rev. A* **23**, 2137 (1981).
- [35] G. Pestka, M. Bylicki, and J. Karwowski, *J. Phys. B: At. Mol. Opt. Phys.* **39**, 2979 (2006).
- [36] G. Pestka, M. Bylicki, and J. Karwowski, *J. Phys. B: At. Mol. Opt. Phys.* **40**, 2249 (2007).

- [37] M. Bylicki, G. Pestka, and J. Karwowski, *Phys. Rev. A* **77**, 044501 (2008).
- [38] N. Brandefelt and E. Lindroth, *Phys. Rev. A* **59**, 2691 (1999).
- [39] A. Derevianko, V. A. Dzuba, and M. G. Kozlov, *Phys. Rev. A* **82**, 022720 (2010).
- [40] S. B. Zhang and D. L. Yeager, *Phys. Rev. A* **85**, 032515 (2012).
- [41] S. B. Zhang and D. L. Yeager, *J. Mol. Struct.* **1023**, 96 (2012).
- [42] Y.-G. Peng, Y. Wu, L.-F. Zhu, S. B. Zhang, J.-G. Wang, H.-P. Liebermann, and R. J. Buenker, *J. Chem. Phys.* **144**, 054306 (2016).
- [43] V. A. Zaytsev, I. A. Maltsev, I. I. Tupitsyn, and V. M. Shabaev, *Phys. Rev. A* **100**, 052504 (2019).
- [44] V. A. Zaytsev, I. A. Maltsev, I. I. Tupitsyn, V. M. Shabaev, and V. Y. Ivanov, *Opt. Spectrosc.* **128**, 307 (2020).
- [45] Y. Sajeev, A. Ghosh, N. Vaval, and S. Pal, *Int. Rev. Phys. Chem.* **33**, 397 (2014).
- [46] F. Matz and T.-C. Jagau, *J. Chem. Phys.* **156**, 114117 (2022).
- [47] D. L. Yeager and M. K. Mishra, *Int. J. Quantum Chem.* **104**, 871 (2005).
- [48] K. Samanta and D. L. Yeager, *J. Phys. Chem. B* **112**, 16214 (2008).
- [49] K. Samanta and D. L. Yeager, *Complex Multiconfigurational Self-Consistent Field-Based Methods to Investigate Electron-Atom/Molecule Scattering Resonances* (Wiley, New York, 2012), pp. 103–142.
- [50] S. A. Blundell, P. J. Mohr, W. R. Johnson, and J. Sapirstein, *Phys. Rev. A* **48**, 2615 (1993).
- [51] I. Lindgren, H. Persson, S. Salomonson, and L. Labzowsky, *Phys. Rev. A* **51**, 1167 (1995).
- [52] P. J. Mohr and J. Sapirstein, *Phys. Rev. A* **62**, 052501 (2000).
- [53] V. A. Yerokhin, A. N. Artemyev, V. M. Shabaev, M. M. Sysak, O. M. Zherebtsov, and G. Soff, *Phys. Rev. A* **64**, 032109 (2001).
- [54] O. Y. Andreev, L. N. Labzowsky, G. Plunien, and G. Soff, *Phys. Rev. A* **64**, 042513 (2001).
- [55] B. Åsén, S. Salomonson, and I. Lindgren, *Phys. Rev. A* **65**, 032516 (2002).
- [56] O. Y. Andreev, L. N. Labzowsky, G. Plunien, and G. Soff, *Phys. Rev. A* **67**, 012503 (2003).
- [57] O. Y. Andreev, L. N. Labzowsky, G. Plunien, and G. Soff, *Phys. Rev. A* **69**, 062505 (2004).
- [58] A. N. Artemyev, V. M. Shabaev, V. A. Yerokhin, G. Plunien, and G. Soff, *Phys. Rev. A* **71**, 062104 (2005).
- [59] Y. S. Kozhedub, A. V. Malyshev, D. A. Glazov, V. M. Shabaev, and I. I. Tupitsyn, *Phys. Rev. A* **100**, 062506 (2019).
- [60] V. A. Yerokhin, V. Patkóš, and K. Pachucki, *Phys. Rev. A* **106**, 022815 (2022).
- [61] V. M. Shabaev and I. G. Fokeeva, *Phys. Rev. A* **49**, 4489 (1994).
- [62] V. M. Shabaev, *Phys. Rep.* **356**, 119 (2002).
- [63] E. Balslev and J. M. Combes, *Commun. Math. Phys.* **22**, 280 (1971).
- [64] B. Simon, *Commun. Math. Phys.* **27**, 1 (1972).
- [65] B. Simon, *Ann. Math.* **97**, 247 (1973).
- [66] J. Sapirstein and W. R. Johnson, *J. Phys. B: At. Mol. Opt. Phys.* **29**, 5213 (1996).
- [67] H. Bachau, E. Cormier, P. Decleva, J. E. Hansen, and F. Martín, *Rep. Prog. Phys.* **64**, 1815 (2001).
- [68] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, *Phys. Rev. Lett.* **93**, 130405 (2004).
- [69] V. A. Yerokhin, A. N. Artemyev, T. Beier, G. Plunien, V. M. Shabaev, and G. Soff, *Phys. Rev. A* **60**, 3522 (1999).
- [70] A. N. Artemyev, T. Beier, G. Plunien, V. M. Shabaev, G. Soff, and V. A. Yerokhin, *Phys. Rev. A* **60**, 45 (1999).
- [71] Y. S. Kozhedub, A. V. Volotka, A. N. Artemyev, D. A. Glazov, G. Plunien, V. M. Shabaev, I. I. Tupitsyn, and Th. Stöhlker, *Phys. Rev. A* **81**, 042513 (2010).
- [72] A. V. Malyshev, D. A. Glazov, A. V. Volotka, I. I. Tupitsyn, V. M. Shabaev, G. Plunien, and Th. Stöhlker, *Phys. Rev. A* **96**, 022512 (2017).
- [73] O. Y. Andreev, L. N. Labzowsky, and A. V. Prigorovsky, *Phys. Rev. A* **80**, 042514 (2009).
- [74] E. Tiesinga, P. J. Mohr, D. B. Newell, and B. N. Taylor, *Rev. Mod. Phys.* **93**, 025010 (2021).
- [75] A. V. Malyshev, A. V. Volotka, D. A. Glazov, I. I. Tupitsyn, V. M. Shabaev, and G. Plunien, *Phys. Rev. A* **90**, 062517 (2014).
- [76] V. A. Yerokhin and V. M. Shabaev, *J. Phys. Chem. Ref. Data* **44**, 033103 (2015).
- [77] Y. S. Kozhedub, O. V. Andreev, V. M. Shabaev, I. I. Tupitsyn, C. Brandau, C. Kozhuharov, G. Plunien, and T. Stöhlker, *Phys. Rev. A* **77**, 032501 (2008).
- [78] A. N. Artemyev, V. M. Shabaev, I. I. Tupitsyn, G. Plunien, A. Surzhykov, and S. Fritzsche, *Phys. Rev. A* **88**, 032518 (2013).
- [79] V. M. Shabaev, *Theor. Math. Phys.* **63**, 588 (1985) [*Teor. Mat. Fiz.* **63**, 394 (1985)].
- [80] V. M. Shabaev, *Sov. J. Nucl. Phys.* **47**, 69 (1988) [*Yad. Fiz.* **47**, 107 (1988)].
- [81] C. W. P. Palmer, *J. Phys. B: At. Mol. Phys.* **20**, 5987 (1987).
- [82] V. M. Shabaev, *Phys. Rev. A* **57**, 59 (1998).
- [83] K. Pachucki and H. Grotch, *Phys. Rev. A* **51**, 1854 (1995).
- [84] A. N. Artemyev, V. M. Shabaev, and V. A. Yerokhin, *Phys. Rev. A* **52**, 1884 (1995).
- [85] A. N. Artemyev, V. M. Shabaev, and V. A. Yerokhin, *J. Phys. B: At. Mol. Opt. Phys.* **28**, 5201 (1995).
- [86] G. S. Adkins, S. Morrison, and J. Sapirstein, *Phys. Rev. A* **76**, 042508 (2007).
- [87] A. V. Malyshev, R. V. Popov, V. M. Shabaev, and N. A. Zubova, *J. Phys. B: At. Mol. Opt. Phys.* **51**, 085001 (2018).
- [88] G. Plunien, B. Müller, W. Greiner, and G. Soff, *Phys. Rev. A* **43**, 5853 (1991).
- [89] G. Plunien and G. Soff, *Phys. Rev. A* **51**, 1119 (1995); **53**, 4614(E) (1996).
- [90] A. V. Nefiodov, L. N. Labzowsky, G. Plunien, and G. Soff, *Phys. Lett. A* **222**, 227 (1996).
- [91] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, *Phys. Rev. A* **88**, 012513 (2013).
- [92] V. M. Shabaev, I. I. Tupitsyn, and V. A. Yerokhin, *Comput. Phys. Commun.* **189**, 175 (2015); **223**, 69 (2018).
- [93] A. V. Malyshev, D. A. Glazov, Y. S. Kozhedub, I. S. Anisimova, M. Y. Kaygorodov, V. M. Shabaev, and I. I. Tupitsyn, *Phys. Rev. Lett.* **126**, 183001 (2021).