

Many-body study of the g factor in boronlike argon

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Highly accurate measurements of the g factor of boronlike Ar are currently implemented within the ARTEMIS experiment at GSI (Darmstadt, Germany) and within the ALPHATRAP experiment at the MPIK (Heidelberg, Germany). A comparison with the corresponding theoretical predictions will allow one to test the modern methods of bound-state QED. However, at least three different theoretical values of the g factor have been published up to date. The systematic study of the g -factor value of $^{40}\text{Ar}^{13+}$ in the ground $[(1s)^2(2s)^22p^1]^2P_{1/2}$ and the first excited $[(1s)^2(2s)^22p^1]^2P_{3/2}$ states is performed within the high-order coupled cluster and configuration interaction theories up to the full configuration interaction treatment. Correlation contributions are discussed and results are compared with previous studies.

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I. INTRODUCTION

Experiments on few-electron ions of heavy atoms are of great importance to test bound-state QED [1,2]. Highly accurate results for g factor [3–9] and hyperfine structure [10,11] have already been obtained for H-like and Li-like systems. In particular, the most accurate value of the electron mass (almost by two orders of magnitude more precise than the value from the independent measurements) has been obtained in the study of g factor of highly charged ions [8]. An independent determination of the fine-structure constant α is expected from the g -factor measurements in few-electron ions [12–14]. Combined experimental and theoretical studies of the g factor and hyperfine structure can be used to obtain the values of the nuclear magnetic moments [15–18].

The ARTEMIS experiment [19,20] at GSI implements the laser-microwave double-resonance technique with the fine or hyperfine structure of highly charged ions. In particular, it can yield the Zeeman splitting in the boronlike argon $^{40}\text{Ar}^{13+}$ ion (with spinless nucleus) in the ground $[(1s)^2(2s)^22p^1]^2P_{1/2}$ and excited $[(1s)^2(2s)^22p^1]^2P_{3/2}$ states at the ppb level of accuracy. Apart from the g factor of these states, it will also provide the possibility to measure the nonlinear Zeeman effect [19,21]. The ALPHATRAP experiment [22] at the Max-Planck-Institut für Kernphysik (MPIK) aims at the high-precision g -factor determination using the Larmor and cyclotron frequency measurements following the earlier experiments performed at the Mainz University [3–9].

Previously several theoretical values of g factor have been reported which are in a certain disagreement between each other: 0.663 647(1) [23], 0.663 728 [24], and 0.663 899(2) [25]. As noted in Ref. [25], the difference between these values is within the accuracy of the ARTEMIS experiment

[19]. This discrepancy can be explained by the different methods used in these works to obtain the electron-electron interaction contributions. All the other terms such as nuclear recoil and high-order (beyond the free-electron part) QED contributions calculated in Refs. [23,26] are much smaller than the difference. Thus, an independent calculation of g factor is of high importance.

It was shown that for such properties as g factor [27], enhancement factors of the electron electric dipole moment, effective electric field, and hyperfine structure [28–35] in atoms and molecules the coupled cluster theory gives very accurate results. It allows one to efficiently sum perturbation theory series up to an infinite order. Even for these neutral (or weakly charged) atoms and molecules the main uncertainty of the results were due to neglect or approximate inclusion of the Breit interaction.

The present paper is focused on the theoretical study of the boronlike Ar ion within the Dirac-Coulomb-Breit Hamiltonian with accounting effects of electron correlations in all orders of perturbation theory.

II. THEORY

The first-order Zeeman shift of the 2P_J state in the spinless-nucleus ion with the angular momentum projection M_J is directly related to the g factor:

$$\Delta E^{(1)} = gM_J\mu_0B, \quad (1)$$

where $\mu_0 = \frac{e\hbar}{2mc}$ is the Bohr magneton. Thus the atomic magnetic moment (and g factor) is determined by the first derivative of the energy with respect to the magnetic field B at zero field.

In the four-component Dirac theory, Zeeman Hamiltonian can be written in the following form:

$$H_Z = \mu_0 \sum_i [\mathbf{r}_i \times \boldsymbol{\alpha}_i] \cdot \mathbf{B}, \quad (2)$$

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where α is the vector of the Dirac matrices and i is an electron index; summation goes over all the electrons in the system.

Contribution of the QED to the atomic magnetic moment (and g factor) outside the Breit approximation can be approximately estimated as an expectation value of the following operator [36]:

$$\mu_0 \frac{g_e - 2}{2} \sum_i \beta_i \Sigma_{z,i}, \quad (3)$$

where $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, Σ_z is the z component of the vector operator $\Sigma = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$, σ are Pauli matrices, and $g_e = 2.002\,319\,3\dots$ is the free-electron g factor.

The frequency-independent Breit interelectronic interaction is given by the following operator:

$$H_B = -\frac{1}{2} \sum_{i < j}^N \left(\frac{(\alpha_i \cdot \alpha_j)}{r_{ij}} + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^3} \right), \quad (4)$$

where α_i and α_j act on variables of i th and j th electrons, correspondingly. This operator is the first QED correction to the Coulomb term and includes both the magnetic interaction (Gaunt) and ‘‘retardation’’ effects. Note that due to the off-diagonal structure of α matrices H_B and H_Z couple large and small bispinor components. Therefore, negative energy states can be of great importance for accurate calculation of g factor. A similar effect is well known in the calculation of the shielding constants (see, e.g., [37,38]).

The coupled cluster (CC) approach [39–42] is one of the most successful methods to consider dynamic electron correlation effects. It is based on the exponential ansatz for the wave function Ψ :

$$\Psi_{CC} = e^{\hat{T}} \Phi_0. \quad (5)$$

For the single-reference case Φ_0 is a one-determinant wave function of a system obtained in some approximation, e.g., within the Dirac-Fock method. \hat{T} is the excitation cluster operator which is expanded in terms of different excitation orders:

$$\hat{T} = \sum_{k=1}^n \hat{T}_k, \quad (6)$$

where

$$\hat{T}_k = \sum_{b_1 < b_2 \dots < b_k; i_1 < i_2 \dots < i_k} t_{i_1 i_2 \dots i_k}^{b_1 b_2 \dots b_k} a_{b_1}^\dagger a_{i_1}^\dagger a_{b_2}^\dagger a_{i_2}^\dagger \dots a_{b_k}^\dagger a_{i_k}^\dagger, \quad (7)$$

indexes i_n correspond to occupied orbitals while b_m correspond to unoccupied ones; a_{i_n} is the annihilation operator of the state i_n and $a_{b_m}^\dagger$ is the creation operator of the state b_m , and $t_{i_1 i_2 \dots i_k}^{b_1 b_2 \dots b_k}$ are unknown cluster amplitudes to be determined [39–42]. Truncation of the \hat{T} operator at \hat{T}_2 leads to the coupled cluster with single and double cluster amplitudes, CCSD, etc. In the coupled cluster technique [39–42] Schrödinger equation $H\Psi_{CC} = E\Psi_{CC}$ is reduced to a nonlinear equation system with unknown cluster amplitudes and energy and is solved iteratively. From the perturbation theory (PT) point of view, even truncated CC methods include some terms of PT (in interelectron interaction) up to an infinite order due to the exponential ansatz. For example, the coupled cluster

with single, double, triple, and quadruple cluster amplitudes, CCSDTQ [or its approximation CCSDT(Q) [43]] which was used in the present paper (see below) includes all terms of PT up to order six and some terms up to an infinite order. The CCSDT theory [and its approximation CCSD(T)] includes all terms of PT of the fourth order (and some terms up to an infinite order). Contrary to the CC theory, the configuration interaction (CI) method uses a linear ansatz instead of the exponential one in Eq. (5). If n in Eq. (6) equals the number of electrons in the system the CC and CI methods will give the same exact (full CI) wave function (within the given basis set, Hamiltonian, and in no-pair approximation).

III. ELECTRONIC STRUCTURE CALCULATION DETAILS

In all calculations we used Gaussian basis sets. For the main Dirac-Coulomb-Breit calculation the Dyal’s ACV4Z basis set [44] with excluded f - and g -type functions has been used. This basis set includes $25s$, $15p$, and $9d$ functions for large component and in the following will be called the MBas basis set. Additionally the correction on the basis set extension was considered within the Dirac-Coulomb approximation using the CCSDT method. The extended basis set, LBAs, included $61s$ -, $50p$ -, $33d$ -, $6f$ - and $4g$ -type functions. Finally, also the truncated version of the MBas basis set, SBas, was used which includes $25s$, $15p$, and $2d$ functions. The Gauss finite nuclear model was used in all of the calculations. All (five) electrons of the considered system were included in all the correlation calculations discussed in the next section.

For the Dirac-Fock-Gaunt calculations and Coulomb integral transformations we used the DIRAC15 code [45]. Relativistic correlation calculations were performed within the MRCC code [46–48]. One-electron bispinors were obtained within the $D_{\infty h}$ point group while correlation calculations were performed employing the D_{2h} symmetry [49]. This suggests possible extensions of these kind of calculations on molecules.

The code to compute matrix elements of the Breit operator (4) over one-electron bispinors generated by the DIRAC15 code has been developed in the present paper. The following algorithm is used. At first Coulomb-type integrals over primitive Gaussian-type basis functions, $x^l y^m z^n e^{-\alpha_i r^2}$, are computed. Then one uses four-index transformation to obtain integrals of the Breit operator (4) over one-electron bispinors. We use a standard technique to reduce the formal complexity of this step from $O(N^8)$ to $O(N^5)$ where N is the number of basis functions. No symmetry is used in the algorithm to be able to use this code in further molecular applications.

IV. RESULTS AND DISCUSSION

Table I gives a positive energy contribution to the g factor of the ground $^2P_{1/2}$ and excited $^2P_{3/2}$ states of Ar^{13+} via different methods within the Breit approximation. In this study the Dirac-Fock-Gaunt method (without the retardation part of the Breit interaction) for the open-shell $^2P_{1/2}$ state of Ar^{13+} has been used to obtain one-electron bispinors for subsequent correlation calculation. In this procedure negative and positive one-electron functions were updated at each iteration of the Dirac-Fock-Gaunt procedure [50]. Correlation calculations

TABLE I. Positive energy contributions to g factor of the ground ${}^2P_{1/2}$ and excited ${}^2P_{3/2}$ states of Ar^{13+} .

Method	${}^2P_{1/2}$	${}^2P_{3/2}$
Dirac-Fock-Gaunt	0.664797	1.331708
MP2(S)	0.664762	1.331609
MP2(SD)	0.665117	1.331589
CCSD	0.664962	1.330711
CCSD(T)	0.664732	1.331075
CCSDT	0.664764	1.331602
CCSDT(Q)	0.664762	1.331603
CCSDTQ	0.664762	1.331603
FullCI – CCSDTQ	0.000000	0.000000

were performed within the Breit approximation – the retardation part was added to the Hamiltonian after the self-consistent stage. MP2(S) (MP2 is the second-order Møller-Plesset perturbation theory) is the first order in the interelectron interaction (with respect to chosen zero-order approximation) contribution to g factor. It can be seen from Table I that higher-order correlation effects within the nondegenerate PT [MP2(SD)] or terms of single-reference CC models also contribute; however, their sum gives a rather small contribution for the problem under consideration [compare the results of the CCSDTQ and MP2(S) approaches]. This can be an indication of slight static correlation effects whose description is of some difficulty for the single-reference CC approaches (e.g., there is some admixture of the $1s^2 2p^3$ configuration to the leading $1s^2 2s^2 2p^1$ configuration — the corresponding cluster amplitude is about 0.1). The CCSD approach overestimates the value of g factor for the ${}^2P_{1/2}$ state and underestimates it for the case of the ${}^2P_{3/2}$ state. Nevertheless, one can see that the treatment of higher-order cluster amplitudes leads to rather fast convergence in the CC series [CCSD, CCSD(T), CCSDT, CCSDT(Q), and CCSDTQ]. According to Table I, already the CCSDT method gives results that almost coincide with the final values for both considered states. The values of g factor obtained within the CCSDT(Q) and CCSDTQ are identical within six digits.

The full CI treatment of all correlation effects for the positive energy spectrum, i.e., in the CISDTQP/CCSDTQP models, was possible within the SBas basis set. As expected, the inclusion of pentuple (quintuple) excitations gave negligible contribution to g factor.

Table II provides results for the g factor of the ${}^2P_{1/2}$ state within the single-reference [47] and multireference (MR) [48] configuration interaction methods. Two different active spaces were used for the multireference treatment. In the MRmin-CI model active space included only $2p_{1/2}$ bispinors. For example, for the MRmin-CISD model the variational problem is solved in the basis of Slater determinants corresponding to $[(1s)^2(2s)^2 2p_{j=1/2, m_j=1/2}^1]$ and $[(1s)^2(2s)^2 2p_{j=1/2, m_j=-1/2}^1]$ configurations and all single and double excitations from these determinants to all virtual orbitals. In the MRsp-CI model the complete active space (CAS) included all $2s$ ($j = 1/2$) and $2p$ ($j = 1/2, 3/2$) bispinors, i.e., determinants with all possible distributions of three electrons over these bispinors were considered as the multireference. For example, in the MRsp-CISDT one considers all possible single, double, and

TABLE II. Positive-energy contributions to g factor of the ground ${}^2P_{1/2}$ state of Ar^{13+} using different configuration interaction methods.

Method	
CISD	0.664755
CISDT	0.664840
CISDTQ	0.664762
FullCI – CISDTQ	0.000000
MRmin-CISD	0.664763
MRmin-CISDT	0.664762
MRmin-CISDTQ	0.664762
FullCI – MRmin-CISDTQ	0.000000
MRsp-CISD	0.664762
MRsp-CISDT	0.664762
MRsp-CISDTQ	0.664762
FullCI – MRsp-CISDTQ	0.000000

triple excitations from these determinants (including excitations from $1s^2$). As can be seen in the present case of five correlated electrons the g -factor value converges very fast for both considered multireference models. Note, that the convergence of the correlation energy is slower. The single-reference series (CISD, CISDT, CISDTQ, FCI) converges much slower.

Table III presents the final value of g factor including the negative energy spectrum contribution which was calculated in the first order of the interelectronic interaction [within the MP2(S) method]. For the positive energy spectrum the CCSDTQ result was taken as the most accurate one (it included 1.3×10^8 cluster amplitudes). We also took into account basis set correction calculated within the Dirac-Coulomb Hamiltonian employing the CCSDT method [43]. This correction is included in the uncertainty of the final value.

QED contribution to the g factors of the considered ${}^2P_{1/2}$ and ${}^2P_{3/2}$ states has been estimated at the same level as g factor using the operator given by Eq. (3) which has also been employed in Refs. [24,25]. The obtained contribution is termed “QED estimation” in Table III. Within the rigorous QED theory in the first order in α the one-electron QED correction is given by the self-energy and vacuum-polarization diagrams. The self-energy contribution was evaluated to all orders in the parameter αZ in effective screening potential in Ref. [23] (see also Ref. [51] for high-accuracy calculations in the Coulomb potential and Ref. [52] for recent extension of the screening-potential calculations to $Z = 10\text{--}20$). These values are presented in Table III as “self-energy correction.” The vacuum-polarization contribution was found to be on the level of 10^{-9} for both considered states [23]. For the two-loop QED correction (of the second order in α) only the free-electron value (zeroth order in αZ) is available [53]; it is termed “free-electron two-loop QED” in Table III. Finally, the first-order interelectronic-interaction contribution was evaluated with the frequency-dependent operator in Refs. [23,52]. The difference between this value and the corresponding term evaluated with the Coulomb and frequency-independent Breit operators is termed “one-photon-exchange QED” in Table III. QED contributions obtained by the approximation operator given by Eq. (3) and rigorous results of Ref. [23] are compared in Table III and found to be in reasonable agreement.

TABLE III. Calculated g factor of the ground ${}^2P_{1/2}$ and excited ${}^2P_{3/2}$ states of Ar^{13+} in comparison with previous studies.

Method	${}^2P_{1/2}$	${}^2P_{3/2}$
Positive, CCSDTQ	0.664762	1.331603
Negative [MP2(S)]	-0.000335	-0.000089
Basis set correction (Coulomb)	-0.000001	-0.000002
Total (w/o QED)	0.664426(3)	1.331512(3)
PT + CI-DFS	0.664427(1)	1.331513(3)
(Ref. [23], w/o QED, w/o recoil)		
QED estimation ^a	-0.000774(3)(6) ^b	0.000773(3)(6) ^b
QED, rigorous approach ^c		
self-energy correction	-0.000770	0.000780
free-electron two-loop QED	0.000001	-0.000001
one-photon-exchange QED	-0.000002	-0.000002
Total + QED estimation ^{a,d}	0.663652(3)(6) ^b	1.332286(3)(6) ^b
PT + CI-DFS + QED ^c	0.663657(1)	1.332290(3)
(Ref. [23], with QED, w/o recoil)		
MCDF + QED ^a	0.663899(2)	1.332372(1)
(Marques <i>et al.</i> [25])		
MRCI + QED ^a	0.663728	1.332365
(Verdebout <i>et al.</i> [24])		
PT + CI-DFS + QED ^c + recoil	0.663647(1)	1.332285(3)
(Glazov <i>et al.</i> [23])		

^aCalculated within the approximation given by the operator in Eq. (3).

^bThe first uncertainty is due to the basis set and correlation; the second is due to the approximate nature of the operator given by Eq. (3).

^cRigorous QED calculation (see text and Ref. [23] for details).

^dThese values include estimation of QED correction (see text) to compare with previous theoretical results in Refs. [24,25] where individual contributions within the Breit approximation are not given.

Our “Total + QED estimation” value in Table III is obtained as a sum of the Breit-approximation result and the QED estimation by Eq. (3). In this way, we can consistently compare our results with those of Refs. [24,25] where the individual contributions within the Breit approximation were not given. The most accurate up-to-date g -factor values should include the rigorous results for the QED [23] and nuclear recoil [26] corrections.

It can be seen that the correlation part of the g factor within the Breit approximation is in perfect agreement with the corresponding values from Ref. [23]. It should be stressed that in the present paper a completely different approach has been used. We employed Gaussian-type basis functions defined above while the Dirac-Fock-Sturm functions were used in [23]. In addition, in our approach different zero-order approximation has been used: Dirac-Fock-Gaunt vs one-particle Dirac in [23]. We have performed additional calculations within the LBas basis set using the one-particle Dirac equation. g -factor values for both considered electronic states obtained within this approach coincide within $\sim 10^{-10}$ with analytic values given by Eqs. (3) and (4) in [23] and presented in Table I of Ref. [23]. This also suggests an additional test of the basis set completeness. Due to completely different zero-order approximations and different practical techniques used in the present correlation calculations and in [23] it is not possible to compare some intermediate values, such as one-photon exchange from [23], with our correlation models and only the final values can be compared. However, as was already noted above, these final values obtained with different

methods to treat electron correlation effects (CC theory up to full CC vs PT+CI-DFS) within the Breit approximations agree on the level of 10^{-6} (within the numerical uncertainty). This is not the case for the other previously obtained results [24,25] (see Table III).

It should be stressed that in the present paper we performed benchmark full CI calculation which includes all correlation effects for the positive-energy states. It means that this result can be used to test different approximate methods. Taking into account the data from Tables I and II one should note that a delicate check of the g -factor value is required in the case when electron correlation effects are taken into account approximately. For example, in the case of the ${}^2P_{1/2}$ state the simplest MP2(S) model gives the same results as the full CI method. At the same time the CCSD(T) method gives results which are in poorer agreement with the full CI results. Unfortunately, in the previous studies only limited data concerning the convergence of the g -factor value with respect to inclusion of correlation effects are presented or only the final result is given. On the other hand, it was shown that the reasonable multireference configuration interaction model can provide accurate results for g factor. Taking into account the data in Table II as well as the above discussion and according to the description given for the multireference CI model in Ref. [24] one may suggest that the model may give reasonable results for the positive energy contribution to g factor. But one should stress that there can also be some dependence on the actual details of the implemented approach in [24]. The latter is also true for Ref. [25].

In the theory section it is noted that the contribution of the negative energy spectrum to g factor is important (the actual value of the contribution depends on the method of the negative energy bispinors construction). According to the description given in Ref. [24] the Breit interaction was added to the Hamiltonian after the multiconfigurational Dirac-Hartree-Fock calculation which was performed within the Dirac-Coulomb Hamiltonian. No influence of the Breit interaction on the negative energy states was considered at this stage. Within the updated Hamiltonian the configuration interaction calculation has been performed including only positive-energy states. In such approach important contribution of the simultaneous treatment of the Breit [Eq. (4)] and Zeeman [Eq. (2)] interactions is not taken into account. This may be (one of) the reason for the discrepancy between our present value and the value from Ref. [24].

V. CONCLUSION

The correlation treatment of g factors of the ground and excited states of the B-like Ar ion within the Dirac-Coulomb-Breit Hamiltonian has been performed. Uncertainty of the result has been tested by performing the full CI calculation (i.e., full inclusion of correlation effects) and considering different basis sets. Obtained g factors of the ground $^2P_{1/2}$ and excited $^2P_{3/2}$ states coincide within the uncertainty with

one of three previous theoretical results [23] and thus can be considered as its independent confirmation. It is shown that high-order correlation effects give non-negligible individual contributions to the value of g factor; however, their sum is small for the problem under consideration.

In this work, the code to compute matrix elements of the Breit interaction has been developed. It does not use atomic symmetry and can be modified to study heavy atoms in external fields and molecules which is already of great interest for precise study of electron electric dipole moment enhancement factors [28–30], hyperfine structure, and related fundamental problems including few-electron systems.

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- [1] A. V. Volotka, D. A. Glazov, G. Plunien, and V. M. Shabaev, *Ann. Phys. (NY)* **525**, 636 (2013).
 - [2] V. M. Shabaev, D. A. Glazov, G. Plunien, and A. V. Volotka, *J. Phys. Chem. Ref. Data* **44**, 031205 (2015).
 - [3] H. Häffner, T. Beier, N. Hermanspahn, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, *Phys. Rev. Lett.* **85**, 5308 (2000).
 - [4] J. Verdú, S. Djekić, S. Stahl, T. Valenzuela, M. Vogel, G. Werth, T. Beier, H.-J. Kluge, and W. Quint, *Phys. Rev. Lett.* **92**, 093002 (2004).
 - [5] S. Sturm, A. Wagner, B. Schabinger, J. Zatorski, Z. Harman, W. Quint, G. Werth, C. H. Keitel, and K. Blaum, *Phys. Rev. Lett.* **107**, 023002 (2011).
 - [6] A. Wagner, S. Sturm, F. Köhler, D. A. Glazov, A. V. Volotka, G. Plunien, W. Quint, G. Werth, V. M. Shabaev, and K. Blaum, *Phys. Rev. Lett.* **110**, 033003 (2013).
 - [7] S. Sturm, A. Wagner, M. Kretzschmar, W. Quint, G. Werth, and K. Blaum, *Phys. Rev. A* **87**, 030501(R) (2013).
 - [8] S. Sturm, F. Köhler, J. Zatorski, A. Wagner, Z. Harman, G. Werth, W. Quint, C. H. Keitel, and K. Blaum, *Nature (London)* **506**, 467 (2014).
 - [9] F. Köhler, K. Blaum, M. Block, S. Chenmarev, S. Eliseev, D. A. Glazov, M. Goncharov, J. Hou, A. Kracke, D. A. Nesterenko *et al.*, *Nat. Commun.* **7**, 10246 (2016).
 - [10] M. Lochmann, R. Jöhren, C. Geppert, Z. Andelkovic, D. Anielski, B. Botermann, M. Bussmann, A. Dax, N. Frömmgen, M. Hammen, V. Hannen, T. Kühl, Y. A. Litvinov, R. López-Coto, T. Stöhlker, R.C. Thompson, J. Vollbrecht, A. Volotka, C. Weinheimer, W. Wen, E. Will, D. Winters, R. Sánchez, and W. Nörtershäuser, *Phys. Rev. A* **90**, 030501(R) (2014).
 - [11] J. Ullmann, Z. Andelkovic, C. Brandau, A. Dax, W. Geithner, C. Geppert, C. Gorges, M. Hammen, V. Hannen, S. Kaufmann *et al.*, *Nat. Commun.* **8**, 15484 (2017).
 - [12] V. M. Shabaev, D. A. Glazov, N. S. Oreshkina, A. V. Volotka, G. Plunien, H.-J. Kluge, and W. Quint, *Phys. Rev. Lett.* **96**, 253002 (2006).
 - [13] A. V. Volotka and G. Plunien, *Phys. Rev. Lett.* **113**, 023002 (2014).
 - [14] V. A. Yerokhin, E. Berseneva, Z. Harman, I. I. Tupitsyn, and C. H. Keitel, *Phys. Rev. Lett.* **116**, 100801 (2016).
 - [15] G. Werth, H. Häffner, N. Hermanspahn, H.-J. Kluge, W. Quint, and J. Verdú, in *The Hydrogen Atom*, edited by S. G. Karshenboim, F. S. Pavone, F. Bassani, M. Inguscio, and T. W. Hänsch (Springer, Berlin, 2001), p. 204.
 - [16] W. Quint, D. L. Moskovkhin, V. M. Shabaev, and M. Vogel, *Phys. Rev. A* **78**, 032517 (2008).
 - [17] V. A. Yerokhin, K. Pachucki, Z. Harman, and C. H. Keitel, *Phys. Rev. Lett.* **107**, 043004 (2011).
 - [18] S. Schmidt, J. Billowes, M. Bissell, K. Blaum, R. G. Ruiz, H. Heylen, S. Malbrunot-Ettenauer, G. Neyens, W. Nörtershäuser, G. Plunien *et al.*, *Phys. Lett. B* **779**, 324 (2018).
 - [19] D. von Lindenfels, M. Wiesel, D. A. Glazov, A. V. Volotka, M. M. Sokolov, V. M. Shabaev, G. Plunien, W. Quint, G. Birkel, A. Martin *et al.*, *Phys. Rev. A* **87**, 023412 (2013).
 - [20] M. Vogel, M. S. Ebrahimi, Z. Guo, A. Khodaparast, G. Birkel, and W. Quint, *Ann. Phys.*, 1800211 (2018), doi: 10.1002/andp.201800211.
 - [21] A. S. Varentsova, V. A. Agababaev, D. A. Glazov, A. M. Volchkova, A. V. Volotka, V. M. Shabaev, and G. Plunien, *Phys. Rev. A* **97**, 043402 (2018).

- [22] S. Sturm, M. Vogel, F. Köhler-Langes, W. Quint, K. Blaum, and G. Werth, *Atoms* **5**, 4 (2017).
- [23] D. A. Glazov, A. V. Volotka, A. A. Schepetnov, M. M. Sokolov, V. M. Shabaev, I. I. Tupitsyn, and G. Plunien, *Phys. Scr.* **T156**, 014014 (2013).
- [24] S. Verdebout, C. Naze, P. Jonsson, P. Rynkun, M. Godefroid, and G. Gaigalas, *At. Data Nucl. Data Tables* **100**, 1111 (2014).
- [25] J. P. Marques, P. Indelicato, F. Parente, J. M. Sampaio, and J. P. Santos, *Phys. Rev. A* **94**, 042504 (2016).
- [26] D. A. Glazov, A. V. Malyshev, V. M. Shabaev, and I. I. Tupitsyn, *Opt. Spectrosc.* **124**, 457 (2018).
- [27] A. N. Petrov, L. V. Skripnikov, and A. V. Titov, *Phys. Rev. A* **96**, 022508 (2017).
- [28] L. V. Skripnikov, D. E. Maison, and N. S. Mosyagin, *Phys. Rev. A* **95**, 022507 (2017).
- [29] L. V. Skripnikov and A. V. Titov, *J. Chem. Phys.* **142**, 024301 (2015).
- [30] L. V. Skripnikov, *J. Chem. Phys.* **145**, 214301 (2016).
- [31] L. V. Skripnikov, A. D. Kudashov, A. N. Petrov, and A. V. Titov, *Phys. Rev. A* **90**, 064501 (2014).
- [32] L. V. Skripnikov, A. N. Petrov, A. V. Titov, and V. V. Flambaum, *Phys. Rev. Lett.* **113**, 263006 (2014).
- [33] L. V. Skripnikov, A. N. Petrov, N. S. Mosyagin, A. V. Titov, and V. V. Flambaum, *Phys. Rev. A* **92**, 012521 (2015).
- [34] L. V. Skripnikov, *J. Chem. Phys.* **147**, 021101 (2017).
- [35] L. V. Skripnikov, A. N. Petrov, A. V. Titov, R. J. Mawhorter, A. L. Baum, T. J. Sears, and J.-U. Grabow, *Phys. Rev. A* **92**, 032508 (2015).
- [36] K. T. Cheng and W. J. Childs, *Phys. Rev. A* **31**, 2775 (1985).
- [37] G. A. Aucar, T. Saue, L. Visscher, and H. J. A. Jensen, *J. Chem. Phys.* **110**, 6208 (1999).
- [38] L. V. Skripnikov, S. Schmidt, J. Ullmann, C. Geppert, F. Kraus, B. Kresse, W. Nörtershäuser, A. F. Privalov, B. Scheibe, V. M. Shabaev *et al.*, *Phys. Rev. Lett.* **120**, 093001 (2018).
- [39] J. Cizek and J. Paldus, *Phys. Scr.* **21**, 251 (1980).
- [40] R. J. Bartlett, *Theor. Chim. Acta* **80**, 71 (1991).
- [41] S. A. Kucharski and R. J. Bartlett, *J. Chem. Phys.* **97**, 4282 (1992).
- [42] R. J. Bartlett and M. Musiał, *Rev. Mod. Phys.* **79**, 291 (2007).
- [43] M. Kállay and J. Gauss, *J. Chem. Phys.* **123**, 214105 (2005).
- [44] K. G. Dyall, *Theor. Chem. Acc.* **135**, 128 (2016).
- [45] R. Bast, T. Saue, L. Visscher, and H. J. Aa. Jensen, with contributions from V. Bakken, K. G. Dyall, S. Dubillard, U. Ekstroem, E. Eliav, T. Enevoldsen, E. Fasshauer, T. Fleig, O. Fossgaard, A. S. P. Gomes, T. Helgaker, J. Henriksson, M. Ilias, Ch. R. Jacob, S. Knecht, S. Komorovsky, O. Kullie, J. K. Laerdahl, C. V. Larsen, Y. S. Lee, H. S. Nataraj, M. K. Nayak, P. Norman, G. Olejniczak, J. Olsen, Y. C. Park, J. K. Pedersen, M. Pernpointner, R. Di Remigio, K. Ruud, P. Salek, B. Schimmelpfennig, J. Sikkema, A. J. Thorvaldsen, J. Thyssen, J. van Stralen, S. Villaume, O. Visser, T. Winther, and S. Yamamoto, *DIRAC, a relativistic ab initio electronic structure program*, Release DIRAC15 (2015), see <http://www.diracprogram.org>.
- [46] M. Kállay, Z. Rolik, I. Ladjánszki, L. Szegedy, B. Ladóczki, J. Csontos, and B. Kornis, MRCC, a quantum chemical program suite; See also Z. Rolik and M. Kállay, *J. Chem. Phys.* **135**, 104111 (2011), as well as www.mrcc.hu.
- [47] M. Kállay and P. R. Surján, *J. Chem. Phys.* **115**, 2945 (2001).
- [48] M. Kállay, P. G. Szalay, and P. R. Surján, *J. Chem. Phys.* **117**, 980 (2002).
- [49] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 3rd ed. (Pergamon, Oxford, 1977).
- [50] M. H. Mittleman, *Phys. Rev. A* **24**, 1167 (1981).
- [51] V. A. Yerokhin and U. D. Jentschura, *Phys. Rev. A* **81**, 012502 (2010).
- [52] V. A. Agababaev, D. A. Glazov, A. V. Volotka, D. V. Zinenko, V. M. Shabaev, and G. Plunien, *J. Phys. Conf. Ser.* **1138**, 012003 (2018).
- [53] H. Grotch and R. Kashuba, *Phys. Rev. A* **7**, 78 (1973).