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Correlated many-body treatment of the Breit interaction with application to cesium atomic properties and parity violation

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Corrections from the Breit interaction to basic properties of atomic ^{133}Cs are determined in the framework of third-order relativistic many-body perturbation theory. The corrections to energies, hyperfine-structure constants, off-diagonal hyperfine $6S$-$7S$ amplitude, and electric-dipole matrix elements are tabulated. It is demonstrated that the Breit corrections to correlations are comparable to the Breit corrections at the Hartree-Fock level. Modification of the parity-nonconserving (PNC) $6S$-$7S$ amplitude due to Breit interaction is also evaluated; the resulting weak charge of ^{133}Cs shows no significant deviation from the prediction of the standard model of elementary particles. The neutron skin correction to the PNC amplitude is also estimated to be -0.2% with an error bound of 30% based on the analysis of recent experiments with antiprotonic atoms. The present work supplements publication [A. Derevianko, Phys. Rev. Lett. **85**, 1618 (2000)] with a discussion of the formalism and provides additional numerical results and updated discussion of parity violation.

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I. INTRODUCTION

To date, the most accurate measurement of parity nonconservation (PNC) [1,2] in atoms has been carried out by Wieman and co-workers using ^{133}Cs [3,4]. The observed weak charge of the nucleus, Q_W, is determined as a combination of the experimental PNC amplitude E_{PNC} of the $6S_{1/2}$-$7S_{1/2}$ transition and a theoretical atomic-structure parameter E_{PNC}/Q_W. Such determined Q_W provides powerful constraints on possible extensions to the standard model (SM) of elementary particles. The achieved precision in experiments [3,4] is 0.35%; however, the required atomic structure parameter has been calculated only with an accuracy of about 1% [5,6], limiting the accuracy of determination of the weak charge. Presently it is understood [7–9] that a detailed account of the Breit corrections to basic atomic properties is required to reach the next level of precision in *ab initio* relativistic calculation of PNC amplitudes. In particular, the Breit correction to the $6S_{1/2}$-$7S_{1/2}$ PNC amplitude in ^{133}Cs accounts for a dominant part of the deviation [4] of determined weak charge from the prediction of the standard model [7–9].

The purpose of this paper is to provide a detailed discussion of the formalism employed in Refs. [7,10] and to tabulate additional numerical results. Since the publication of Refs. [7,10] several calculations of the Breit correction to properties of cesium atom have been carried out [8,9,11] and a comparison between different approaches is also presented here. We also calculate a value for the neutron "skin" correction to the PNC amplitude based on the analysis of experiments with antiprotonic atoms [12].

The major difference between the present analysis and earlier works on the Breit interaction in multielectron atoms [13–19] is the systematic treatment of correlation effects, i.e., contributions beyond self-consistent Breit-Coulomb-Hartree-Fock (BCHF) formulation [14,17,18]. These correlation effects are estimated here in the framework of relativistic many-body perturbation theory. It is demonstrated that these additional contributions are comparable to the lowest-order BCHF corrections for almost all considered atomic properties.

The paper is organized as follows. In Sec. II we describe the employed many-body formalism. Numerical results are tabulated and discussed in Sec. III. We consider Breit corrections to energies, hyperfine-structure constants, off-diagonal hyperfine $6S$-$7S$ amplitude, and electric-dipole matrix elements. The Breit correction to parity nonconserving $6S$-$7S$ amplitude is also evaluated in Sec. IV.

II. METHOD

The Breit interaction [20–22] is a two-particle interaction caused by an exchange of transverse photons between atomic electrons. Qualitatively, it describes a magnetic interaction between electrons (so-called Gaunt interaction) and retardation effect. Its low-frequency form in the Coulomb gauge, employed here, is given by[1]

$$B=\sum_{i<j} -\frac{1}{2r_{ij}}\{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j+(\boldsymbol{\alpha}_i\cdot\hat{r}_{ij})(\boldsymbol{\alpha}_j\cdot\hat{r}_{ij})\}, \qquad (2.1)$$

where α are Dirac matrices and r_{ij} is a distance between electrons. In this paper, we disregard the frequency dependence in the Breit interaction. It is worth noting that a consistent inclusion of the frequency dependence in the Breit interaction would require simultaneous treatment of QED self-energy correction [18].

A. Many-body perturbation theory and Breit interaction

The many-body Hamiltonian of an atomic system can be generally represented as

$$H=H_0+T=\sum_i h_0(i)+\frac{1}{2}\sum_{ij} t(i,j), \qquad (2.2)$$

where

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[1] Unless specified otherwise, atomic units $\hbar=|e|=m_e=1$ are used throughout the paper.

$$h_0(i)=c(\boldsymbol{\alpha}_i\cdot\mathbf{p}_i)+\beta c^2+V_{\mathrm{nuc}}(i) \tag{2.3}$$

is a one-particle Dirac Hamiltonian for an electron including Coulomb interaction with the nucleus $V_{\mathrm{nuc}}(i)$ and $t(i,j)$ represents two-particle interactions. To effectively minimize the perturbing two-particle interactions, one introduces a potential $U(i)$ and rewrites the Hamiltonian as

$$H=\sum_i \{h_0(i)+U(i)\}+\left\{\frac{1}{2}\sum_{ij} t(i,j)-\sum_i U(i)\right\}. \tag{2.4}$$

For atoms with one valence electron v outside a closed-shell core a many-body wave function $|\Psi_v\rangle$ in the independent-particle approximation is a Slater determinant constructed from core and valence single-particle orbitals ϕ_i. These orbitals satisfy the one-particle Dirac equation

$$(h_0+U)\phi_i=\varepsilon_i\phi_i . \tag{2.5}$$

The potential U is usually chosen to be spherically symmetric and label i is a list of conventional quantum numbers $\{n_i,j_i,l_i,m_i\}$ for bound states, with n_i replaced by ε_i for continuum. With the complete set of single-particle states ϕ_i, the Hamiltonian, Eq. (2.4), can be recast into the second-quantized form

$$H=\sum_i \varepsilon_i a_i^\dagger a_i+\sum_{ij}(-U)_{ij}a_i^\dagger a_j+\frac{1}{2}\sum_{ijkl} t_{ijkl}a_i^\dagger a_j^\dagger a_l a_k . \tag{2.6}$$

Only certain combinations of positive- and negative-energy solutions of the Dirac equation (2.5) are retained in relativistic many-body Hamiltonian (*no-pair* approximation [23]). The reader is directed to Refs. [24,25] and references therein for a detailed discussion of the problem of negative-energy states.

We follow a convention of Ref. [26] and label core orbitals as $a,b,\ldots,$ excited (virtual) orbitals as $m,n,\ldots,$ and valence orbitals as v,w. Indexes *i,j,k,l* range over both core and virtual (including valence) orbitals. In this notation the lowest-order wave function is $|\Psi_v\rangle^{(0)}=a_v^\dagger|0_{\mathrm{core}}\rangle$, where quasivacuum state $|0_{\mathrm{core}}\rangle=(\Pi_{a\in\mathrm{core}}a_a^\dagger)|0\rangle$ represents a closed-shell atomic core. Introducing normal form of operator products, $:\cdots:$, defined with respect to $|0_{\mathrm{core}}\rangle$ one can rewrite a two-particle operator T as a sum of zero-, one-, and two-body contributions [26]

$$T^{(0)}=\frac{1}{2}\sum_h t_{bb},$$

$$T^{(1)}=\sum_{ij} t_{ij}:a_i^\dagger a_j:,$$

$$T^{(2)}=\frac{1}{2}\sum_{ijkl} t_{ijkl}:a_i^\dagger a_j^\dagger a_l a_k:,$$

with $t_{ij}=\Sigma_a(t_{iaja}-t_{iaaj})$. In this notation the Hamiltonian reads

$$H'=\Sigma_i\varepsilon_i:a_i^\dagger a_i:+\Sigma_{ij}\{t_{ij}-U_{ij}\}:a_i^\dagger a_j:$$
$$+\frac{1}{2}\Sigma_{ijkl}t_{ijkl}:a_i^\dagger a_j^\dagger a_l a_k:. \tag{2.7}$$

Zero-body contribution to the total Hamiltonian H has been discarded since it does not affect the properties of valence states. It is worth emphasizing that the Breit and Coulomb interactions are of course two-*particle* operators; reference to zero-, one-, and two-*body* parts arises due to the separation into the normal forms of operator products and is just a matter of convenience.

In the case at hand, the two-particle interaction

$$T=C+B$$

is a sum of the instantaneous Coulomb interaction $C=\Sigma_{i<j}(1/r_{ij})$ and the Breit interaction B, Eq. (2.1). Corresponding two-particle matrix elements are designated as c_{ijkl} and b_{ijkl}. The Coulomb interaction dominates and we distinguish two possibilities in defining the effective potential U in Eq. (2.5): traditional Coulomb-Hartree-Fock (CHF) potential U^{CHF} and BCHF potential U^{BCHF}, where the Breit and Coulomb interactions are treated on the same footing. To differentiate between the two resulting eigensystems of Eq. (2.5) we will add bar to the quantities pertaining to the BCHF case, e.g., $\overline{\varepsilon_i},\overline{a_i},\overline{a_i^\dagger}$.

The conventional CHF equation reads

$$(h_0+U^{\mathrm{CHF}})\phi_i=\varepsilon_i\phi_i , \tag{2.8}$$

U^{CHF} being mean-field Hartree-Fock potential; this potential contains direct and exchange Coulomb interactions of electron i with core electrons. A set of CHF equations is solved self-consistently for core orbitals; valence wave functions and energies are determined subsequently by "freezing" the core orbitals. The BCHF approximation constitutes introduction of the Breit interaction simultaneously with the Coulomb interaction into the above CHF equation

$$(h_0+U^{\mathrm{BCHF}})\overline{\phi_i}=\overline{\varepsilon_i}\overline{\phi_i} . \tag{2.9}$$

Compared to the CHF equations, energies, wave functions, and the Hartree-Fock potential are modified. We discuss a relation between CHF and BCHF methods and the associated relaxation effect in Sec. II B.

To simplify the second-quantized Hamiltonian, Eq. (2.7), we use the fact that matrix elements of the Hartree-Fock potentials are $\langle\phi_i|U^{\mathrm{CHF}}|\phi_j\rangle=c_{ij}$ and $\langle\overline{\phi_i}|U^{\mathrm{BCHF}}|\overline{\phi_j}\rangle=\overline{c_{ij}}+\overline{b_{ij}}$. In the Coulomb-Hartree-Fock case the Hamiltonian reduces to a sum of the conventional Coulomb Hamiltonian

$$H_C'=\sum_i \varepsilon_i:a_i^\dagger a_i:+\frac{1}{2}\sum_{ijkl} c_{ijkl}:a_i^\dagger a_j^\dagger a_l a_k: \tag{2.10}$$

and the Breit correction

$$\delta_B H_C'=\sum_{ij} b_{ij}:a_i^\dagger a_j:+\frac{1}{2}\sum_{ijkl} b_{ijkl}:a_i^\dagger a_j^\dagger a_l a_k:. \tag{2.11}$$

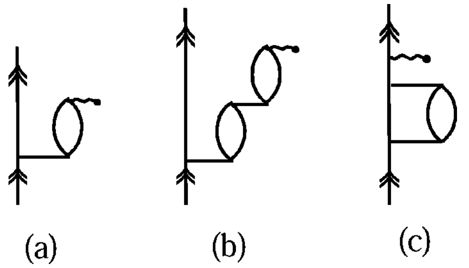

FIG. 1. Sample second- and third-order Brueckner-Goldstone diagrams representing many-body contributions to matrix elements. Diagrams (a) and (b) arise in the random-phase approximation and (c) is the Brueckner-orbital correction.

In the case of equivalent treatment of the Breit and Coulomb interactions (BCHF case) the corresponding Hamiltonian is less complicated,

$$H'_{C+B}=\sum_i \overline{\varepsilon}_i :\overline{a}_i^\dagger \overline{a}_i: + \frac{1}{2}\sum_{ijkl} (\overline{c}_{ijkl}+\overline{b}_{ijkl}) :\overline{a}_i^\dagger \overline{a}_j^\dagger \overline{a}_l \overline{a}_k:, \tag{2.12}$$

since the effective one-body Breit term in Eq. (2.11) has been "transformed away" by a proper choice of one-particle states.

Of course, finding a solution of the Shrödinger equation even with the traditional many-body Coulomb Hamiltonian, Eq. (2.10), is a nontrivial problem. Many-body perturbation theory [26] has proven to be very successful in treating contributions beyond the Hartree-Fock level. In particular, *ab initio* relativistic many-body calculations for alkali-metal atoms have been performed by Notre Dame and Novosibirsk (Sydney) groups. These and other calculations have been reviewed recently in Ref. [27]. An accurate description of the correlations (i.e., contributions beyond Hartree-Fock value) plays a crucial role in high-precision calculations. One of the most striking examples of the importance of correlations in ^{133}Cs is the magnetic-dipole hyperfine-structure (HFS) constant A of $5D_{5/2}$ level. Here the Coulomb-Hartree-Fock value, $+7.47$ MHz, has a sign opposite to that of experimental value $-21.24(5)$ MHz from Ref. [28]. The dominant correlation corrections to matrix elements arise because of core-shielding of externally applied fields (e.g., nuclear fields for HFS constants) and an additional attraction of a valence electron by an induced dipole moment of the core [29]. The former effect is described by contributions beginning at second order [random-phase approximation (RPA)] and the latter in third order (Brueckner corrections) of many-body perturbation theory. Representative many-body diagrams are shown in Fig. 1. Qualitatively, the Breit correction to a certain Coulomb diagram is proportional to the value of the Coulomb diagram. Therefore, in addition to lowest-order corrections we consider the Breit contributions to the dominant RPA and Brueckner diagrams. It will be demonstrated that these *correlated* Breit corrections in many cases are comparable to the lowest-order ones. In the BCHF basis the correlated Breit correction to valence energies appears in the second order; a sample diagram is drawn in Fig. 2. The corrections to this class of diagrams is comparable to the modification at the Hartree-Fock level.

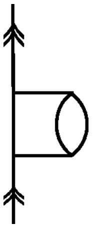

FIG. 2. Representative second-order contribution to an energy of valence electron.

In the present paper we employ many-body perturbation theory (MBPT). Explicit expressions for contributions to matrix elements up to the third order were tabulated by Blundell *et al.* [30]. These authors provide formulas for a general perturbing potential with one- and two-body parts. In the second and third orders there are 31 distinct diagrams involving one-body part of the perturbation and 28 diagrams containing only two-body part. Certainly, calculations of the Breit corrections are less complicated in the Breit-Coulomb-Hartree-Fock basis, where the one-body perturbation is absent. Another advantage of the BCHF basis is an automatic inclusion of important relaxation effect discussed below. An adequate account for the relaxation effect correction in the CHF basis would have required fifth-order calculations for matrix elements.

The generalization of MBPT expressions to a simultaneous treatment of Coulomb and Breit interactions is straightforward: Coulomb interaction lines are replaced by a sum of Coulomb and Breit interactions and particle (hole) lines by Breit-Coulomb-Hartree-Fock states (see Figs. 1 and 2.) Together with the corrections linear in the Breit interaction such approach introduces terms nonlinear in the Breit interaction. Strictly speaking, these nonlinear terms have no meaningful theoretical basis and therefore have to be omitted. However, the Breit contribution to atomic properties is relatively small and the much smaller terms nonlinear in the Breit interactions can be neglected at the present level of accuracy.

B. Relaxation effect

In the CHF basis the first-order corrections to valence energies ε_v and matrix elements Z_{wv} due to the one-body part of the Breit interaction are given by

$$\delta\varepsilon_v = b_{vv}, \tag{2.13}$$

$$\delta Z_{wv}=\sum_{i\neq v}\frac{z_{wi}b_{iv}}{\varepsilon_v-\varepsilon_i}+\sum_{i\neq w}\frac{b_{wi}z_{iv}}{\varepsilon_w-\varepsilon_i}.$$

Similar one-body Breit corrections can be calculated as differences between lowest-order values found in the Breit-Coulomb-and Coulomb-Hartree-Fock approximations

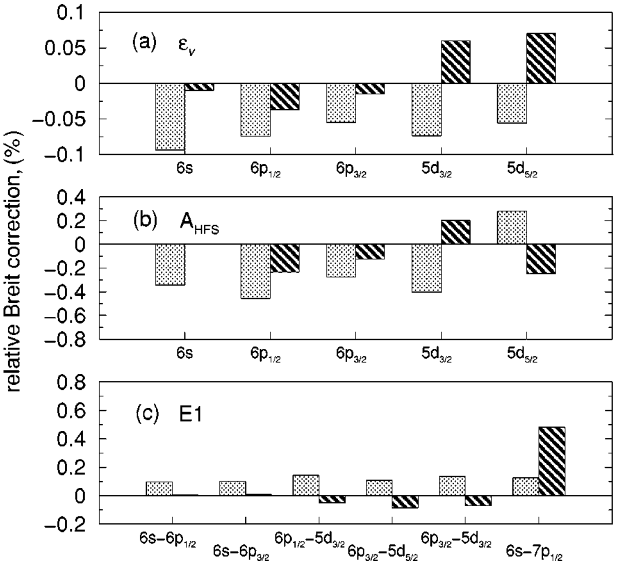

FIG. 3. Comparison of Hartree-Fock and first-order relative one-body Breit corrections to (a) energies of valence states, (b) hyperfine-structure (HFS) constants *A*, and (c) electric-dipole transition amplitudes. The dotted and striped bars represent first-order and Hartree-Fock corrections, respectively. The relative corrections to the energies and HFS constants are defined with respect to experimental values, and electric-dipole amplitudes with respect to Coulomb-Hartree-Fock values.

$$\delta\varepsilon_v^{\mathrm{HF}} = \overline{\varepsilon_v} - \varepsilon_v\,, \tag{2.14}$$

$$\delta Z_{wv}^{\mathrm{HF}} = \langle \overline{\phi_w} | z | \overline{\phi_v} \rangle - \langle \phi_w | z | \phi_v \rangle .$$

In Fig. 3 we present a comparison of the lowest-order one-body Breit corrections to valence energies, HFS constants *A* and electric-dipole transition amplitudes. The dotted and striped bars represent first-order, Eq. (2.13), and Hartree-Fock corrections, Eq. (2.14), respectively. There is a striking discrepancy between the two corrections for all these quantities. For example, the first-order correction to the $6s$ HFS constant is -0.4%, while at the Hartree-Fock level the Breit correction almost vanishes.

These large discrepancies are explained by a "relaxation" effect, i.e., modification of the Hartree-Fock potential through adjustment of core orbitals [18]. To illustrate this effect we rewrite the BCHF equation, Eq. (2.9), as

$$(h_0 + U^{\mathrm{CHF}} + \Delta U)\overline{\phi_i} = \overline{\varepsilon_i}\,\overline{\phi_i}\,, \tag{2.15}$$

where the perturbing potential is $\Delta U = U^{\mathrm{BCHF}} - U^{\mathrm{CHF}}$. Further, $\overline{\phi_j} = \phi_j + \chi_j$, where χ_j is a correction to a CFH wave function ϕ_j due to the Breit interaction. In the lowest order these corrections can be expressed as

$$\chi_j = \sum_i{}' \ \phi_i \frac{\langle i | \Delta U | j \rangle}{\varepsilon_j - \varepsilon_i}. \tag{2.16}$$

To the first order in the Breit interaction,

$$\begin{aligned}\Delta U(1) \approx & \sum_a \int \phi_a^\dagger(2) b(1,2) \phi_a(2) d\tau_2 \\ & + \sum_a \int \chi_a^\dagger(2) c(1,2) \phi_a(2) d\tau_2 \\ & + \sum_a \int \phi_a^\dagger(2) c(1,2) \chi_a(2) d\tau_2 + \ \dots\end{aligned} \tag{2.17}$$

with the proper exchange terms. Here the first term is an explicit Breit contribution, while in the second and the third terms the Breit interaction enters implicitly through corrections to core orbitals. Only the first term (and its exchange form) are included in the first-order correction, Eq. (2.13). As demonstrated by Lindroth *et al.* [18] for Breit corrections to the energy levels of Hg, the residual "relaxation" terms are large and substantially modify the first-order corrections. Similar observation has been made by Johnson *et al.* [31] in calculations of Breit corrections to energies of sodiumlike ions. Independent of the present analysis (partially published in Ref. [7]), the relaxation effect in Cs has been recently discussed by Kozlov *et al.* [32].

At this point it is clear that the inclusion of Breit interaction in the Coulomb-Hartree-Fock equations (i) greatly simplifies many-body perturbation expansions, and (ii) automatically accounts for the significant relaxation effects. In other words, compared to the traditional Coulomb-Hartree-Fock formulation, the transformation to the Breit-CHF basis sums many-body diagrams involving the effective one-body Breit interaction to all orders of perturbation theory.

C. Construction of Breit-Coulomb Hartree-Fock basis

Several methods can be devised for constructing the Breit-CHF single-particle basis. For example, one can determine the Breit corrections to wave functions by substituting Eq. (2.17) into Eq. (2.16). It is convenient to express the resulting equations in terms of expansion coefficients $\xi_{ij} = \langle \phi_i | \chi_j \rangle$

$$(\varepsilon_j - \varepsilon_i)\xi_{ij} = \sum_a \overline{b}_{iaja} + \sum_{ka} \{ \xi_{ka}^* \tilde{c}_{kiaj} + \xi_{ka} \tilde{c}_{aikj} \} \tag{2.18}$$

Here $\tilde{t}_{ijkl}$ is an antisymmetrized two-particle matrix element $\tilde{t}_{ijkl} = t_{ijkl} - t_{ijlk}$. Once the equations (2.18) are solved the "Breit-dressed basis" can be determined as $\overline{\phi_j} = \phi_j + \Sigma_i' \xi_{ij} \phi_i$. The derived equations are essentially equivalent to the random-phase approximation or the self-consistent-field method, with an effective one-body Breit interaction serving as an external perturbation. The many-body diagrams for the amplitudes ξ_{ij} are shown in Fig. 4. By iterating these equations one sums a certain class of many-body diagrams to all orders in the Coulomb interaction.

The resulting equations (2.18) are *linear* in the Breit interaction. It is worth noting that the Breit interaction, Eq. (2.1), is an approximation and terms nonlinear in the Breit interaction have no meaningful theoretical basis. Therefore, linearized equations (2.18) are conceptually more attractive

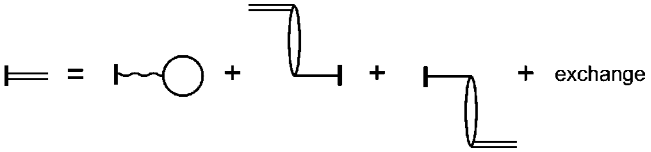

FIG. 4. Diagrammatic representation of Eq. (4). Here horizontal solid (wavy) lines represent the Coulomb (Breit) interactions. Double horizontal lines are expansion coefficients ξ and little "stumps" indicate places where particle or hole lines are to be attached.

than the self-consistent BCHF method based on an integration of Eq. (2.9). However, the Breit contribution to atomic properties is relatively small and the much smaller nonlinear terms in the Breit interaction can be safely neglected at the present level of accuracy.

An alternative approach to generating the BCHF basis set has proven to be more numerically robust and was employed in the present work. Two complete basis sets, CHF $\{\phi_i\}$ and BCHF $\{\overline{\phi_i}\}$ sets, can be related by a unitary transformation

$$\overline{\phi_j} = \sum_i d_{ij} \phi_i .$$

Using Eq. (2.15) one determines expansion coefficients d_{kj} and one-particle BCHF energies $\overline{\varepsilon_j}$ from secular equations

$$(\varepsilon_k - \overline{\varepsilon_j}) d_{kj} + \sum_i (\Delta U)_{ki} d_{ij} = 0, \ \forall j . \tag{2.19}$$

In this paper the difference between the two Hartree-Fock potentials ΔU was generated using finite-difference methods. The radial Coulomb-Hartree-Fock basis was approximated with B splines [19] and then transformed into the radial BCHF basis employing Eq. (2.19). Negative-energy states, $\varepsilon_i < -m_e c^2$, were included in the diagonalization procedure.

To summarize, third-order many-body calculations were performed in the Breit-Coulomb-Hartree-Fock basis with the two-body Breit interaction $B^{(2)}$ treated on equal footing with the residual Coulomb interaction. Sample many-body diagrams are presented in Figs. 2 and 1. Contributions of negative-energy states, discussed, for example, in Ref. [24], were also included and found to be relatively small [10]. Two series of third-order calculations were performed, first with the Breit and Coulomb interactions fully included using the Breit-CHF basis set, and second in the CHF basis set without the Breit interaction and negative-energy states. The obtained differences are the Breit corrections analyzed in the following sections.

Numerical calculations were performed using B-spline basis sets generated in a cavity of radius 75 a.u. This cavity size has been chosen for numerical consistency with the previous determination of parity-nonconserving amplitudes by Blundell *et al.* [5]. The numerical quasispectrum was represented by 100 negative-and 100 positive-energy states for each angular quantum number κ. The intermediate-state summations were performed over 75 lowest-energy positive-energy states and 75 highest-energy negative-energy states for each partial wave $s_{1/2}$-$h_{11/2}$.

III. ATOMIC PROPERTIES

A. Energies of valence states

At the Hartree-Fock level, the Breit interaction contributes less than 0.1% to all the energy levels considered in Fig. 3. Numerical values for Breit correction at the Hartree-Fock level are given in Table I; these were obtained as differences between one-particle energies in Breit-CHF and CHF approximations, i.e., $\overline{\varepsilon_v} - \varepsilon_v$. As in the traditional CHF calculations, the first-order many-body contributions to valence energies vanish identically in the BCHF basis. In the second order the corrections arise due to self-energy diagrams. For each valence state we perform two calculations with and without the Breit interaction and take a difference between the two values. Further, we distinguish between two classes of Breit modifications, one-body and two-body corrections, as illustrated for a diagram in Fig. 5. The one-body contribution arises from a transformation of the one-particle basis from Coulomb-Hartree-Fock to Breit-CHF.

The calculated values and breakdown on various contributions are presented in Table I. Apparently the Breit correction to the *correlation* part of the energy, δE_{BO}, is equally important as the modification in the lowest order, δE_{HF}. The

TABLE I. Contributions of the Breit interaction to energies of valence electrons in cm^{-1}. E_{CHF} are the energies in the Coulomb-Hartree-Fock approximation. δE_{HF} column lists corrections at the Hartree-Fock level defined as $\overline{\varepsilon_v} - \varepsilon_v$. Columns $\delta E_{\mathrm{BO}}, B^{(1)}$ and $\delta E_{\mathrm{BO}}, B^{(2)}$ are the contributions in the second order due to one-body and two-body Breit interactions, respectively.

State	E_{CHF}	δE_{HF}	$\delta E_{\mathrm{BO}}, B^{(1)}$	$\delta E_{\mathrm{BO}}, B^{(2)}$	$\delta E_{\mathrm{Total}}$
$6S_{1/2}$	-27954	3.2	-4.98	-0.83	-2.6
$7S_{1/2}$	-12112	1.1	-1.1	-0.28	-0.26
$6P_{1/2}$	-18791	7.5	-0.08	-0.28	7.1
$7P_{1/2}$	-9223	2.7	-0.1	-0.10	2.5
$6P_{3/2}$	-18389	2.9	-1.8	-0.25	0.84
$7P_{3/2}$	-9079	1.0	-0.56	-0.09	0.38
$5D_{3/2}$	-14138	-10.2	-12	-0.35	-22
$5D_{5/2}$	-14163	-11.8	-14	-0.33	-26

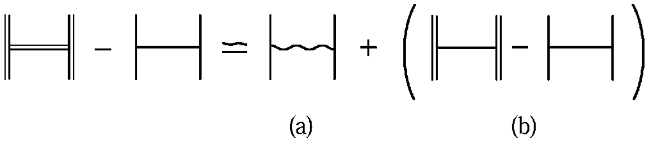

FIG. 5. Separation of Breit correction into (a) two-body and (b) one-body (basis shift) parts. Here horizontal solid and wavy lines represent Coulomb and Breit interactions respectively; double horizontal line is a sum of Coulomb and Breit interactions. Vertical solid lines correspond to Coulomb-Hartree-Fock states and vertical double lines to Breit-CHF states.

interplay of Breit corrections to various many-body diagrams for the energy of the $7S_{1/2}$ state is remarkable. Here the two terms $\delta E_{\rm HF}$ and $\delta E_{\rm BO},B^{(1)}$ are almost equal and have opposite signs, the resulting modification being determined by relatively smaller two-body Breit correction $\delta E_{\rm BO},B^{(2)}$. From Table I we see that generally the two-body Breit contributions are smaller than the one-body corrections; the $B^{(2)}$ corrections become important when the cancellations are involved.

The first study of correlated Breit corrections to the energies of Cs and other alkali-metal atoms has been performed in Refs. [33,34]. Based on formalism developed in Ref. [35], the corrections have been determined as an expectation value of the Breit correction to the Coulomb-Hartree-Fock many-body Hamiltonian, Eq. (2.11),

$$\delta E_v = \langle \Psi_v^{SD} | \delta_B H'_C | \Psi_v^{SD} \rangle. \tag{3.1}$$

Here $|\Psi_v^{SD}\rangle$ is the linearized coupled-cluster wave function limited to single and double excitations from the reference Slater determinant $a_v^\dagger|0_{\rm core}\rangle$. The correlations are built into these wave functions. The coupled-cluster singles-doubles (CCSD) formalism accounts for a complete third order of MBPT with certain classes of diagrams summed to all orders. However, the random-phase-approximation sequence of diagrams, important for the self-consistent treatment of the Breit interaction, is missed starting from the fourth order. The approach employed by Kozlov *et al.* [9] is similar to the present method, but in Ref. [9] the full Breit interaction has been approximated by the Gaunt term and contribution due to effective two-body interaction $B^{(2)}$ has been neglected.

TABLE II. Comparison of Breit corrections to energies of valence electrons in cm^{-1}.

State	This work	CCSD [33]	Gaunt, no $B^{(2)}$ [9]
$6S_{1/2}$	−2.6	−1.1	−4
$7S_{1/2}$	−0.26	0.72	0
$6P_{1/2}$	7.1	6.9	9
$7P_{1/2}$	2.5	2.6	2
$6P_{3/2}$	0.84	0.29	2
$7P_{3/2}$	0.38	0.45	0

Comparison of our results with the CCSD values and results of Ref. [9] is presented in Table II. The best agreement is for $P_{1/2}$ states where there is no cancellation between corrections $\delta E_{\rm HF}$ and $\delta E_{\rm BO}$, $B^{(1)}$. The values differ significantly for $S_{1/2}$ states where strong cancellations, emphasizing higher orders of MBPT, are present. One should keep in mind that these discrepancies arise only when the Breit corrections, due to cancellation effects, are small and do not have an enhanced effect on evaluation of parity-nonconserving amplitudes, discussed in Sec. IV. Calculations [9] are less consistent with the present and CCSD results, with discrepancies caused by approximation of full Breit interaction by Gaunt term and neglect of two-body part of the Breit interaction.

B. Magnetic-dipole hyperfine structure constants

To reiterate discussion in Sec. II, we performed two series of computations: (i) traditional Coulomb and (ii) fully including Breit interaction. The difference between resulting values defines the Breit correction. From parametrical argument it is assumed that the leading Breit corrections arise from induced modifications of the dominant traditional Coulomb diagrams. Therefore the calculations were limited to the RPA and Brueckner diagrams (see Fig. 1). Further, the RPA sequence was truncated at the third order.

In calculations of Breit corrections to ^{133}Cs HFS magnetic-dipole constants A nucleus was modeled by a uniformly magnetized ball of radius $R_m = 5.6748$ fm. The gyromagnetic ratio for ^{133}Cs nucleus is $g_I = 0.737\,89$ [36].

The breakdown of Breit corrections to various classes of many-body diagrams is given in Table III. Clearly, the Breit

TABLE III. Breit corrections to magnetic-dipole hyperfine structure constants A of ^{133}Cs in MHz. Column CHF lists Coulomb-Hartree-Fock values. Breit corrections to a class X of many-body diagrams of order N are designated as δA_X^N. Total Breit correction $\delta A_{\rm Total}$ is a sum of modifications δA_X^N.

State	CHF	$\delta A_{\rm HF}^{\rm I}$	$\delta A_{\rm RPA}^{\rm II+III}$	$\delta A_{\rm BO}^{\rm III}$	$\delta A_{\rm Total}$
$6S_{1/2}$	1425.3	0.011	4.1	0.79	4.87
$7S_{1/2}$	391.6	−0.029	1.1	0.08	1.15
$6P_{1/2}$	160.9	−0.68	0.39	−0.24	−0.52
$7P_{1/2}$	57.62	−0.23	0.14	−0.059	−0.15
$6P_{3/2}$	23.92	−0.06	0.10	−0.008	0.034
$7P_{3/2}$	8.642	−0.022	0.038	−0.0020	0.014
$5D_{3/2}$	18.23	0.099	0.10	0.11	0.31

TABLE IV. Comparison of contributions of Breit interaction to magnetic-dipole hyperfine-structure constants A of ^{133}Cs in MHz.

	$6S_{1/2}$	$7S_{1/2}$	$6P_{1/2}$	$7P_{1/2}$
This work[a]	4.87	1.15	−0.52	−0.15
Kozlov *et al.* [9][b]	5.0	0.8	−0.2	0.0
Sushkov [11][c]	4.6	1.09		
Safronova *et al.* [33][d]	−4.64	−0.83	−0.87	−0.29
Blundell *et al.* [37][e]	0.00	−0.05	−1.25	−0.39

[a] Third-order calculations in the BCHF basis, Ref. [7].

[b] Full Breit interaction is approximated by the Gaunt term.

[c] Analytical αZ expansion with $Z=55$.

[d] Second-order calculations in the CHF basis. See Ref. [10] for details.

[e] RPA sequence of diagrams in one-body Breit interaction.

correction to correlations ($\delta A_{\rm RPA}^{\rm II+III}, \delta A_{\rm BO}^{\rm III}$) is equally important as the modifications in the lowest order $\delta A_{\rm HF}^{\rm I}$. As an extreme case, almost entire Breit correction to HFS constants of $6S$ and $7S$ states comes from correlations. There is a cancellation of various contributions to the HFS constants of $P_{1/2}$ and $P_{3/2}$ states. For these states the contribution of higher-order diagrams not included in the present third-order analysis can become enhanced. At the same time the total Breit corrections to A_{6S} and A_{7S} are expected to be insensitive to higher-order contributions.

A comparison of our results, partially published in Ref. [7], with other calculations is presented in Table IV. The correction to hyperfine constants is very sensitive to correlations: e.g., Ref. [37] found a numerically insignificant modification for A_{6S}, while Refs. [10,33] determined the modification to be large (−4.64 MHz), and the approach reported here yields +4.87 MHz. In the calculation of Ref. [37] the correction was determined as a difference of the Breit-CHF and CHF values; however, such approach misses two-body Breit corrections of comparable size. In Refs. [10, 33] a second-order perturbation analysis was used for the Breit interaction, but the important relaxation effect discussed earlier was omitted. The present calculation incorporates all mentioned diagrams and is also extended to third order. Motivated by strong dependence of results [7,33,37] on many-body corrections, Sushkov [11] derived an analytical expression for Breit correction to HFS constants of S states. His results for $6S$ and $7S$ states are in an excellent agreement with the present calculations. Kozlov *et al.* [9] used an approach similar to Ref. [7]. There is a cancellation of various contributions for the P states; both higher-order diagrams and an approximation of the full Breit interaction by the Gaunt term in Ref. [9] are the sources of discrepancies between our results for $6P_{1/2}$ and $7P_{1/2}$ states.

Hyperfine structure constants sample atomic wave functions close to the nucleus and provide a unique way of testing atomic-structure calculations of parity-nonconserving amplitudes. In Table V we combine the Breit corrections with the results of *ab initio* all-order Coulomb-correlated calculations [37] and compare the results with experimental values. It is clear that the Breit corrections uniformly improve the agreement. In particular, the theoretical HFS constants are improved to 0.1% for $6S_{1/2}$, $7S_{1/2}$, and $7P_{1/2}$ states except for $6P_{1/2}$ where the discrepancy becomes 0.5%. While the achieved agreement in Table V is encouraging, one should keep in mind the omitted QED corrections and higher-order contributions in Coulomb interaction. For example, an estimate [38,39] for *hydrogenlike* Cs ion results in a QED correction to HFS constant A of S states at a few 0.1%. Due to electron-electron interaction in *atomic* Cs QED corrections can be significantly modified. Correlated calculations of QED corrections would be beneficial for reaching 0.1% level of accuracy needed for interpretation of parity-nonconservation and also for understanding the role of high-order Coulomb diagrams at 0.1% precision.

C. Off-diagonal $6S$-$7S$ hyperfine-structure matrix element

Experiments [3] on PNC in ^{133}Cs determine the ratio of $6S$-$7S$ PNC amplitude $E_{\rm PNC}$ to vector transition polarizability β. The value of β is difficult to calculate reliably since it vanishes in the nonrelativistic limit. Following suggestion [40], Bennett and Wieman [4] determined a supporting ratio of β to off-diagonal magnetic-dipole matrix element $M_{\rm hf}$ with a precision of 0.16%. Such an approach eliminates β from the analysis, but requires an accurate value for $M_{\rm hf}$.

The quantity $M_{\rm hf}$ can be expressed in terms of the off-diagonal magnetic-dipole hyperfine-structure constant $A_{6S\text{-}7S}$. This constant can be well approximated by a semi-empirical geometric-mean formula [41]

$$A_{6S\text{-}7S}^{\rm s.e.} \approx \sqrt{A_{6S}A_{7S}}, \qquad (3.2)$$

where A_{6S} and A_{7S} are precise experimental hyperfine-structure constants. The accuracy of this expression was investigated in Refs. [42–44]. Most recently, Dzuba and Flambaum [44] employed several many-body techniques of increasing accuracy in the Coulomb interaction between

TABLE V. Comparison of theoretical and experimental hyperfine constants A of ^{133}Cs. All-order Coulomb-correlated values by Blundell *et al.* [37] are supplemented with Breit corrections. Deviations from experimental values are placed in square brackets.

	$6S_{1/2}$	$7S_{1/2}$	$6P_{1/2}$	$7P_{1/2}$
Coulomb [37]	2291.00[−0.3%]	544.09[−0.3%]	293.92[0.7%]	94.60[0.3%]
Breit	4.87	1.15	−0.52	−0.15
Total	2295.87[−0.1%]	545.24[−0.1%]	293.40[0.5%]	94.45[0.1%]
Experiment	2298.16	545.90	291.93(2)	94.35(4)

TABLE VI. Breit corrections to reduced electric-dipole matrix elements for transitions between low-lying valence states of Cs atom. Column $\delta D,\%$ represents a ratio (in %) of the total Breit correction to a matrix element calculated in a third order of MBPT. See caption of Table III for description of other columns.

Transition	CHF	$\delta D^{\mathrm{I}}_{\mathrm{HF}}$	$\delta D^{\mathrm{II+III}}_{\mathrm{RPA}}$	$\delta D^{\mathrm{III}}_{\mathrm{BO}}$	$\delta D_{\mathrm{Total}}$	$\delta D,\%$
$6S_{1/2}$-$6P_{1/2}$	5.278	0.00035	−0.00022	−0.0011	−0.00097	−0.02
$6S_{1/2}$-$6P_{3/2}$	7.426	0.00078	−0.00045	−0.0014	−0.0011	−0.02
$6S_{1/2}$-$7P_{1/2}$	0.3717	0.0018	−0.00013	0.00021	0.0019	0.5
$6S_{1/2}$-$7P_{3/2}$	0.6947	0.00059	−0.00020	0.00011	0.00049	0.07
$7S_{1/2}$-$6P_{1/2}$	4.413	0.0046	−0.000067	0.00038	0.0049	0.1
$7S_{1/2}$-$6P_{3/2}$	6.671	0.0019	−0.000011	−0.00030	0.0016	0.02
$7S_{1/2}$-$7P_{1/2}$	11.01	−0.0011	−0.000050	−0.0018	−0.0029	−0.03
$7S_{1/2}$-$7P_{3/2}$	15.34	0.0007	−0.00013	−0.0019	−0.0013	−0.009
$5D_{3/2}$-$6P_{1/2}$	8.978	−0.0044	−0.00035	−0.0082	−0.013	−0.2
$5D_{3/2}$-$6P_{3/2}$	4.062	−0.0028	−0.00019	−0.0035	−0.0065	−0.2

electrons and found that this geometric-mean formula is accurate to a fraction of 10^{-3}. Here we extend their analysis and rigorously consider the additional effect of the correlated Breit interaction. The Breit correction to hyperfine-structure constants A_{6S} and A_{7S} is in the order of 0.2% and it can affect the sub-0.1% accuracy of the Coulomb analysis [44].

Breit corrections are relatively small. If Eq. (3.2) holds, the following relation between the Breit corrections (δA) has to be satisfied

$$\frac{\delta A^{\text{s.e.}}_{6S\text{-}7S}}{A^{\text{s.c.}}_{6S\text{-}7S}} \approx \frac{1}{2}\left\{\frac{\delta A_{6S}}{A_{6S}} + \frac{\delta A_{7S}}{A_{7S}}\right\}. \tag{3.3}$$

As a result of the correlated Breit calculations we find $\delta A_{6S\text{-}7S} = 2.4\,\mathrm{MHz}$. With $A_{6S\text{-}7S} = 1120.1\,\mathrm{MHz}$, the ratio $(\delta A_{6S\text{-}7S})/(A_{6S\text{-}7S}) = 2.1\times10^{-3}$. Using the Breit corrections to HFS constants A_{6S} and A_{7S} from Table III, the semiempirical rhs of the above equation is also 2.1×10^{-3}. Clearly, the accuracy of the geometric-mean formula (3.2) is not affected by the Breit correction. Qualitatively, this can be explained by a close proportionality of $6S$ and $7S$ wave functions in the vicinity of the nucleus, where the main contribution to the HFS constants of S states is accumulated.

D. Electric-dipole transition amplitudes

Calculated Breit corrections to reduced electric-dipole matrix elements of various transitions in Cs are presented in Table VI. We note that the Breit corrections to the random-phase approximation diagrams are small compared to the lowest-order and Brueckner-orbital corrections. Generally the total corrections are rather small (~0.1%), with an exception of $6S_{1/2}$-$7P_{1/2}$ electric-dipole matrix element. Using the *ab initio* all-order Coulomb-correlated value by Blundell *et al.* [37], $\langle 6S_{1/2}\|D\|7P_{1/2}\rangle = 0.279$, and adding the Breit correction of 0.0019, one finds $\langle 6S_{1/2}\|D\|7P_{1/2}\rangle = 0.281$ in a better agreement with the 0.284(2) experimental value of Shabanova *et al.* [45]. The relatively large Breit correction is caused both by an accidentally small matrix element and by admixture into $\langle 6S_{1/2}|D|7P_{1/2}\rangle$ from a 30 times larger $7S_{1/2}$-$7P_{1/2}$ matrix element.

IV. PARITY-NONCONSERVING AMPLITUDE $6S_{1/2}\rightarrow 7S_{1/2}$

The parity-nonconserving amplitude for the $6S_{1/2}\rightarrow 7S_{1/2}$ transition in ^{133}Cs can be represented as a sum over intermediate states $mP_{1/2}$

$$E_{PNC} = \sum_m \frac{\langle 7S|D|mP_{1/2}\rangle\langle mP_{1/2}|H_W|6S\rangle}{E_{6S} - E_{mP_{1/2}}} + \sum_m \frac{\langle 7S|H_W|mP_{1/2}\rangle\langle mP_{1/2}|D|6S\rangle}{E_{7S} - E_{mP_{1/2}}}. \tag{4.1}$$

Here D and H_W are electric-dipole amplitudes and weak interaction matrix elements, and E_i are atomic energy levels. The PNC amplitude is expressed in units of $10^{-11} i|e|a_0(-Q_W/N)$, where $N = 78$ is the number of neutrons in the nucleus of ^{133}Cs and Q_W is the weak charge. In these units the results of past calculations for ^{133}Cs are $E_{\mathrm{PNC}} = -0.905$, Ref. [5], and $E_{\mathrm{PNC}} = -0.908$, Ref. [6]. The former value includes a partial Breit contribution $+0.002$, and the latter includes none. The reference many-body Coulomb-correlated amplitude

$$E^C_{\mathrm{PNC}} = -0.9075 \tag{4.2}$$

is determined as an average, with the partial Breit contribution removed from the value of Ref. [5]. The major difference between present and previous calculation [5] of Breit correction to the PNC amplitude is an additional incorporation of effective two-body part of the Breit interaction and Breit correction to the correlations.

It is convenient to break the total Breit correction δE_{PNC} into three distinct parts due to corrections in the weak interaction and dipole matrix elements, and energy denominators, respectively

$$\delta E^B_{\mathrm{PNC}} = E_{\mathrm{PNC}}(\delta H_W) + E_{\mathrm{PNC}}(\delta D) + E_{\mathrm{PNC}}(\delta E). \tag{4.3}$$

For example, the modification of the PNC amplitude due to the Breit corrections to energies δE_{nS}, $\delta E_{mP_{1/2}}$ can be expressed as

TABLE VII. Breit corrections to matrix elements of weak interaction for ^{133}Cs in units of $10^{-11} i|e|a_0(-Q_W/N)$. See caption of Table III for description of columns.

Transition	CHF	$\delta(H_W)^{\rm I}_{\rm HF}$	$\delta(H_W)^{\rm II+III}_{\rm RPA}$	$\delta(H_W)^{\rm III}_{\rm BO}$	$\delta(H_W)_{\rm Total}$
$6S_{1/2}$-$6P_{1/2}$	0.03159	−0.00010	−0.00015	−0.000029	−0.00028
$6S_{1/2}$-$7P_{1/2}$	0.01891	−0.000058	−0.000091	−0.000014	−0.00016
$7S_{1/2}$-$6P_{1/2}$	0.01656	−0.000053	−0.000081	−0.000013	−0.00015
$7S_{1/2}$-$7P_{1/2}$	0.00991	−0.000031	−0.000048	−0.0000061	−0.000085

$$E_{\rm PNC}(\delta E) = -\sum_m \frac{\langle 7S|D|mP_{1/2}\rangle\langle mP_{1/2}|H_W|6S\rangle}{(E_{6S}-E_{mP_{1/2}})^2} \times(\delta E_{6S}-\delta E_{mP_{1/2}}) + \text{c.c.}(7S\leftrightarrow 6S), \quad (4.4)$$

where the last term stands for the complex conjugate of the first term with $6S$ and $7S$ states interchanged. The Breit corrections to energies and dipole matrix elements were discussed in the preceding sections; here we focus on corrections to the weak matrix elements.

The overwhelming contribution from parity-violating interactions arises from the Hamiltonian

$$H_W = \frac{G_F}{\sqrt{8}} Q_W \rho_{\rm nuc}(r)\gamma_5, \quad (4.5)$$

where G_F is the Fermi constant, γ_5 is the Dirac matrix, and $\rho_{\rm nuc}(r)$ is the *neutron* density distribution. To be consistent with the previous calculations the $\rho_{\rm nuc}(r)$ is taken to be a *proton* Fermi distribution employed in Ref. [5]. The slight difference between the neutron and proton distributions will be addressed in the conclusion of this section. The dominant contribution to the PNC amplitude, Eq. (4.1), comes from intermediate states $6P_{1/2}$ and $7P_{1/2}$. In Table VII we present calculated third-order Breit corrections to the relevant matrix elements of weak interaction. Apparently, the dominant part of the Breit correction arises from modifications at the Hartree-Fock level and in RPA. All the corrections add coherently, and we do not expect omitted higher-order diagrams to be important. In fact, third-order RPA corrections are a few times smaller than those in the second order, hinting at a good convergence of the present technique.

The Breit correction to the PNC amplitude is determined by combining induced modifications in matrix elements and energy denominators. The required corrections are summarized in Table VIII. The tabulated dipole amplitudes are related to the reduced matrix elements in Table VI as

$$\langle nS_{1/2}|D|n'P_{1/2}\rangle = \langle nS_{1/2}\|D\|n'P_{1/2}\rangle/\sqrt{6}.$$

Before proceeding to the correlated calculations, it is worth examining the Breit contribution to the PNC amplitude at the Hartree-Fock level. Most of the Breit contribution to the PNC amplitude can be determined by limiting the summation over intermediate states in Eq. (4.1) to the two lowest valence $P_{1/2}$ states: $6P_{1/2}$ and $7P_{1/2}$. In the CHF approximation one then finds $E_{\rm PNC} = -0.6888$ (90% of the total value). The lowest-order corrections to matrix elements and energy denominators calculated as differences between Breit-CHF and CHF values are listed in Table VIII. The resultant BCHF corrections to $E_{\rm PNC}$ are

$$E^{\rm HF}_{\rm PNC}(\delta H_W) = 0.0022\,(0.32\%),$$
$$E^{\rm HF}_{\rm PNC}(\delta D) = 0.0020(0.29\%), \quad (4.6)$$
$$E^{\rm HF}_{\rm PNC}(\delta E) = -0.0019(-0.28\%).$$

Here the percentage values in parentheses are taken with respect to the CHF value of PNC amplitude. The sum of these three terms leads to $\delta E_{\rm PNC} = 0.0023$. Inclusion of intermediate states beyond $6P_{1/2}$ and $7P_{1/2}$ leads to a small ad-

TABLE VIII. Breit corrections to electric-dipole amplitudes, weak-interaction matrix elements, and energy intervals; δX, I$\equiv$X$_{\rm BCHF}-$X$_{\rm CHF}$, and δX, I+II+III are the differences in the third order of MBPT. Weak matrix elements are expressed in units of $10^{-11} i|e|a_0(-Q_W/N)$ and energies and dipole amplitudes in atomic units.

	$6S_{1/2}$-$6P_{1/2}$	$6S_{1/2}$-$7P_{1/2}$	$7S_{1/2}$-$6P_{1/2}$	$7S_{1/2}$-$7P_{1/2}$
H_W, CHF	0.03159	0.01891	0.01656	0.009913
δH_W, I	−0.00010	−0.00006	−0.00005	−0.000031
δH_W, I+II+III	−0.00028	−0.00016	−0.00015	−0.000085
D, CHF	2.1546	0.15176	1.8017	4.4944
δD, I	0.0001	0.00073	0.0019	−0.0004
δD, I+II+III	−0.0004	0.00077	0.0020	−0.0012
ΔE, CHF	−0.041752	−0.085347	0.030429	−0.013166
$\delta\Delta E$, I	−0.000020	0.000003	−0.000030	−0.000007
$\delta\Delta E$, I+II	−0.000045	−0.000023	−0.000034	−0.000012

ditional modification to $\delta E_{\rm PNC}$ of $-0.000\,04$. The obtained lowest-order result is in agreement with the 0.002 correction found by Blundell *et al.* [5]. In addition to the lowest-order the Breit correction in Ref. [5] also contained small random-phase-approximation diagrams in the Coulomb interaction for matrix elements of the weak interaction. The two-body Breit interaction has been disregarded in Ref. [5]. In the following discussion we will include these omitted effects. Note that if experimental energies (which effectively include the Breit interaction) are used in the energy denominators of Eq. (4.1), then the $E_{\rm PNC}(\delta E)$ term must be excluded and the total correction becomes twice as large: $\delta E_{\rm PNC}=0.0042$.

With further examination of the modifications of *individual* uncorrelated matrix elements summarized in Table VIII, one notices the following.

(i) Weak interaction matrix elements are each reduced in absolute value by 0.3%, which is directly reflected in a 0.3% correction to the PNC amplitude.

(ii) Modification of dipole amplitudes is strongly nonuniform. There are substantial corrections only to the $6S_{1/2}$-$7P_{1/2}$ (0.5%) and $7S_{1/2}$-$6P_{1/2}$ (0.1%) matrix elements. The large 0.5% Breit correction to $\langle 6S_{1/2}|D|7P_{1/2}\rangle$ provides partial resolution to a long-standing 1.5% discrepancy of spectroscopic experiment [45] and *ab initio* Coulomb-correlated calculations [33,37,46].

(iii) The largest modification in the energy denominators is 0.1% for E_{7S}-E_{6P}; however, this leads to a 0.3% correction $E_{\rm PNC}(\delta E)$. As recently emphasized by Dzuba *et al.* [47], such large sensitivity of the resulting PNC amplitude to small variations in individual atomic properties entering Eq. (4.1) arises due to a cancellation of relatively large terms in the sum over states.

It is well known that correlations caused by residual Coulomb interactions not included in the Hartree-Fock equations can lead to substantial modifications of the lowest-order values. For example, the weak matrix element $\langle 6S_{1/2}|H_W|6P_{1/2}\rangle$ is increased by a factor of 1.8 by correlations due to residual Coulomb interactions. As demonstrated in the previous sections, correlations are also important for a proper description of the Breit corrections. Examination of the third-order corrections listed in Table VIII reveals that the corrections to weak interaction matrix elements become three times larger than those in the lowest order. Using third-order matrix elements and second-order energies the following *ab initio* corrections are determined:

$$E_{\rm PNC}(\delta H_W)=0.0043,$$

$$E_{\rm PNC}(\delta D)=0.0035,$$

$$E_{\rm PNC}(\delta E)=-0.0028.$$

Thus the lowest-order corrections given in Eq. (4.6) are amplified in higher orders. The calculated Breit corrections to the PNC amplitude is expected to be insensitive to the omitted higher-order diagrams. Such uncertainty can arise if the calculated Breit corrections to leading classes of many-body diagrams cancel. Indeed, the calculated Breit corrections always add coherently for matrix elements of weak interaction. There are also no strong cancellations between various Breit corrections to the relevant dipole amplitudes $\langle nS_{1/2}|D|n'P_{1/2}\rangle$ (see Table VI). Corrections to energy denominators are also stable with respect to the omitted higher-order contributions. For example, in Sec. III A we found that the Breit correction to the energy of $7S_{1/2}$ valence state due to cancellations of calculated contributions is small (-0.26 cm^{-1}) enhancing possible effect of smaller higher-order corrections. However, in the calculation of the term $E_{\rm PNC}(\delta E)$ this (unstable) correction substantially appears only in a combination with a 25 times larger and stable Breit correction (7.1 cm^{-1}) to the energy of $6P_{1/2}$ state.

We further improve the accuracy of the calculation by combining all-order Coulomb-correlated matrix elements and experimental energy denominators tabulated in Ref. [5] with the present third-order Breit corrections. The results are

$$\begin{aligned} E_{\rm PNC}(\delta H_W)&=0.0047\,(0.5\%),\\ E_{\rm PNC}(\delta D)&=0.0037\,(0.4\%),\\ E_{\rm PNC}(\delta E)&=-0.0030\,(-0.3\%). \end{aligned} \tag{4.7}$$

Here the values in parentheses are defined relative to the Coulomb-correlated PNC amplitude, Eq. (4.2). The total Breit correction to the PNC amplitude is $\delta E^B_{\rm PNC}=0.0054$. This result was first reported in Ref. [7]. Similar correction of 0.0053 was obtained by Dzuba *et al.* [8]. Kozlov *et al.* [9] found a 20% smaller correction of 0.004; this discrepancy is most likely due to the omission of the retarded part of the Breit interaction in the calculations [9].

If the experimental energies (which incorporate Breit corrections by definition) are used in the energy denominators the term $E_{\rm PNC}(\delta E)$ should be excluded and the semiempirical Breit correction becomes $\delta E^{\rm B,s.e.}_{\rm PNC}=0.0084$. A minor difference of our treatment [7] of the Breit correction to $E_{\rm PNC}$ and Refs. [8,9] is the *interpretation* of results of previous Coulomb-correlated calculations [5,6]. Authors [8,9] assert that the *ab initio* 0.6% correction (0.4% in Ref. [9]) should be used to augment $E^{\rm C}_{\rm PNC}$, Eq. (4.2). Our approach is to exclude the term $E_{\rm PNC}(\delta E)$. The difference in the two *interpretations* arises due to the difficulty of accounting for higher-order Coulomb diagrams. Some semiempirical "fitting" or "scaling" procedure is used in practice to mimic the effect of the omitted contributions. Since only energies are known with a very high precision from experiments, experimental energies play a central role in such analysis. For example, the experimental energies were employed in eight out of ten test cases in the scatter analysis in the Table IV of Ref. [5] (Phys. Rev. D) based on Eq. (4.1).

The above discussion demonstrates some arbitrariness encountered in the analysis of theoretical values and assignment of theoretical uncertainty when a semiempirical adjustment of *ab initio* values is attempted. We notice that authors of Ref. [8,9] argue that the theoretical uncertainty of the PNC amplitude is in the order of 1%, therefore a 0.3% difference between the two different interpretations of the Breit correction is irrelevant at this level. We believe that the most convincing error estimate would be a repetition of the scatter analysis originally performed in Ref. [5] but with a Breit correction to the involved quantities included. Such calculation is beyond the scope of the present work. However, we expect that the resulting uncertainty would be better than the original 1% assigned to the results [5,6] because of the better theory-experiment agreement for dipole amplitudes (see [4]) and hyperfine-structure constants (see Table V). Additional QED and especially neutron skin effects can further modify the value of E_{PNC} in a way that cannot be mimicked by the suggested analysis.

The parity violation in atoms is dominated by the *Z*-boson exchange between atomic electrons and *neutrons*. However, the reference value $E^{\mathrm{C}}_{\mathrm{PNC}}$ Eq. (4.2), is based on the empirically deduced *proton* distribution. The difference between the proton and neutron distributions is visualized as the neutron "skin" or "halo." Here we update our previous treatment of the neutron skin correction with the most recent data from the literature. This correction was estimated in Ref. [5] but was not included in the final value for the PNC amplitude. It can be shown that the neutron skin correction $\delta E^{\mathrm{n.s.}}_{\mathrm{PNC}}$ does not depend on the electronic structure, therefore it can be parametrized as

$$\frac{\delta E^{\mathrm{n.s.}}_{\mathrm{PNC}}}{E_{\mathrm{PNC}}} \approx -\frac{3}{7}(\alpha Z)^2 \frac{\Delta R_{np}}{R_p}. \quad (4.8)$$

Here R_p is the root-mean-square (rms) radius of proton distribution and ΔR_{np} is the difference between rms radii of neutron and proton distributions. This expression can be easily derived from analysis by Fortson *et al.* [48]. From nonrelativistic nuclear-structure calculations Pollock and Welliver [49] concluded $\Delta R_{np}/R_p = 0.016$ or 0.022 depending on the model of nuclear forces. The calculations [50,51] of nuclear distributions were *relativistic* and the corrections twice as large $\Delta R_{np}/R_p = 0.043$–$0.053$ were found. Therefore, nonrelativistic calculations led to $\delta E^{\mathrm{n.s.}}_{\mathrm{PNC}}/E_{\mathrm{PNC}}$ of -0.1% and relativistic determinations to the range of -0.3 to -0.4%. The latter values are comparable to the experimental error bar of the PNC amplitude [3,4] and unfortunately it is difficult to assess the accuracy of the nuclear-structure calculations.

Here we propose an alternative analysis of the neutron skin correction allowing to estimate the error bar. Indeed Trzcinska *et al.* [12] very recently deduced neutron density distributions from experiments with antiprotonic atoms and concluded that

$$\Delta R_{np} = (-0.04 \pm 0.03) + (1.01 \pm 0.15)\,\frac{N-Z}{A}\ \mathrm{fm}. \quad (4.9)$$

Here N and A are the neutron and the mass numbers. Although experimental data for ^{133}Cs do not enter the analysis [12], a wide range of stable nuclei was investigated. Assuming that this relation holds for ^{133}Cs we find $\Delta R_{np} = 0.13(4)$ fm. For ^{133}Cs $R_p = 4.807$ fm [52] leading to

$$\frac{\delta E^{\mathrm{n.s.}}_{\mathrm{PNC}}}{E_{\mathrm{PNC}}} = -0.0019(6). \quad (4.10)$$

Therefore, the neutron skin corrects the PNC amplitude by -0.2% with an error bar of 30%. This uncertainty contributes only 0.06% to an error budget of the observed weak charge, i.e., the proposed determination of the neutron skin correction will be adequate until the 0.1% level of overall accuracy is reached.

Combining the calculated semiempirical 0.9% Breit correction with the reference Coulomb-correlated value, Eq. (4.2), and the neutron skin correction, Eq. (4.10), one obtains the parity-nonconserving amplitude

$$E_{\mathrm{PNC}}(^{133}\mathrm{Cs}) = -0.8974 \times 10^{-11} i(-Q_W/N). \quad (4.11)$$

In Sec. III C we concluded that the result for the off-diagonal hyperfine structure matrix element M_{hf} by Dzuba and Flambaum [44] is not affected by the Breit correction. Using their value of M_{hf} together with the experimental results [3,4] we arrive at

$$E_{\mathrm{PNC}}(^{133}\mathrm{Cs}) = -0.8354(33) \times 10^{-11}\ \mathrm{a.u.} \quad (4.12)$$

From the values above, the observed weak charge is

$$Q_W(^{133}\mathrm{Cs}) = -72.61(28)_{\mathrm{expt}}(73)_{\mathrm{theor}}.$$

This value differs from the prediction [53] of the standard model $Q^{\mathrm{SM}}_{\mathrm{W}} = -73.20(13)$ by 0.7σ, vs 2.5σ of Ref. [4], where σ is calculated by taking experimental and theoretical uncertainties in quadrature. Here we assigned 1% uncertainty to the theoretical PNC amplitude, Eq. (4.11). The deviation stands at 1.3σ if 0.4% theoretical uncertainty is assumed as discussed by Bennett and Wieman [4]. Following Ref. [7], a similar conclusion has been reached in Refs. [8,9].

V. CONCLUSION

In this paper we presented a relativistic many-body formalism for treating correction from the Breit interaction. Numerical evaluation of the Breit corrections to a number of properties of cesium atom were carried out. In particular, we considered energies, hyperfine-structure constants, electric-dipole transition amplitudes and $6S$-$7S$ parity-violating amplitude. We demonstrated that the Breit corrections to correlations are as important as the modifications at the lowest-order Hartree-Fock level. This work supplements Ref. [7] with additional numerical results. The present treatment has been based on third-order relativistic many-body perturbation theory. In a few cases we observed intricate cancellations between the lowest-order and higher-order corrections. These are the counterintuitive cases where the most advanced methods of many-body perturbation theory originally developed for residual Coulomb interaction, which will have to be employed to obtain an adequate description of a small Breit correction.

Is it possible to test the accuracy of the theoretical treatment of the Breit contribution for alkali-metal structure? One could consider the nonrelativistically forbidden magnetic-dipole transitions $nS_{1/2}$-$n'S_{1/2}$. A second-order analysis [24] demonstrated exceptionally large contributions from the Breit interaction and negative-energy states for such transitions; more accurate all-order calculations would be desirable. At the same time, an accurate experimental value for the $7S$-$6S$ transition in Cs is available [4].

We determined Breit correction to parity nonconserving (PNC) amplitude of the $6S$-$7S$ transition. The calculated correction resolves most of the discrepancy [4] between the standard model prediction and atomic PNC determination of the ^{133}Cs weak charge.

Breit correction to the PNC amplitude is one of the smaller contributions that needed to be addressed in order to reach the next level of accuracy in *ab initio* calculations required for refined interpretation of parity violation. In this paper we also evaluated and constrained the neutron ‘‘skin’’ or ‘‘halo’’ correction. As discussed in Refs. [8,9,11], the remaining corrections that may contribute at a few 0.1% are due to higher-order many-body diagrams in the Coulomb interaction and QED corrections.

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