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Theoretical overview of atomic parity violation

Recent developments and challenges

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Abstract. Recent advances in interpreting the most accurate-to-date measurement of atomic parity violation in Cs are reviewed. The inferred nuclear weak charge, $Q_W(^{133}\mathrm{Cs}) = -72.65(28)_{\mathrm{expt}}(36)_{\mathrm{theor}}$, agrees with the prediction of the standard model at 1σ level. Further improved interpretation is limited by an accuracy of solving the basic correlation problem of the atomic structure. We report on our progress in solving this problem within the relativistic coupled-cluster formalism. We include single, double and triple electronic excitations in the coupled-cluster expansion. Numerical results for energies, electric-dipole matrix elements, and hyperfine-structure constants of Cs are presented.

PACS. 32.80.Ys Weak-interaction effects in atoms – 31.15.Dv Coupled-cluster theory – 32.10.Fn Fine and hyperfine structure – 32.70.Cs Oscillator strengths, lifetimes, transition moments

1 Introduction

This year, 2006, marks 50 years of the fall of parity conservation, one of the hallmark discoveries of the 20th century physics. The field has started with the seminal Lee and Yang paper [1] and the discovery of parity violation in the nuclear β-decay [2]. Soon after this discovery, Zel'dovich [3] contemplated the possibility of observing the parity-nonconserving (PNC) signal in atoms. He concluded that the effect was too small to be of experimental significance. In 1974, however, M.-A. Bouchiat and C. Bouchiat [4] realized that the PNC is amplified in *heavy* atoms. They showed that the relevant PNC amplitude scales steeply with the nuclear charge Z. In atomic physics, the first P-violating signal has been observed in 1978 by Barkov and Zolotorev [5] in the Bi atom. Over the following decades the experiments were refined, with PNC signal observed in several atoms. So far the most accurate measurement has been carried out in ^{133}Cs by the Boulder group [6].

Rich history of atomic parity violation is examined in a number of review articles, *e.g.*, refs. [7,8] and a book [9]. Here, due to the space limitation, we restrict our attention to recent developments in interpreting P-violation in the Cs atom and report on the progress towards a more accurate interpretation of atomic PNC in this atom.

The PNC measurements are interpreted in terms of the weak nuclear charge Q_W, which quantifies the strength of the electroweak coupling between atomic electrons and quarks in the nucleus. The relation between Q_W and the PNC amplitude, E_{PNC}, can be represented as

$$E_{\mathrm{PNC}} = k\, Q_W\,, \tag{1}$$

where k is an atomic-structure factor. Apparently, the interpretation requires atomic-structure calculations of k with an accuracy that matches the experimental uncertainty in E_{PNC}. In particular, in Cs, the present theoretical uncertainty dominates over the experimental error bar resulting in an overall 0.6% uncertainty in the inferred value of $Q_W(^{133}\mathrm{Cs})$.

The underlying theory of the electroweak interactions is well established and its predictions have been verified in a variety of experiments. Much of the present efforts are driven by searches for "new physics" beyond the standard model (SM). We may distinguish between two approaches to such searches: low- and high-energy experiments. Atomic parity violation probes the low-energy electroweak sector of the SM. While the relevant momentum transfer is just $\sim 30\,\mathrm{MeV}$, the exquisite accuracy of the interpretation constrains new physics at much higher energies. Indeed, following arguments of ref. [10], we find that the present 0.6% determination of the $Q_W(^{133}\mathrm{Cs})$ probes the new physics at a mass scale of

$$\left\{8\sqrt{2}\,\pi\,\frac{1}{G_F}\left|\frac{Q_W}{\delta Q_W}\right|\right\}^{1/2} \approx 20\,\mathrm{TeV},$$

where G_F is the Fermi constant. Apparently by reducing the uncertainty in the determination of the weak charge,

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Table 1. Present status of the 2.5σ deviation of the inferred $Q_W(^{133}\mathrm{Cs})$ from the prediction of the standard model. In the bulk of the table, we summarize the recent theoretical progress on computing "small" sub-1% corrections to the $6s$-$7s$ PNC amplitude. These corrections directly affect the inferred value of the weak charge of Cs. For illustrative purposes all the corrections (pulls) are tabulated in terms of the original Bennet and Wieman [16] uncertainty, $\sigma = \{\sigma^2_{\mathrm{expt}} + \sigma^2_{\mathrm{theor}}\}^{1/2} \approx 0.5\%$.

Deviation (1999) Bennet and Wieman [16]	2.5σ	Based on calculations by Dzuba *et al.* (1989) [14] and Blundell *et al.* (1990) [15]
Theoretical correction	Pull	Reference
Breit interaction	-1.2σ	Derevianko (2000) [20] Dzuba *et al.* (2001) [21] Kozlov *et al.* (2001) [22]
Vacuum polarization ($+0.8\sigma$) Vertex/self-energy (-1.3σ)	-0.5σ	Johnson *et al.* (2002) [23] Milstein *et al.* (2002) [24,25] Kuchiev and Flambaum (2002) [26] Sapirstein *et al.* (2003) [27] Shabaev *et al.* (2005) [28]
Neutron skin	-0.4σ	Derevianko (2002) [29]
Updated correlated E_{PNC} and β	$+0.7\sigma$	Dzuba *et al.* (2002) [30]
e-e P-violating interaction, Renormalization $Q \to 0$, Giant nuclear resonance	-0.08σ	Sushkov and Flambaum (1978) Milstein *et al.* (2002) [24]
Total deviation (agreement)	1σ	

$|\delta Q_W|$, we may access even higher mass scales. Such a reduction in the uncertainty of Q_W is the goal of our present efforts outlined in sect. 3.

While discussing the impact of atomic PNC on particle physics, it is worth noting that colliders are blind to certain "new physics" scenarios [10]. For example, atomic PNC is uniquely sensitive to extra Z bosons predicted in grand unified theories, technicolor models, SUSY, and string theories. Generally, atomic PNC is one of a few probes of electroweak coupling below the Z-pole. Competing and at the same time complementary experiments include determination of the weak charge of the electron at SLAC [11] and ν-nucleus deep inelastic scattering by the NuTeV Collaboration [12]. With an upgrade at Jefferson Lab, an even more accurate constraint on electroweak coupling is expected to come from a P-violating e-p scattering experiment (Q-weak Collaboration) [13]. Still, the atomic PNC will continue to play an important complementary role, as the atomic PNC is sensitive to electron-neutron couplings, while the Q-weak experiment will probe electron-proton coupling, *i.e.*, a different linear combination in terms of the up and down quark-electron couplings.

2 Deviation from the standard model and recent theoretical progress

Parity violation in Cs has been the subject of a recent controversy. To infer the value of the weak charge, one needs to combine measurements with atomic-structure calculations. The uncertainty in the value of the inferred Q_W is usually determined by summing experimental and theoretical uncertainties in quadrature,

$$\sigma = \left\{\sigma^2_{\mathrm{expt}} + \sigma^2_{\mathrm{theor}}\right\}^{1/2} . \qquad (2)$$

In 1997, the most accurate to date (0.35%) measurement of PNC has been carried out by the Boulder group [6]. At that time, the accuracy of calculations [14,15] has been estimated to be 1%. In 1999, Bennet and Wieman [16], in light of new lifetime data which improved theory-experiment agreement, have reduced the theoretical error bar to 0.4%. While compared with the prediction of the SM, the resulting value of Q_W differed by 2.5σ, one of the largest deviations in the recent history. The deviation has prompted a substantial interest from the particle physics community (see, *e.g.*, [10,17–19]). At the same time the reduced theoretical uncertainty raised the questions whether some "small" sub-1% atomic-structure effects could be the reason for the deviation.

Over the last few years, there has been an important progress in understanding "small" corrections, such as Breit, radiative, and neutron-skin corrections. These advances are summarized in table 1.

Taking into account the tabulated "small" corrections, the revised value of vector transition polarizability and the somewhat improved value of E_{PNC} [30], we arrive at the following revised value of the weak charge (the assigned theoretical uncertainty of 0.5% is consistent with an estimate of ref. [30] and the central value with that of ref. [28]):

$$Q_W(^{133}\mathrm{Cs}) = -72.65(28)_{\mathrm{expt}}(36)_{\mathrm{theor}}\,. \qquad (3)$$

This value agrees with the SM value [19] of $-73.19(13)$ at 1σ level.

The present theoretical uncertainty in PNC calculations is estimated to be 0.5%. Since the overall error is obtained with quadrature (2), reducing σ_{theor} below the experimental uncertainty of 0.35% will either reveal new physics or set important constraints on competing extensions to the SM. In addition, it will set a stage for further experimental efforts, such as those by the Paris group [31, 32]. Other experimental efforts which will benefit from the improved calculations are PNC measurements with Ba^+ [33,34], Tl [35], and Fr [36].

3 High-accuracy atomic-structure calculations

The present accuracy in the determination of the weak charge of Cs is limited by the accuracy of solving the basic correlation problem. The many-body problem is hard. Even classically, the three-body problem cannot be solved in closed form. While adequate numerical approaches (*e.g.*, configuration interaction and variational methods) were developed for few-electron atoms, accurate solution of the many-body problem for atoms with many electrons still remains a challenge.

In a particular case of the PNC problem in Cs, we need to evaluate the PNC amplitude for the $6S_{1/2} \to 7S_{1/2}$ transition

$$E_{\mathrm{PNC}} = \sum_n \frac{\langle 7S|D|nP_{1/2}\rangle\langle nP_{1/2}|H_W|6S\rangle}{E_{6S}-E_{nP_{1/2}}} + \sum_n \frac{\langle 7S|H_W|nP_{1/2}\rangle\langle nP_{1/2}|D|6S\rangle}{E_{7S}-E_{nP_{1/2}}}\,. \qquad (4)$$

Here D and H_W are the electric-dipole and the weak interaction matrix elements, and E_i are the atomic energy levels. The effective weak interaction, averaged over quarks is accumulated inside the nucleus

$$H_W = -\frac{G_F}{\sqrt{8}}\,Q_W\,\gamma_5\,\rho(\mathbf{r})\,, \qquad (5)$$

where $\rho(\mathbf{r})$ is the neutron-density distribution. One could easily recast eqs. (4) and (5) in terms of the structure factor k of eq. (1).

We wish to evaluate accurately the sum (4). Let us comment on the pre-requisites for such calculations. i) Due to the particular characters of the involved operators in summation (4), the approximate wave functions have to reproduce the short-range (close to the nucleus) and long-range atomic properties simultaneously. The accurate short-range description requires *ab initio* relativistic approach, as the ratio of the velocity of the electron to the speed of light near the nucleus is $\sim \alpha Z \sim 0.4$ for Cs. ii) With respect to the accuracy, we notice that simple Dirac-Hartree-Fock (DHF) calculations for the hyperfine-structure (HFS) constant of the ground state are about 50% off from the experimental value. This constant describes the strength of the coupling of the electron to the nuclear magnetic moment and its short-distance nature mimics the behavior of the weak matrix elements. Therefore we arrive at the conclusion that so-called correlation corrections (those beyond the DHF approximation) have to be addressed. We treat the correlations within the systematic and successful methods of many-body perturbation theory.

How do we estimate the accuracy of calculating E_{PNC}? Ultra-precise experimental data are available for Cs. These data have accuracy better than our anticipated theoretical uncertainty thus allowing us to calibrate our calculations. Atomic energies are known to many significant figures. The Ultra-precise (0.01% accurate) value of the lifetime of the $6P_{3/2}$ state of Cs has been recently inferred from photoassociation spectroscopy [37,38] with ultracold atoms. The HFS constants for Cs are also measured to a good accuracy (the HFS constant A_{6S} of ^{133}Cs is known *exactly* by the definition of the second).

To reiterate, to further improve the interpretation of atomic parity violating signals, we need a high-accuracy *ab initio* relativistic many-body method capable of reaching the accuracy level of 0.1% for Cs.

4 Relativistic coupled-cluster method

Many-body perturbation theory (MBPT) provides a systematic way of treating correlation corrections, the critical issue for an improved interpretation of atomic PNC. First, we review main ideas of MBPT and the all-order coupled-cluster (CC) method. Then, we describe our present CC-inspired computational scheme and illustrate it with numerical results for the basic atomic properties of the Cs atom.

4.1 Generalities

In MBPT the atomic Hamiltonian is partitioned as

$$H = \left(\sum_i h_{\mathrm{nuc}}(\mathbf{r}_i) + \sum_i U_{\mathrm{DHF}}(\mathbf{r}_i)\right) + \left(\frac{1}{2}\sum_{i\neq j}\frac{1}{r_{ij}} - \sum_i U_{\mathrm{DHF}}(\mathbf{r}_i)\right),$$

where h_{nuc} includes the kinetic energy of an electron and its interaction with the nucleus, U_{DHF} is the DHF potential, and the last term represents the residual Coulomb interaction between electrons. In MBPT the first part of the Hamiltonian is treated as the lowest-order Hamiltonian H_0 and the residual Coulomb interaction as a perturbation. The perturbative expansion is built in powers of residual interaction and the derivations typically involve methods of second quantization and diagrammatic techniques.

One of the mainstays of practical applications of MBPT is the assumption of the convergence of series in powers of the residual interaction. Sometimes the convergence is poor and then one sums certain classes of diagrams to "all orders" using the iterative techniques. One of the most popular all-order methods is the coupled-cluster (CC) formalism [39,40]. It is widely employed in atomic and nuclear physics, and quantum chemistry [41]. The *relativistic* atomic-structure CC-type calculations were carried out, for example, in refs. [42–47].

The Hamiltonian in the second quantization (based on the DHF basis) reads

$$H = H_0 + G = \sum_i \varepsilon_i \left\{ a_i^\dagger a_i \right\} + \frac{1}{2} \sum_{ijkl} g_{ijkl} \left\{ a_i^\dagger a_j^\dagger a_l a_k \right\}, \tag{6}$$

where H_0 is the lowest-order Hamiltonian and the residual Coulomb interaction G is treated as a perturbation. The operators a_i and $a_i^\dagger$ are annihilation and creation operators, and $\{\ldots\}$ stands for a normal product of operators with respect to the core quasivacuum state $|0_c\rangle$. In the lowest order the atomic wave function with the valence electron in an orbital v reads $|\Psi_v^{(0)}\rangle = a_v^\dagger |0_c\rangle$. For example, v can represent the ground state $6s$ orbital of the Cs atom. Formally, we can introduce a wave operator Ω that produces the exact many-body wave function, $|\Psi_v\rangle = \Omega\, |\Psi_v^{(0)}\rangle$.

Central to the CC method is the realization that the wave operator can be represented via the exponential ansatz [48]

$$\Omega = \{\exp(K)\} = 1 + K + \frac{1}{2!}\{K^2\} + \ldots. \tag{7}$$

The operator K can be compellingly separated into cluster operators combining simultaneous excitations of core and valence electrons from the reference state $|\Psi_v^{(0)}\rangle$ to all orders of MBPT,

$$K = S + D + T + \cdots, \tag{8}$$

i.e., K is separated into single (S), double (D), triple (T), and higher-rank excitations. For the univalent systems it is convenient to subdivide cluster operators into core and valence classes

$$K = K_c + K_v\,. \tag{9}$$

Clusters K_c involve excitations from the core orbitals only, while K_v describe simultaneous excitations of the core and valence electrons. Then $S = S_c + S_v$, $D = D_c + D_v$, etc. The cluster operators satisfy so-called Bloch equations [48].

While the CC formulation is exact, in practice the full cluster operator K is truncated at a certain level of excitations. If we restrict it to single and double excitations,

$$K \equiv K^{(\mathrm{SD})} \approx S_c + D_c + S_v + D_v\,, \tag{10}$$

we arrive at the widely employed coupled-cluster single-double (CCSD) method.

The linearized version of the CCSD method was employed by the Notre Dame group for high-accuracy calculations of various atomic properties [42,43,46,47]. In this approximation, one discards nonlinear terms in the expansion of the exponent in eq. (7), $\Omega \approx 1 + K^{(\mathrm{SD})}$. We will refer to this approximation as the singles-doubles (SD) method. The resulting SD equations are written out in ref. [42]. A typical *ab initio* accuracy attained for properties of heavy alkali-metal atoms is at the level of 1%.

Since the present goal is to reduce theoretical uncertainties to the level of 0.1–0.2% we have to go beyond the SD approach. A systematic step in improving the SD method would be an additional inclusion of triple and nonlinear double excitations. However, considering the present state of available computational power, the full incorporation of triples (specifically, core triples) seems to be unmanageable for heavy atoms. For instance, for Cs storing and manipulating core triple amplitudes would require $\sim 100\,\mathrm{Gb}$ of memory.

To motivate next-generation formalism, we have explicitly computed 1648 fourth-order diagrams for matrix elements that appear due to triple excitations and nonlinear terms (*i.e.*, those omitted in the SD method) [49, 50]. We observe from numerical results for electric-dipole matrix elements in Na [50] and Cs [51] that the contributions from *valence* triples T_v and nonlinear doubles D_{nl} are much larger than those from *core* triples T_c. This leads to our present level of approximation: we discard core triples and core nonlinear terms and incorporate the *valence triples* and *valence nonlinear terms* into the SD formalism. The resulting approximation will be referred to as CCSDvT method.

4.2 Driving equations in the CCSDvT approximation

Below we write down the CC equations for cluster amplitudes in the CCSDvT approximation. Here we present the topological structure of the equations only. A detailed tabulation of the formulas can be found in our paper [52]. The equations in the SD approximation are presented in explicit form in ref. [42]. The CCSDvT equations for the core cluster amplitudes S_c and D_c are the same as in the SD approximation.

For valence triple amplitudes we obtain symbolically

$$-[H_0, T_v] + \delta E_v T_v \approx T_v[D_c] + T_v[D_v]. \tag{11}$$

Here $[H_0, T_v]$ is a commutator, and δE_v is the correlation valence energy defined as

$$\delta E_v = \delta E_{\mathrm{SD}} + \delta E_{\mathrm{CC}} + \delta E_{\mathrm{vT}}\,, \tag{12}$$

where the correction δE_{SD} is obtained within the SD approach, the correction δE_{CC} comes from nonlinear CC contributions and δE_{vT} is due to valence triples. Contributions $T_v[D_c]$ and $T_v[D_v]$ denote the effect of core and valence doubles on valence triples, respectively. At present we include only these effects omitting the effect of valence and core triples on valence triples ($T_v[T_v]$ and $T_v[T_c]$) and nonlinear CC contributions. These are higher-order effects which computationally are much more demanding.

The topological structure of the valence singles equation is

$$
\begin{aligned}
&-[H_0, S_v] + \delta E_v S_v \approx \mathrm{SD} \\
&+S_v[S_c \otimes S_v] + S_v[S_c \otimes S_c] \\
&+S_v[S_c \otimes D_v] + S_v[S_v \otimes D_c] + S_v[T_v]. \qquad (13)
\end{aligned}
$$

Here $S_v[S_c \otimes S_v]$ stands for a contribution from the excitations of core and valence electrons resulting from a product of clusters S_c and S_v. All other terms are defined in a similar fashion.

Finally, equation for valence doubles can be symbolically represented as

$$
\begin{aligned}
&-[H_0, D_v] + \delta E_v D_v \approx \mathrm{SD} \\
&+D_v[S_c \otimes S_v] + D_v[S_c \otimes S_c] \\
&+D_v[S_c \otimes D_v] + D_v[S_v \otimes D_c] + D_v[S_c \otimes D_c] \\
&+D_v[D_c \otimes D_v] + D_v[S_c \otimes T_v] \\
&+D_v[S_v \otimes T_c] + D_v[T_v]. \qquad (14)
\end{aligned}
$$

Solution of the above equations provides us with the cluster amplitudes and correlation energies. Numerical results for the energies will be presented in sect. 4.4. At this point, with the obtained wave functions we proceed to evaluating matrix elements.

4.3 Matrix elements

The SD method has already proven to be successful in calculations of various atomic properties. For heavy alkali-metal atoms the attained level of agreement with experimental data for the hyperfine constants is at 5% and the accuracy of a similar calculation for the electric-dipole amplitudes is 0.5% (see, *e.g.*, [47]). At the same time the accuracy required for our goals should be at the level of 0.1–0.2%. In order to improve the overall accuracy we develop the technique of relativistic calculations of matrix elements beyond the SD approach.

Given two computed CCSDvT wave functions, we may evaluate matrix elements of one-electron operator Z as

$$
Z_{wv} = \frac{\langle \Psi_w | \sum_{ij} z_{ij}\, a_i^\dagger a_j | \Psi_v \rangle}{\sqrt{\langle \Psi_w | \Psi_w \rangle \langle \Psi_v | \Psi_v \rangle}}\,. \qquad (15)
$$

The explicit expressions are given in ref. [52]. Compared to the SD approximation, we include contribution of valence triples T_v. They contribute both directly via explicit contributions to matrix element formula and indirectly through the modification of the SD amplitudes.

It is worth pointing out, that the importance of the valence triples has been realized earlier by the Notre Dame group [43]. They have shown that at the SD level, the error for the HFS constants is as large as 5% for Cs. To rectify this problem, they proposed and implemented a scheme that approximates the effect $S_v[T_v]$, *i.e.*, the effect of valence triples on valence singles. While improving the agreement for the HFS constants, their approximation leads to a poorer agreement (compared to SD method) for the dipole matrix elements. The advantage of the Notre Dame scheme is that it avoided expensive storing of triple excitations. Due to improved computational resources, we are able to store triples. Accounting for the triples in a rigorous fashion leads to a better agreement between theory and experiment.

Compared to the Notre Dame approximation we also include dressing of matrix elements based on the CC ansatz. The idea of our method [51] is as follows. When the CC exponent is expanded in eq. (15), we encounter an infinite number of terms. We devised a method of partial summation (dressing) of the resulting series. Our formalism is built upon an expansion of the product of cluster amplitudes into a sum of n-body insertions. We considered two types of insertions: the particle (hole) line insertion (line "dressing") and the two-particle (two-hole) random-phase-approximation-like insertion. We demonstrated how to "dress" these insertions and formulated iterative equations.

Another formal improvement over Notre Dame calculations comes from including the CC nonlinear terms in the equations for valence singles (13) and doubles (14). We also include the contribution of the core triples to matrix elements from a direct fourth-order calculation.

4.4 Numerical results

Our developed numerical CCSDvT code is an extension of the relativistic SD code [46] which employs a B-spline basis set. This basis numerically approximates a complete set of single-particle atomic states. Here we use 35 out of 40 positive-energy basis functions. Basis functions with $l_{\max} \le 5$ are used for singles and doubles. For triples we employ a more limited set of basis functions with $l_{\max}(T_v) \le 4$. Excitations from core sub-shells $[4s, \ldots, 5p]$ are included in the calculations of triples while excitations from sub-shells $[1s, \ldots, 3d]$ are discarded.

Computed removal energies of $6s$, $6p_{1/2}$, and $6p_{3/2}$ states of atomic cesium are presented in table 2. The dom-

Table 2. Contributions to removal energies of $6s$, $6p_{1/2}$, and $6p_{3/2}$ states for Cs in cm^{-1} in various approximations. $\delta E^{\mathrm{tot}}_{\mathrm{extrapolated}}$ correction is obtained by computing SD properties with increasingly larger basis sets and interpolating them to $l = \infty$ [53]. A comparison with experimental values is presented in the lower panel.

	$6s$	$6p_{1/2}$	$6p_{3/2}$
E_{DHF}	27954	18790	18389
δE_{SD}	3869	1611	1623
$\delta E_{\mathrm{CCSDvT}}$	3350	1387	1220
$E^{\mathrm{tot}}_{\mathrm{CCSDvT}}$	31304	20178	19608
QED[1]	18	−0.4	0
$\delta E^{\mathrm{tot}}_{\mathrm{extrapolated}}$	30	20	20
$\mathrm{E}^{\mathrm{tot}}_{\mathrm{final}}$	31352	20198	19628
E_{experim}[2]	31407	20228	19675

[1] Reference [54].

[2] Reference [55].

Table 3. Magnetic-dipole hyperfine structure constants A (in MHz) and matrix elements of the electric-dipole moment (in a.u.) for ^{133}Cs. Results of calculations and comparison with experimental values are presented. See text for the explanation of entries.

	$A(6s)$	$A(6p_{1/2})$	$\langle 6p_{1/2}\|D\|6s\rangle$	$\langle 6p_{3/2}\|D\|6s\rangle$
DHF	1425.4	160.94	5.2777	7.4264
SD	2438.0	310.71	4.4829	6.3075
Δ(CCSDvT)	−136.9	−20.92	0.0256	0.0363
Complementary corrections				
Line dressing	−12.5	−2.16	0.0094	0.0107
Vertex dressing	4.3	0.29	−0.0067	−0.0088
MBPT-IV (core triples, ...)	7.8	1.14	0.0001	0.0001
Breit + QED	-6.5^1		0.0024^2	
Extrapolation for $l=\infty^3$	5.0	0.37	−0.004	−0.006
Final CCSDvT + corrections	2299.2	289.43	4.5097	6.3398
Experiment	2298.2	$291.89(8)^4$	$4.5049(17)^5$	$6.3404(3)^6$

[1] Reference [56].

[2] References [20,54].

[3] Reference [53].

[4] Reference [57].

[5] References [58,38].

[6] Reference [38].

inant contribution to the energies comes from the DHF values. The remaining (correlation) contribution is given by eq. (12). We computed this correlation correction in SD and CCSDvT approximations. As it follows from the table the agreement with experiment is at the level of 0.1–0.2% for all considered states. We anticipate that including other corrections missed at this stage (*e.g.*, nonlinear corrections to core amplitudes and core triples) can further improve the agreement with the experimental results.

With the computed wave functions of the $6s$, $6p_{1/2}$ and $6p_{3/2}$ states we determine matrix elements. Numerical results for magnetic-dipole hyperfine-structure constants A and electric-dipole transition amplitudes are presented in table 3. This table is organized as follows. First we list the DHF and SD values, and the differences between CCSDvT and SD values, Δ(CCSDvT) = CCSDvT − SD. We base our final *ab initio* results on the most sophisticated CCSDvT values. These values also include all-order dressing, and corrections due to core triples, computed in the the fourth order of MBPT. QED corrections are included where available. The results for the HFS constants include finite nuclear size (Born-Weisskopf) effect.

We find an excellent, 0.1% level, agreement for dipole matrix elements and the HFS constant of the ground state. The agreement for the the HFS constant of the $6p_{1/2}$ is only at 1% level. We are presently working on testing the sensitivity of this constant to higher-order effects.

We would like to emphasize that presently the correlation corrections at the level of a few 0.1% are comparable to radiative corrections. In this regard it would be useful to carefully compute them to unmask the remaining many-body effects.

5 Summary and outlook

Atomic parity violation plays an important role in testing the low-energy electroweak sector of the standard model. The interpretation of experiments in terms of nuclear weak charge requires calculations challenging the capabilities of modern atomic theory. Over the last few years, we have witnessed a substantial advance in evaluating corrections to parity-violating amplitudes in heavy atoms. These small (sub-1%), but important corrections include Breit, radiative (vacuum polarization, self-energy, and vertex) and neutron skin corrections. As a result of this progress, the most accurate-to-date measurement of atomic parity violation in Cs has been brought into substantial agreement with the prediction of the standard model.

Presently, the theoretical interpretation is clouded by uncertainties in solving the basic correlation problem of the atomic structure. In this paper we outlined our next-generation many-body formalism for solving this problem. We tested our coupled-cluster-inspired method by computing basic atomic properties of the Cs atom. All the computed properties are important for quantifying the accuracy of the calculations of parity-violating amplitudes. We find an agreement at 0.1% for the ground-state hyperfine structure constant, $E1$ transition amplitudes, and energies. However, a relatively poor 1% agreement of the HFS constant A for the $6P_{1/2}$ state with experiment requires further improvements of the method. The advantage of the employed coupled-cluster method is that it allows for such systematic improvements. It is anticipated that the further theoretical progress will refine constraints on new physics beyond the standard model and enable the next round of experimental studies.

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