Constraints on new physics from an improved calculation of parity violation in $^{133}$Cs

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We report the result of our calculation of the nuclear spin-independent parity violating electric dipole transition amplitude ($E1_{PV}$) for the $6s^2\, ^2S_{1/2} \rightarrow 7s^2\, ^2S_{1/2}$ transition in $^{133}$Cs to an accuracy of 0.3% using a variant of the perturbed relativistic coupled-cluster (RCC) theory. In the present work, we treat the contributions of both the low-lying and high-lying excited states to the above mentioned amplitude on the same footing, thereby overcoming the limitations of previous high accuracy RCC calculations. We obtain an accurate value for the vector polarizability ($\beta$) for the above transition and by combining it with the results from our present calculation of $E1_{PV}$ and the latest measurement of $\text{Im}(E1_{PV}/\beta)$, we extract the nuclear weak charge ($Q_W$); and analyze its deviation from its value in the Standard Model (SM) in order to constrain certain scenarios of new physics beyond the SM.

I. INTRODUCTION

Atomic processes are usually studied by considering the exchange of photons ($\gamma$) between the bound electrons and the nucleus and the bound electrons themselves. The longitudinal $\gamma$s are responsible for the Coulomb interaction, which is the dominant contribution to electromagnetic interactions in atomic systems. However, the Breit interaction [1] due to the transverse $\gamma$s and quantum electrodynamics (QED) effects must also be considered in high precision atomic calculations. All these interactions preserve parity symmetry, and these systems are described conveniently using spherical coordinates [2]. Inclusion of the neutral current weak interactions due to the exchange of the $Z_0$ boson in atomic systems leads to parity violation [3], and this phenomenon has been referred to as atomic parity violation (APV). Depending on the electron-nucleus vector–axial-vector (V-A) or the axial-vector–vector (A-V) currents, APV interactions can be nuclear spin ($I$) independent or dependent. In addition to the $Z_0$ exchange interactions, the possible interaction of the nuclear anapole moment with electrons can give rise to APV that depends on $I$ [4]. The $I$ dependent APV contributions are relatively smaller than its NSI counterpart, as the odd-nucleon contributes primarily to APV. In the case of the nuclear spin independent (NSI) interaction, the nucleons which ultimately arise from the up- and down-quarks, contribute coherently, and these contributions are several orders of magnitude larger than those due to the exchange of $Z_0$ between the electrons [5]. Nonetheless, the NSI APV interaction is too weak to be detected using typical spectroscopic measurements, and therefore, special techniques have been developed in different laboratories to observe effects due to it [7][11].

Heavier atomic systems are preferred for measuring the subtle NSI APV effects owing to the fact that the weak interaction causing them in atomic systems scales slightly faster than $Z^3$ [3], where $Z$ is the atomic number. These measurements in combination with high-precision atomic calculations have the potential to probe physics beyond the Standard Model (SM) of elementary particles [12][16].

APV has been measured to an accuracy of 0.35% in the $6s^2\, ^2S_{1/2} \rightarrow 7s^2\, ^2S_{1/2}$ transition in $^{133}$Cs [5]. This is the most accurate APV measurement to date. New experiments have been proposed to measure APV in Cs [17][18], which have the potential to surpass the accuracy of this measurement. The stage is now clearly set to take the APV calculations in Cs to the next level, which would lead to an improvement in the accuracy of $Q_W$, thereby making it possible to probe new physics beyond the SM. This indeed provides the motivation for our present work. The principal quantity of interest in the APV studies is the nuclear weak charge ($Q_W$), which is a linear combination of the coupling coefficients between electrons, and up- and down-quarks in an atomic system [3][10]. The difference in the model independent value of $Q_W$ obtained from APV and that obtained from the SM could, in principle, shed light on new physics beyond the SM. The APV study in $^{133}$Cs currently yields $\sin^2 \theta_W^\text{exp} = 0.2356(20)$ [10] and the value predicted by the SM is $\sin^2 \theta_W^\text{SM} = 0.23857(5)$ [20] for the Weinberg angle $\theta_W$, at the zero momentum transfer in the $\overline{\text{MS}}$ scheme. The difference in the values of $Q_W$ also gives the lower mass limit of an extra $Z'$ boson as $M_{Z'} > 710$ GeV/$c^2$ and weak isospin conserving parameter $S = -0.81(54)$ at the $1\sigma$ level [10]. It has been argued that the signature of a dark boson ($Z_d$) (also referred to as dark photon in the...
literature) can be obtained from the above mentioned difference \[21\] \[23\]. Direct experimental signature suggests its value to be less than 0.2 GeV \[23\]. A fairly recent manuscript \[24\] suggests that the limit on an effective electron-nucleus coupling describing new physics beyond the SM expressed as $\lambda^{eff} < 4 \times 10^{-5}$ GeV$^{-2}$ with a new energy scale $\Lambda$ and emphasizes that the bound on the effective couplings inferred from AV is more stringent than the ones from the neutrino-nucleus coherent scattering processes.

State-of-the-art relativistic atomic many-body theories have been applied to $^{133}$Cs APV calculations in the last four decades \[19\] \[20\] \[31\]. The accuracy of the calculations have steadily improved, as the theoretical methods have been able to incorporate larger classes of higher-order effects during this time due to advances in high performance computing. The latest two high precision calculations have been reported in Refs. \[19\] \[31\]. These calculations divided the entire electron correlation contribution into three parts and they are calculated by mixed many-body methods. Further, the dominant part was evaluated through sum-over-states approach and the other contributions were not treated on the same footing. Contributions from the Breit and QED effects were taken from the earlier works, but not double core-polarization (DCP) effects \[32\]. Some of these issues triggered discussions recently \[16\] \[33\], and therefore, it is necessary to revisit this problem. In this work, we intend to circumvent the above mentioned limitations of the previous calculations by solving the first-order perturbed wave functions due to the APV interaction for atomic states in the framework of the relativistic coupled-cluster (RCC) theory. Thus, it considers both the electromagnetic and weak interactions simultaneously in addition to accounting for Coulomb, Breit and QED interactions using the same many-body method. Most importantly, it treats all the three different parts of the total correlation contribution mentioned above on the same footing.

II. THEORY

Neglecting the A-V interaction, the short range effective Lagrangian corresponding to the V-N weak neutral current interaction of an electron with up- and down-quarks in an atomic system is given by \[6\] \[7\]

$$\mathcal{L}_{eq}^{VA} = \frac{G_F}{\sqrt{2}} \sum_{u,d} \left[ C_{1u} \bar{\psi}_u \gamma_\mu \psi_u + C_{1d} \bar{\psi}_d \gamma_\mu \psi_d \right] \bar{\psi}_e \gamma^\mu \gamma^5 \psi_e$$

$$= \frac{G_F}{\sqrt{2}} \sum_{n} C_{1n} \bar{\psi}_u \gamma_\mu \psi_u \bar{\psi}_e \gamma^\mu \gamma^5 \psi_e,$$  

(1)

where $G_F = 1.16632 \times 10^{-5}$ GeV$^{-2}$ is the Fermi constant, sums $u$, $d$ and $n$ stand for up-quark, down-quark and nucleons respectively, and $C_{i=1,2,3}$ represent coupling coefficients of the interaction of an electron with quarks and nucleons. Adding them coherently and taking the non-relativistic approximation for nucleons, the temporal component gives the NSI weak interaction Hamiltonian

$$H_{en}^{VA} = -\frac{G_F}{2\sqrt{2}} \left[ Q_W \rho(r) + (NC_{1N} - ZC_{1P}) \Delta \rho(r) \right] \gamma^5,$$  

(2)

where $N$ and $P$ representing for neutron and proton respectively, $\rho(r) = (\rho_N(r) + \rho_P(r))/2$ is the average nucleon density with normalized proton density $\rho_P(r)$ and normalized neutron density $\rho_N(r)$, $\Delta \rho(r) = \rho_N(r) - \rho_P(r)$, and $Q_W = 2[ZC_{1P} + NC_{1N}]$ is known as the nuclear weak charge. In the atomic calculations, contribution from $\Delta \rho(r)$ is neglected at first, but is added later as “nuclear skin” correction. The nuclear skin correction to $Q_W$ is expressed as \[34\]

$$\Delta Q_W^{N-P} = 0.9857 N (Z \alpha_e)^2 \frac{232}{255} \frac{t}{r_P},$$  

(3)

where $\alpha_e$ is the fine-structure constant, $r_{i-P[N]}$ are the root mean square radius of proton (neutron), $t = r_N - r_P$ is the neutron skin, and $q_P$ is defined as

$$q_P = \int d^3r f(r) \rho_P(r)$$  

(4)

with the electronic form factor $f(r)$ that describes the spatial variation of the electronic axial-vector matrix element over the size of the nucleus.

The NSI weak interaction Hamiltonian for atomic calculations, thus, is given by \[3\]

$$H_{APV}^{NSI} = \sum_{\kappa} H_{en}^\kappa - \frac{G_F}{2\sqrt{2}} Q_W^{\kappa} \sum_{\kappa} \gamma^5 \rho(r),$$  

(5)

where $Q_W^{\kappa} = Q_W - \Delta Q_W^{N-P}$. It is obvious that $Q_W$ is a model dependent quantity. Thus, the difference of its actual value from the SM, given by $\Delta Q_W = Q_W^{exp} - Q_W^{SM}$, can provide signatures about new physics. In the SM, $C_{1u} = \frac{1}{2} [1 - \frac{8}{3} \sin^2 \theta_W^{SM}]$ and $C_{1d} = -\frac{1}{2} [1 - \frac{4}{3} \sin^2 \theta_W^{SM}]$ \[6\] \[8\] \[10\]. This follows $C_{1N} = 2C_{1d} + C_{1u} = -1/2$ and $C_{1P} = 2C_{1u} + C_{1d} = (1 - 4 \sin^2 \theta_W^{SM})/2 \approx 0.04$.

Moreover, $\sin^2 \theta_W$ varies with energy scale (denoted by $Q$) and is parameterized in the MS scheme as \[11\]

$$\sin^2 \theta_W(Q^2) = \kappa(Q^2) \sin^2 \theta_W(M_{Z_0})_{\text{MS}}.$$  

(6)

where $M_{Z_0}$ is the mass of $Z_0$-boson and $\kappa(Q^2)$ denotes perturbative $\gamma-Z_0$-boson mixing. For the normalization $\kappa(Q^2 = M_{Z_0}^2) = 1.0$, it corresponds to $\kappa(0) \approx 1.03$ \[13\]. In the one-loop radiative correction, the mass of $W$-boson and $\sin^2 \theta_W(M_{Z_0})_{\text{MS}}$ are given by \[11\]

$$M_{W} = 80.362(6)[1 - 0.0036S + 0.0056T] \text{ GeV}/c^2,$$  

(7)

and

$$\sin^2 \theta_W(M_{Z_0})_{\text{MS}} = 0.23124(6)[1 + 0.0157S - 0.0112T],$$  

(8)

where $c$ is speed of light, and $S$ and $T$ are the isospin conserving and isospin breaking parameters, respectively.
By comparing the above expression for $M_W$ with its experimental value of 80.379(12) GeV/c$^2$ [20], it gives [22]

$$S = 0.07 \pm 0.09 \quad \text{and} \quad T = 0.10 \pm 0.09.$$  \hspace{1cm} (9)

Also, $M_{Z'}$ can be obtained in the SO(10) model as [12]

$$\Delta Q_W \approx 0.4 \times (2N + Z)(M_W/M_{Z'})^2.$$  \hspace{1cm} (10)

In the $Z_0$ and $Z_4$ mixing of two-Higgs doublet model scenario, we get [12, 22, 23]

$$\sin^2 \theta_W^0(0) - \sin^2 \theta_W^{SM}(0) \approx -0.42 \varepsilon \delta M_{Z_0}/M_{Z_4},$$  \hspace{1cm} (11)

where $\varepsilon$ and $\delta$ are the model dependent parameters, and $M_{Z_4}$ is mass of $Z_4$.

Accounting for all the aforementioned possible physics beyond the SM, the weak charge of $^{133}$Cs atom can be expressed in terms of all the combined parameters as

$$Q_W(^{133}\text{Cs}) = Q_W^{SM}(^{133}\text{Cs}) \times \left[1 + 0.011S - 0.008T - 0.9(M_{Z_0}^2/M_{Z_4}^2) - 1.265\varepsilon \delta (M_{Z_0}/M_{Z_4})\right],$$  \hspace{1cm} (12)

where $Q_W^{SM}(^{133}\text{Cs}) = -N + Z(1 - 4\sin^2 \theta_W^{SM}) = -73.23$ is the nuclear weak charge of $^{133}$Cs in the SM [20].

In an effective description [24], $\Delta Q_W$ is encoded using a new energy scale $\Lambda$ as

$$\Delta Q_W = \frac{2\sqrt{2}}{G_F} \frac{3}{\Lambda^2} f_{VQ}^{\text{eff}}(Z + N),$$  \hspace{1cm} (13)

where

$$f_{VQ}^{\text{eff}} = \frac{C_{1a}(2Z + N) + C_{1d}(Z + 2N)}{3(Z + N)}.\hspace{1cm} (14)$$

Similarly, $Q_W$ can be expressed in terms of the nucleon-electron V-A couplings as [20]

$$Q_W = -2\left[Ng^{np} + Ng^{nn} + 0.00743 \left(1 - \frac{\alpha_s}{\pi}\right)\right],$$  \hspace{1cm} (15)

where $g^{np(n)}$ are the electron-proton(neutron) coupling constants. The SM offers $55g^{np} + 78g^{nn} = 36.70(1)$ [20].

### III. ATOMIC CALCULATIONS

#### A. General aspects

The atomic wave function ($|\Psi_v\rangle$) of a state in Cs atom is calculated by dividing the total Hamiltonian as

$$H = H_{em} + \lambda H_w,$$  \hspace{1cm} (16)

where $H_{em}$ represents the dominant electromagnetic interactions in the atom and $H_{AP}^{NSI} \equiv \lambda H_w$ with $\lambda = \frac{G_F Q_{AP}}{2\sqrt{2}}$. The electric dipole transition amplitude between the same nominal parity states $|\Psi_i\rangle$ and $|\Psi_f\rangle$ states due to the presence of $H_{AP}^{NSI}$ can be written as

$$E_{1PV} = \frac{\langle \Psi_f | D | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}}.$$  \hspace{1cm} (17)

Since the strength of $H_{AP}^{NSI}$ is much weaker than that of the $H_{em}$ in an atomic system, the wave function for a state (say, $|\Psi_v\rangle$) corresponding to the total Hamiltonian $H = H_{em} + \lambda H_w$ and its energy (say, $E_v$) can be expressed as

$$|\Psi_v\rangle = |\Psi_v^{(0)}\rangle + \lambda |\Psi_v^{(1)}\rangle + O(\lambda^2)$$  \hspace{1cm} (18)

and

$$E_v = E_v^{(0)} + \lambda E_v^{(1)} + O(\lambda^2),$$  \hspace{1cm} (19)

where the superscripts 0 and 1 stand for the zeroth-order and first-order contributions due to $H_w$, respectively. By neglecting $O(\lambda^3)$ contributions, we get

$$E_{1PV} \approx \lambda \frac{\langle \Psi_{f}^{(1)} | D | \Psi_{i}^{(0)} \rangle + \langle \Psi_{f}^{(0)} | D | \Psi_{i}^{(1)} \rangle}{\sqrt{\langle \Psi_{f}^{(0)} | \Psi_{f}^{(0)} \rangle \langle \Psi_{i}^{(0)} | \Psi_{i}^{(0)} \rangle}}.$$  \hspace{1cm} (20)

As mentioned before, the previous two high-precision calculations of $E_{1PV}$ were evaluated using the sum-over-states approach by expanding the first-order wave function as

$$|\Psi_{v}^{(1)}\rangle = \sum_{I \neq v} |\Psi_{i}^{(0)}\rangle \frac{\langle \Psi_{f}^{(0)} | H_{AP}^{SI} | \Psi_{i}^{(0)} \rangle}{E_{v}^{(0)} - E_{I}^{(0)}},$$  \hspace{1cm} (21)

where $I$ denotes all possible intermediate states, that can be divided into core states (contributions from these states are designated as “Core”), low-lying bound states (contributions from these states are given as “Main”), and the remaining high-lying states including continuum (whose contributions are mentioned as “Tail”) for computational simplicity. The drawback of this approach is that in an actual calculation, it is possible to evaluate “Main” contributions from only a few low-lying valence excited bound states accurately by calculating them individually using a powerful many-body method, and the “Core” and “Tail” contributions are estimated using less rigorous many-body methods. Therefore, the results from the latter two sectors are less accurate. In other words, this approach of evaluating correlation effects in a piecemeal manner does not take into account certain types of correlation effects. As a consequence, contributions from effects such as the DCP are completely excluded. Keeping in mind the high accuracy needed for APV to achieve its ultimate objective of probing new physics beyond the SM, it is desirable to include contributions from all the intermediate states on an equal footing. This can be accomplished not by summing over intermediate states, but rather by obtaining the first-order perturbed wave functions for the initial and final states directly.

From the equation $H|\Psi_v\rangle = E_v|\Psi_v\rangle$, the inhomogeneous equation for the first-order wave function is obtained as

$$(H_{em} - E_v^{(0)})|\Psi_v^{(1)}\rangle = (E_v^{(1)} - H_w)|\Psi_v^{(0)}\rangle,$$  \hspace{1cm} (22)

where $E_v^{(1)} = 0$ in the present case owing to the odd-parity nature of $H_w$. Obtaining $|\Psi_v^{(1)}\rangle$ directly by solving the above equation can implicitly include contributions.
from all the intermediate states $I$ of Eq. [21], thereby, overcoming the problem of unequal treatment of various electron correlation effects from different sectors as mentioned above. Moreover, it is also necessary to account for correlation effects involving both the weak and electromagnetic interactions. Therefore, it is very important to consider a powerful and versatile many-body theory to obtain both $|\Psi_1^{(0)}\rangle$ and $|\Psi_v^{(1)}\rangle$ accurately. Since Cs is a heavy atom, it is necessary to employ a relativistic method for computing the wave functions of this atom. The coupled-cluster (CC) theory is currently considered to be one of the leading quantum many-body methods and has been referred to as the gold standard for treating electron correlation effects in atomic and molecular systems [35–37]. Thus, the relativistic version of the CC (RCC) theory is very well suited for the accurate evaluation of the correlation effects in $E1_{PV}$ for the $6s^2 2S1/2 - 7s^2 2S1/2$ transition in $^{133}$Cs.

**B. Atomic Hamiltonian**

The starting point of our calculation is the Dirac-Coulomb (DC) Hamiltonian [38] representing the leading order contributions to $H_{em}$ to calculate the zeroth-order wave functions and energies which in atomic units (a.u.) is given by

$$H_{DC} = \sum_i [\mathbf{\alpha}_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_n(r_i)] + \sum_{i,j>i} \frac{1}{r_{ij}} \tag{23}$$

where $\alpha$ and $\beta$ are the usual Dirac matrices, $\mathbf{p}$ is the single particle momentum operator, $V_n(r)$ denotes the nuclear potential, and $\sum_{i,j>i} \frac{1}{r_{ij}}$ represents the Coulomb potential between the electrons located at the $i^{th}$ and $j^{th}$ positions. It should be noted that the above Hamiltonian is scaled with respect to the rest mass energies of electrons. Contributions from the Breit interaction [39] to $H_{em}$ is determined by including the following potential

$$V^B = -\sum_{j>i} \frac{\mathbf{\alpha}_i \cdot \mathbf{\alpha}_j + (\mathbf{\alpha}_i \cdot \mathbf{r}_{ij})(\mathbf{\alpha}_j \cdot \hat{\mathbf{r}}_{ij})}{2r_{ij}} \tag{24}$$

where $\hat{\mathbf{r}}_{ij}$ is the unit vector along $\mathbf{r}_{ij}$.

Contributions from the QED effects to $H_{em}$ are estimated by considering the lower-order vacuum polarization (VP) interaction ($V_{VP}$) and the self-energy (SE) interactions ($V_{SE}$). We account for $V_{VP}$ through the Uehling [40] and Wichmann-Kroll [41] potentials ($V_{VP} = V_{Uehl}^{VP} + V_{WK}^{VP}$), given by

$$V_{Uehl}^{VP} = -\frac{2}{3} \sum_i \frac{\alpha_i^2}{r_i} \int_0^\infty dx \rho(x) \int_1^\infty dt \sqrt{t^2 - 1} \times \left( \frac{1}{t^3} + \frac{1}{2t^5} \right) e^{-2ct|\mathbf{r}_i - \mathbf{x}|} - e^{-2ct(\mathbf{r}_i + \mathbf{x})} \tag{25}$$

and

$$V_{WK}^{VP} = \sum_i \frac{0.368 Z^2}{9\pi c^5 (1 + (1.62cr_i)^4)} \rho(r_i), \tag{26}$$

respectively.

The SE contribution $V_{SE}$ is estimated by including two parts [42]

$$V_{SE}^{ef} = A_1 \int_0^\infty \frac{2\pi Z\alpha_e}{r_i} f(r_i) - B_1 \sum_i \frac{\alpha_e I_{ef}^n(r_i)}{r_i} \tag{27}$$

known as the effective electric form factor part and

$$V_{SE}^{mg} = -\sum_k \frac{i\alpha^3 e^2}{4} \nabla_k \frac{1}{r_k} \int_0^\infty dx \rho_n(x) \int_1^\infty dt \frac{1}{\sqrt{t^2 - 1}} \times \left[ e^{-2ct|\mathbf{r}_k - \mathbf{x}|} - e^{-2ct(\mathbf{r}_k + \mathbf{x})} - 2ct (\mathbf{r}_k + \mathbf{x} - |\mathbf{r}_k - \mathbf{x}|) \right], \tag{28}$$

known as the effective magnetic form factor part. In the above expressions, we use [43]

$$A_1 = \begin{cases} 0.074 + 0.35Z\alpha_e & \text{for } l = 0, 1 \\ 0.056 + 0.05Z\alpha_e + 0.195Z^2\alpha_e^2 & \text{for } l = 2, \tag{29} \end{cases}$$

and

$$B_l = \begin{cases} 1.071 - 1.97x^2 - 2.128x^3 + 0.169x^4 & \text{for } l = 0, 1 \\ 0 & \text{for } l \geq 2. \tag{30} \end{cases}$$

The integrals are given by

$$R_{1}^{ef}(r) = \int_0^\infty dx \rho_n(x)[(Z|\mathbf{r} - \mathbf{x}| + 1)e^{-Z|\mathbf{r} - \mathbf{x}|} - (Z(r + x) + 1)e^{-2ct(r+x)}] \tag{31}$$

and

$$I_{2}^{ef}(r) = \int_0^\infty dx \rho_n(x) \int_1^\infty dt \frac{1}{\sqrt{t^2 - 1}} \left\{ \left( 1 - \frac{1}{2t^2} \right) \times \left[ \ln(t^2 - 1) + 4 \ln \left( \frac{1}{Z\alpha_e} + \frac{1}{2} \right) \right] - \frac{3}{2} + \frac{1}{t^2} \right\} \times \left\{ \frac{\alpha_c}{t} \left[ e^{-2ct|\mathbf{r}_i - \mathbf{x}|} - e^{-2ct(\mathbf{r}_i + \mathbf{x})} \right] + 2r_A e^{2r_A ct} \times \left[ E_1(2ct(|\mathbf{r} - \mathbf{x}| + r_A)) - E_1(2ct(r + x + r_A)) \right] \right\} \tag{32}$$

with the orbital quantum number $l$ of the system, $x = (Z - 80)\alpha_e$, $r_A = 0.07Z^2\alpha_e^3$, and the exponential integral $E_1(r) = \int_r^\infty ds e^{-s}/s$.

We have determined the nuclear potential and density by assuming a Fermi-charge distribution given by [44]

$$\rho_n(r) = \frac{\rho_0}{1 + e^{(r-b)/a}} \tag{33}$$

for the normalization factor $\rho_0$, the half-charge radius $b = 5.670729105$ fm [43] and $a = 2.3/4(\ln3)$ is related to the skin thickness.
C. RCC theory for unperturbed wave function

In the RCC theory framework, the unperturbed wave function of an atomic system with a closed-core and a valence orbital like in the case of Cs atom due to \( H_{em} \) can be expressed as \[36\]

\[ |\Phi_v^{(0)}\rangle = e^{-T^{(0)}} \left\{ 1 + S_v^{(0)} \right\} |\Phi_v\rangle, \]  

(34)

where \( |\Phi_v\rangle \) is the reference wave function, which is obtained by solving Dirac-Hartree-Fock (DHF) wave function of the closed-core (\(|\Phi_0\rangle\)), and then, appending the corresponding valence orbital \( v \) to it as \( |\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle \). \( T^{(0)} \) and \( S_v^{(0)} \) are the core and the valence excitation operators with the superscript 0 represents absence of any external perturbation. The amplitudes of the unperturbed RCC operators and energies are obtained by solving the following equations (see, e.g. \[37\]

\[ \left\langle \Phi_0^K \right| H_{em} \left| \Phi_0 \right\rangle = \delta_{K,0} E_0^{(0)} \]  

(35)

and

\[ \left\langle \Phi_v^M \right| H_{em} \left\{ 1 + S_v^{(0)} \right\} \right| \Phi_v \rangle = E_v^{(0)} \left\langle \Phi_v^M \right| \left\{ \delta_{M,v} + S_v^{(0)} \right\} \right| \Phi_v \rangle \]  

(36)

where \( H_{em} = e^{-T^{(0)}} H_{em} e^{T^{(0)}} \), the superscripts \( K \) and \( M \) represent the \( K^{th} \) and \( M^{th} \) excited state determinants with respect to their respective reference states \(|\Phi_0\rangle \) and \(|\Phi_v\rangle\), \( E_0 \) is the energy of the closed-core (i.e. Cs\(^{+}\)) and \( E_v \) is the energy of a neutral state of Cs atom. These energies are determined by

\[ E_0^{(0)} = \left\langle \Phi_0^K \right| H_{em} \left| \Phi_0 \right\rangle \]  

(37)

and

\[ E_v^{(0)} = \left\langle \Phi_v^M \right| H_{em} \left\{ 1 + S_v^{(0)} \right\} \right| \Phi_v \rangle \]  

(38)

\( \Delta E_v = E_v^{(0)} - E_0^{(0)} \) is the electron binding energy and is the negative of the electron affinity (EA) for the valence \( v \) orbital. We have incorporated one-particle and one-hole (single), two-particle and two-hole (double) and three-particle three-hole (triple) excitations in our calculations through the RCC operators by defining

\[ T^{(0)} \simeq T_1^{(0)} + T_2^{(0)} + T_3^{(0)} \]  

(39)

and

\[ S_v^{(0)} \simeq S_{1v}^{(0)} + S_{2v}^{(0)} + S_{3v}^{(0)} \]  

(40)

where the subscripts \( K \) and \( M \) run over 1, 2 and 3 which are referred to as single, double and triple excitations respectively. To assess the importance of the triple excitations, we have performed calculations considering single and double excitations in the RCC theory (RCCSD method) after exciting all the core electrons, and then with single, double and triple excitations in the RCC theory (RCCSDT method). In addition, we have also carried out calculations using the second-order relativistic many-body theory (RMP(2) method), considering two-orders of the residual interaction and only keeping linear terms from the RCCSD method (RLCCSD method) as

\[ |\Psi_v^{(0)}\rangle \simeq \left\{ 1 + T^{(0)} + S_v^{(0)} \right\} |\Phi_v\rangle. \]  

(41)

Intermediate results from the RMP(2) and RLCCSD methods can demonstrate the propagation of electron correlation effects from lower- to all-order methods systematically in order to understand the role of electron correlation effects in the accurate calculations of EAs of valence electrons in different states of the Cs atom.

D. RCC theory for perturbed wave function

Extending the RCC theory ansatz of atomic wave function, the first-order perturbed wave function due to \( H_w \) can be expressed as \[50\]

\[ |\Psi_v^{(1)}\rangle = e^{T^{(0)}} \left\{ S_v^{(1)} + T^{(1)} \left( 1 + S_v^{(0)} \right) \right\} |\Phi_v\rangle, \]  

(42)

where \( T^{(1)} \) and \( S_v^{(1)} \) are the core and the valence excitation operators with the superscript 1 representing order of perturbation in \( H_w \). After obtaining the amplitudes of the unperturbed RCC operators, we obtain the amplitudes of their perturbed counterparts by solving the following equations

\[ \left\langle \Phi_0^K \right| H_{em} T^{(1)} + H_w \left| \Phi_0 \right\rangle = 0 \]  

(43)

and

\[ \left\langle \Phi_v^M \right| (H_{em} - E_v^{(0)}) S_v^{(1)} + (H_{em} T^{(1)} + H_w) \times \left( 1 + S_v^{(0)} \right) |\Phi_v\rangle = 0, \]  

(44)
where $\tilde{H}_w = e^{-T^{(0)}} H_w e^{T^{(0)}}$. Here, the subscripts $K$ and $M$ run again over 1, 2 and 3 which are referred to as single, double and triple excitations respectively. The important difference between the amplitude determining equations for unperturbed and perturbed wave functions is that the projected determinantal states (denoted by superscripts $K$ and $M$) have even and odd parities, respectively. The RCC operators representing perturbed single, double and triple excitations are denoted by

$$T^{(1)} \simeq T^{(0)}_1 + T^{(1)}_2 + T^{(1)}_3$$

and

$$S^{(1)}_v \simeq S^{(1)}_{1v} + S^{(0)/(1)}_{2v} + S^{(1)}_{3v}.$$  

(46)

Along with the calculations using the RCCSD and RCCSDT methods, we also determine perturbed wave functions in the RLCCSD approximation by considering the expression

$$|\Phi^{(1)}_v\rangle \simeq \left\{ \left(1 + T^{(0)}_1\right) S^{(1)}_v + T^{(1)}_1 \left(1 + S^{(0)}_v\right) \right\} |\Phi_v\rangle. \quad (47)$$

The differences in the results from these methods will demonstrate the role of non-linear in $T^{(0)}$ terms and triple excitations to the amplitudes of the first-order perturbed wave functions.

E. Evaluation of atomic properties

To test the accuracies of the wave functions, we also evaluate other relevant properties apart from the binding energies and compare them with their high precision experimental values. The accuracies of the calculated energies are sensitive to the quality of the wave functions slightly away from the nuclear region of atomic systems. For testing the accuracies of the wave functions in the nuclear region and the far nuclear region, we evaluate the magnetic dipole hyperfine structure constants ($A_{hf}$) and the electric dipole (E1) transition amplitudes, and compare them with their respective experimental values. These quantities were evaluated using the expression

$$\langle O \rangle_{fi} = \frac{\langle \Psi^{(0)}_f | O | \Psi^{(0)}_i \rangle}{\sqrt{\langle \Psi^{(0)}_f | \Psi^{(0)}_f \rangle \langle \Psi^{(0)}_i | \Psi^{(0)}_i \rangle}}$$

$$\simeq \frac{\langle \Phi_f | \{S^{(0)}_i + 1\} O \{1 + S^{(0)}_i\} | \Phi_i \rangle}{\langle \Phi_f | \{S^{(0)}_i + 1\} N \{1 + S^{(0)}_i\} | \Phi_i \rangle}, \quad (48)$$

where $\sigma = e^{T^{(0)}} O e^{T^{(0)}}$ for the operator $O$ representing the respective property and $\overline{N} = e^{T^{(0)}_{RMP}} e^{T^{(0)}}$. In the evaluation of $A_{hf}$, we set $|\Psi^{(0)}_f\rangle = |\Psi^{(0)}_i\rangle$. Both $\overline{O}$ and $\overline{N}$ are the non-terminating series, which are evaluated by adopting iterative procedures as described in Refs. $^{48}$ $^{49}$ $^{54}$. We also present results from the RMP(2) and RLCCSD methods to make a comparative analysis of trend of correlation effects in the determination of the aforementioned properties. We have used $g_I = \mu_I / I = 0.737885714$ with nuclear magnetic moment

| Method       | 6S  | 6P1/2 | 7S  | 7P1/2 | 8P1/2 |
|--------------|-----|-------|-----|-------|-------|
| Dirac-Coulomb contributions |
| DHF          | 1433.96 | 161.07 | 394.12 | 57.69 | 27.01 |
| RMP(2)       | 2317.02 | 267.09 | 559.62 | 89.08 | 40.95 |
| RLCCSD       | 2492.22 | 311.80 | 571.67 | 98.45 | 44.21 |
| RCCSD        | 2328.40 | 286.48 | 548.65 | 92.52 | 41.79 |
| RCCSDT       | 2308.52 | 290.21 | 548.48 | 94.03 | 41.65 |

Corrections from Breit interaction

| Method       | 6S  | 6P1/2 | 7S  | 7P1/2 | 8P1/2 |
|--------------|-----|-------|-----|-------|-------|
| DHF          | 0.01 | 0.01  | -1.18 | 0.004 | \(\sim \) 0.0 |
| RMP(2)       | -7.29 | -0.05 | -1.61 | 0.02  | 0.01  |
| RLCCSD       | -8.22 | -0.06 | -1.69 | 0.01  | \(\sim \) 0.0 |
| RCCSD        | -7.58 | -0.05 | -1.65 | 0.01  | \(\sim \) 0.0 |
| RCCSDT       | -7.28 | -0.05 | -1.51 | 0.01  | \(\sim \) 0.0 |

$\Delta$BW

-6.74 $\sim$ -0.09 $\sim$ -1.62 $\sim$ -0.02 $\sim$ 0.02

Extra

7.98 $\sim$ 0.65 $\sim$ 0.86 $\sim$ 0.39 $\sim$ 0.0

Final

2306(10) $\sim$ 291(2) $\sim$ 547(2) $\sim$ 94(1) $\sim$ 42(1)

Experiment

2298.16$^a$ $\sim$ 291.91$^b$ $\sim$ 545.82$^c$ $\sim$ 94.03$^d$ $\sim$ 42.97$^e$

$^a$ $^{62}$; $^b$ $^{63}$; $^c$ $^{64}$; $^d$ $^{65}$; $^e$ $^{66}$.

$\mu_I$ for the evaluation of $A_{hf}$ values. We have also taken into account the Bohr-Weisskopf (BW) effect by defining the nuclear magnetization function ($F(r)$) in the Fermi nuclear charge distribution approximation as

$$F(r) = \frac{f_{WS}}{N}(r/b)^3 - 3(a/b)(r/b)^2 R_1((b - r)/a)$$

$$+ 6(a/b)^2(r/b) R_2((b - r)/a) - 6(a/b)^3$$

$$\times R_3((b - r)/a) + 6(a/b)^3 R_3(b/a),$$

(49)

for $r \leq b$ and

$$F(r) = 1 - \frac{1}{N} \left[ 3(a/b)(r/b)^2 R_1((r - b)/a)$$

$$+ 6(a/b)^2(r/b) R_2((r - b)/a) \right]$$

(50)

for $r > b$, where

$$N = 1 + (a/b)^2 \pi^2 + 6(a/b)^3 R_3(b/a),$$

and

$$R_k(x) = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{e^{-nx}}{n^k}.$$  

(52)
TABLE III. Magnitudes of the reduced E1 matrix elements in atomic units (a.u.) are given at different levels approximations of many-body theory. Corrections from the Breit and QED interactions are given as $\Delta$Breit and $\Delta$QED, respectively, and extrapolated contributions are given as “Extra”. The final values are given along with the uncertainties and compared with the extracted values from the latest experiments.

| Transition   | DHF  | RMP(2) | RLCCSD | RCCSD | RCCSDT | $\Delta$Breit | $\Delta$QED | Extra | Final | Experiment |
|--------------|------|--------|--------|-------|--------|--------------|-------------|-------|------|-----------|
| $6P_{1/2} \rightarrow 6S$ | 5.2777 | 4.5877 | 4.4740 | 4.5445 | 4.5023 | −0.0002 | 0.0011 | 0.0035 | 4.5067(40) | 4.508 [67] |
| $7P_{1/2} \rightarrow 6S$ | 0.3717 | 0.2233 | 0.2962 | 0.2989 | 0.2804 | 0.0006 | −0.0008 | 0.0003 | 0.2805(20) | 0.27810 [68] |
| $8P_{1/2} \rightarrow 6S$ | 0.1321 | 0.8996 | 0.0902 | 0.0919 | 0.0817 | 0.0007 | −0.0005 | 0.0005 | 0.0824(10) |               |
| $6P_{1/2} \rightarrow 7S$ | 4.4131 | 4.4428 | 4.2925 | 4.2528 | 4.2510 | 0.0041 | −0.0017 | 0.0025 | 4.2559(30) | 4.249 [69] |
| $7P_{1/2} \rightarrow 7S$ | 11.0121 | 10.2646 | 10.2481 | 10.2921 | 10.2795 | −0.0015 | 0.0025 | 0.0110 | 10.2915(100) | 10.308 [70] |
| $8P_{1/2} \rightarrow 7S$ | 0.9336 | 0.9437 | 0.9431 | 0.9501 | 0.9602 | 0.0028 | −0.0015 | 0.0005 | 0.9623(20) |               |

In Eq. (54), $f_{WF}$ takes into account the Woods-Saxon (WS) potential correction and is estimated after neglecting the spin-orbit interaction within the nucleus using the following expressions:

$$f_{WS} = 1 - \left( \frac{3}{\mu I} \right) \ln \left( \frac{r}{b} \right) \left[ \frac{2I - 1}{8(I + 1)} g_S + (I - 1/2) g_L \right]$$

for $I = L + \frac{1}{2}$ and

$$f_{WS} = 1 - \left( \frac{3}{\mu I} \right) \ln \left( \frac{r}{b} \right) \left[ \frac{2I + 3}{8(I + 1)} g_S + \frac{I(2I + 3)}{2(I + 1)} g_L \right]$$

for $I = L - \frac{1}{2}$ with the total orbital angular momentum $L$ of the nucleus. We have used the nuclear parameters $g_L = 1$ and $g_S = 4.143$ for $^{133}$Cs atom [52].

F. Evaluation of E1$_{PV}$

In the RCC theory framework, Eq. (20) is given by

$$E1_{PV} \simeq \left< \Phi_f \right| \left( S_f^{(1)} + S_f^{(0)} + 1 \right) T(1) \left| \Phi_i \right> \overline{D} \{1 + S_i^{(0)} \} \Phi_i + \left< \Phi_f \right| \left( S_f^{(0)} + 1 \right) \overline{D} \{T(1)(1 + S_i^{(0)}) + S_i^{(1)} \} \Phi_i \Phi_i$$

where $\overline{D} = e^{T(0)} D e^{T(0)}$ and $\overline{N} = e^{T(0)} N e^{T(0)}$. Contributions from the non-terminating expressions $\overline{D}$ and $\overline{N}$ are estimated by an iterative approach similar to that used in the expression for evaluating properties, which is given in Eq. (48). The “Core” contributions for the initial and final states originate from $T(1) \left| \Phi_i \right>$ and $\left| \Phi_i \right>$, respectively, and the rest of the RCC terms involving $S_f^{(0)}$ and $S_i^{(0)}$ give rise to valence contributions from the ‘final’ and ‘initial’ states, respectively. The simultaneous presence of both the electromagnetic and NSI weak interactions through the RCC operators account for core and valence correlation contributions, including the DCP correlation effects.

G. Basis functions

We have used Gaussian type orbitals (GTOs) [57] to construct the single particle DHF wave functions. The radial components for the large and small components of DHF orbitals are expressed using these GTOs as

$$P(r) = \sum_{k=1}^{N_k} c_k \zeta_k r^l e^{-\alpha_0 \beta^k r^2}$$

and

$$Q(r) = \sum_{k=1}^{N_k} c_k \zeta_k \zeta S \left( \frac{d}{dr} + \frac{\kappa}{r} \right) r^l e^{-\alpha_0 \beta^k r^2},$$

where $P(r)$ and $Q(r)$ are the large and small radial components of the DHF orbitals, $l$ is the orbital quantum number, $\kappa$ is the relativistic angular momentum quantum number, $c_k$ are the expansion coefficients, $\zeta_k$ are the normalization factors of GTOs, $\alpha_0$ and $\beta$ are optimized GTO parameters for a given orbital, and $N_k$ represents the number of GTOs used. We have considered 40 GTOs for each symmetry up to $l = 6$ for the RCC calculations and up to $l = 9$ for analyzing results using the RMP(2) method. For the construction of GTOs, the values of $\alpha_0$ we use are 0.0009, 0.0008, 0.001, 0.004 and 0.005 for the $s$, $p$, $d$, $f$ and other higher angular momentum symmetry orbitals, respectively. The corresponding $\beta$ values we have used are 2.15, 2.15, 2.15, 2.25 and 2.35 for the $s$, $p$, $d$, $f$ and other higher symmetry orbitals, respectively. Since our orbitals are not bounded by a cavity, we carry out the numerical integration of radial integrals up to $r = 500$ a.u. using a 10-point Newton-Cotes Gaussian quadrature formula on grids. Non-linear grids are defined, as in Ref. [58], for the numerical calculations with the step-size 0.0199 a.u. over 1200 grid points. We have considered excitations from all the occupied orbitals, but limited the virtual space to excitations of orbitals in that space with energies less than 2000 a.u. This includes 1–19s, 2–19p, 3–19d, 4–18f, 5–16g, 6–15h and 7–15i-symmetry orbitals. These orbitals will be referred to as the “active orbitals” hereafter.
TABLE IV. List of the experimental values of $E_1$ matrix elements (in a.u.) for a few low-lying transitions reported over the years using different measurement techniques.

| Transition | Value     | Reference | Year |
|------------|-----------|-----------|------|
| $6P_{1/2} \leftrightarrow 6S$ | 4.5097(74) | [71]  | 1994 |
|           | 4.4890(65) | [72]  | 1999 |
|           | 4.505(2)   | [73]  | 2015 |
|           | 4.508(4)   | [74]  | 2015 |
| $7P_{1/2} \leftrightarrow 6S$ | 0.2825(20) | [75]  | 2002 |
|           | 0.2789(16) | [76]  | 2013 |
|           | 0.27810(45) | [77] | 2019 |
| $8P_{1/2} \leftrightarrow 6S$ | Not available yet | | |
| $6P_{1/2} \leftrightarrow 7S$ | 4.233(22) | [78]  | 1984 |
|           | 4.249(4)   | [79]  | 2019 |
| $7P_{1/2} \leftrightarrow 7S$ | 10.308(15) | [80]  | 1999 |
| $8P_{1/2} \leftrightarrow 7S$ | Not available yet | | |

IV. RESULTS AND DISCUSSION

A. Cs APV calculations & context of present work

The main thrust of our present work is a high-precision calculation of $E_{1 PV}$ for the $6s^2S_{1/2} \rightarrow 7s^2S_{1/2}$ in $^{133}$Cs; the transition on which the most accurate APV measurement (0.35% accuracy) has been carried out to date [8]. As mentioned earlier, a considerable amount of effort has also gone into performing very accurate calculations on $E_{1 PV}$ using state-of-the-art relativistic many-body theories (e.g. see [19] and references therein). At the time of the last Cs APV measurement, the accuracies of the atomic calculations were about 1% [20,27]. Later by using the amended values of the $E_1$ matrix elements inferred from the high precision measurements of lifetimes and polarizabilities of atomic states, the uncertainty in the calculation was reduced to 0.4% [50]. This yielded a $Q_{WS}^0$ that disagreed with its SM value by 2.5σ. Subsequently, the leading order relativistic correction from the Breit interaction and the lower-order QED effects and the neutron skin were included in the atomic calculations (refer to [28,30] for discussions). As pointed out before, there has been a renewed interest in the inclusion of the neglected correlation effects in Cs APV since about a decade. (e.g. see discussions in [16,33]). The latest calculations including the effect of the valence triple excitations were investigated by employing the RCC theory, and it was found that their contributions to the atomic properties of $^{133}$Cs were relatively important in reducing the uncertainty in the $E_{1 PV}$ amplitude to 0.27% [31].

This result is in good agreement with the SM, however the calculation on which it is based had used a sum-over-states approach in which the leading contributions from the excited states up to the principal quantum number $n = 9$ were estimated by using matrix elements, calculated using the RCC theory and referred to as “Main” contribution. The rest were classified into “Core” and “Tail”, and they were evaluated using mixed many-body methods [31]. Later, Dzuba et al. reported another result with 0.5% accuracy by evaluating the “Main” contribution, again, using a sum-over-states approach but with different “Core” (opposite sign than [31]) and “Tail” contributions by taking into account certain sub-classes of correlation effects [19]. This resulted in a difference of about 0.8% between the $E_{1 PV}$ calculations of Porsev et al [31] and Dzuba et al. [19].

Following these works, Roberts et al. have reported the contributions from QED and DCP effects [52,56]. There are still unresolved issues in the determination of electron correlation in Cs APV due to the disparate approaches that have been used in the treatment of different physical effects in the low- and high-lying excited states. In other words, the “Main”, “Tail” and “Core” contributions have not been evaluated on par with each other. Also, the Breit interaction and the effective QED interactions have not been treated at the same level as the DC interaction in Refs. [19,31]. The contributions from the triple excitations involving core orbitals were not determined in Ref. [31].

In contrast to the previous previous works, our calculation of the $E_{1 PV}$ amplitude adopts an approach based on the perturbed RCC theory as outlined above. We excite all the core electrons in our RMP(2), RLCSSD and RCCSD calculations to account for the electron correlation effects. However, we correlate all the electrons except the $1 - 3s$, $2 - 3p$, and $3d$ occupied orbitals and beyond $n = 15$ virtual orbitals for triple excitations due to limitations in the available computational resources.

B. Ancillary Properties

At the outset, we would like to reemphasize that it is customary to compare the results of the calculations of energies, $E_1$ matrix elements and $A_{hyf}$ values based on a many-body theory with the available experimental data to assess the accuracy of the $E_{1 PV}$ amplitude. We give values for all these quantities by taking into account contributions from the DC Hamiltonian, the Breit interaction, and the QED effects at different levels of approximation in the many-body methods systematically. We have also estimated the contributions to different properties by extrapolating our basis functions to infinite-size, which we have referred to as “Extra”, and given their values. The uncertainties in our calculations are estimated by analyzing the optimized GTOs used in the calculations and contributions from the higher level excitations that are neglected here.

In Table II we give the final EA values from our calculations and these values are compared with the precise measurements listed in the National Institute of Science and Technology (NIST) database [61]. Following this, we have given the $A_{hyf}$ values in Table III using different methods. After adding up all the contributions along with corrections from the BW effect, the final values are compared with the high-precision experimental values [52,56]. It can be seen that the triple excitations
TABLE V. Magnitudes of the $H_{APV}^{NSI}$ matrix elements in $-i(Q_W/N) \times 10^{-11}$ from different methods. Corrections from the Breit and QED interactions are given as $\Delta$Breit and $\Delta$QED, respectively. The final values after including “Extra” contributions are given along with the uncertainties in the parentheses. The quantity $\chi$ is defined as $\chi = |[R_{th}/R_{ex}] - 1| \times (\Psi^0_k|H_{APV}^{NSI}|\Psi^0_v)$ for the corresponding theoretical (denoted with subscript th) and experimental (denoted with subscript ex) values, where $\mathcal{R} = \sqrt{A_{hyf}^k A_{hyf}^v}$ with superscripts $k$ and $v$ designated for the states with valence orbitals $k$ and $v$, respectively.

| $|\Psi^0_k\rangle \rightarrow |\Psi^0_v\rangle$ | DHF | RMP(2) | RLCCSD | RCCSD | RCCSDT | $\Delta$Breit | $\Delta$QED | Extra | Final | $\chi$ |
|-----------------|------|-------|--------|--------|---------|---------------|-------------|--------|--------|--------|
| $6P_{1/2} \rightarrow 6S$ | 0.7286 | 1.1955 | 1.3536 | 1.2567 | 1.2725 | -0.0066 | -0.0055 | 0.0010 | 1.2648(15) | 0.0002 |
| $7P_{1/2} \rightarrow 6S$ | 0.4362 | 0.6009 | 0.7628 | 0.7164 | 0.7268 | -0.0036 | -0.0030 | 0.0008 | 0.7210(15) | 0.0004 |
| $8P_{1/2} \rightarrow 6S$ | 0.2985 | 0.3782 | 0.5117 | 0.4823 | 0.4821 | -0.0024 | -0.0021 | 0.0007 | 0.4783(10) | 0.0010 |
| $6P_{3/2} \rightarrow 7S$ | 0.3820 | 0.5891 | 0.6456 | 0.6094 | 0.6205 | -0.0032 | -0.0022 | 0.0010 | 0.6161(15) | 0.0005 |
| $7P_{3/2} \rightarrow 7S$ | 0.2287 | 0.3393 | 0.3624 | 0.3458 | 0.3493 | -0.0019 | -0.0015 | 0.0005 | 0.3464(10) | 0.0010 |
| $8P_{3/2} \rightarrow 7S$ | 0.1565 | 0.2117 | 0.2425 | 0.2321 | 0.2314 | -0.0012 | -0.0009 | 0.0003 | 0.2296(05) | 0.0013 |

TABLE VI. Correlation contribution to the $E1_{PV}$ amplitude (in $-i(Q_W/N)\sigma_0 \times 10^{-11}$) of the $6s^2 2S_1/2 - 7s^2 2S_1/2$ transition in $^{133}$Cs from different terms of the RLCCSD, RCCSD and RCCSDT methods. ‘Others’ are the terms including correction due to normalization of wave functions that are not mentioned explicitly. Contributions corresponding to “Core” and “Valence” correlations are given separately to distinguish them. $\mathcal{T} \equiv D$ in the RLCCSD method approximation.

| RCC term | RLCCSD | RCCSD | RCCSDT |
|-----------|--------|--------|--------|
| Core contributions | $D_{S_0}^{(1)}$ | -0.0534 | -0.0410 | -0.0410 |
| Others | $T_{1}^{(1)}$ | 0.0519 | 0.0392 | 0.0392 |
| Total | $\mathcal{T}$ | -0.0016 | -0.0019 | -0.0018 |

Valence (Main+Tail) contributions

| $T_{1}^{(1)}$ | -0.1663 | -0.1913 | -0.1874 |
| $S_{1}^{(1)}$ | 2.0603 | 1.8064 | 1.7925 |
| $S_{2}^{(1)}$ | -0.3045 | -0.2336 | -0.2288 |
| $S_{1}^{(0)}$ | -0.5529 | -0.4218 | -0.4417 |
| $T_{2}^{(0)}$ | -0.0357 | -0.0263 | -0.0254 |
| $T_{3}^{(0)}$ | 0.0006 | 0.0009 | 0.0004 |
| $S_{2}^{(0)}$ | -0.0019 | -0.0007 | -0.0006 |
| Total | 0.9407 | 0.8980 | 0.8985 |

C. $E1_{PV}$ results

In Table [V] we present and compare our $E1_{PV}$ results for the $6s^2 2S_1/2 - 7s^2 2S_1/2$ transition in $^{133}$Cs from different terms of the RLCCSD, RCCSD and RCCSDT approximations. For the sake of brevity, we present contributions from terms representing “Core” correlations and valence correlations separately in the same table. It should be noted that these valence correlation contributing terms contain both “Main” and “Tail” contributions of the sum-over-states approach implicitly. As can be calculations and the experimental values [69–72] is found to be quite good. However, we would like to mention that the experimental values of these matrix elements have been reported differently over the time [69–72]; sometime they do not even agree within the quoted error bars as can be found from the list given in Table [V]. Nonetheless, it can be seen from Table [III] that the DHF values of E1 matrix elements are large in magnitude and they reduce successively after the inclusion of the correlation effects at the RCCSD and RCCSDT levels. The triples contributions to the E1 matrix elements are more significant than those in the case of other properties for $^{133}$Cs. Similarly, the matrix elements of $H_{APV}^{NSI}$ are given in Table [VI]. As can be seen from this table, the correlation trends in the matrix elements of $H_{APV}^{NSI}$ are completely different than those for the E1 matrix elements but almost similar to those of $A_{hyf}$. We analyze the accuracies of $\mathcal{R} = \sqrt{A_{hyf}^k A_{hyf}^v}$, the superscripts $k$ and $v$ denoting for states with valence orbitals $k$ and $v$ respectively, by comparing our theoretical values with the experimental results. This is used to determine the accuracy of the $\langle \Psi_k|H_{APV}^{NSI}|\Psi_v \rangle$ matrix elements and their accuracies are quantified by evaluating $\chi = |[R_{th}/R_{ex}] - 1| \times (\Psi^0_k|H_{APV}^{NSI}|\Psi^0_v)$ values, with subscripts th and ex referring to our theoretical values and experimental results respectively, for important low-lying states. These values are found to be very small, implying that the $H_{APV}^{NSI}$ matrix elements are obtained quite accurately by us.

improve the $A_{hyf}$ results of the $P_{1/2}$ states quite significantly. Contributions from the Breit and QED interactions are non-negligible for achieving high precision results. We give the values of the reduced matrix elements of $D$ of important transitions along with their error bars in Table [III]. The extracted E1 matrix elements from the latest precise measurements of lifetimes and Stark shifts are given in the same table. The agreement between our
and that there are significant changes in that the
D and compared are also quoted.

Using the Dirac-Coulomb Hamiltonian in the DHF, RCCSD and RCCSDT methods. Valence contributions are given in the continuum. Contributions from the extrapolated basis function, “Extra” and neutral weak interactions among electrons \((e-e)\) are also quoted.

| Method | Core | Main | Tail | Extra | \(e-e\) |
|--------|------|------|------|-------|---------|
| DHF    | -0.0017 | 0.7264 | 0.0137 |
| RCCSD  | -0.0019 | 0.8623 | 0.0357 |
| RCCSDT | -0.0018 | 0.8594 | 0.0391 | 0.0026 | 0.0003 |

\(^†\) Contains additional contribution from the 9p \(^2\)\(P_{1/2}\) state.

seen from the table, the RLCCSD result seems to be relatively large, but the rather small difference between the RCCSD and RCCSDT values suggests the convergence of the results after the inclusion of higher level particle-hole excitations. The fairly large RLCCSD value is not entirely surprising, given that in this method there have been quite significant deviations of various spectroscopic properties from their experimental values as discussed in the previous subsection. The differences in the spectroscopic properties at the RCCSD and RCCSDT levels are somewhat large, and their trends are nonuniform. For example, it can be seen from Tables I and III that the calculated energies and E1 matrix elements decrease in going from the RCCSD method to the RCCSDT method, while the matrix elements of \(H_{\text{APV}}^{\text{NSI}}\), given in Table IV increase. This is the reason for the small difference between the RCCSD and RCCSDT E1\(PV\) values. It can be seen from Table VI that there are significant changes in the core contributions through the individual RCC terms in the RLCCSD and RCCSD methods, but the differences in the RCCSD and RCCSDT methods are negligibly small. However, we find that changes in the valence correlations from different RCC terms in all the three approximations are relatively large. Compared to contributions from the first-order perturbed \(\mathbf{T}S_{1i}^{(1)}\) term of the ground state, the perturbed \(S_{1f}^{(1)}\)\(T\) term of the excited \(7S_{1/2}\) state contributes predominantly, which correspond to contributions mainly from the one-particle one-hole excitations. The contributions from the two-particle two-hole excitations to E1\(PV\) are found to be small, which are represented by \(\mathbf{T}S_{2i}^{(1)}\) and \(S_{2f}^{(1)}\)\(T\) for the perturbed wave functions of the ground and excited states, respectively. As mentioned above, there is a small difference between the final results from the RCCSD and RCCSDT methods. However, a comparison of the contributions of the individual terms obtained from both these methods reveals that there are significant differences among them. This is because the RCCSD wave functions change when triple excitations are added, due to the change in the coupled cluster amplitudes. However, this change leads to large cancellations among the net contributions of the individual terms arising through the initial and final perturbed wave functions resulting in a small difference in their final values. This is also in accordance with our analysis of energies and E1 matrix elements changing differently than the matrix elements of \(H_{\text{APV}}^{\text{NSI}}\) in both the methods, which are manifested in the contributions from the individual RCC terms in a different form. Nonetheless, the convergence of E1\(PV\) amplitude with the higher-level excitations in the framework of the RCC theory strongly suggests that the neglected correlation effects are indeed small.

By using the calculated energies, E1 matrix elements and amplitudes of \(H_{\text{APV}}^{\text{NSI}}\) for the intermediate \(n=6,7,8)P_{1/2}\) states at different levels of approximations in the tables previously discussed, we estimated the “Main” contributions for a qualitative comparison of its value with other results reported using the sum-over-states approach. Combining the “Main” contributions with the “Core” contributions, contributions from the “Tail” are estimated in the DHF, RCCSD and RCCSDT methods. This breakdown from the DHF, RCCSD and RCCSDT methods are given in Table VII and compared with the previously reported values from the sum-over-states approach. Our core contributions are in agreement with the values reported in [27, 31], but it differs from the latest calculation reported in [19]. Since the contribution from the \(9P_{1/2}\) state is not included in our “Main” contribution and contained in the “Tail”, it would be more appropriate to make comparison among the total valence correlation contributions (“Main+Tail”) from different calculations. We find that our valence correlation contributions are 0.8980 and 0.8985 from the RCCSD and RCCSDT methods, respectively, against the values 0.911 [27], 0.9018 [31], and 0.8916 [19] in units of \(10^{-11}i(-Q_W/N)e\alpha\). This shows that our valence correlation contribution is closer to that of [19]. In Table VII we also present contributions from the extrapolated basis functions, denoted as “Extra”, and a small contribution to E1\(PV\) from Ref. [27] due to possible neutral weak interactions among electrons \((e-e)\) that was not included in our calculation.

In Table VIII we also give contributions from the Breit and QED interactions using the RCCSDT method and compare them with the values reported by other approaches earlier [28, 30, 32, 60, 78]. We have also mentioned the many-body method employed by other works in the same table to estimate contributions from the Breit and QED interactions to E1\(PV\) of the \(6s^27S_{1/2}-7s^27S_{1/2}\) transition in \(^{133}\)Cs. We find consistency in the results obtained from various works. This means that these relativistic corrections are not influenced significantly by the electron correlation effects. Nonetheless, our method
is more rigorous than the previous calculations of these corrections to the above $E1_{PV}$ amplitude.

After taking into account contributions from the DC Hamiltonian, Breit interaction and QED effects from the RCCSDT method, the estimated value of “Extra” and small correction from the $e-e$ contribution, we obtain the $E1_{PV}$ amplitude of the $6s^2 S_{1/2} - 7s^2 S_{1/2}$ transition in $^{133}$Cs as $0.8914 \times 10^{-11} i(-Q_W/N)e\alpha$. To estimate its uncertainty, we adopt the following approach: We have taken the difference between the RCCSD and RCCSDT values to estimate the uncertainties in the core and valence contributions to $E1_{PV}$. The major source of error for this transition amplitude comes from the finite size of the basis used in our calculation, which is extrapolated to be $0.0026 \times 10^{-11} i(-Q_W/N)e\alpha$. We assume this as the maximum uncertainty arising from the incomplete basis functions. This approach to the estimation of the error is more rigorous than the one adopted in Ref. [31]. In the latter work, an uncertainty of 10% is assigned to the “Core” and “Tail” contributions based on the spread of their results in different approximations, and the uncertainty in “Main” is taken to be 0.18% by analyzing results from a calculation using an ab initio calculation and another obtained from scaled wave functions. We have also estimated the uncertainties from the Breit and QED contributions. Adding all the uncertainties mentioned above in quadrature, we find that the final uncertainty in $E1_{PV}$ is $0.0027 \times 10^{-11} i(-Q_W/N)e\alpha$.

We have given a list of the calculated $E1_{PV}$ amplitude of the $6s^2 S_{1/2} - 7s^2 S_{1/2}$ transition in $^{133}$Cs over the years in Table IX. We also mention the approaches used in the previous works to determine this quantity. As can be seen, apart from a few calculations, most of the previous results were reported either using the sum-over-states approach or by considering mixed many-body methods. The last two high-precision calculations were carried out by adopting the sum-over-states approach, and estimating “Core” and “Tail” contributions using different types of many-body methods. Our ab initio calculation has similar accuracy to those are obtained using the sum-over-states approach, but our error estimation is more rigorous than that of the latter. The most important feature of our work is that it treats correlation contributions from the “Core”, “Main” and “Tail” sectors at par with each other, thereby resolving the large discrepancy in the “Core” contribution between the works reported in Refs. [19] and [31] in an unambiguous manner.

D. Vector polarizability

An accurate determination of the vector ($\beta$) dipole polarizability of the $6s^2 S_{1/2} - 7s^2 S_{1/2}$ transition in $^{133}$Cs is imperative so that it can be combined with the measured value of $\text{Im}(E1_{PV}/\beta)$ and our high accuracy calculation of $E1_{PV}$ to extract $Q_V^\alpha$. A very precise measurement of $\alpha/\beta = -9.905(11)$ has been reported by Cho et al. [81], where $\alpha$ is the scalar dipole polarizability of the transi-

\begin{table}[h]
\centering
\caption{Comparison of contributions from the Breit and QED interactions to the $E1_{PV}$ amplitude (in $-i(Q_W/N)e\alpha \times 10^{-11}$) of the $6s^2 S_{1/2} - 7s^2 S_{1/2}$ transition in $^{133}$Cs from various methods employed by different works.}
\begin{tabular}{|c|c|c|c|}
\hline
Breit & QED & Method & Reference \\
\hline
-0.0055(5) & -0.0028(3) & RCCSDT & This work \\
-0.0029(3) & Correlation potential & Ref. [42] \\
-0.0054 & RMP(3) & Ref. [28] \\
-0.004 & Optimal energy & Ref. [29] \\
-0.33(4)% & Radiative potential & Ref. [60] \\
-0.0055 & Correlation potential & Ref. [70] \\
-0.0045 & Local DHF potential & Ref. [30] \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Progresses in the atomic calculation of the $E1_{PV}$ amplitude (in $-i(Q_W/N)e\alpha \times 10^{-11}$) of the $6s^2 S_{1/2} - 7s^2 S_{1/2}$ transition in $^{133}$Cs over the years by adopting various approaches.}
\begin{tabular}{|c|c|c|c|}
\hline
Year & Result & Approach & Reference \\
\hline
1989 & 0.908(9) & Ab initio & Ref. [26] \\
1990 & 0.909(4) & Sum-over-states & Ref. [27] \\
2000 & 0.8991(36) & Ref. [27] + Breit & Ref. [28] \\
2001 & 0.901 & Scaled optimal energy & Ref. [29] \\
2002 & 0.904(5) & Ab initio & Ref. [70] \\
2005 & 0.904 & Ref. [70] + QED corr. & Ref. [30] \\
2009 & 0.8906(24) & Sum-over-states & Ref. [31] \\
2012 & 0.8977(40) & Ref. [31] + core corr. & Ref. [19] \\
2020 & 0.8914(27) & Ab initio & This work \\
\hline
\end{tabular}
\end{table}

\begin{table}[h]
\centering
\caption{Contributions to the scalar dipole polarizability ($\alpha$) of the $6s^2 S_{1/2} - 7s^2 S_{1/2}$ transition in $^{133}$Cs using the most precise $E1$ matrix element amplitudes from the available measurements and our calculations. We have used experimental energies from the NIST database [61] to reduce the uncertainty in the result. Estimated uncertainties from the $E1$ matrix element amplitudes are quoted within the parentheses.}
\begin{tabular}{|c|c|c|c|c|}
\hline
Intermediate state & Initial state & Final state & Contribution & (in a.u.) \\
$6s^2 S_{1/2}$ & $7s^2 S_{1/2}$ & & & \\
\hline
$\rightarrow 6p^2 P_{1/2}$ & 4.5067(40) & -4.2559(30) & -32.60(6) \\
$\rightarrow 6p^2 P_{3/2}$ & 6.345(8) & -6.8890(50) & -93.01(15) \\
$\rightarrow 7p^2 P_{1/2}$ & 0.27810(45) & 10.2095(100) & -37.22(10) \\
$\rightarrow 7p^2 P_{3/2}$ & 0.57417(57) & -14.2703(120) & -101.53(18) \\
$\rightarrow 8p^2 P_{1/2}$ & 0.0824(10) & -0.19623(20) & -0.52(1) \\
$\rightarrow 8p^2 P_{3/2}$ & 0.2294(15) & 1.17115(20) & -2.54(2) \\
$\rightarrow 9p^2 P_{1/2}$ & -0.0424(15) & -0.3896(15) & -0.08(1) \\
$\rightarrow 9p^2 P_{3/2}$ & 0.1268(10) & 1.7388(20) & -0.50(1) \\
\hline
Core & & & 0.1999(50) & 0.8547(500) \\
$n > 9$ & & & -268.65(27) \\
\hline
Total & & & & \\
\hline
\end{tabular}
\end{table}

References: [67]; [68]; [69].
tion. The $\alpha$ value for the transition $|\Psi_i\rangle \rightarrow |\Psi_f\rangle$ can be expressed as

$$
\alpha = \sum_k \frac{\langle \Psi_f^{(0)} | D | \Psi_i^{(0)} \rangle \langle \Psi_i^{(0)} | D | \Psi_f^{(0)} \rangle}{\sqrt{\langle \Psi_f^{(0)} | \Psi_f^{(0)} \rangle \langle \Psi_i^{(0)} | \Psi_i^{(0)} \rangle}} \times \left[ \frac{1}{E_f^{(0)} - E_k^{(0)}} + \frac{1}{E_i^{(0)} - E_k^{(0)}} \right]. \quad (56)
$$

As in the case of $E_{1\nu}$, the contributions to $\alpha$ come from the “Core”, “Main” and “Tail” regions. We have included the $E_1$ matrix elements up to the $9P$ states in this estimation. Most of these matrix elements were calculated in the present work using the RCCSDT method, except a few for which very accurate experimental data are available $[27, 28]$. We have also used measured values of the energies in our calculations. The contributions from the “Core” and “Tail” were estimated to be small using the RMP(2) method. The individual contributions from “Main” that come from the low-lying intermediate states, “Core” and “Tail” are given in Table XI. The matrix elements used from different works are presented in the same table. As can be seen from the table, the maximum contribution to $\alpha$ of the $6s \ 2S_{1/2} - 7s \ 2S_{1/2}$ transition in $^{133}\text{Cs}$ comes from the $7p \ 2P_{3/2}$ state followed by the $6p \ 2P_{3/2}$ state. The contributions from the $8P$ state onwards are found to be small. Our final value is $\alpha = -268.65(27) e a_0^3$. Another recent study has found this value to be $-268.82(30) e a_0^3$ $[80]$, where contributions from many matrix elements were included explicitly by analyzing them from the literature. They had estimated the “Core” and “Tail” contributions using the DHT method, whereas we have done so using the RMP(2) method. Nonetheless, we find very good agreement between both the results. By combining our value for $\alpha$ with the measured ratio of $\alpha/\beta = -9.905(11)$ $[81]$, we obtain the vector polarizability for this transition as $\beta = 27.12(4) e a_0^3$. The accuracy of this quantity is about 0.15%; even better than the accuracy of our calculated $E_{1\nu}$ for the above transition. In Ref. $[80]$, a summary of the results for $\beta$ have been presented, the variation in these values covers a wide range. Our result is in agreement with all those values, but with a precision similar to the most accurate one $[81]$.

E. Inferred $Q_W$ value and its implications

Combining our results of $E_{1\nu}$ and $\beta$ with the precisely measured $\text{Im}(E_{1\nu}/\beta) = 1.5935(56)$ mV/cm $[8]$, where $\text{Im}$ means imaginary part, for the $6s \ 2S_{1/2} - 7s \ 2S_{1/2}$ transition in $^{133}\text{Cs}$, we get $Q_W^{\nu} = -73.54(26)_{es}(22)_{th}$. After accounting for the nuclear skin effect $[24]$, we get

$$
Q_W = Q_W^{\nu} + \Delta Q_W^{N-P} = -73.54(26)_{es}(22)_{th} + 0.064 = -73.48(20)_{es}(23)_{th}. \quad (57)
$$

This result in the difference between the value of $Q_W$ obtained from our calculation and the SM value $Q_W^{\text{SM}} = -73.23(1) [24]$ as $\Delta Q_W = Q_W - Q_W^{\text{SM}} = -0.25(34)$ at 1σ level.

From the relation $Q_W = -N + Z(1 - 4\sin^2 \theta_W)$, we can derive as

$$
Q_W \approx -N + Z[1 - 4(\sin^2 \theta_W^{\text{SM}} + \Delta \sin^2 \theta_W)] = Q_W^{\text{SM}} - 4\Delta \sin^2 \theta_W.
$$

$$
\Rightarrow \Delta Q_W \approx -4Z\Delta \sin^2 \theta_W. \quad (58)
$$

This gives change in $\sin^2 \theta_W$ as $\Delta(\sin^2 \theta_W) = 0.0011(15)$. Accounting for this correction along with its SM value $\sin^2 \theta_W^{\text{SM}} = 0.23857(5)$ at the zero momentum transfer in the MS scheme $[21]$, we get a new value for $\sin^2 \theta_W(0) = 0.23967(150)$. In Fig. 1 we plot deviation in running of $\Delta \sin^2 \theta_W(Q^2)$ with respect to $\sin^2 \theta_W(m_Z, )^{\text{SM}}$ from the SM and the deviation obtained in this work at $Q^2 = 30$ MeV corresponding to the experiment on $^{133}\text{Cs} [77]$. It can be seen that the $\Delta \sin^2 \theta_W$ value obtained from the present study agrees quite well with the SM.

From the above $\Delta Q_W$ value, we constrain the isospin conserving parameter $S \approx 0.31(43)$ after neglecting the contribution from the isospin breaking parameter $T$ from the relation $\Delta Q_W \approx -0.8S - 0.007T [12]$. Furthermore, in the SO(10) model $[12]$

$$
\Delta Q_W \approx 0.4(2N + Z) \frac{M^2_W}{M^2_{Z^*}}, \quad (59)
$$

we get a lower limit $M_{Z^*} > 961$ GeV/c^2 compared to 3.5 TeV/c^2 from the observation using the ATLAS detector $[82]$. Furthermore, $\Delta Q_W$ can be expressed in the dark photon model characterized by $U(1)_d$ gauge symmetry as $[21]$

$$
\Delta Q_W = 220 \left( \frac{\varepsilon}{\varepsilon_z} \right) \sin \theta_W \cos \theta_W \delta^2 - Q_W^{\text{SM}} \delta^2, \quad (60)
$$

FIG. 1. Plot demonstrating deviation of $\Delta \sin^2 \theta_W(Q^2)$ (in percentage) in the SM from $\sin^2 \theta_W(m_Z, )^{\text{SM}} = 0.23124(6)$ with energy scale $(Q)$ in GeV. The value obtained using the present APV study in $^{133}\text{Cs}$ is shown at $Q^2 = 30$ MeV, which shows good agreement with the SM.
where $\varepsilon$ is a dimensionless parameter, $\varepsilon_z = \delta M_{Zd}/M_{Zd}$, and $\delta$ is a model dependent quantity. Substituting the aforementioned SM values, we get

$$\left[1.28(1) \left(\frac{\varepsilon}{\varepsilon_z}\right) - 1\right] \delta^2 \simeq 0.0034(46). \quad (61)$$

Using the effective field theory, suggested in Ref. [22], we obtain

$$f^{ff}_{Vq}/\Lambda^2 \simeq -26(35) \times 10^{-10} \text{GeV}^{-2}. \quad (62)$$

Similarly, in terms of the nucleon-electron V-A couplings, defined in Ref. [20], it yields $55g^{ep} + 78g^{em} = 36.82(25)$.

V. SUMMARY

We have revisited the calculation of electric dipole amplitude due to the nuclear spin independent neutral weak interaction for the $6s^2 S_1/2 - 7s^2 S_1/2$ transition in $^{133}\text{Cs}$ by employing the relativistic coupled-cluster theory. In our approach, we solve an inhomogeneous equation to obtain the first-order perturbed wave function due to the weak interaction in order to account for the correlation effects of the electrons from the occupied, valence and virtual orbitals on an equal footing. This resolves the large discrepancy, including sign, for the core electron correlation contribution to the above amplitude between the two latest high accuracy calculations. Moreover, it includes contributions from correlation effects due to the double core-polarization, the Breit interaction and lower-order quantum electrodynamics effects by the same method used to incorporate contributions from the Dirac-Coulomb atomic Hamiltonian. Relevant spectroscopic properties have been evaluated at different levels of many-body approximations and the role of electron correlation effects arising from higher-level particle-hole excitations, in particular the triple excitations, have been demonstrated to be non-negligible. By analyzing the differences between these calculated results and their respective high-precision experimental values, the accuracy of the above electric dipole transition amplitude is estimated and found to be of the order of 0.3%. This is slightly better than the reported accuracy of the corresponding measurement. We have determined the vector polarizability of the above transition with an accuracy of 0.15%. Combining all our calculated values with the measurement, we have obtained the nuclear weak charge $Q_W = -73.48(26)_{ex}(23)_{th}$ for $^{133}\text{Cs}$, which differs from the Standard Model value by $-0.25(34)$. By considering certain extensions of the Standard Model of current interest, we have discussed the salient implications of this discrepancy in the nuclear weak charge for possible new physics. Our findings are in agreement with the Standard Model predictions.

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