$E1$ parity-nonconserving transition amplitudes of the hyperfine components for $^2S_{1/2}$-$^2D_{3/2}$ transitions of $^{137}Ba^+$ and $^{87}Sr^+$

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In this paper, we have calculated parity nonconserving electric dipole amplitudes of the hyperfine components for the transitions between the ground and first excited states of $^{137}Ba^+$ and $^{87}Sr^+$ using sum-over-states technique. The results are presented to extract the constants associated with the nuclear spin-dependent amplitudes from experimental measurements. The wave functions to calculate the most dominant part of the sums are constructed using highly correlated coupled-cluster theory based on the Dirac-Coulomb-Gaunt Hamiltonian.

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I. INTRODUCTION

The anapole moment (AM) is a parity-violating electromagnetic moment of a nucleus [1–3]. Calculations and measurements on parity-nonconservation- (PNC-) induced electric dipole ($E1$) transitions in atomic systems are being considered as an excellent way to estimate this moment [4,5]. It is the nuclear spin-dependent (NSD) part of the PNC that provides the value of the AM of a nucleus [1–4], whereas the dominant contribution to PNC arises from the nuclear spin-independent (NSI) part [6]. The NSI part depends on the weak nuclear charge. Investigation on the anapole values of various nuclei is a promising tool to put constraints on the PNC meson-nucleon coupling constants [1,3,7]. The anapole constant of the ^{133}Cs nucleus, which has a valence proton, was measured with near about 15% accuracy [3,8] by Wood *et al.* [9]. However, this anapole value is found to be inconsistent with some results obtained through different nuclear many-body theories [3] and also with the anapole value of the ^{205}Tl nucleus [3,10]. However, the latter was measured with very large uncertainty [10]. Therefore, in the present situation, it is necessary to perform highly accurate PNC calculations and measurements on several species including systems having a neutron as a valence nucleon to resolve this issue [3,7]. Also, the anapole values of this kind of systems can infer about the weak potential between the neutron and nuclear core [1,3].

Isotopes of several singly ionized heavier ions like Ba^+, Ra^+, and Yb^+, having a valence neutron in the nucleus, are considered as potential candidates for estimating anapole values through the PNC calculations and measurements [4,11]. The experimental technique of reaching very accurate PNC measurement for the $6s\ ^2S_{1/2}$-$5d\ ^2D_{3/2}$ transition of Ba^+ was suggested by Fortson [12]. This work is going on at Seattle [13–15]. Theoretical calculations on a few isotopes of Ba^+ in this regard were performed by Dzuba *et al.* [4,16] and Sahoo *et al.* [11,17]. The most recent PNC results of Dzuba *et al.* are presented in the form of a ratio (R) of NSD to NSI amplitudes [4]. The wave functions used in the their PNC calculations reflect considerable discrepancies in the hyperfine A values from precise experimental measurements for few relevant states [4]. The hyperfine A values are the most important tools to judge the accuracy of the wave functions of the states in contact with the nuclear region where PNC interaction takes place. Nevertheless, as mentioned by them, such inaccuracies are canceled out largely in the R value associated with a hyperfine component if both the NSI and NSD amplitudes are calculated by a similar approach considering all the leading contributions are accounted in a same way [4,18].

In spite of, the PNC effects are prominent in heavier systems, their theoretical accuracies are limited due to enhancement of the quantum electrodynamics (QED) correction [19,20], neutron skin effects [21], etc. Moreover, computational complexity for these systems to achieve desirable accuracy is increased. Hence, it is reasonable to choose PNC candidates where both theory and experiment can keep conclusive accuracy. Recently PNC calculations were carried out on a relatively lighter system like ^{85,87}Rb [19]. Following a similar trend, a stable isotope like $^{87}Sr^+$ having a valence neutron in the nucleus may be considered as good candidate for anapole estimation. PNC measurement on the $5s\ ^2S_{1/2}$-$4d\ ^2D_{3/2}$ transition of Sr^+ was also proposed by Fortson using a similar technique as used for Ba^+ [12].

In the present work, we calculate the $E1$ PNC amplitudes of the hyperfine components (HCs) for the $6s\ ^2S_{1/2}$-$5d\ ^2D_{3/2}$ transition of $^{137}Ba^+$ using improved wave functions with respect to those used by Dzuba *et al.* [4]. Also, we calculate these amplitudes of the HCs for the $5s\ ^2S_{1/2}$-$4d\ ^2D_{3/2}$ transition of $^{87}Sr^+$. The results are presented with the aim of extracting the constants associated with the NSD PNC interactions using ongoing and future experiments [5]. The anapole contributions to these constants can be extracted using a similar approach as discussed in detail in Refs. [1,8]. In the present work, the sum-over-states technique is used where the main part or the dominating part [22–24] of the sum is calculated with high accuracy using relativistic coupled-cluster (RCC) theory [25–27] and the experimental transition energies. The nonlinear RCC theory with single, double, and partial triple excitations [CCSD(T)] [27] is applied here to generate the $E1$ and weak matrix elements of this part in a correlation exhaustive way. Also, these matrix elements are generated from the solutions of the Dirac-Coulomb-Gaunt (DCG) Hamiltonian [28]. Note that the Gaunt interaction [29] is the unretarded approximation of the well-known Breit interaction [30]. A comparatively less accurate method is used for calculation of the rest of the sum, where the core polarization effect is included on top of the Dirac-Fock approximation based on the Dirac-Coulomb (DC) Hamiltonian. The good quality of the present RCC wave functions is established by comparisons of few relevant results

for PNC calculations with the other accurate theoretical and experimental results. The PNC results of $^{137}Ba^{+}$ as obtained from the recent work of Dzuba *et al.* [4] are compared with the present results, as both works are aiming at extraction of the anapole values using a similar technique [5].

II. THEORY

A brief discussion about the nonlinear version of the coupled-cluster theory with the inclusion of the partial triple excitation is discussed in Refs. [27,31,32]. Also, the implementation of the Gaunt interaction in the atomic calculations using the coupled-cluster framework is discussed in detail in Ref. [28].

The PNC interaction Hamiltonian due to both NSI and NSD interactions is given by $H_{\rm PNC} = H_{\rm NSI} + H_{\rm NSD} = \frac{G_F}{\sqrt{2}}\left(-\frac{Q_W}{2}\gamma_5 + \frac{\kappa}{I}\boldsymbol{\alpha}\cdot\boldsymbol{I}\right)\rho(r)$ [4]. Here G_F is the Fermi constant of the weak interaction; Q_W is the weak nuclear charge, which is nearly equal to $-0.9877N + 0.0716Z$, where N and Z are the number of neutrons and protons, respectively, inside the nucleus [4]; $\boldsymbol{\alpha}$ and γ_5 are the Dirac matrices; $\rho(r)$ is the normalized nuclear density distribution function, which is considered Fermi type here [8]; and κ is a dimensionless constant which accounts for the contributions from the anapole moment, electron-nucleus spin-dependent weak interaction, and combined action of the NSI PNC and hyperfine interaction [8]. Using the sum-over-states technique, the spin-independent and spin-dependent $E1$ reduced matrix elements between the states $|J_f F_f\rangle$ and $|J_i F_i\rangle$ are derived as [4,8,33]

$$\langle J_f F_f||d_{\rm NSI}||J_i F_i\rangle = (-1)^{I+F_i+J_f+1}\sqrt{[F_f][F_i]}\begin{Bmatrix} J_i & J_f & 1\\ F_f & F_i & I\end{Bmatrix}\sum_n\left[\frac{\langle J_f||d||J_n\rangle\langle J_n||H_{\rm NSI}||J_i\rangle}{E_i - E_n}[J_i]^{-1/2} + \frac{\langle J_f||H_{\rm NSI}||J_n\rangle\langle J_n||d||J_i\rangle}{E_f - E_n}[J_f]^{-1/2}\right] \tag{2.1}$$

and

$$\langle J_f F_f||d_{\rm NSD}||J_i F_i\rangle = \frac{\kappa}{I}\sqrt{I(I+1)(2I+1)[F_i][F_f]}\sum_n\left[(-1)^{J_i-J_f+1}\begin{Bmatrix} F_f & F_i & 1\\ J_n & J_f & I\end{Bmatrix}\begin{Bmatrix} I & I & 1\\ J_n & J_i & F_i\end{Bmatrix}\times\frac{\langle J_f||d||J_n\rangle\langle J_n||K||J_i\rangle}{E_i - E_n} + (-1)^{F_i-F_f+1}\begin{Bmatrix} F_f & F_i & 1\\ J_i & J_n & I\end{Bmatrix}\begin{Bmatrix} I & I & 1\\ J_n & J_f & F_f\end{Bmatrix}\times\frac{\langle J_f||K||J_n\rangle\langle J_n||d||J_i\rangle}{E_f - E_n}\right], \tag{2.2}$$

where $[F] = 2F + 1$ and $[J] = 2J + 1$. The single-particle reduced matrix elements of the operators d, $H_{\rm NSI}$, and K are given in Refs. [8,33].

III. RESULTS AND DISCUSSIONS

To judge the accuracy of our wave functions based on the DCG Hamiltonian, we compare a few results of the relevant properties of and among the most important states for the PNC calculations with the highly accurate theoretical and most accurate experimental results. Table I and Table II depict the comparisons of these results for the hyperfine A constants and $E1$ transition amplitudes, respectively. These tables also contain the theoretical results calculated by Dzuba *et al.* [4]. Here the highly accurate theoretical results are estimated using the all-order single-double with partial triple (SDpT) excitations method in linearized approximation by Safronova for both of the systems Ba^{+} [34] and Sr^{+} [35]. However, in addition to the linear terms, our present theory incorporates some nonlinear terms. Also, we use Gaussian-type orbital (GTO) bases to construct the Dirac-Fock orbitals, whereas Safronova used B-spline bases to generate these orbitals. The experimental values are found from various earlier measurements where uncertainties were claimed to be lowest [36–46]. However, the $E1$ amplitude of the $5d\,^2D_{3/2}$-$6p\,^2P_{1/2}$ transition is measured differently: 2.90(9) [41], 3.03(9) [43], and 3.14(8) [14] a.u. by different groups with almost the same precision. Moreover, in a few cases, the experimental $E1$ transition amplitudes are estimated with large error bars. Therefore, we choose the SDpT results of the $E1$ transitions as standard to estimate the uncertainty in our PNC calculations as discussed later. Nevertheless, the good agreements among our RCC results with the SDpT results and the experimental

TABLE I. Calculated hyperfine A constants in MHz and their comparisons with the SDpT results of Safronova ($^{137}Ba^{+}$: [34], $^{87}Sr^{+}$: [35]), theoretical results of Dzuba *et al.* [4] and experimentally measured values (Expt.). The results of Dzuba *et al.* [4] for $^{137}Ba^{+}$ are calculated by scaling their results for $^{135}Ba^{+}$ using the experimental ratio: $\frac{(A)_{^{137}Ba^{+}}}{(A)_{^{135}Ba^{+}}}$.

Ions	States	Present	[34,35]	[4]	Expt.
$^{137}Ba^{+}$	$6s\,^2S_{1/2}$	4112.31	3997.39	4106	4018.87(0) [36]
	$6p\,^2P_{1/2}$	731.13	733.98	747	743.7(0.3) [37]
	$6p\,^2P_{3/2}$	123.13	121.35	147	127.2(0.2) [37]
	$5d\,^2D_{3/2}$	194.18	191.53	180	189.73(0) [38]
$^{87}Sr^{+}$	$5s\,^2S_{1/2}$	1009.18	997.85		1000.47(0) [39]
	$5p\,^2P_{1/2}$	175.85	177.33		
	$5p\,^2P_{3/2}$	35.11	35.26		36.00(0.4) [40]
	$4d\,^2D_{3/2}$	46.66	46.70		

TABLE II. Calculated $E1$ transition amplitudes in a.u. and their comparisons with the SDpT results of Safronova (Ba^+: [34], Sr^+: [35]), theoretical results of Dzuba *et al.* [4], and experimental values (Expt.). The Expt. of Sr^+ are calculated using the oscillator strengths given in the references and excitation energies from National Institute of Standards and Technology (NIST) [46].

Ions	Transition	Present	[34,35]	[4]	Expt.
Ba^+	$6s\ ^2S_{1/2}$-$6p\ ^2P_{1/2}$	3.3749	3.3710	3.32	3.36(4) [41]
	$6s\ ^2S_{1/2}$-$6p\ ^2P_{3/2}$	4.7586	4.7569	4.69	4.72(4) [42]
	$5d\ ^2D_{3/2}$-$6p\ ^2P_{1/2}$	3.0337	3.0957	3.06	3.03(9) [43]
	$5d\ ^2D_{3/2}$-$6p\ ^2P_{3/2}$	1.3217	1.3532	1.34	1.36(4) [43]
Sr^+	$5s\ ^2S_{1/2}$-$5p\ ^2P_{1/2}$	3.1059	3.0967		3.12 [44]
	$5s\ ^2S_{1/2}$-$5p\ ^2P_{3/2}$	4.3891	4.3768		4.40 [44]
	$4d\ ^2D_{3/2}$-$5p\ ^2P_{1/2}$	3.0794	3.1193		3.47(32) [45]
	$4d\ ^2D_{3/2}$-$5p\ ^2P_{3/2}$	1.3669	1.3858		1.45(14) [45]

measurements (within the limits of the uncertainties) as seen from these tables can ensure good quality of the RCC wave functions for all states. Moreover, we have checked the Gaunt contributions to the A constants of the $6s\ ^2S_{1/2}$ and $5s\ ^2S_{1/2}$ states of $^{137}Ba^+$ and $^{87}Sr^+$, respectively. These values are $+8.13$ and $+1.40$ MHz, respectively, and are consistent with the Breit contributions $+8.33$ and $+1.39$ MHz, respectively, as obtained from Sushkov's analytic expression $\delta A = 0.68ZA\alpha^2$ [47].

In Table III we present the $E1$ PNC transition amplitudes for the NSI interaction of $^{137}Ba^+$ and $^{87}Sr^+$ calculated by the present approach. In these calculations, the sums are considered for intermediate $np\ ^2P_{1/2}$ and $np\ ^2P_{3/2}$ states having values of n from 2 to 25. The main parts or the dominant parts of the sums contain $n = 6, 7$, and 8 for Ba^+ and $n = 5, 6$, and 7 for Sr^+. These values of n for the corresponding systems represent bound excited states at the Dirac-Fock (DF) level. The RCC theory is used here to construct the wave functions and as a consequence the matrix elements of this part accurately. This theory can account for the core correlation, core polarization, and pair correlation contributions [48] to the matrix elements in an all-order way [49]. The next contributions to the PNC amplitudes arise from the core or the autoionization states parts of the sums [23]. These parts take the values of n from 2 to 5 for Ba^+ and 2 to 4 for Sr^+. The remaining part or the tail part contributes little compare to the main and the core parts for both the ions. In the core and tail sectors, the core polarization (CP) effect is included in the matrix elements to provide sufficient accuracy in the final PNC amplitudes [22,23]. To include the CP effect in the core sector, we consider the second-order diagram in many-body perturbation theory (MBPT) from Ref. [50] and replace this diagram by an equivalent all-order diagram [51] using Ref. [49]. Similarly, in the highly excited valence sector or tail sector, we use a combination of all-order and second-order diagrams [52] to incorporate the CP effect [48,49]. With this treatment of the CP effect, for $^{137}Ba^+$, the core and tail contributions become 3.415 and 0.701, respectively, at the DF + CP level, which are 2.886 and 1.008, respectively, at the DF level using the unit $10^{-12}iea_0Q_W/(-N)$. A large cancellation is seen to happen between the CP corrections to the core and the tail sectors. A similar kind of cancellation is seen to occur in the calculation of the $E1$ NSI PNC amplitude for the $7s\ ^2S_{1/2}$-$6d\ ^2D_{3/2}$ transition of $^{223}Ra^+$ by Pal *et al.* [23]. They included the CP corrections in the core and the tail regions using the random phase approximation (RPA) method. For $^{87}Sr^+$ also, the CP effect increases the core value from 3.732 to 4.364, but decreases the tail value from 0.863 to -0.166 using the unit $10^{-13}iea_0Q_W/(-N)$. After including the exhaustive correlation in the main part and the CP correction in the remaining part, two further corrections are performed for the NSI PNC amplitudes. First, we include the Gaunt interaction in the main part only. The contributions from this interaction change the NSI PNC amplitudes by around -0.4% and -0.3% for $^{137}Ba^+$ and $^{87}Sr^+$, respectively. Second, to increase the accuracy further, the experimental transition energies [46] are used at the denominators of this part. On the top of the Gaunt corrected *ab initio* results, the replacement of our RCC energies by the experimental energies change the amplitudes by $+1.2\%$ to $^{137}Ba^+$ and by $+1.1\%$ to $^{87}Sr^+$. The main parts yield results 1.896 for the former ion and 0.260 for latter ion in the unit of $10^{-11}iea_0Q_W/(-N)$.

TABLE III. Calculated $E1$ NSI PNC amplitudes for the $6s\ ^2S_{1/2}$-$5d\ ^2D_{3/2}$ transition of $^{137}Ba^+$ and $5s\ ^2S_{1/2}$-$4d\ ^2D_{3/2}$ transition of $^{87}Sr^+$ in the unit of $10^{-11}iea_0Q_W/(-N)$. The present result of $^{137}Ba^+$ is compared with the corresponding results of Dzuba *et al.* [4,16] and Gopakumar *et al.* [24].

Ions	Present	[4,16]	[24]
$^{137}Ba^+$	2.308	2.34	2.35
$^{87}Sr^+$	0.302		

In Table III, we also compare the present $E1$ NSI PNC amplitude of $^{137}Ba^+$ with the other calculations obtained by the sum-over-states technique, but using different strategies. The result of Gopakumar *et al.* was evaluated by treating the main part at the RCC level, but the core and tail parts at the DF level [24]. Their DF orbitals are based on the hybridization of the analytical GTO bases and numerical bases [24], whereas we use analytical GTO bases only to construct these orbitals. Theoretically, for a more accurate treatment, the CP effect should be included at these less contributing parts, which is performed in the present approach. Dzuba *et al.* used correlation potential method to generate the Bruckner-type orbitals and included a CP effect (using RPA method) in the relevant matrix elements for the PNC calculations including the hyperfine constants [4,5,16]. As seen from Table I, their method produces the hyperfine A constants of the $6p\ ^2P_{3/2}$ and $5d\ ^2D_{3/2}$ states with a considerably large discrepancy from the experimental measurements and the SDpT values. These discrepancies in the $J = 3/2$ states appear due to the inaccuracies in the correlation corrections (mainly from the core polarization effects) [18]. As a consequence, these inaccuracies can be significantly reflected in the weak matrix elements associated with these states [23]. This is the reason that the term associated with the weak matrix element having $6p\ ^2P_{3/2}$ and $5d\ ^2D_{3/2}$ states gives the results -0.130 as calculated by us and results -0.264 as calculated by Dzuba *et al.* [16] using the unit $10^{-11}iea_0Q_W/(-N)$ for the $E1$ NSI PNC amplitude. However, for the $6s\ ^2S_{1/2}$ and $6p\ ^2P_{1/2}$

TABLE IV. Calculated $\sqrt{A_f \times A_i}$ values for $^{137}Ba^+$ and $^{87}Sr^+$ in MHz and their comparisons with theoretical results of Safronova (Ba^+: [34], Sr^+: [35]), and Dzuba *et al.* [4], and experimental values (Expt.). The references of the experimental hyperfine values are given in Table I.

Ions	$f - i$	Present	[34,35]	[4]	Expt.
$^{137}Ba^+$	$6s\ ^2S_{1/2}$-$6p\ ^2P_{1/2}$	1733.96	1712.89	1751.34	1728.82
	$6s\ ^2S_{1/2}$-$6p\ ^2P_{3/2}$	711.58	696.48	776.91	714.98
	$5d\ ^2D_{3/2}$-$6p\ ^2P_{1/2}$	376.79	374.94	366.69	375.64
	$5d\ ^2D_{3/2}$-$6p\ ^2P_{3/2}$	154.63	152.45	162.67	155.35
$^{87}Sr^+$	$5s\ ^2S_{1/2}$-$5p\ ^2P_{1/2}$	421.27	420.65		
	$5s\ ^2S_{1/2}$-$5p\ ^2P_{3/2}$	188.23	187.57		189.78
	$4d\ ^2D_{3/2}$-$5p\ ^2P_{1/2}$	90.58	91.00		
	$4d\ ^2D_{3/2}$-$5p\ ^2P_{3/2}$	40.48	40.58		

states, the A values obtained from all three theories and the experiments exist in a reasonably good agreement. Therefore, the term associated with the weak matrix element having these two states yields 1.962 and 2.036 as obtained by the calculations of ourselves and Dzuba *et al.* [16], respectively, using the unit $10^{-11} iea_0 Q_W/(-N)$ for the $E1$ NSI PNC amplitude. A measurable parameter, which is supposed to determine the accuracy of a weak matrix element, can be considered by the factor $\sqrt{A_f \times A_i}$ [4,18,53]. A comparison of these factors as calculated by the different theories and the experiments is presented in Table IV for both $^{137}Ba^+$ and $^{87}Sr^+$. This table clearly shows that the present calculations of these factors associated with the $J = 3/2$ states are more accurate compared to the corresponding factors as calculated by Dzuba *et al.* Furthermore, the calculations of both Gopakumar *et al.* and Dzuba *et al.* did not consider the Gaunt correction, which is considered in the present approach. Nevertheless, our $E1$ NSI PNC amplitude agrees well with both the other results. This can be the consequence of cancellations between the various contributions to the sum.

The results of Table V are the major focus in the present work. These results are presented in the form of $\langle J_f F_f || d_{\rm NSI} || J_i F_i \rangle [1 + R\kappa]$, where the ratio $R = \frac{\langle J_f F_f || d_{\rm NSI} || J_i F_i \rangle}{\kappa \langle J_f F_f || d_{\rm NSI} || J_i F_i \rangle}$ [4]. The NSD PNC amplitudes are calculated in the identical strategy that is adopted to calculate the NSI PNC amplitudes as explained earlier. To the former

TABLE V. Calculated $E1$ PNC amplitudes (reduced matrix elements) for the $|6s\ ^2S_{1/2}, F_i\rangle$-$|5d\ ^2D_{3/2}, F_f\rangle$ transition of $^{137}Ba^+$ and $|5s\ ^2S_{1/2}, F_i\rangle$-$|4d\ ^2D_{3/2}, F_f\rangle$ transition of $^{87}Sr^+$ in 10^{-11} a.u. The results of $^{137}Ba^+$ are compared with the corresponding results of Dzuba *et al.* [4].

Ions	F_f	F_i	Present	[4]
$^{137}Ba^+$	3	2	$-7.0166(1-0.0233\kappa)$	$-7.15(1-0.0239(2)\kappa)$
	2	2	$4.1932(1-0.0231\kappa)$	$4.27(1-0.022(1)\kappa)$
	2	1	$-4.1932(1+0.0386\kappa)$	$-4.27(1+0.038(1)\kappa)$
	1	2	$-1.8753(1-0.0229\kappa)$	$-1.93(1-0.021(2)\kappa)$
	1	1	$4.1932(1+0.0387\kappa)$	$4.29(1+0.0392(4)\kappa)$
	0	1	$-2.6520(1+0.0388\kappa)$	$-2.70(1+0.0398(3)\kappa)$
$^{87}Sr^+$	6	5	$-1.2436(1-0.0335\kappa)$	
	5	5	$0.8861(1-0.0351\kappa)$	
	5	4	$-0.7235(1+0.0433\kappa)$	
	4	5	$-0.5343(1-0.0364\kappa)$	
	4	4	$0.8861(1+0.0420\kappa)$	
	3	4	$-0.9126(1+0.0409\kappa)$	

amplitudes, the main, core, and tail parts contribute about 80%, 16.5%, and 4.0%, respectively, in case of Ba^+ and about 82%, 17.5% to 18.5% and −0.3% to 0.7%, respectively, in case of Sr^+. The results calculated by the present technique are compared with the corresponding results of Dzuba *et al.* for $^{137}Ba^+$ [4]. In their paper, the values are presented in the z-component matrix element forms of hyperfine states [4]. However, in the present comparison, we keep their results in reduced matrix element forms. Also, we invert the signs of all their NSI and NSD amplitudes to make these consistent with our sign conventions.

Using the DC Hamiltonian, we have found that the magnitudes of the R values are changed by about −9.5% to −11.0% for $^{137}Ba^+$ and by about −17% to −24% for $^{87}Sr^+$ from the pure *ab initio* DF results to the correlation corrected results (RCC for the main sectors and DF + CP for the remaining sectors). The correlations in the ratios can be understood from the unequal correlation contributions to the NSI and NSD amplitudes. In order to analyze the unequal correlation contributions, let us split the $E1$ PNC amplitudes as presented in Eq. (2.1) and Eq. (2.2) into two parts. These parts are named according to their contributions to the total $E1$ NSI and NSD PNC amplitudes and are as follows:

$$\text{Large Part} = C_1 \sum_n \frac{\langle (m-1)d^2 D_{3/2} || d || np^2 P_{1/2} \rangle \langle np^2 P_{1/2} || \text{weak} || ms^2 S_{1/2} \rangle}{E_{ms^2 S_{1/2}} - E_{np^2 P_{1/2}}},$$

$$\text{Small Part} = C_2 \sum_n \frac{\langle (m-1)d^2 D_{3/2} || d || np^2 P_{3/2} \rangle \langle np^2 P_{3/2} || \text{weak} || ms^2 S_{1/2} \rangle}{E_{ms^2 S_{1/2}} - E_{np^2 P_{3/2}}}$$

$$+ C_3 \sum_n \frac{\langle (m-1)d^2 D_{3/2} || \text{weak} || np^2 P_{1/2} \rangle \langle np^2 P_{1/2} || d || ms^2 S_{1/2} \rangle}{E_{(m-1)d^2 D_{3/2}} - E_{np^2 P_{1/2}}}$$

$$+ C_4 \sum_n \frac{\langle (m-1)d^2 D_{3/2} || \text{weak} || np^2 P_{3/2} \rangle \langle np^2 P_{3/2} || d || ms^2 S_{1/2} \rangle}{E_{(m-1)d^2 D_{3/2}} - E_{np^2 P_{3/2}}}.$$

Here the sums run over all the intermediate states indicated by n. C_1, C_2, C_3, and C_4 are the associated coefficients, which are different for the $E1$ NSI and NSD amplitudes [see Eq. (2.1) and Eq. (2.2)]. The Large Parts to the PNC amplitudes arise from the sum of the terms having weak matrix elements of the type $^2S_{1/2}$-$^2P_{1/2}$. The corresponding weak matrix elements of this type for both the NSI and NSD PNC interactions are similar in nature. The percentage impacts of correlations to the Large Parts are almost identical for both the $E1$ NSI and NSD PNC amplitudes. However, the same thing is not true for the rest or the Small Parts of the sums. These parts contain the sum of all the terms involved with the $^2S_{1/2}$-$^2P_{3/2}$, $^2P_{1/2}$-$^2D_{3/2}$, and $^2P_{3/2}$-$^2D_{3/2}$ type of weak matrix elements. The weak matrix elements of the type $^2S_{1/2}$-$^2P_{3/2}$ and $^2P_{1/2}$-$^2D_{3/2}$ are zero for NSI PNC as the initial and final states of these matrix elements do not have the same J values [8]. However, this restriction is not there in the weak matrix elements for NSD PNC. Furthermore, these Small Parts in both the NSI and NSD amplitudes mainly arise due to correlations as their DF values are too little or nearly zero. The Small Parts are found to be responsible for about -5.5% and -15% to -16.5% correlation corrections to the $E1$ NSI PNC and NSD PNC amplitudes, respectively, of $^{137}Ba^+$. Similarly, the Small Parts provide about -13% and -28.5% to -35% correlation corrections to the $E1$ NSI PNC and NSD PNC amplitudes, respectively, of $^{87}Sr^+$. Therefore, the Small Parts, which contain the weak matrix elements having $J = 3/2$ states, are the major responsible factor for providing correlations in the ratios. As a consequence, good accuracy in the correlation corrections of the weak matrix elements associated with the $J = 3/2$ states is very much important for the accurate calculations of the ratios.

After including the correlation corrections in a pure *ab initio* environment, we investigate the variations of the ratios from the inclusions of the Gaunt corrections in the $E1$ and weak matrix elements and from the substitutions of the RCC energies by the experimental energies. These change the R values by about $+0.5\%$ to $+1\%$ and $+1.5\%$ to $+2\%$ for $^{137}Ba^+$ and $^{87}Sr^+$, respectively.

Both the $E1$ NSI and NSD PNC amplitudes of $^{137}Ba^+$ and $^{87}Sr^+$ are calculated within theoretical uncertainty of about 3%. These uncertainties are calculated using a usual procedure [4,23,53] of replacing the $E1$ amplitudes obtained from the RCC theory by the $E1$ amplitudes calculated from the SDpT approximation and scaling a weak amplitude $\langle f|\text{weak}|i\rangle$ by the factor $\frac{\sqrt{(A_f \times A_i)_{\text{SDpT}}}}{\sqrt{(A_f \times A_i)_{\text{RCC}}}}$ and $\frac{\sqrt{(A_f \times A_i)_{\text{Expt.}}}}{\sqrt{(A_f \times A_i)_{\text{RCC}}}}$ in the main part. Also, a rough approximation from the QED [20], neutron skin effects [21], and more complete calculations in the core sectors are considered here. The QED and neutron skin corrections are considered when the SDpT results are used. Nevertheless, precise experimental data are necessary in few cases to judge the accuracy in the present values of the $E1$ NSI and NSD PNC amplitudes in a more perfect way.

The R values for both ions are calculated within theoretical uncertainty of about 0.5% considering the scaling and replacements of the matrix elements as mentioned above. More complete calculations in the core and the tail parts are expected for better accuracy in the ratios. However, such parts are supposed to largely arise from the sum of the terms having weak matrix elements of the type $^2S_{1/2}$-$^2P_{1/2}$. Therefore, according to the explanations given earlier, the uncertainties due to the incompleteness in the core and the tail sectors have the possibility of being canceled largely between the numerator and denominator of a ratio. Consideration of such incompleteness can predict the present R values at the uncertainty level 1% to 1.5%. As a consequence, the ratio of two different precise PNC measurements corresponding to two different hyperfine components and its comparison with the present theoretical value can lead to a very accurate interpretation of the κ value [5].

IV. CONCLUSION

The $E1$ PNC amplitudes of $^{137}Ba^+$ and $^{87}Sr^+$ have been calculated for the purpose of extracting the constants associated with the NSD PNC interactions with high accuracy from the ongoing experiment for the former ion and the proposed experiment for the latter ion.

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[1] V. V. Flambaum and D. W. Murray, Phys. Rev. C **56**, 1641 (1997).
[2] V. V. Flambaum, I. B. Khriplovich, and O. P. Sushkov, Phys. Lett. B **146**, 367 (1984).
[3] V. F. Dmitriev and I. B. Khriplovich, arXiv:nucl-th/0201041v1.
[4] V. A. Dzuba and V. V. Flambaum, Phys. Rev. A **83**, 052513 (2011).
[5] V. A. Dzuba, V. V. Flambaum, and C. Harabati, Phys. Rev. A **84**, 052108 (2011).
[6] V. A. Dzuba, J. C. Berengut, V. V. Flambaum, and B. Roberts, Phys. Rev. Lett. **109**, 203003 (2012).
[7] C. P. Liu, AIP Conf. Proc. **675**, 262 (2003).
[8] W. R. Johnson, M. S. Safronova, and U. I. Safronova, Phys. Rev. A **67**, 062106 (2003).
[9] C. S. Wood *et al.*, Science **275**, 1759 (1997).
[10] P. A. Vetter, D. M. Meekhof, P. K. Majumder, S. K. Lamoreaux, and E. N. Fortson, Phys. Rev. Lett. **74**, 2658 (1995).
[11] B. K. Sahoo, P. Mandal, and M. Mukherjee, Phys. Rev. A **83**, 030502(R) (2011).
[12] N. Fortson, Phys. Rev. Lett. **70**, 2383 (1993).
[13] J. A. Sherman, T. W. Koerber, A. Markhotok, W. Nagourney, and E. N. Fortson, Phys. Rev. Lett. **94**, 243001 (2005).
[14] J. A. Sherman, A. Andalkar, W. Nagourney, and E. N. Fortson, Phys. Rev. A **78**, 052514 (2008).

[15] S. R. Williams, A. Jayakumar, M. R. Hoffman, B. B. Blinov, and E. N. Fortson, Phys. Rev. A **88**, 012515 (2013).
[16] V. A. Dzuba, V. V. Flambaum, and J. S. M. Ginges, Phys. Rev. A **63**, 062101 (2001).
[17] B. K. Sahoo, R. Chaudhuri, B. P. Das, and D. Mukherjee, Phys. Rev. Lett. **96**, 163003 (2006).
[18] B. M. Roberts, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **89**, 012502 (2014).
[19] V. A. Dzuba, V. V. Flambaum, and B. Roberts, Phys. Rev. A **86**, 062512 (2012).
[20] B. M. Roberts, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **87**, 054502 (2013).
[21] B. A. Brown, A. Derevianko, and V. V. Flambaum, Phys. Rev. C **79**, 035501 (2009).
[22] S. A. Blundell, J. Sapirstein, and W. R. Johnson, Phys. Rev. D **45**, 1602 (1992).
[23] R. Pal, D. Jiang, M. S. Safronova, and U. I. Safronova, Phys. Rev. A **79**, 062505 (2009).
[24] G. Gopakumar, B. P. Das, R. K. Chaudhuri, D. Mukherjee, and K. Hirao, J. Chem. Phys. **126**, 014301 (2007).
[25] R. F. Bishop and H. G. Kümmel, Phys. Today **40**, 52 (1987).
[26] I. Lindgren and D. Mukherjee, Phys. Rep **151**, 93 (1987).
[27] C. Sur, B. K. Sahoo, R. K. Chaudhuri, B. P. Das, and D. Mukherjee, Eur. Phys. J. D **32**, 25 (2005).
[28] N. N. Dutta and S. Majumder, Phys. Rev. A **85**, 032512 (2012).
[29] J. A. Gaunt, Proc. R. Soc. London A **122**, 513 (1929).
[30] G. Breit, Phys. Rev. **34**, 553 (1929); **36**, 383 (1930); **39**, 616 (1932).
[31] B. K. Mani, K. V. P. Latha, and D. Angom, Phys. Rev. A **80**, 062505 (2009).
[32] B. K. Mani and D. Angom, Phys. Rev. A **83**, 012501 (2011).
[33] B. M. Roberts, V. A. Dzuba, and V. V. Flambaum, Phys. Rev. A **89**, 042509 (2014).
[34] U. I. Safronova, Phys. Rev. A **81**, 052506 (2010).
[35] U. I. Safronova, Phys. Rev. A **82**, 022504 (2010).
[36] R. Blatt and G. Werth, Z. Phys. A **299**, 93 (1981).
[37] P. Villemoes, A. Arnesen, F. Heijkenskjöld, and A. Wännström, J. Phys. B: At. Mol. Opt. Phys. **26**, 4289 (1993).
[38] R. E. Silverans, G. Borghs, P. De Bisschop, and M. Van Hove, Phys. Rev. A **33**, 2117 (1986).
[39] H. Sunaoshi *et al.*, Hyperfine Interact. **78**, 241 (1993).
[40] F. Buchinger *et al.*, Phys. Rev. C **41**, 2883 (1990); **42**, 2754 (1990).
[41] M. D. Davidson, L. C. Snoek, H. Volten, and A. Dönszelmann, Astron. Astrophys. **255**, 457 (1992).
[42] N. Kurz, M. R. Dietrich, G. Shu, R. Bowler, J. Salacka, V. Mirgon, and B. B. Blinov, Phys. Rev. A **77**, 060501(R) (2008).
[43] A. Kastberg, P. Villemoes, A. Arnesen, F. Heijkenskjöld, A. Langereis, P. Jungner, and S. Linnaeus, J. Opt. Soc. Am. B **10**, 1330 (1993); **11**, 523 (1994).
[44] E. H. Pinnington, R. W. Berends, and M. Lumsden, J. Phys. B: At. Mol. Opt. Phys. **28**, 2095 (1995)
[45] A. Gallagher, Phys. Rev. **157**, 24 (1967).
[46] A. Kramida, Yu. Ralchenko, J. Reader, and NIST ASD Team. *NIST Atomic Spectra Database* (ver. 5.1), http://physics.nist.gov/asd.
[47] O. P. Sushkov, Phys. Rev. A **63**, 042504 (2001).
[48] N. N. Dutta and S. Majumder, Phys. Rev. A **88**, 062507 (2013).
[49] B. K. Sahoo, S. Majumder, R. K. Chaudhuri, B. P. Das, and D. Mukherjee, J. Phys. B: At. Mol. Opt. Phys. **37**, 3409 (2004).
[50] M. Kutzner, J. A. Robertson, and P. Pelley, Phys. Rev. A **62**, 062717 (2000).
[51] M. Kutzner, Z. Altun, and H. P. Kelly, Phys. Rev. A **41**, 3612 (1990).
[52] S. Garpman, I. Lindgren, J. Lindgren, and J. Morrison, Phys. Rev. A **11**, 758 (1975).
[53] B. K. Sahoo, G. Gopakumar, R. K. Chaudhuri, B. P. Das, H. Merlitz, U. S. Mahapatra, and D. Mukherjee, Phys. Rev. A **68**, 040501(R) (2003).