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Theoretical studies of the $6s^2S_{1/2}\rightarrow 5d^2D_{3/2}$ parity-nonconserving transition amplitude in Ba$^+$ and associated properties

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It is widely believed that the standard model of particle physics is just an intermediate step in understanding the properties of the elementary physics in nature and the interactions between them. Over the past twenty years, studies of the parity nonconservation in atomic systems based on nonaccelerator methods have made remarkable progress. An experiment to measure parity nonconservation in singly ionized barium has been proposed as an independent test of the standard model. We have employed the relativistic coupled-cluster theory to calculate the parity nonconserving $6s^2S_{1/2}\rightarrow 5d^2D_{3/2}$ transition amplitude and associated properties. We have also shown contributions from various intermediate states which play a significant role in the determination of this transition amplitude.

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I. INTRODUCTION

Our present understanding of elementary particle physics is encapsulated in the standard model (SM). Despite the remarkable success of this model, it is widely considered as an intermediate step towards a complete theory of matter [1]. Parity nonconservation (PNC) in atomic systems which arises primarily from the neutral weak interaction between the electrons and the nucleus has the potential to probe new physics beyond the SM [1,2]. By combining the results of high precision measurements and many-body calculations of atomic PNC observables, it is possible to extract the nuclear weak charge (Q_W), and compare with its corresponding value in the SM [1]. A discrepancy between these two values could reveal the possible existence of new physics. The most accurate data on atomic PNC currently comes from the $6s^2S_{1/2}\rightarrow 7s^2S_{1/2}$ transition in cesium (Cs), where the claimed experimental and theoretical accuracies are 0.35% [3] and 0.5% [4], respectively, and the deviation from the SM is about one standard deviation (1σ) [4]. It would indeed be desirable to consider other candidates, which could yield accurate values of Q_W. Fortson has proposed an experiment [5] to measure PNC in $6s^2S_{1/2}\rightarrow 5d^2D_{3/2}$ transition of the singly ionized barium (^{137}Ba$^+$) using the techniques of laser cooling and ion trapping. The observable that would be measured in this experiment is a PNC induced light shift, which depends on the electric dipole transition amplitude caused by the parity nonconserving neutral weak interaction ($E1_{\text{PNC}}$) and the electric quadrupole ($E2$) transition amplitude for the $6s^2S_{1/2}\rightarrow 5d^2D_{3/2}$ transition. One can determine the value of Q_W by combining the measured light shift and the values of the $E1_{\text{PNC}}$ and $E2$ amplitudes [6]. Therefore, from a theoretical point of view, accurate calculations of $E1_{\text{PNC}}$ and $E2$ amplitudes are of special importance. Other important physical quantities like excitation energies, $E1$ transition amplitudes and hyperfine structure constants can be used to determine the error associated with the above mentioned $E1_{\text{PNC}}$ amplitude and therefore, are necessary to be calculated very accurately. The $5d$ states of this system are also important for the studies of the nuclear anapole moment [7], optical frequency standard [8] and astrophysics [9]. The relativistic coupled-cluster (RCC) theory, which is an all order theory [10,11] and based on an exponential ansatz, is known to produce high quality results for atomic and molecular properties. It has been successfully applied to a wide range of problems; prominent among them are high precision calculations of transition probabilities [12] and hyperfine interaction constants [13,14] in heavy atomic systems.

In this paper, we present in detail our $E1_{\text{PNC}}$ calculation for the $6s^2S_{1/2}\rightarrow 5d^2D_{3/2}$ transition in Ba$^+$ using the RCC theory that has been reported recently [15]. It is the first application of this theory to atomic PNC. Blundell had used this theory in the linear approximation to calculate $E1_{\text{PNC}}$ amplitude for the $6s^2S_{1/2}\rightarrow 7s^2S_{1/2}$ transition in Cs by a sum-over-states approach [16,17]. Dzuba *et al.* [18] and Geetha [19] have calculated this PNC amplitude for the $6s^2S_{1/2}\rightarrow 5d^2D_{3/2}$ transition in Ba$^+$. Our calculation of Ba$^+$ PNC is more rigorous than those two calculations and has an accuracy of better than 1%. If the accuracy of this result can be matched by that of experiment on PNC in Ba$^+$, it can provide an independent atomic probe of physics beyond the SM.

II. THEORY OF $E1_{\text{PNC}}$

PNC in atoms arises primarily due to the exchange of the neutral Z_0 boson between the nucleus and the electrons [20]. The dominant contribution arises from the nuclear spin inde-

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TABLE I. Ionization potential energies (cm^{-1}) for different states of Ba^{+}.

	Guet and Johnson	Eliav *et al.*	Dzuba *et al.*	Geetha *et al.*	This work	Expt.
$6s\,^2S_{1/2}$	81882	80871	80813	80797	80794	80686.3(1)
$7s\,^2S_{1/2}$			38333		38291	38331.13
$6p\,^2P_{1/2}$	60887	60476	60581	60505	60384	60424.74
$7p\,^2P_{1/2}$			31332		31216	31296.48
$8p\,^2P_{1/2}$			19378		19213	19354.87
$6p\,^2P_{3/2}$	59140	58769	58860	58778	58690	58733.90
$7p\,^2P_{3/2}$			30704		30597	30674.96
$5d\,^2D_{3/2}$	77194	75605	76404	75989	75481	75812.45
$5d\,^2D_{5/2}$	76263	74779	75525	75084	74346	75011.49
$4f\,^2F_{5/2}$					32169	32427.68
$4f\,^2F_{7/2}$					31272	32202.97

pendent (NSI) neutral weak interaction [20]. The corresponding interaction Hamiltonian is given by

$$H_{\mathrm{PNC}}^{\mathrm{NSI}}=\frac{G_F}{2\sqrt{2}}Q_w\gamma_5\rho_N(r), \tag{2.1}$$

where G_F is the Fermi constant, $\rho_N(r)$ is the nuclear density function and $\gamma_5(=i\gamma_0\gamma_1\gamma_2\gamma_3)$ which is the product of the four Dirac matrices. The quantity Q_w is known as the nuclear weak charge which is equal to $2(Zc_p+Nc_d)$, with c_p and c_n representing electron-proton and electron-neutron coupling constants for atomic number Z and neutron number N of the system, respectively. The values predicted by the SM in the lowest order of electroweak interaction for these coupling constants are [1]

$$c_p=\frac{1}{2}(1-4\sin^2\theta_W)\approx 0.04, \quad \text{and} \quad c_n=-\frac{1}{2}, \tag{2.2}$$

where θ_W is the Weinberg angle and experimentally it's value is $\sin^2\theta_W\approx 0.23$ [21].

The reduced matrix element of $H_{\mathrm{PNC}}^{\mathrm{NSI}}$ in terms of single particle orbitals is given by

TABLE II. Excitation energies (cm^{-1}) for different states of Ba^{+}.

Transition States	This work (cm^{-1})	Experiment (cm^{-1})
$6p\,^2P_{1/2}\rightarrow 6s\,^2S_{1/2}$	20409.60	20261.561
$7p\,^2P_{1/2}\rightarrow 6s\,^2S_{1/2}$	49577.78	49389.822
$5d\,^2D_{3/2}\rightarrow 6s\,^2S_{1/2}$	5312.38	4873.852
$5d\,^2D_{5/2}\rightarrow 6s\,^2D_{1/2}$	6441.58	5674.807
$5d\,^2D_{3/2}\rightarrow 6p\,^2P_{3/2}$	16791.35	17078.55
$5d\,^2D_{3/2}\rightarrow 7p\,^2P_{3/2}$	44883.88	45137.49

TABLE III. Hyperfine structure constants for different states of Ba^{+} in MHz.

	This work		Experiment	
State	A	B	A	B
$6s\,^2S_{1/2}$	4078.20		4018.8708(3)[a] 4018.871(2)[b]	
$7s\,^2S_{1/2}$	1196.30			
$6p\,^2P_{1/2}$	740.77		743.7(3)[c] 741.9(1.3)[d]	
$7p\,^2P_{1/2}$	264.92			
$8p\,^2P_{1/2}$	109.93			
$6p\,^2P_{3/2}$	128.27	92.87	127.2(2)[c] 127.1(6)[e]	92.5(2)[c] 89.7(15)[e]
$7p\,^2P_{3/2}$	45.77	32.91		
$5d\,^2D_{3/2}$	189.92	46.23	189.7288(6)[e] 189.6(4)[f]	44.5417(16)[e] 44.9(6)[f]
$5d\,^2D_{5/2}$	−11.67	62.17	−12.028(11)[g] −11.9(10)[g]	59.533(43)[g] 62.5(40)[g]

[a] Reference [35].
[b] Reference [36].
[c] Reference [37].
[d] Reference [38].
[e] Reference [39].
[f] Reference [40].
[g] Reference [41].

TABLE IV. Calculated absolute values of $E1$ reduced matrix elements in a.u. for different states.

Transition states	This work (a.u.)
$6s\,^2S_{1/2}\rightarrow 6p\,^2P_{1/2}$	3.37
$6s\,^2S_{1/2}\rightarrow 7p\,^2P_{1/2}$	0.09
$6s\,^2S_{1/2}\rightarrow 8p\,^2P_{1/2}$	0.11
$6s\,^2S_{1/2}\rightarrow 6p\,^2P_{3/2}$	4.72
$6s\,^2S_{1/2}\rightarrow 7p\,^2P_{3/2}$	0.17
$7s\,^2S_{1/2}\rightarrow 6p\,^2P_{1/2}$	2.45
$7s\,^2S_{1/2}\rightarrow 7p\,^2P_{1/2}$	7.11
$7s\,^2S_{1/2}\rightarrow 8p\,^2P_{1/2}$	0.37
$7s\,^2S_{1/2}\rightarrow 6p\,^2P_{3/2}$	3.80
$7s\,^2S_{1/2}\rightarrow 7p\,^2P_{3/2}$	9.92
$6p\,^2P_{1/2}\rightarrow 5d\,^2D_{3/2}$	3.08
$7p\,^2P_{1/2}\rightarrow 5d\,^2D_{3/2}$	0.28
$8p\,^2P_{1/2}\rightarrow 5d\,^2D_{3/2}$	0.13
$6p\,^2P_{3/2}\rightarrow 5d\,^2D_{3/2}$	1.36
$7p\,^2P_{3/2}\rightarrow 5d\,^2D_{3/2}$	0.16
$6p\,^2P_{3/2}\rightarrow 5d\,^2D_{5/2}$	4.19
$7p\,^2P_{3/2}\rightarrow 5d\,^2D_{5/2}$	0.46
$5d\,^2D_{3/2}\rightarrow 4f\,^2F_{5/2}$	3.73
$5d\,^2D_{5/2}\rightarrow 4f\,^2F_{5/2}$	1.08
$5d\,^2D_{5/2}\rightarrow 4f\,^2F_{7/2}$	4.59

$$\langle \phi_i \| H_{\mathrm{PNC}}^{\mathrm{NSI}} \| \phi_j \rangle = i \frac{G_F}{2\sqrt{2}} \sqrt{2j_i + 1}\, \delta(\kappa_i, -\kappa_j) \int_0^\infty [P_i(r) Q_j(r) - Q_i(r) P_j(r)] \rho_N(r) dr. \tag{2.3}$$

$H_{\mathrm{PNC}}^{\mathrm{NSI}}$ is responsible for mixing atomic states of opposite parities, but with the same angular momenta. Its strength is sufficiently weak for it to be considered as a first-order perturbation. It is therefore possible to write a general atomic wave function as

$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + G_F |\Psi_n^{(1)}\rangle, \tag{2.4}$$

where $|\Psi_n^{(0)}\rangle$ is an eigenstate of the atomic Hamiltonian, $H^{(0)}$, in the absence of PNC and $|\Psi_n^{(1)}\rangle$ is the first order correction of the above wave function due to the PNC weak interaction.

Using Eq. (2.4), the explicit form of $E1_{\mathrm{PNC}}$ is given by

$$E1_{\mathrm{PNC}} = \frac{\langle \Psi_f | D | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}} = \frac{\langle \Psi_f^{(0)} | D | \Psi_i^{(1)} \rangle + \langle \Psi_f^{(1)} | D | \Psi_i^{(0)} \rangle}{\sqrt{\langle \Psi_f^{(0)} | \Psi_f^{(0)} \rangle \langle \Psi_i^{(0)} | \Psi_i^{(0)} \rangle}}, \tag{2.5}$$

where D is the electric dipole ($E1$) operator. The subscripts i and f are used for the initial and final valence electrons, respectively. Using the explicit expression for the first order perturbed wave function, we get

$$E1_{\mathrm{PNC}} = \sum_{I \neq i} \frac{\langle \Psi_f^{(0)} | D | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | H_{\mathrm{PNC}}^{\mathrm{NSI}} | \Psi_i^{(0)} \rangle}{E_i^{(0)} - E_I^{(0)}} + \sum_{I \neq f} \frac{\langle \Psi_f^{(0)} | H_{\mathrm{PNC}}^{\mathrm{NSI}} | \Psi_I^{(0)} \rangle \langle \Psi_I^{(0)} | D | \Psi_i^{(0)} \rangle}{E_f^{(0)} - E_I^{(0)}}, \tag{2.6}$$

where I represents the intermediate states and $E^{(0)}$'s are the energy eigenvalues of $H^{(0)}$.

It is obvious from the above equation that the accuracy of the calculated $E1_{\mathrm{PNC}}$ amplitude depends on the excitation energies of the different intermediate states, the matrix elements of $H_{\mathrm{PNC}}^{\mathrm{NSI}}$ and D. Therefore, accurate calculations of these quantities require accurate determination of the ground state and the excited states atomic wave functions.

Blundell *et al.* have used the above equation to determine $E1_{\mathrm{PNC}}$ for the $6s\,^2S_{1/2} \rightarrow 7s\,^2S_{1/2}$ transition in Cs by considering the most important intermediate states [16,17]. The drawback of this approach is that the summation can be performed only over a finite set of intermediate states which limits the accuracy of the calculation. This could be overcome by getting the first order wave functions as the solution of the following equation

$$(H^{(0)} - E^{(0)}) |\Psi_v^{(1)}\rangle = (E^{(1)} - H_{\mathrm{PNC}}^{\mathrm{NSI}}) |\Psi_v^{(0)}\rangle, \tag{2.7}$$

where $E^{(1)}$ vanishes for the first order correction.

III. RCC THEORY OF SINGLE VALENCE ATOMIC SYSTEMS

A. Without perturbation

In the RCC theory, the atomic wave function $|\Psi_v^{(0)}\rangle$ for a single valence (v) open-shell system is expressed as [10,22]

$$|\Psi_v^{(0)}\rangle = e^{T^{(0)}} \{1 + S_v^{(0)}\} |\Phi_v\rangle, \tag{3.1}$$

where we define $|\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle$, with $|\Phi_0\rangle$ as the Dirac-Fock (DF) state for the closed-shell system. The curly bracket in the above expression represents normal order form.

In the single and double excitations approximation coupled-cluster (CCSD) method, we have

$$T^{(0)} = T_1^{(0)} + T_2^{(0)},$$

$$S_v^{(0)} = S_{1v}^{(0)} + S_{2v}^{(0)}, \tag{3.2}$$

where $T_1^{(0)}$ and $T_2^{(0)}$ are the single and double hole-particle excitation operators for the core electrons and $S_{1v}^{(0)}$ and $S_{2v}^{(0)}$ are the single and double excitation operators for the valence electron, respectively. The amplitudes corresponding to these operators can be determined by solving the relativistic coupled-cluster singles and doubles equations as given below:

$$\langle \Phi_0^L | \widehat{H^{(0)} e^{T^{(0)}}} | \Phi_0 \rangle = \delta_{L,0} E_0^{(0)}, \tag{3.3}$$

$$\langle \Phi_v^K | \widehat{H^{(0)} e^{T^{(0)}}} S_v^{(0)} | \Phi_v \rangle = - \langle \Phi_v^K | \widehat{H^{(0)} e^{T^{(0)}}} | \Phi_v \rangle + \langle \Phi_v^K | \{1 + S_v^{(0)}\} | \Phi_v \rangle E_v^{(0) = - \langle \Phi_v^K | \widehat{H^{(0)} e^{T^{(0)}}} | \Phi_v \rangle + E_v^{(0)} + \langle \Phi_v^K | S_v^{(0)} | \Phi_v \rangle \langle \Phi_v | \widehat{H^{(0)} e^{T^{(0)}}} \{1 + S_v^{(0)}\} | \Phi_v \rangle}, \tag{3.4}$$

where $L = 1, 2$ represents single and double excitations from the closed-shell state and $K = 1, 2$ represents single and double excitations from a single valence state. For $L = 0$, we get the closed-shell energy $E_0^{(0)}$ and for $K = 0$, we get the energy $E_v^{(0)}$ with the valency electron $'v'$. The difference between these two energies give the ionization potential (IP) energy of the corresponding valence electron. In the above equation, the wide-hat notation represents contraction and we have used the relation $(e^{-T^{(0)}} H^{(0)} e^{T^{(0)}})_c = \widehat{H^{(0)} e^{T^{(0)}}}$, where the subscript "$c$" represents only the connected terms for the expression of the left-hand side.

We consider the Dirac-Coulomb (DC) Hamiltonian in our calculation given by

$$H^{(0)} = [H_0^{(0)}] + [V_{es}^{(0)}] = \sum_i^N [c\alpha \cdot p_i + (\beta - 1)c^2 + V_n(r_i) + U(r_i)] + \left[\sum_{i>j}^N \frac{1}{r_{ij}} - \sum_i^N U(r_i)\right], \tag{3.5}$$

where $H_0^{(0)}$ is the DF Hamiltonian and $V_{es}^{(0)}$ is the Coulomb residual term in atomic unit (au) obtained using the mean field potential $U(r_i)$. Here α and β are universal Dirac matrices.

The most important triple excitations have been considered by constructing excitation operators [23,24]

$$S_{vbc}^{pqr(0)} = \frac{\widehat{V_{es}^{(0)}T_2^{(0)}} + \widehat{V_{es}^{(0)}S_{v2}^{(0)}}}{\varepsilon_v + \varepsilon_b + \varepsilon_c - \varepsilon_p - \varepsilon_q - \varepsilon_r}, \tag{3.6}$$

where ε's are the orbital energies. The above operators are used to construct the single and double open-shell cluster amplitudes by connecting further with the CCSD operators and they are solved self-consistently.

The general expression for calculating the transition amplitude corresponding to any physical operator, O, using the RCC method is given by

$$\langle O\rangle_{f\leftarrow i} = \frac{\langle\Psi_f^{(0)}|O|\Psi_i^{(0)}\rangle}{\sqrt{\langle\Psi_f^{(0)}|\Psi_f^{(0)}\rangle\langle\Psi_i^{(0)}|\Psi_i^{(0)}\rangle}} = \frac{\langle\Phi_f^{(0)}|\{1 + S_f^{(0)^\dagger}\}e^{T^{(0)^\dagger}}Oe^{T^{(0)}}\{1 + S_i^{(0)}\}|\Phi_i^{(0)}\rangle}{\sqrt{\langle\Phi_f^{(0)}|\{1 + S_f^{(0)^\dagger}\}e^{T^{(0)^\dagger}}e^{T^{(0)}}\{1 + S_f^{(0)}\}|\Phi_f^{(0)}\rangle\langle\Phi_i^{(0)}|\{1 + S_i^{(0)^\dagger}\}e^{T^{(0)^\dagger}}e^{T^{(0)}}\{1 + S_i^{(0)}\}|\Phi_i\rangle^{(0)}}}, \tag{3.7}$$

while evaluating expectation values, we consider the special case $f=i$.

For computational simplicity, we compute the expression given by Eq. (3.7) in two steps. We define $\overline{O}(=e^{T^{(0)^\dagger}}Oe^{T^{(0)}})$, which can be expanded using the Wick's general theorem [10] as

$$\overline{O} = \overline{O}_{\text{f.c.}} + \overline{O}_{\text{o.b.}} + \overline{O}_{\text{t.b.}} + \cdots, \tag{3.8}$$

where we have used the abbreviations f.c., o.b., and t.b. for fully contracted, effective one-body, and effective two-body terms, respectively. In this expansion of $\overline{O}$, the effective one-body terms are computed first keeping terms up to

$$\overline{O}_{\text{o.b.}} = O + T^{(0)^\dagger}O + OT^{(0)} + T^{(0)^\dagger}OT^{(0)}. \tag{3.9}$$

Obviously, the fully contracted terms (f.c.) will not contribute in the calculation based on the linked-diagram theorem [10]. The calculation procedure for these effective one-body terms is given by Geetha *et al.* [12]. These terms are finally contracted with the $S_v^{(0)}$ and $S_v^{(0)^\dagger}$ operators in the property calculation. Contributions from the effective two-body terms of $\overline{O}$ are computed directly in the final property calculation. The following types of RCC terms are considered for the construction of effective two-body terms:

$$\overline{O}_{\text{t.b.}} = OT_1^{(0)} + T_1^{(0)^\dagger}O + OT_2^{(0)} + T_2^{(0)^\dagger}O. \tag{3.10}$$

Other effective terms correspond to higher order in residual Coulomb interaction and are neglected for the present calculation. A similar procedure has been followed to account for the normalization terms. Contributions from normalization factors, which are given later in Table VII, are obtained using the following relation

$$\text{norm} = \langle\Psi_f|D|\Psi_i\rangle\left\{\frac{1}{\sqrt{(1 + N_f^{(0)})(1 + N_i^{(0)})}} - 1\right\}, \tag{3.11}$$

with $N_v^{(0)}=\{S_v^{(0)^\dagger}e^{T^{(0)^\dagger}}e^{T^{(0)}}S_v^{(0)}\}$ for the valence electron v.

B. Presence of weak interaction

In the presence of the PNC weak interaction, the exact atomic wave function can be written as

$$|\Psi_v\rangle = e^T\{1 + S_v\}|\Phi_v\rangle, \tag{3.12}$$

where the cluster amplitudes are given by

$$T = T^{(0)} + G_F T^{(1)},$$

$$S_v = S_v^{(0)} + G_F S_v^{(1)}. \tag{3.13}$$

The $T^{(1)}$ and $S_v^{(1)}$ operators are the corrections to the cluster operators $T^{(0)}$ and $S^{(0)}$, respectively. Since G_F is very small, one can consider only the first order terms in Eq. (3.13). Therefore, Eq. (3.12) can be written as

$$|\Psi_v\rangle = [e^{T^{(0)}}T^{(1)}\{1 + S_v^{(0)}\} + e^{T^{(0)}}\{S_v^{(1)}\}]|\Phi_v\rangle, \tag{3.14}$$

which can be explicitly separated as given in Eq. (2.4).

The perturbed amplitudes for $T^{(1)}$ and $S_v^{(1)}$ operators are solved using the following equations:

$$\langle\Phi_0^L|\widehat{\overline{H^{(0)}}T^{(1)}} + \overline{H_{\text{PNC}}^{\text{NSI}}}|\Phi_0\rangle = 0, \tag{3.15}$$

$$\langle \Phi_v^K | \widehat{(\overline{H^{(0)}} - E_v^{(0)}) S_v^{(1)}} + \widehat{\overline{H^{(0)}} T^{(1)}} + \widehat{\overline{H^{(0)}} T^{(1)} S_v^{(0)}} + \overline{H_{\mathrm{PNC}}^{\mathrm{NSI}}} + \widehat{\overline{H_{\mathrm{PNC}}^{\mathrm{NSI}}} S_v^{(0)}} | \Phi_v \rangle = 0, \qquad (3.16)$$

where $L,K=1,2$ and the effective Hamiltonian operators with overline defined as $\overline{H^{(0)}}=(e^{-T^{(0)}} H^{(0)} e^{T^{(0)}})_c$. These are computed after determining $T^{(0)}$. The wide-hat symbol as usual represents the connected terms.

Using the above relations, the $E1_{\mathrm{PNC}}$ amplitude can be expressed as

$$\begin{aligned} E1_{\mathrm{PNC}} &= \frac{\langle \Phi_f | \{1 + S_f^{(1)^\dagger} + T^{(1)^\dagger} S_f^{(0)^\dagger} + T^{(1)^\dagger}\} e^{T^{(0)^\dagger}} \mathrm{D} e^{T^{(0)}} \{1 + T^{(1)} + T^{(1)} S_i^{(0)} + S_i^{(1)}\} | \Phi_i \rangle}{\sqrt{(1 + N_f^{(0)})(1 + N_i^{(0)})}} \\ &= \frac{\langle \Phi_f | S_f^{(1)^\dagger} \overline{\mathrm{D}^{(0)}} \{1 + S_i^{(0)}\} + \{1 + S_f^{(0)^\dagger}\} \overline{\mathrm{D}^{(0)}} S_i^{(1)} + S_f^{(0)^\dagger} (T^{(1)^\dagger} \overline{\mathrm{D}^{(0)}} + \overline{\mathrm{D}^{(0)}} T^{(1)}) S_i^{(0)} + (T^{(1)^\dagger} \overline{\mathrm{D}^{(0)}} + \overline{\mathrm{D}^{(0)}} T^{(1)}) S_i^{(0)} | \Phi_i \rangle}{\sqrt{(1 + N_f^{(0)})(1 + N_i^{(0)})}}, \qquad (3.17) \end{aligned}$$

where we have defined $\overline{D^{(0)}}=e^{T^{(0)^\dagger}} D e^{T^{(0)}}$ and the above equation is calculated using the similar procedure followed for Eq. (3.7).

IV. BASIS FUNCTIONS

We have calculated hyperfine structure constants earlier in different atoms using Gaussian type orbitals (GTOs) and they are capable of producing accurate results [13,14]. As a matter of fact both PNC and hyperfine interactions arise from interactions between the atomic nucleus and electrons. Therefore, it would be appropriate to use GTOs to calculate $E1_{\mathrm{PNC}}$. The GTOs are expressed as [25]

$$F_{i,k}(r) = r^k e^{-\alpha_i r^2}, \qquad (4.1)$$

where $k=0,1,\ldots$ for $s,p,\ldots$ type orbital symmetries, respectively. For the exponents, we have used

$$\alpha_i = \alpha_0 \beta^{i-1}. \qquad (4.2)$$

It has been found that effects of the core electrons are important for very accurate calculations, especially, for the d states [26,27]. Therefore, we consider all occupied (holes) orbitals in both the DF and RCC calculations. In order to achieve high precision in our calculations, we have considered orbitals up to g symmetries. The GTOs are defined on a grid and the DF matrix is constructed and diagonalized. The eigenvectors obtained from this diagonalization together with GTOs are used to construct the occupied and unoccupied orbitals on the grid. We have used $\alpha_0=0.00525$ and $\beta=2.73$ in our calculations. The finite size of the nucleus has been accounted by considering a two-parameter Fermi nuclear charge distribution approximation given by

$$\rho = \frac{\rho_0}{1 + e^{(r-c)/a}}. \qquad (4.3)$$

We use values of ρ_0, c and a as given by Parpia and Mohanty [28]. Contributions from the protons and neutrons asymmetry in this system has been evaluated in a separate work by Panda and Das in Ba^+ using the relativistic mean field (RMF) model [29]; the contribution is about 0.3% to the present system.

V. RESULTS AND DISCUSSIONS

To justify the accuracy of the calculated wave functions, we have carried out important physical quantities whose experimental results are known. Our calculated results in one hand test the potential of the method used in the system to produce accurate results and in other hand they provide support to the precision of the experimental results. We first present the IP, magnetic dipole hyperfine constants (A), electric quadrupole hyperfine structure constants (B), $E1$ amplitudes and $E2$ amplitudes for the low-lying states and compare with other works along with the experimental results. We deduced the excitation energies from our IP results for various states. We give the $E1_{\mathrm{PNC}}$ contributions from different RCC terms and investigate the importance of various low-lying states through these terms. The accuracy of $E1_{\mathrm{PNC}}$ has been estimated in a rigorous approach by considering difference between results obtained from two approximations at the same level of excitations.

A. Ba^+ properties

We have calculated the IPs of the first eleven low-lying states and presented them in Table I. In the same table, these results are compared with other calculated results by Guet and Johnson [30], Eliav *et al.* [31], Dzuba *et al.* [18] and Geetha *et al.* [24] along with the experimental data [32,33]. Dzuba *et al.* have used a variant of all order relativistic many-body perturbation theory. Guet and Johnson had used the second order relativistic MBPT theory to calculate their results. Both Eliav *et al.* and Geetha *et al.* had used the RCC method in their calculations.

We have determined the excitation energies of a few transitions, which will be used later for evaluating other quantities, by subtracting the IP results of the corresponding states. These results are tabulated in Table II. It is obvious from this table that this work provides very accurate results and can be

TABLE V. Transition probabilities A_{if}, where i is the initial and f is the final state, of $E1$ transition amplitudes from different works in $10^8\ \mathrm{s}^{-1}$.

Transition states	Guet and Johnson[a]	Dzuba *et al.*[b]	Geetha *et al.*[c]	This work	Expt.
$6s\,^2S_{1/2} \rightarrow 6p\,^2P_{1/2}$	0.918	0.923	0.937	0.978	0.95(9)[d] 0.955(10)[e] 0.95(7)[f]
$6s\,^2S_{1/2} \rightarrow 6p\,^2P_{3/2}$	1.163	1.171	1.194	1.218	1.06(9)[d] 1.17(4)[e] 1.18(8)[f]
$5d\,^2D_{3/2} \rightarrow 6p\,^2P_{1/2}$	0.334	0.370	0.326	0.331	0.338(19)[d] 0.33(8)[e] 0.33(4)[f]
$5d\,^2D_{3/2} \rightarrow 6p\,^2P_{3/2}$	0.044	0.045	0.043	0.044	0.0469(29)[d] 0.048(5)[e] 0.048(6)[f]
$5d\,^2D_{5/2} \rightarrow 6p\,^2P_{3/2}$	0.360	0.345	0.349	0.342	0.377(24)[d] 0.37(4)[e] 0.37(4)[f]

[a] Reference [30].
[b] Reference [18].
[c] Reference [7].
[d] Reference [43].
[e] Reference [44].
[f] Reference [45].

used for *ab initio* calculations for PNC amplitudes and lifetimes of different states.

A knowledge of the hyperfine structure constants is necessary in many areas of atomic physics. For example, the error associated with the PNC matrix elements can be determined from the accuracies of these constants [42] as their behavior is determined by the wave functions near the nuclear region [10] and they are also useful in determining shift of the resonance frequency in atomic clocks [8]. We have calculated the magnetic dipole (A) and electric quadrupole (B) hyperfine structure constants for few low-lying states in $^{137}\mathrm{Ba}^+$ and presented in Table III. We have used nuclear Lande g factor, g_I, as 0.6249 [34] and nuclear quadrupole moment, Q, equal to $0.246b$ [41] $(1b=10^{-24}\ \mathrm{cm}^2)$ in the present calculations. There are many experimental results available for these quantities, but we have compared our results with the best data [35–41]. Some of the A results were published in our earlier work [42], where orbitals with g-symmetry were not included. It is clear from the present work that these orbitals are important for accurate calculations of the hyperfine structure constants for p and d states. In our earlier work, we have also discussed the trends of the correlation effects arising from the RCC terms and also compared with other works [42].

As given in Table III, the hyperfine structure constants for the $6s\,^2S_{1/2}$, $6p\,^2P_{1/2}$, $6p\,^2P_{3/2}$, and $5d\,^2D_{3/2}$ states are close to the experimental results suggesting that the wave functions used in these calculations can give us accurate $H_{\mathrm{PNC}}^{\mathrm{NSI}}$ matrix elements between the above states.

Our reduced matrix elements for the $E1$ operator (in a.u.) is presented in Table IV. Expression for the $E1$ transition probability is given by

$$A_{i\leftarrow f}^{E1} = \frac{2.02613 \times 10^{18}}{[J_f]\lambda^3} S_{i\leftarrow f}^{E1}, \tag{5.1}$$

where i and f represent the initial and final states, λ is the corresponding wavelength, $[J]=2J+1$ is the degeneracy of the state, and $S_{i\leftarrow f}^{E1}$ is the square of the transition amplitude due to $E1$ operator given in Table IV. We have calculated A^{E1} for different transitions and presented in Table V. Here λ is derived from our calculated excitation energies given in Tables I and II for an *ab initio* study.

In Table V, we also compare the A_{if} values from different calculations by Guet and Johnson [30], Dzuba *et al.* [18], and Geetha *et al.* [7]. There are three different set of experimental data [43–45] available for these quantities, but Kastberg *et al's* results are more accurate than others. In the first two calculations, they had used experimental wavelengths whereas we have used the results of our *ab initio* calcula-

TABLE VI. Reduced matrix element of $E2$ transition of $5d\,^2D_{5/2}$ state.

Transition states	Guet and Johnson[a]	Geetha *et al.*[b]	This work	Expt.
$5d\,^2D_{3/2} \rightarrow 6s\,^2S_{1/2}$	13.7	12.63	12.74	12.40(74)[c]
$5d\,^2D_{5/2} \rightarrow 6s\,^2S_{1/2}$	16.0	16.0	15.96	16.86 ± 1.18[d] 13.91 ± 3.22[e] 16.25 ± 0.77[f]

[a] Reference [30].
[b] Reference [7].
[c] Reference [46].
[d] Reference [47].
[e] Reference [48].
[f] Reference [49].

TABLE VII. Contributions to the $E1_{\mathrm{PNC}}$ calculation in $\times 10^{-11} iea_0(-Q_W/N)$ using RCC calculation.

Initial pert. terms	$6s\,^2S^{(1)}_{1/2} \to 5d\,^2D^{(0)}_{3/2}$	Final pert. terms	$6s\,^2S^{(0)}_{1/2} \to 5d\,^2D^{(1)}_{3/2}$
$DH^{\mathrm{NSI}}_{\mathrm{PNC}}$	2.018	$H^{\mathrm{NSI}}_{\mathrm{PNC}}$ D	−0.2 $\times 10^{-5}$
$\overline{D^{(0)}}T^{(1)}_1$	0.0003	$T^{(1)\dagger}\overline{D^{(0)}}$	0.418
$\overline{D^{(0)}}S^{(1)}_{1i}$	2.634	$S^{(1)\dagger}_{1f}\overline{D^{(0)}}$	−0.179
$\overline{D^{(0)}}S^{(1)}_{2i}$	−0.242	$S^{(1)\dagger}_{2f}\overline{D^{(0)}}$	−0.166
$S^{(0)\dagger}_{1f}\overline{D^{(0)}}S^{(1)}_{1i}$	0.149	$S^{(1)\dagger}_{1f}\overline{D^{(0)}}S^{(0)}_{1i}$	0.003
$S^{(0)\dagger}_{1f}\overline{D^{(0)}}S^{(1)}_{2i}$	0.007	$S^{(1)\dagger}_{1f}\overline{D^{(0)}}S^{(0)}_{2i}$	0.008
$S^{(0)\dagger}_{2f}\overline{D^{(0)}}S^{(1)}_{1i}$	−0.116	$S^{(1)\dagger}_{2f}\overline{D^{(0)}}S^{(0)}_{1i}$	−0.009
$S^{(0)\dagger}_{2f}\overline{D^{(0)}}S^{(1)}_{2i}$	−0.001	$S^{(1)\dagger}_{2f}\overline{D^{(0)}}S^{(0)}_{2i}$	0.001
Norm	−0.046		−0.001
Total	2.375		0.087

tions. Geetha *et al.* had carried out their calculations using the RCC method, but they had omitted many nonlinear terms.

In Table VI, we present the $E2$ reduced matrix elements of the $5d\,^2D_{3/2} \to 6s\,^2S_{1/2}$ and $5d\,^2D_{5/2} \to 6s\,^2S_{1/2}$ transitions. These results are compared with Guet and Johnson [30] and Geetha *et al.* [7], which are derived from their lifetime calculations. We have also compared these results with the experimental results obtained from the lifetime measurements of the corresponding states. Using our results, we obtain the quadrupole polarizability of 6s state due to $5d$ states, $\alpha^0_2 = 1844 a_0^5$, which agrees with the experimental value $\alpha^0_2 = 1828(88) a_0^5$ [50].

B. $E1_{\mathrm{PNC}}$ result of the $6s\ ^2S_{1/2} \to 5d\,^2D_{3/2}$ transition

The main goal of this work is to obtain an accurate value of the parity nonconserving electric dipole transition amplitude for the $6s\,^2S_{1/2} \to 5d\,^2D_{3/2}$ based on RCC theory. As has been mentioned before, it is necessary to test the excitation energies, $E1$ transition amplitudes and magnetic dipole (A) hyperfine structure constants, in order to determine an approximate error for the PNC transition amplitude of our interest.

TABLE VIII. Reduced $E1$ matrix elements for different intermediate states.

	$\langle 5d_{3/2} \lVert D \rVert np_{1/2} \rangle_{\mathrm{DF}}$	$\langle np_{3/2} \lVert D \rVert 6s \rangle_{\mathrm{DF}}$
$n=4$	0.75	0.07
$n=5$	1.94	0.91
$n=6$	3.73	5.48
$n=7$	0.36	0.31
$n=8$	0.19	0.18
$n=9$	0.47	0.07
$n=10$	0.23	0.08
$n=11$	0.04	0.04

TABLE IX. Contributions to the $E1_{\mathrm{PNC}}$ calculation at Dirac-Fock level in $\times 10^{-11} iea_0(-Q_W/N)$.

	$\langle 5p_{3/2}\lvert D\rvert np_{1/2}\rangle_{\mathrm{DF}} \times \langle np_{1/2}\lvert H^{NSI}_{\mathrm{PNC}}\rvert 6s\rangle_{\mathrm{DF}}$	$\langle 5d_{3/2}\lvert H^{\mathrm{NSI}}_{\mathrm{PNC}}\rvert np_{3/2}\rangle_{\mathrm{DF}} \times \langle np_{3/2}\lvert D\rvert 6s\rangle_{\mathrm{DF}}$
$n=6$	1.860	-2.6×10^{-6}
$n=7$	0.045	-2.9×10^{-8}
$n=8$	0.013	-9.5×10^{-8}
$n=9$	0.075	8.1×10^{-9}
$n=10$	0.024	5.1×10^{-9}
$n=11$	0.002	1.1×10^{-9}

The contributions from different terms in the $E1_{\mathrm{PNC}}$ amplitude calculation for the $6s\,^2S_{1/2} \to 5d\,^2D_{1/2}$ transition are presented in Table VII. It is clear that the largest contribution comes from $\overline{D^{(0)}}S^{(1)}_1$, which represents the DF term and a certain subclass of core polarization as well as pair correlation effects. This is due to the relatively large $(6s_{1/2} - 6p_{1/2})$ $S^{(1)}_1$ cluster amplitude. Two different types of core polarization effects, $\overline{D^{(0)}}T^{(1)}_1$ and $\overline{D^{(0)}}S^{(1)}_2$ as well as its conjugate, also make significant contributions. The former is mediated by the neutral weak interaction and involves the $6s$ valence and core electrons. Correlation effects corresponding to $S^{(0)\dagger}_1\overline{D^{(0)}}S^{(1)}_1$ and $S^{(0)\dagger}_2\overline{D^{(0)}}S^{(1)}_1$are non negligible, but their signs are opposite. Contributions from the other terms are comparatively small.

It is important to understand the role of different intermediate states in the calculation of the $E1_{\mathrm{PNC}}$ amplitude of the $6s\,^2S_{1/2} \to 5d\,^2D_{3/2}$ transition in Ba$^+$. It is also possible to determine the error in this quantity by identifying important intermediate states and estimating the accuracies of the different properties of those states that are related to the above PNC amplitude. As has been mentioned, our method includes implicitly all the intermediate states through the RCC theory with the PNC interaction as a first order perturbation. It is therefore not possible to find the individual contribution from different intermediate states in this approach. However, we have made a special effort to investigate their contributions by computing the first order perturbed wave functions, which involves summing over various intermediate states. In Tables IX to XII, we present these contributions at various levels. In Table VIII, we present the reduced $E1$ matrix elements for different transitions at the DF level, which are used to calculate the contributions from excited states from RCC terms to the above $E1_{\mathrm{PNC}}$ amplitude.

As given in Table IX, the major contributions to the DF calculation of $E1_{\mathrm{PNC}}$ come from the $6p_{1/2}$ and $7p_{1/2}$ states. Nevertheless, contributions from the continuum orbitals,

TABLE X. Contributions to the $E1_{\mathrm{PNC}}$ calculation from core-excitation operators in $\times 10^{-11} iea_0(-Q_W/N)$ using RCC calculation.

	$\langle 6s\lvert T^{\dagger(1)}_1\rvert np_{1/2}\rangle \times\langle np_{1/2}\lvert D\rvert 5d_{3/2}\rangle_{\mathrm{DF}}$	$\langle 6s\lvert D\rvert np_{3/2}\rangle_{\mathrm{DF}} \times\langle np_{3/2}\lvert T^{(1)}_1\rvert 5d_{3/2}\rangle$
$n=4$	−0.0005	−0.00003
$n=5$	0.4188	0.0004

TABLE XI. Contributions to the $E1_{\rm PNC}$ calculation from leading DF and pair-correlation diagrams in $\times 10^{-11} iea_0(-Q_W/N)$ using RCC calculation.

	$\langle 5d_{3/2}\|D\|np_{1/2}\rangle_{\rm DF} \times \langle np_{1/2}\|S^{(1)}_{1i}\|6s\rangle$	$\langle 5d_{3/2}\|S^{\dagger(1)}_{1f}\|np_{3/2}\rangle \times \langle np_{3/2}\|D\|6s\rangle_{\rm DF}$
$n=6$	2.407	−0.181
$n=7$	0.066	−0.003
$n=8$	0.019	−0.001
$n=9$	0.111	0.008
$n=10$	0.032	4×10^{-4}
$n=11$	0.003	2×10^{-5}

$10p_{1/2}$ and $11p_{1/2}$ orbitals, are also significant. We shall now consider the contributions from the important intermediate states at the RCC level.

As explained before, the $\overline{D^{(0)}}T_1$ and its conjugate term correspond to a part of the core-polarization effects. The leading contributions come from these terms are DT_1 and its conjugate term. From Table X, it is clear that the $4p$ and $5p$ occupied orbitals contribute significantly to the $E1_{\rm PNC}$ amplitude.

The most important correlation contributions to the $E1_{\rm PNC}$ amplitude are $DS^{(1)}_{1i}$ and $S^{(1)\dagger}_{1f}D$ from $\overline{D^{(0)}}S^{(1)}_{1i}$ and $S^{(1)\dagger}_{1f}\overline{D^{(0)}}$, respectively. We present contributions from different intermediate states arising from these terms in Table XI. As seen in this table the $6p$, $7p$, $10p$ and $11p$ states made the most important contributions.

Core-polarization effects arising through $DS^{(1)}_{2i}$ and $S^{(1)\dagger}_{2f}D$ from different intermediate states are quoted in Table XII. It can be seen from this table that the most important contributions come from the p states. We have also made special effort to see contributions from various combinations of orbitals through $S^{(1)\dagger}_{1f}DS^{(0)}_{1i}$ and $S^{(0)\dagger}_{1f}DS^{(1)}_{1i}$ terms. These results are presented in Table XII.

C. Estimation of $E1_{\rm PNC}$ accuracy through the calculated quantities

As has been shown in Table II, the agreement with the experiment of the most important excitation energy $(6p\,^2P_{1/2})$ for the calculation of $E1_{\rm PNC}$ is better than one percent. The accuracy of the next important state $(7p\,^2P_{1/2})$ for the initial PNC perturbed state is just 0.5%. The excitation energy of $5d\,^2D_{3/2}-6p\,^2P_{3/2}$ is around 1.6%. But this will not affect the $E1_{\rm PNC}$ result very much as the $5d\,^2D_{3/2}$ state does not contribute significantly to the PNC amplitude.

TABLE XII. Contributions to the $E1_{\rm PNC}$ calculation from pair-correlation from Coulomb and PNC interactions in $\times 10^{-11} iea_0(-Q_W/N)$ using RCC calculation.

	$\langle 5d_{3/2}\|S^{\dagger(1)}_{1f}\|mp_{3/2}\rangle \times \langle mp_{3/2}\|D\|ns\rangle_{\rm DF} \times \langle ns\|S^{(0)}_{1i}\|6s\rangle$		$\langle 5d_{3/2}\|S^{\dagger(0)}_{1f}\|kd_{3/2}\rangle \times \langle kd_{3/2}\|D\|lp_{1/2}\rangle_{\rm DF} \times \langle lp_{1/2}\|S^{(1)}_{1i}\|6s\rangle$
For,	$n=7$	and	$k=6$
$m=6$	0.007	$l=6$	0.175
$m=7$	−0.005	$l=7$	−0.089
$m=8$	−0.0002	$l=8$	−0.0004
For,	$n=8$	and	$k=7$
$m=6$	0.001	$l=6$	0.024
$m=7$	0.002	$l=7$	0.349
$m=8$	−0.002	$l=8$	−0.041

TABLE XIII. Square root of the magnetic dipole hyperfine constants (MHz) and their deviations from experimental results.

	Experiment	This work	Deviation (%)
$\sqrt{A_{6s^2S_{1/2}}A_{6p^2P_{1/2}}}$	1728.83	1738.1	0.5
$\sqrt{A_{6p^2P_{3/2}}A_{5d^2D_{3/2}}}$	155.35	156.08	0.5

From the transition probability calculations presented in Table V, it is obvious that our $E1$ transition amplitudes given in table IV, are very accurate. This is an indication that these amplitudes are included accurately in the $E1_{\rm PNC}$ amplitude calculation. It is also clear that most of the other calculated results do not fall within the experimental error and are farther away from the central values than ours.

There is no direct procedure to determine the accuracy of the calculated PNC matrix elements between different states. An alternative method has been followed to calculate the error associate with this quantity, i.e., by calculating the square root of the product of the corresponding states connecting to the PNC operator as shown in [42]. In Table XIII, we present the values of the square root of the product of $\sqrt{A_{6s^2S_{1/2}}A_{6p^2P_{1/2}}}$ and $\sqrt{A_{6p^2P_{3/2}}A_{5d^2D_{3/2}}}$. The accuracies of these two quantities give an indication of the accuracies of the PNC matrix elements between $6s\,^2S_{1/2}$ and $6p\,^2P_{1/2}$ states as well as the $6p\,^2P_{3/2}$ and $5d\,^2D_{3/2}$ states. Both of them are in excellent agreement with experiment, suggesting that the two leading PNC matrix elements for the $E1_{\rm PNC}$ calculation are very accurate.

D. Comparison between different works

The result of $E1_{\rm PNC}$ for the $6s\,^2S_{1/2}\rightarrow 5d\,^2D_{3/2}$ transition from our calculation is $2.46\times 10^{-11} iea_0(-Q_W/N)$. In Table XIV, we compare it with other calculations. Our result is larger in magnitude than those obtained by Dzuba *et al.* [18] and Geetha [19]. The former work is based on a variant of all order many-body perturbation theory, but it has some semiempirical features. It is carried out using two different approaches: One of them is similar to the sum-over-states (SS) approach and the other is known as the mixed-parity (MP) approach, where the PNC interaction explicitly mixes states of opposite parities. However, both calculations do not in-

TABLE XIV. Comparison of $E1_{\rm PNC}$ results from different calculations in $\times 10^{-11} iea_0(-Q_W/N)$.

Dzuba *et al.*		Geetha	This work
(MP)	(SS)		
2.17	2.34	2.35	2.46(2)

clude contributions from certain correlation effects; i.e., structural radiation, weak correlation potential and normalization of states, that are included in our calculation. Their $6p\,^2P_{1/2} \rightarrow 5d\,^2D_{3/2}$ $E1$ matrix element, which is important for the above mentioned PNC transition amplitude, is not as accurate as ours. Furthermore, the accuracies of their PNC matrix elements are not known, as they have not performed calculations of the hyperfine constants of the relevant states. The reason for the discrepancy between our calculation and Geetha's is that our approach implicitly includes several intermediate states; particularly doubly excited opposite parity states, which her sum-over-states approach omits.

The error accrued in our calculation of $E1_{\mathrm{PNC}}$ can be determined from the errors in the excitation energies, $E1$ transition amplitudes, and hyperfine constants. We have not estimated the errors in the calculated values of these quantities by comparing with measurements, since the error bars in the $E1$ transition amplitudes are rather large. Instead, we have taken the differences of our RCC calculations to single, double and leading triple excitations [CCSD(T)] and also just to single and double excitations (CCSD) as the errors. We have shown the variation between different results for the important contributing intermediate states using these two methods in Table XIV. The quadrature formula used for estimating error is given below. By expressing $E1_{\mathrm{PNC}}$ as

$$X = \frac{AB}{C}, \tag{5.2}$$

the error can be evaluated using the relationship

$$\Delta X = \sqrt{\frac{B^2}{C^2}\Delta A^2 + \frac{A^2}{C^2}\Delta B^2 + \frac{A^2B^2}{C^4}\Delta C^2}, \tag{5.3}$$

where the Δ values are the results of the differences between CCSD(T) and CCSD for the quantities given in Table XV. The error (0.018) in $E1_{\mathrm{PNC}}$ has been obtained by adding the errors for the different quantities it depends on in quadrature given in the above formula, for the leading intermediate states $6p\,^2P_{1/2}$ and $6p\,^2P_{3/2}$. We have considered slightly bigger value for the error associate with other states, which contributes comparatively very small.

TABLE XV. Differences (Δs) of the CCSD(T) and CCSD results for the excitation energy (cm^{-1}), $E1$ transition amplitudes (a.u.), and magnetic dipole hyperfine structure constant (MHz) for different low-lying states of Ba$^+$.

Excitation	$6s\,^2S_{1/2} \rightarrow 6p\,^2P_{1/2}$	$5d\,^2D_{3/2} \rightarrow 6p\,^2P_{3/2}$
Energy	−19.89	12.45
$E1$ transition	$6s\,^2S_{1/2} \rightarrow 6p\,^2P_{3/2}$	$5d\,^2D_{3/2} \rightarrow 6p\,^2P_{1/2}$
amplitude	−0.004	−0.01
Hyperfine	$\sqrt{A_{6s\,^2S_{1/2}} A_{6p\,^2P_{1/2}}}$	$\sqrt{A_{6p\,^2P_{3/2}} A_{5d\,^2D_{3/2}}}$
constants (A)	10.26	1.28

VI. CONCLUSION

A significant feature of our work is that it is concerned with two different fundamental interactions (electromagnetic and weak) and their interplay. We apply the full fledged RCC theory which incorporates all the single, double, and leading triple excitations to calculate atomic wave functions. Our approach implicitly takes into account all the intermediate states in the PNC perturbed wave functions. Our present calculation of the $E1_{\mathrm{PNC}}$ amplitude for the $6s\,^2S_{1/2} \rightarrow 5d\,^2D_{3/2}$ transition in Ba$^+$ is more accurate than the previous calculations by Dzuba *et al.* and Geetha *et al.*, since it includes larger range of physical effects. The difference between the calculations for different properties related to $E1_{\mathrm{PNC}}$ based on the single, double and leading triple excitations and just the single and double excitations have been computed and added in quadrature to determine the error bars for $E1_{\mathrm{PNC}}$. The error in our $E1_{\mathrm{PNC}}$ calculation was found to be less than one percent by this procedure.

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