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Relativistic coupled-cluster calculations of parity nonconservation in Ba$^+$ by the sum-over-states approach

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The authors present the results of their calculation for the parity nonconserving $5p^6 6s_{1/2} \rightarrow 5p^6 5d_{3/2}$ transition in Ba$^+$ using the relativistic coupled-cluster theory in the singles, doubles, and partial triples approximation. The contributions from the leading intermediate states are explicitly considered. It is found that the largest contribution comes from the $|5p^6 6p_{1/2}\rangle$ state. Their results are in reasonable agreement with other calculations. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2404664]

I. INTRODUCTION

Parity nonconservation (PNC) in atoms and ions is an important area of atomic physics where combined sub-1% accurate relativistic many-body calculations and experiments provide important information about the possible existence of new physics beyond the standard model in the regime of small momentum transfer.[1] To this date, such a precision has been achieved only for atomic Cs,[2] where the result of the PNC calculation combined with the experiment on atomic Cs by Wood *et al.*[3] is found to be consistent with the standard model.

A variety of *ab initio* and semiempirical methods has been employed to compute the PNC induced electric dipole transition amplitude ($E1_{\mathrm{PNC}}$) in various atoms and ions in the past few decades. Among them the order-by-order many-body perturbation theory (MBPT) is the method that is most widely used. In this method, apart from the residual Coulomb interaction [difference of the two-electron Coulomb interaction and the one electron Dirac-Fock (DF) potential], the PNC interaction arising from the neutral weak currents is also considered as a perturbation. For atoms with strongly interacting configurations, it would be appropriate to use a hybrid approach consisting of configuration interaction (CI) and MBPT or coupled-cluster (CC) approaches. Examples of such atoms are bismuth and ytterbium.

The quantity that is measured in a PNC experiment is related to the interference of $E1_{\mathrm{PNC}}$ and an allowed electromagnetic transition amplitude.[4] Experiments that have been successful so far are based on fluorescence and optical rotation.[3,5] In the former case the interference is between $E1_{\mathrm{PNC}}$ and a Stark-induced electric dipole transition amplitude. In the latter it is between $E1_{\mathrm{PNC}}$ and an allowed magnetic dipole transition amplitude. Precise measurements of optical rotation have been carried out for the $6p_{1/2} \rightarrow 6p_{3/2}$ transition in ^{205}Tl in Oxford[6] and Seattle,[5] for the $6^3P_0 \rightarrow 6^3P_1$ transition in ^{208}Pb in Seattle[7] and Oxford,[8] and for the $^4S_{3/2} \rightarrow {}^2D_{3/2}$ transition in ^{209}Bi in Oxford.[9] The other stream of experiments based on fluorescence has led to very accurate predictions in atomic cesium [10%,[10] 2%,[11] 0.35% (Ref. 3)] which in comparison with the theoretical calculations by Blundell *et al.*[12] using the linearized CC method and the most recent all order MBPT approach of Dzuba *et al.*[2] are found to be consistent with the standard model. For the past two decades a number of ingenious experimental techniques (e.g., laser cooling and trapping of atoms) have been used in the study of symmetry violations in atomic systems.

Our interest is mainly on Ba$^+$ for which an experiment to observe PNC using the $|5p^6 6s\rangle_{1/2} \rightarrow |5p^6 5d\rangle_{3/2}$ transition has been proposed by Fortson.[13] For this ion we have performed step by step relativistic CC calculations for various properties of interest such as the ionization potentials/excitation energies,[14] lifetimes,[15] and hyperfine constants,[16] and the results are very promising. The hyperfine constant calculations using different single particle orbitals by Sahoo[17] reveal the importance of the accuracy of the basis functions in such calculations. All these tests are essential as the accuracy of $E1_{\mathrm{PNC}}$ depends on the accuracies of certain atomic properties close to and far away from the nucleus. In this paper, we have evaluated $E1_{\mathrm{PNC}}$ using the sum over states approach in which we have taken the contributions from the dominant low-lying states using the relativistic CC theory and the rest by the DF method.

The outline of the paper is as follows. First we present the basic formalism of the relativistic CC method and then describe briefly the two different approaches to compute $E1_{\mathrm{PNC}}$, viz., the sum over intermediate states approach and

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the mixed parity approach. This is followed by the application of sum over intermediate states approach for the computation of $E1_{\rm PNC}$ in Ba$^+$ which is compared with other calculations of this quantity.

II. METHOD OF CALCULATION

Let us consider the atomic Hamiltonian to be the exact no-virtual pair Dirac-Coulomb (DC) Hamiltonian as discussed in Refs. 18 and 19 and given by

$$H_{\rm DC}=\sum_{i}^{N}[c\alpha_i\cdot p_i+(\beta_i-1)c^2+V_{\rm nuc}(r_i)]+\sum_{i<j}\frac{1}{r_{ij}}. \tag{1}$$

The contributions due to the Breit interaction, negative-energy states, and radiation corrections are omitted in the present calculation as they are rather small compared to the terms present in the DC Hamiltonian. The CC theory is based on the exponential wave function

$$|\Psi_{\rm CC}\rangle=e^{T}|\Phi_o\rangle, \tag{2}$$

where $|\Phi_o\rangle$ is the DF reference state and the operator T generating excitations from it. One can choose a non-DF reference state instead of the DF state, and for a multireference method it is replaced by a linear combination of determinants. In the present case, we start with the DF reference state corresponding to $(N-1)$ electron closed-shell configuration (in the present case it is Ba^{++}). In the single reference case, the operator T is given by

$$T=\sum_{i=1}T_i, \tag{3}$$

where

$$T_1=\sum_{a,p}t_a^p a_p^\dagger a_a, \tag{4}$$

$$T_2=\frac{1}{(2!)^2}\sum_{a,b,p,q}t_{ab}^{pq}a_p^\dagger a_q^\dagger a_b a_a, \tag{5}$$

and so on. Here a,b and p,q represent core and virtual orbitals. These operators act on the $N-1$ electron ($|\Phi_o\rangle$) reference state function to give single and double excited states with respect to reference state and they can be represented as $|\Phi_a^p\rangle$ and $|\Phi_{a,b}^{p,q}\rangle$. Once we solve the $N-1$ electron closed-shell configuration we add one electron to the kth virtual orbital and obtain the N electron system as

$$|\Phi_k^N\rangle=a_K^\dagger|\Phi_o\rangle, \tag{6}$$

where $|\Phi_k^N\rangle$ represents the N electron system. Any general state in the open-shell CC method[20] is written as

$$|\Psi_k^N\rangle=e^{T^{(0)}}\{e^{S_k^{(0)}}\}|\Phi_k^N\rangle. \tag{7}$$

Similar to the definition of T amplitudes, we define the S amplitudes as

$$S=\sum_i S_i, \tag{8}$$

where

$$S_1=\sum_p s_v^p a_p^\dagger a_v, \quad S_2=\frac{1}{(2!)^2}\sum_{a,p,q}s_{va}^{pq}a_p^\dagger a_q^\dagger a_a a_v,$$

and so on. Here in addition to a, p, and q (as defined earlier) v defines a valence orbital. These operators act on the N electron reference state function, thereby generating $|\Phi_v^p\rangle$, $|\Phi_{a,v}^{p,q}\rangle$ which are singly and doubly excited states with respect to $|\Phi_k^N\rangle$. Using the mathematical simplifications given in detail in Refs. 14 and 21, we can arrive at two different equations for determining the cluster amplitudes corresponding to T and S in the CC formalism.

In the present work we have used the nonlinear coupled-cluster singles, doubles, and partial triples [CCSD(T)] formalism for determining the T and S amplitudes. The approximations for the closed and open shell cluster amplitudes are described in our previous publication.[14] $E1_{\rm PNC}$ induced by weak interactions can be expressed as

$$E1_{\rm PNC}=\frac{\langle\tilde{\Psi}_f|D|\tilde{\Psi}_i\rangle}{\sqrt{\langle\tilde{\Psi}_i|\tilde{\Psi}_i\rangle}\sqrt{\langle\tilde{\Psi}_f|\tilde{\Psi}_f\rangle}}, \tag{9}$$

where D denotes dipole operator and $|\tilde{\Psi}_i\rangle$ and $|\tilde{\Psi}_f\rangle$ are the initial and final atomic states of mixed parity given by

$$|\tilde{\Psi}_i\rangle=|\Psi_i^{(0)}\rangle+|\Psi_i^{(1)}\rangle, \quad |\tilde{\Psi}_f\rangle=|\Psi_f^{(0)}\rangle+|\Psi_f^{(1)}\rangle.$$

Here $|\Psi\rangle$ with the superscripts 0 and 1 denote the unperturbed and perturbed atomic states. The neutral weak interaction Hamiltonian[22] given below is considered as the perturbation.

$$H_{\rm PNC}=\frac{G_F}{2\sqrt{2}}Q_W\sum_e\gamma_5\rho(r_e), \tag{10}$$

where G_F is the Fermi constant and Q_W is the weak nuclear charge given by $Q_W=2[ZC_{1p}+NC_{1n}]$. Z and N are the numbers of protons and neutrons, respectively. C_{1p} and C_{1n} are the vector (nucleon)-axial vector (electron) coupling coefficients, $\rho(r_e)$ is the normalized nucleon number density, and γ_5 is the usual pseudoscalar Dirac matrix.

We now focus on the important features of the two different approaches to compute $E1_{\rm PNC}$ using the above CC amplitudes.

A. Evaluation of $E1_{\rm PNC}$ using the sum over intermediate states approach

In this approach, we consider contributions from the bound low-lying states as allowed by the angular momentum selection rules using the CC method and the rest by the DF method. In the present case, we have taken the DF contributions from the singly excited states comprising of bound core and continuum virtual orbitals. Electric dipole transition amplitude induced by the PNC interaction from

$|5p^6 6s_{1/2}\rangle \rightarrow |5p^6 5d_{3/2}\rangle$ for Ba$^+$ using the sum over states approach[12] can be written as

$$E1_{\mathrm{PNC}} = \frac{1}{(\sqrt{\langle\Psi_i^{(0)}|\Psi_i^{(0)}\rangle}\sqrt{\langle\Psi_f^{(0)}|\Psi_f^{(0)}\rangle})} \times \sum_I \left(\frac{\langle\Psi_f^{(0)}|D|\Psi_I^{(0)}\rangle\langle\Psi_I^{(0)}|\mathrm{PNC}|\Psi_i^{(0)}\rangle}{(E_i - E_I)} + \frac{\langle\Psi_f^{(0)}|H_{\mathrm{PNC}}|\Psi_I^{(0)}\rangle\langle\Psi_I^{(0)}|D|\Psi_i^{(0)}\rangle}{(E_f - E_I)} \right), \tag{11}$$

where

$$|\Psi_i\rangle = |5p^6 6s\rangle_{1/2}, \quad |\Psi_f\rangle = |5p^6 5d\rangle_{3/2}.$$

From angular momentum considerations, we know that the nuclear spin independent neutral weak[23] PNC interaction (rank zero tensor) can connect only states of the same angular momentum. Hence, the first term in the $E1_{\mathrm{PNC}}$ expression can have intermediate atomic state functions with angular momentum $j=\frac{1}{2}$ and the second term with angular momentum $j=\frac{3}{2}$, respectively. That leads to intermediate atomic state functions to be only

$$|\Psi_I\rangle = |5p^6 np\rangle_{(1/2,3/2)},$$

with $n=6,7,\ldots,n_{\max}$, where $n_{\max}$ is the number of bound p virtual orbitals for the chosen basis. Using the all order closed and open shell CC amplitudes denoted by $T^{(0)}$ and $S^{(0)}$, all order dipole and PNC matrix elements between various intermediate bound states and initial and final states of interest can be computed. These matrix elements are used in Eq. (11) along with other quantities such as the energy denominators and the normalization factor to obtain $E1_{\mathrm{PNC}}$.

B. Evaluation of $E1_{\mathrm{PNC}}$ using mixed parity approach

In this approach, the all order CC amplitudes for closed- and open-shell systems are first computed without and with PNC as the perturbation. Later the PNC amplitude $E1_{\mathrm{PNC}}$ is constructed with just one order in PNC and all orders in the residual Coulomb perturbation at the singles, doubles, and partial triples level. The basic equations for obtaining these full fledged cluster amplitudes are described in detail in the literature[17,24] including its application to Ba$^+$ (Ref. 25) PNC, which is an important breakthrough in the computation of weak interactions in atoms. The important correlation effects incorporated in this method, but excluded in the summation over intermediate states, will be mentioned later in Sec. III. A somewhat similar approach based on MBPT (taking core polarization effects to all orders with important pair correlation effects to lowest order instead of all orders as in CC) when applied to Ba$^+$ PNC (Ref. 26) points to the importance of the pair correlation effects in the evaluation of $E1_{\mathrm{PNC}}$. The result obtained by this method is in good agreement with the mixed parity MBPT approach of Dzuba *et al.*[27]

Substituting the form of the CC wave function constructed from the unperturbed and perturbed T and S CC amplitudes, respectively, $E1_{\mathrm{PNC}}$ given in Eq. (9) takes the form

$$E1_{\mathrm{PNC}} = \frac{\langle\Phi_f^{(0)}|e^{\{\tilde{S}_f^\dagger\}}e^{\tilde{T}^\dagger}De^{\tilde{T}}e^{\{\tilde{S}_i\}}|\Phi_i^{(0)}\rangle}{\sqrt{\langle\Psi_i^{(0)}|\Psi_i^{(0)}\rangle}\sqrt{\langle\Psi_f^{(0)}|\Psi_f^{(0)}\rangle}}. \tag{12}$$

To obtain a nonzero electric dipole transition amplitude between initial and final states of the same parity, we need to consider terms which are at least linear in λ (zero order λ terms vanishes as per Laport's[28] rule). All the higher order terms in λ are negligible as λ scales as G_F the Fermi constant (10^{-14}).

TABLE I. Ionization potential (IP) and excitation energy (EE) calculations using pure GTOs and hybrid basis using $9s9p10d9f9g7h$ basis in units of a.u. Errors are given in parentheses.

Orbital	Analytical basis	Hybrid basis	Expt.
$6s(1/2)$	0.369 91(0.62%)	0.368 14(0.14%)	0.367 64
$5d(3/2)$	0.347 06(0.47%)	0.346 23(0.23%)	0.345 43
$5d(5/2)$	0.342 94(0.34%)	0.342 11(0.1%)	0.341 78
$6p(1/2)$	0.275 91(0.22%)	0.275 68(0.12%)	0.275 34
$6p(3/2)$	0.268 05(0.16%)	0.267 81 (0.07%)	0.267 62
$6s$-$5d(3/2)$	0.022 84(2.9%)	0.021 91(1.4%)	0.022 21
$6s$-$5d(5/2)$	0.026 97(4.3%)	0.026 03(0.66%)	0.025 86
$6s$-$6p(1/2)$	0.094 00(1.8%)	0.092 46(0.17%)	0.092 30
$6s$-$6p(3/2)$	0.101 85(1.8%)	0.100 33(0.31%)	0.100 02

III. RESULTS AND DISCUSSION

An experiment to observe PNC in the $|5p^6 6s\rangle_{1/2} \rightarrow |5p^6 5d\rangle_{3/2}$ transition in Ba$^+$ has been proposed by Fortson.[13] Previous calculations on this ion using different approaches based on the CI method[23] and MBPT by Dzuba *et al.*[27] and Gopakumar *et al.*[26] have shown the importance of the contribution from low-lying bound orbitals. Here we employ the CC method to calculate $E1_{\mathrm{PNC}}$ using the sum over intermediate states approach.

We first generate the single particle DF orbitals with Ba$^{++}(5p^6)$ as the starting potential. We make use of the hybrid approach[29] where we consider a part numerical and part analytical Gaussian-type orbitals (GTOs) on a grid. Technical details related to orthogonalization and completeness of the above basis set can be found from this reference. The advantage of choosing such a hybrid basis over purely analytical GTO basis is explained in detail taking a test calculation, computing ionization potential (IP) and excitation energy (EE) using CCSD(T) method for the low-lying levels of Ba$^+$ ion. The results of the calculation using the above two different bases consisting of $9s_{1/2}[3,\ldots,11]/[(3,\ldots,8)(9,\ldots,11)]$, $9p_{1/2,3/2}[3,\ldots,11]/[(3,\ldots,8)(9,\ldots,11)]$, $10d_{3/2,5/2}[3,\ldots,12]/[(3,\ldots,7)(8,\ldots,12)]$, $9f_{5/2,7/2}[4,12]/[(4,5)(6,\ldots,12)$, $9g_{7/2,9/2}[5,\ldots,13]/[(-),(5,\ldots,13)$, and $7h_{9/2,11/2}[6,\ldots,12]/[(-)(6,\ldots,12)]$ single particle orbitals are tabulated in Table I. Here $9s$ determines the number of s symmetry orbitals in the above two bases with $j=1/2$ angular momentum. Principal quantum number (n) of the orbitals starting from 3 to 11 belongs to pure analytical basis set, whereas for the hybrid basis $n=3-8$ are taken as numerical

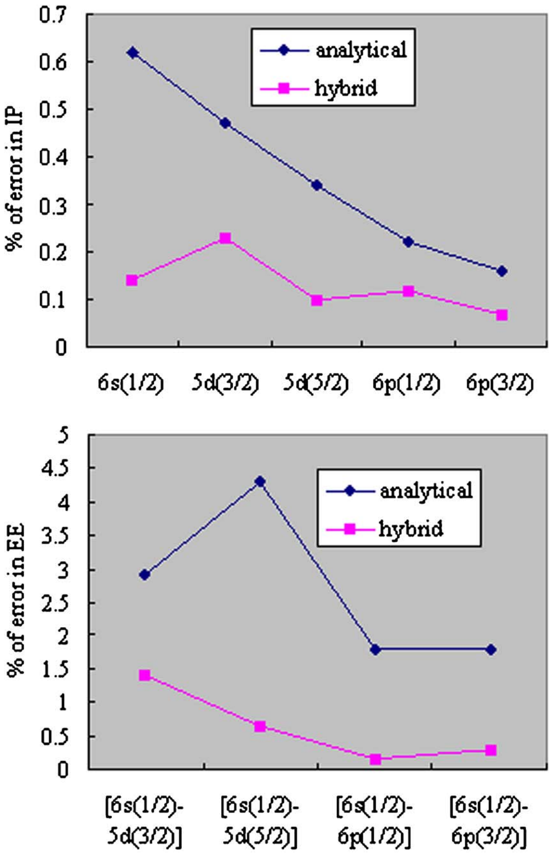

FIG. 1. Percentage of error in IPs and EEs for Ba^+ with analytical and hybrid (partly analytical and numerical) orbital bases.

TABLE II. Number of single particle orbitals (numerical+analytical) used in the calculation.

Symmetry	Analytical (generation)	Numerical orbitals	Analytical orbitals
$s(\frac{1}{2})$	32	$1s\ldots 8s(8)$	$9s..32s(24)$
$p(\frac{1}{2},\frac{3}{2})$	28	$2p..8p(7)$	$9p$-$29p(21)$
$d(\frac{3}{2},\frac{5}{2})$	25	$3d..7d(5)$	$8d..27d(20)$
$f(\frac{5}{2},\frac{7}{2})$	20	$4f,5f(2)$	$6f..23f(18)$
$g(\frac{7}{2},\frac{9}{2})$	15	$\cdots$	$5g..19g(15)$
$h(\frac{9}{2},\frac{11}{2})$	10	$\cdots$	$6h..15h(10)$

orbitals followed by analytical orbitals from $n=9$ to 11. For all other orbitals with the same symmetry but different angular momenta, the same kind of basis set is used.

The errors in IP and EE using the two different basis sets are schematically represented in Fig. 1. The average errors in IP and EE for Ba^+ using the hybrid basis are 0.1% and 0.6% as against the analytical basis with 0.4% and 2.7%. The major difference in the accuracies of the above quantities can only be attributed to the choice of the basis. By representing the core, valence, and the appropriate virtual single particle states by numerical DF/V^{N-1} orbitals, we have been able to obtain the best physical description for them.

The number of analytical orbitals used for the generation of basis using the finite basis-set expansion method[30] and the actual number of analytical and numerical orbitals used in the present calculation are given in Table II.

Examining the single particle orbital energies of $p(\frac{1}{2},\frac{3}{2})$ orbitals generated by the above method, we find that there are three bound virtual orbitals $(6p,7p,8p(\frac{1}{2},\frac{3}{2}))$ and the lowest continuum orbitals are $9p(\frac{1}{2},\frac{3}{2})$ orbitals. Hence we consider the contribution from $6p-8p$ orbitals by the CC method and the rest from $2p-5p$ and $9p-29p$ by lowest order MBPT, i.e., the DF approximation. Due to the presence of nuclear density in the PNC Hamiltonian, the PNC matrix element will be nonzero only when they are connected by $s(\frac{1}{2})$ and $p(\frac{1}{2})$ orbitals. The expression for the lowest order $E1_{\mathrm{PNC}}$ in terms of single particle orbitals and energies can be written as

$$E1_{\mathrm{PNC}} = \sum_n \frac{\langle 5d_{3/2}|D|np_{1/2}\rangle\langle np_{1/2}|H_{\mathrm{PNC}}|6s_{1/2}\rangle}{(\epsilon_{6s_{1/2}} - \epsilon_{np_{1/2}})} + \sum_n \frac{\langle 5d_{3/2}|H_{\mathrm{PNC}}|np_{3/2}\rangle\langle np_{3/2}|D|6s_{1/2}\rangle}{(\epsilon_{5d_{3/2}} - \epsilon_{np_{1/2}})},$$

where the first term represents PNC admixtures into the initial state and the second to the final state. The contributions from the bound and some of the continuum virtual $p_{1/2}$ orbitals at the DF level are tabulated in Table III.

From Table III it is clear that the core $5p_{1/2}$ and the lowest virtual $6p_{1/2}$ orbitals are the largest two contributors to the lowest order $E1_{\mathrm{PNC}}$ calculation. Even though the PNC matrix elements between the inner core $p_{1/2}$ and $6s_{1/2}$ are relatively large, the electric dipole matrix elements are small and the energy denominators are large. The overall contributions are therefore small. For the other bound virtual orbitals, the electric dipole as well as the PNC matrix elements reduce in size, and this with the increasing energy differences results in a rather small value of the total contribution from these orbitals. Examining the specific contributions from continuum $9p_{1/2}$ with bound $7p_{1/2}$ orbital as tabulated above, we can clearly identify the importance of continuum orbitals in the calculation of $E1_{\mathrm{PNC}}$. Comparing with the total contribution from the continuum orbitals starting from $9p_{1/2}$ to $29p_{1/2}$, we find that 99% of the contribution to $E1_{\mathrm{PNC}}$ comes from $9p_{1/2}$ and $10p_{1/2}$ orbitals. Hence the total contribution from the lowest order $E1_{\mathrm{PNC}}$ is $2.30\times 10^{-11} iea_0 Q_W/(-N)$ with 96% from the bound orbitals and the rest from the continuum orbitals. The Hermitian conjugate term connecting

TABLE III. DF contributions from bound (core, virtual) and continuum virtual orbitals in units of $10^{-11} iea_o(-Q_W/N)$. Here $p\star$ denotes $p_{1/2}$ orbitals.

$np\star$	$\langle 5d\|D\|np\star\rangle$	$\langle np\star\|H_{\mathrm{PNC}}\|6s\rangle$	$E1_{\mathrm{PNC}_i}$	Total
$2p\star$	0.002	4.825	0.000	0.000
$3p\star$	0.007	2.284	0.000	0.000
$4p\star$	0.003	1.038	0.000	0.000
$5p\star$	−0.792	0.378	0.286	0.286
$6p\star$	1.529	0.101	1.872	2.158
$7p\star$	0.143	0.063	0.044	2.202
$8p\star$	0.080	0.044	0.014	2.215
$9p\star$	−0.192	−0.242	0.072	2.287
$10p\star$	−0.055	−0.658	0.011	2.298
$11p\star$	0.009	1.952	0.001	2.299
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
$29p\star$	0.11×10^{-7}	-0.76×10^{3}	-0.33×10^{-12}	2.300

TABLE IV. Contribution to $E1_{\rm PNC}$ in Ba$^+$ from the intermediate states $I=6p-8p_{1/2,3/2}$. PNC and the final matrix elements using present method and calculations by Dzuba *et al.* are given in units of $10^{-11}iea_o(-Q_W/N)$. Dipole matrix elements and energy are in a.u. Normalization=1.005 494.

n $j=\frac{1}{2}$	$\langle 5d\|D\|np\rangle$ (a.u.)	$\langle np\|H_{\rm PNC}\|6s\rangle$	$E_{6s}-E_{np}$ (a.u.)	This work	Dzuba *et al.* (Ref. 27)
6	3.00	−2.51	−0.09	2.10	2.036
7	0.31	−1.46	−0.22	0.05	0.045
8	0.11	−0.94	−0.28	0.01	0.012
n $j=\frac{3}{2}$	$\langle np\|D\|6s\rangle$ (a.u.)	$\langle 5d\|H_{\rm PNC}\|np\rangle$	$E_{5d}-E_{np}$ (a.u.)	This work	Dzuba *et al.* (Ref. 27)
6	−4.80	−0.14	−0.10	−0.18	−0.264
7	−0.34	−0.10	−0.23	−0.08	−0.001
8	0.53	−0.06	−0.28	0.0	0.0

the initial state $6s_{1/2}$ through dipole to intermediate $p_{3/2}$ and then through $H_{\rm PNC}$ to final state $5d_{3/2}$ is zero due to the fact that the $H_{\rm PNC}$ matrix element vanishes in this case. However, this term is not zero when correlation effects are taken into account.

Our present approach is similar to that of Blundell *et al.*[12] for cesium, for which the largest contribution to $E1_{\rm PNC}$ is from the $6p_{1/2}$ and $7p_{1/2}$ intermediate states. A sum over states calculation based on MBPT for Ba$^+$ by Dzuba *et al.* clearly shows that the dominant contribution comes from the intermediate $6p_{1/2}$ state. The results of our work on Ba$^+$ with *ab initio* computed matrix elements and energy differences are tabulated in Table IV. We obtain good agreement with the values obtained by Dzuba *et al.*[27]

The DF contributions to $E1_{\rm PNC}$ from the bound core $(2p-5p)$ and the continuum $(9p-29p)$ virtual $p_{1/2}$ orbitals are found to be $0.28iea_0(-Q_W/N)\times10^{-11}$ and $0.08iea_0(-Q_W/N)\times10^{-11}$, respectively. The all order contribution from $(6p-8p)$ virtual $\left(\frac{1}{2},\frac{3}{2}\right)$ intermediate states to $E1_{\rm PNC}$ is $1.98iea_0(-Q_W/N)\times10^{-11}$. Hence the total contribution to $E1_{\rm PNC}$ from $2p-5p$ and $9p-29p$ at zeroth order and $6p-8p$ to all order is found to be $2.35iea_0(-Q_W/N)\times10^{-11}$. Dzuba *et al.*[27] using the experimental dipole matrix elements in the sum over intermediate states calculation find the value of $E1_{\rm PNC}$ to be $2.34iea_0(-Q_W/N)\times10^{-11}$. The total contribution to $E1_{\rm PNC}$ using the sum over states approach as compared to the results got by Dzuba *et al.*[27] is given in Table V. Another calculation based on the CC method using the mixed parity approach[25] gives the total contribution to be $2.46iea_0(-Q_W/N)\times10^{-11}$. The discrepancy of the above result with respect to the mixed parity approach based on MBPT of Dzuba *et al.* is because the latter does not include contributions from certain correlation effects such as structural radiation, weak correlation potential, and normalization correction of states which are automatically present in the CC method, whereas the discrepancy between the present calculation with the mixed parity approach[25] is due to the noninclusion of doubly excited opposite parity intermediate states which are implicitly added in the latter approach.

In order to determine the accuracy of the above calculations, it is necessary to know the accuracy to which one can compute the electric dipole/PNC matrix elements and the excitation energies. All these quantities, except the PNC matrix elements, can be obtained experimentally. The connection between the PNC matrix elements and hyperfine constants in terms of dependence on the wave functions at regions close to nucleus has been the yardstick for the determination of the accuracy of PNC matrix elements.[25] The above quantities are computed by CC method using the same basis and the results are tabulated in Table VI.

As emphasized in the previous paper on electric quadrupole transition calculations,[15] the accuracy of this method depends mainly on the matrix elements; $\langle 5p^65d_{3/2}|D|5p^66p_{1/2}\rangle$, $\langle 5p^66p_{3/2}|D|5p^66s_{1/2}\rangle$, $\langle 5p^66p_{1/2}|H_{\rm PNC}|5p^66s_{1/2}\rangle$, $\langle 5p^65d_{3/2}|H_{\rm PNC}|5p^66p_{3/2}\rangle$, and the energy differences $E_{5p^66s_{1/2}}-E_{5p^66p_{1/2}}$, $E_{5p^65d_{3/2}}-E_{5p^66p_{3/2}}$, respectively. Apart from this, the electric quadrupole transition amplitude $(E2)$ between $|5p^66s_{1/2}\rangle$ and $|5p^65d_{3/2}\rangle$ is also important as it is closely related to the physical quantity that will be measured in the proposed PNC experiment on Ba$^+$. Comparing the electric dipole matrix elements and the energy differences with available experimental quantities we find

TABLE V. Contribution to $E1_{\rm PNC}$ in Ba$^+$ in units of $10^{-11}iea_o(-Q_W/N)$.

Intermediate states	Present (DF+CC)	Dzuba *et al.* (Ref. 27) MBPT	Sahoo *et al.* (Ref. 25) CC
$2p-5p$ (DF)	0.28	⋯	
$9p-29p$ (DF)	0.08	⋯	
$6p-8p$ (CC)	1.99	⋯	
Total	2.35	2.34	2.46

TABLE VI. Excitation energy (cm^{-1}) and $E1$ transition amplitudes (a.u.) for different low-lying states of Ba$^+$ ion.

Initial state → final state	$6s(1/2)$ $-6p(1/2)$	$6s(1/2)$ $-6p(3/2)$	$5d(3/2)$ $-6p(1/2)$	$5d(3/2)$ $-6p(3/2)$
Excitation energy	20 293	22 020	15 383	17 077
Expt.	20 262	21 952	15 388	17 079
$E1$ transition amplitude	3.33	4.70	2.94	1.28
Expt.	3.36(0.16)	4.67(0.08)	3.03(0.08)	1.36(0.04)

that the accuracy of the wave functions in the large radial distances from the nucleus is well described and is better than 1%. The $E2$ electric quadrupole amplitude for the $6s_{1/2} \rightarrow 5d_{3/2}$ transition as shown in the previous paper[15] is also well within the experimental bounds. The results of the H_{PNC} matrix elements as deduced from the relativistic CC calculations of the hyperfine constants are also accurate.[16] The error in $E1_{\mathrm{PNC}}$ can be estimated either by comparing with measured quantities ($E1$ transition amplitudes, excitation energies, and hyperfine constants) or by looking at different contributions to $E1_{\mathrm{PNC}}$ in the framework of the method used. Here we consider the second approach. The error arising from all the intermediate states not included in the present calculation (two hole two particle states) is likely to be smaller than the total contribution from the continuum states ($9p-29p$) which is about 3%. Contributions from the Breit interaction to $E1_{\mathrm{PNC}}$ in Ba^+ was found to be less than 0.1% (Ref. 17) at the DF level and about the same for the relativistic CC calculation. The contributions from the QED effects are likely to be even smaller and can therefore be neglected in the present work.

IV. CONCLUSION

We have calculated $E1_{\mathrm{PNC}}$ for Ba^+ using an *ab initio* approach which takes into account the contribution of the important intermediate states, i.e., $6p-8p(\frac{1}{2},\frac{3}{2})$, by relativistic CC theory and the rest by the DF approximation. It is evident from our calculation that the dominant contribution comes from the $|5p^6 6p(\frac{1}{2})\rangle$ intermediate state. The good agreement of the relevant excitation energies, electric dipole transition amplitudes, and hyperfine constants of the relativistic CC calculations with the corresponding measured values suggests that our calculated PNC transition amplitude is reliable.

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