Calculation of nuclear-spin-dependent parity nonconservation in s-d transitions of Ba\textsuperscript{+}, Yb\textsuperscript{+} and Ra\textsuperscript{+} ions.

V. A. Dzuba and V. V. Flambaum

School of Physics, University of New South Wales, Sydney, NSW 2052, Australia
(Dated: January 18, 2013)

We use correlation potential and many-body perturbation theory techniques to calculate spin-independent and nuclear spin-dependent parts of the parity nonconserving amplitudes of the transitions between the 6s_{1/2} ground state and the 5d_{3/2} excited state of Ba\textsuperscript{+} and Yb\textsuperscript{+} and between the 7s_{1/2} ground state and the 6d_{3/2} excited state of Ra\textsuperscript{+}. The results are presented in a form convenient for extracting of the constants of nuclear-spin-dependent interaction (such as, e.g., anapole moment) from the measurements.

PACS numbers: 11.30.Er, 31.15.A-

I. INTRODUCTION

The study of the parity nonconservation (PNC) in atoms is a low-energy, relatively inexpensive alternative to high-energy search for new physics beyond the standard model (see, e.g. [1]). The most significant recent achievement on this path is the very precise measurements of the PNC in cesium [2]. The cesium PNC experiment together with its interpretation [3–5] in terms of nuclear weak charge provides the best current atomic test of the standard model (see also review [6]). It is also the only measurement of the nuclear anapole moment which is produced by the PNC nuclear forces in the weak nuclear charge from the PNC measurements relies on atomic calculations. Cesium atom has the simplest electron structure among all heavy atoms which were used or considered for the PNC measurements. Still it took considerable efforts of several groups of theorists to bring the accuracy of the calculations in line with the accuracy of measurements and provide reliable interpretation of the measurements in terms of the standard model and possible new physics beyond it [3–5]. It is widely believed now that it would be hard to compete with cesium experiment in terms of accuracy of interpretation of the PNC measurements. Therefore, the study of PNC in atoms is mostly focused now in two directions: (i) the measurements of the PNC ratio for a chain of isotopes which was first proposed in Ref. [8], and (ii) the measurements of the nuclear-spin-dependent PNC, like e.g. the contribution from nuclear anapole moment (see, e.g. reviews [6, 7]). The study of the PNC for a chain of isotopes does not require atomic calculations and can deliver useful information about either neutron distribution or new physics beyond standard model (see, e.g. 10, 11). The measurements of anapole moment does require atomic calculations but high accuracy is not critical here.

Ba\textsuperscript{+}, Yb\textsuperscript{+} and Ra\textsuperscript{+} ions considered in present paper are good candidates for both types of the experimental studies. Ba and Yb both have seven stable isotopes with large difference in neutron numbers $\Delta N_{\text{max}} = 8$. Radium has several long-living isotopes. There are two stable isotopes for each of the Ba and Yb atoms (\textsuperscript{135}Ba, \textsuperscript{139}Ba, \textsuperscript{171}Yb and \textsuperscript{173}Yb) which have non-zero nuclear spin. There are also isotopes of Ra with non-zero nuclear spin (\textsuperscript{223}Ra, \textsuperscript{225}Ra, \textsuperscript{229}Ra). In all cases nuclear spin is provided by valence neutron. This is especially interesting since it allows one to measure the strength of the neutron-nucleus PNC potential [2] (the anapole moment has been measured only for the \textsuperscript{133}Cs nucleus which has valence proton).

Finally, Ba\textsuperscript{+} and Ra\textsuperscript{+} ions have electron structure similar to those of cesium atom. This means that the accuracy of the interpretation of the PNC measurements can be on the same level as for cesium. Moreover, it can be further improved with the use of the experimental data [12].

The use of Ba\textsuperscript{+} in the PNC measurements was first suggested by Fortson [14]. The work is in progress at Seattle (see, e.g. [15, 16]) but no PNC results have been reported yet. Similar approach is now considered for the measurements of PNC in Ra\textsuperscript{+} ion at KVI [18, 19]. It is important that in Ra\textsuperscript{+} the PNC effects are about 20 times larger than in Ba\textsuperscript{+}. There are plans to measure PNC in Yb\textsuperscript{+} at Los Alamos [20]. Note that the PNC measurements for neutral ytterbium are in progress at Berkeley and first PNC results were recently reported [21]. The PNC measurements for the Yb\textsuperscript{+} ion would provide an important consistency test for the measurements and their interpretation.

Calculations of the spin-independent PNC amplitude for Ba\textsuperscript{+} and Ra\textsuperscript{+} were performed in our early work [12] and in [17]. Calculations for Ra\textsuperscript{+} were later performed in [18] and [22]. The only calculation of the spin-dependent PNC in Ra\textsuperscript{+} was recently reported by Sahoo et al [23]. To the best of our knowledge, no PNC calculations for Yb\textsuperscript{+} have been published so far.

In present paper we calculate both spin-independent and spin-dependent PNC amplitudes simultaneously using the same procedure and the same wave functions. In this approach the relative sign of the amplitudes is fixed. This allows for unambiguous determination of the sign.
of the spin-dependent contribution. The constant of the spin-dependent interaction can be expressed via the ratio of the two amplitudes. This brings an extra advantage of more accurate interpretation of the measurements. The accuracy of the calculations for the ratio of the PNC amplitudes is usually higher than that for each of the amplitudes. This is because the amplitudes are often very similar in structure and most of the theoretical uncertainty cancels out in the ratio.

Since we focus on the calculation of the nuclear-spin-dependent PNC amplitudes where high accuracy of calculations is not needed, we don’t include some small corrections, like some classes of diagrams for higher-order correlations, Breit and quantum electrodynamical (QED) corrections, etc. Instead, we make sure that all leading contributions are included exactly the same way for both spin-independent and spin-dependent PNC amplitudes which is important for the cancelation of the uncertainty in the ratio.

II. THEORY

Hamiltonian describing parity-nonconserving electron-nuclear interaction can be written as a sum of spin-independent (SI) and spin-dependent (SD) parts (we use atomic units: \( h = |e| = m_e = 1 \)):

\[
H_{\text{PNC}} = H_{\text{SI}} + H_{\text{SD}} = \frac{G_F}{\sqrt{2}} \left( -\frac{Q_W}{2} \gamma_5 + \frac{\alpha}{I} \sigma I \right) \rho(r),
\]

where \( G_F \approx 2.2225 \times 10^{-14} \text{ a.u.} \) is the Fermi constant of the weak interaction, \( Q_W \) is the nuclear weak charge, \( \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \) and \( \gamma_5 \) are the Dirac matrices, \( I \) is the nuclear spin, and \( \rho(r) \) is the nuclear density normalized to 1. The strength of the spin-dependent PNC interaction is proportional to the dimensionless constant \( \alpha \) which is to be found from the measurements. There are three major contributions to \( \alpha \) arising from (i) electromagnetic interaction of atomic electrons with nuclear anapole moment \( \Delta \), (ii) electron-nucleus spin-dependent weak interaction, and (iii) combined effect of spin-independent weak interaction and magnetic hyperfine interaction \( \Delta \) (see, also review [2]). In this work we do not distinguish between different contributions to \( \alpha \) and present the results in terms of total \( \alpha \) which is the sum of all possible contributions.

Within the standard model the weak nuclear charge \( Q_W \) is given by [20]

\[
Q_W \approx -0.9877N + 0.0716Z.
\]

Here \( N \) is the number of neutrons, \( Z \) is the number of protons.

The PNC amplitude of an electric dipole transition between states of the same parity \(|i\) and \(|f\) is equal to:

\[
\begin{align*}
E_{1_{fi}}^{\text{PNC}} &= \sum_n \left[ \frac{\langle f | d | n \rangle \langle n | H_{\text{PNC}} | i \rangle}{E_i - E_n} + \frac{\langle f | H_{\text{PNC}} | n \rangle \langle n | d_q | i \rangle}{E_f - E_n} \right], \\
&= \frac{(f | H_{\text{PNC}} | n) \langle n | d_q | i \rangle}{E_f - E_n},
\end{align*}
\]

where \( d = -e \sum_i r_i \) is the electric dipole operator, \(|a \rangle \equiv |J_a F_a M_a \rangle\) and \( F = I + J \) is the total angular momentum.

Applying the Wigner-Eckart theorem we can express the amplitudes via reduced matrix elements

\[
\begin{align*}
E_{1_{fi}}^{\text{PNC}} &= (-1)^{F_f - M_f} \left( \begin{array}{c} F_f \\ -M_f \\ q \\ M_i \end{array} \right) \\
&\times \langle J_f F_f | | d_{\text{PNC}} | | J_i F_i \rangle.
\end{align*}
\]

Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found e.g. in Refs. [27] and [28]. For the SI amplitude we have

\[
\langle J_f, F_f | | d_{\text{SI}} | | J_i, F_i \rangle = (-1)^{I_f + I_i + J_f + J_i} \\
\times \sqrt{(2F_f + 1)(2F_i + 1)} \sum J_f J_i \frac{\langle J_f | d | n, J_n \rangle \langle n, J_n | H_{\text{SI}} | J_i \rangle}{E_i - E_n} \\
+ \langle J_f | H_{\text{SI}} | n, J_n \rangle \langle n, J_n | d | J_i \rangle \frac{1}{E_f - E_n}.
\]

For the SD PNC amplitude we have

\[
\langle J_f, F_f | | d_{\text{SD}} | | J_i, F_i \rangle = \frac{G_F}{\sqrt{2}} \times \sum J_f J_i \frac{\langle J_f | d | n, J_n \rangle \langle n, J_n | \alpha \rho | J_i \rangle}{E_i - E_n} \\
+ \langle J_f | \alpha \rho | n, J_n \rangle \langle n, J_n | d | J_i \rangle \frac{1}{E_n - E_f}.
\]

For the case of the 5d – 6s transitions considered in present paper (or 6d – 7s in the case of Ra+ ) it is convenient to break expression (10) into four parts:

\[
\langle 5d_{3/2}, F_f | | d_{\text{SD}} | | 6s, F_i \rangle = S_1 + S_2 + S_3 + S_4,
\]

(7)
where

\[ S_1 = c_1(F_f, F_i) \]
\[ \times \sum_n \langle 5d_{i/2}|d|np_{1/2}\rangle \langle np_{1/2}|\alpha p|6s \rangle \]
\[ \times \sum_n \langle 5d_{i/2}|\alpha p|np_{1/2}\rangle \langle np_{1/2}|d|6s \rangle / (E_{np_{1/2}} - E_{6s}), \]
\[ S_2 = c_2(F_f, F_i) \]
\[ \times \sum_n \langle 5d_{i/2}|np_{3/2}\rangle \langle np_{3/2}|\alpha p|6s \rangle \]
\[ \times \sum_n \langle 5d_{i/2}|\alpha p|np_{3/2}\rangle \langle np_{3/2}|d|6s \rangle / (E_{np_{3/2}} - E_{6s}), \]
\[ S_3 = c_3(F_f, F_i) \]
\[ \times \sum_n \langle 5d_{i/2}|\alpha p|np_{1/2}\rangle \langle np_{1/2}|d|6s \rangle \]
\[ \times \sum_n \langle 5d_{i/2}|\alpha p|np_{3/2}\rangle \langle np_{3/2}|d|6s \rangle / (E_{np_{1/2}} - E_{5d_{i/2}}), \]
\[ S_4 = c_4(F_f, F_i) \]
\[ \times \sum_n \langle 5d_{i/2}|\alpha p|np_{3/2}\rangle \langle np_{3/2}|d|6s \rangle / (E_{np_{3/2}} - E_{5d_{i/2}}). \]

Here \( c_m(F_f, F_i) \) (\( m = 1, 2, 3, 4 \)) are coefficients which can be reconstructed using (8). The terms \( S_1, S_2, S_3, S_4 \) differ by the order of the operators \( d \) and \( \alpha p \) and by the states in the summation which are either \( np_{1/2} \) or \( np_{3/2} \) states. To know the relative values of these terms is important for the analysis of the accuracy of the calculations.

### III. CALCULATIONS

To perform the calculations we follow an \textit{ab initio} approach which uses the correlation potential method and the technique to include higher-order correlations developed in Refs. [30–32].

Calculations start from the relativistic Hartree-Fock (RHF) method in the \( V^{N-1} \) approximation. This means that the initial RHF procedure is done for a closed-shell atomic core with the valence electron removed. After that, the states of the external electron are calculated in the field of the frozen core. Correlations are included by means of the correlation potential method [29]. For \( \text{Ba}^+ \) and \( \text{Ra}^+ \) we use the all-order correlation potential \( \Sigma(\infty) \) which includes two classes of the higher-order terms: screening of the Coulomb interaction and hole-particle interaction (see, e.g. [30] for details). For \( \text{Yb}^+ \) we use the second-order correlation potential \( \Sigma^{(2)} \). The reason for different approaches is due to different electron structures of the ions. The all-order technique developed in [31, 32] works very well for alkali atoms and similar ions in which the valence electron is far from the atomic core and higher-order correlations are dominated by screening of the core-valence residual Coulomb interaction by the core electrons. For atoms and ions similar to \( \text{Yb}^+ \), in which an external electron is close to the core and strongly interacts with its electrons, a different higher-order effect described by the \textit{ladder diagrams} becomes important. The applicability of the technique of Ref. [32] to \( \text{Yb}^+ \) needs further investigation. Meanwhile, the use of the second-order \( \Sigma^{(2)} \) leads to sufficiently good results. Note that an external electron in \( \text{Ba}^+ \) and \( \text{Ra}^+ \) ions is also closer to atomic core than in neutral alkali atoms \( \text{Cs} \) and \( \text{Fr} \). This means that inclusion of ladder diagrams might be a way to improve the accuracy of calculations for the ions as well. This question also needs further investigation.

To calculate \( \Sigma (\Sigma(\infty) \text{ or } \Sigma^{(2)}) \text{ we need a complete set of the single-electron orbitals. We use the B-spline technique [34] to construct the basis. The orbitals are built as linear combinations of 50 B-splines of order 9 in a cavity of radius 40\( a_B \). The coefficients are chosen from the condition that the orbitals are the eigenstates of the RHF Hamiltonian \( H_0 \) of the closed-shell core. The second-order operator \( \Sigma^{(2)} \) is calculated via direct summation over B-spline basis states. The all-order \( \Sigma(\infty) \) is calculated with the technique which combines solving equations for the Green functions (for the direct diagram) with the summation over complete set of states (exchange diagram) [30].

The correlation potential \( \Sigma \) is then used to build a new set of single-electron states, the so-called Brueckner orbitals. This set is to be used in the summation in equations (5), (6). Here again we use the B-spline technique to build the basis. The procedure is very similar to constructing of the RHF B-spline basis. The only difference is that new orbitals are now the eigenstates of the \( H_0 + \Sigma \) Hamiltonian.

Brueckner orbitals which correspond to the lowest valence states are good approximations to the real physical states. Their quality can be tested by comparing experimental and theoretical energies. The energies of the lowest states of \( \text{Ba}^+ \), \( \text{Yb}^+ \) and \( \text{Ra}^+ \) in RHF and Brueckner approximations are presented in Table I. One can see that inclusion of the correlations leads to significant

| Ion   | State | RHF  | Brueckner | Experiment [36] |
|-------|-------|------|------------|------------------|
| \text{Ba}^+ | 6s_{1/2} | 75340 | 80815 | 80687 |
|        | 6p_{1/2} | 57266 | 60571 | 60425 |
|        | 6p_{3/2} | 55873 | 58848 | 58735 |
|        | 5d_{3/2} | 68139 | 76318 | 75813 |
| \text{Yb}^+ | 6s_{1/2} | 90789 | 99477 | 98297 |
|        | 6p_{1/2} | 66087 | 70728 | 71145 |
|        | 6p_{3/2} | 63276 | 67101 | 67815 |
|        | 5d_{3/2} | 66517 | 75551 | 75246 |
| \text{Ra}^+ | 7s_{1/2} | 75898 | 82032 | 81842 |
|        | 7p_{1/2} | 56878 | 60715 | 60491 |
|        | 7p_{3/2} | 52906 | 55753 | 55633 |
|        | 6d_{3/2} | 62356 | 70091 | 69758 |

| Ion   | \( s_{1/2} \) | \( p_{1/2} \) | \( p_{3/2} \) | \( d_{3/2} \) |
|-------|---------------|---------------|---------------|---------------|
| \text{Ba}^+ | 0.978       | 0.960        | 0.964        | 0.941        |
| \text{Yb}^+ | 0.862       | 1.081        | 1.170        | 0.968        |
| \text{Ra}^+ | 0.970       | 0.946        | 0.960        | 0.959        |
improvement of the accuracy in all cases. The deviation of the theory from experiment is just fraction of a per cent in the case of Ba\(^+\) and Ra\(^+\) where an all-order \(\Sigma(\infty)\) is used and does not exceed 1.3\% for Yb\(^+\) where the second-order \(\Sigma(2)\) is used.

The quality of the Brueckner orbitals can be further improved by rescaling the correlation potential \(\hat{\Sigma}\) to fit the experimental energies exactly. We do this by replacing the \(H_0 + \hat{\Sigma}\) with the \(H_0 + \lambda \hat{\Sigma}\) Hamiltonian in which the rescaling parameter \(\lambda\) is chosen for each partial wave to fit the energy of the first valence state. The values of \(\lambda\) are presented in Table I. Note that these values are very close to unity. This means that even without rescaling the accuracy is good and only a small adjustment of the value of \(\hat{\Sigma}\) is needed. Note also that since the rescaling procedure affects not only energies but also the wave functions, it usually leads to improved values of the matrix elements of external fields. In fact, this is a semi-empirical method to include omitted higher-order correlation corrections.

Matrix elements of the \(H_{SI}\), \(H_{SD}\) and electric dipole operators are found by means of the time-dependent Hartree-Fock (TDHF) method \([29, 35]\) extended to Brueckner orbitals. This method incorporates to the well-known random-phase approximation (RPA) diagrams including exchange. In the TDHF method, the single-electron wave functions are presented in the form \(\psi = \psi_0 + \delta \psi\), where \(\psi_0\) is the unperturbed wave function. It is an eigenstate of the RHF Hamiltonian \(H_0\): \((\hat{H}_0 - \epsilon_0)\psi_0 = 0\). \(\delta \psi\) is the correction due to external field. It can be found by solving the TDHF equation

\[
(\hat{H}_0 - \epsilon_0)\delta \psi = -\delta \epsilon \psi_0 - \hat{F} \psi_0 - \delta \hat{V}^{-N-1} \psi_0, \tag{12}
\]

where \(\delta \epsilon\) is the correction to the energy due to external field (\(\delta \epsilon = 0\) for all above mentioned operators but it is not zero for the hyperfine interaction which we will need for the analysis of accuracy), \(\hat{F}\) is the operator of the external field, and \(\delta \hat{V}^{-N-1}\) is the correction to the self-consistent potential of the core due to external field.

The TDHF equations are solved self-consistently for all states in the core. Then the matrix elements between any (core or valence) states \(n\) and \(m\) are given by

\[
(\psi_n|\hat{F} + \delta \hat{V}^{-N-1}|\psi_m). \tag{13}
\]

The best results are achieved when \(\psi_n\) and \(\psi_m\) are the Brueckner orbitals computed with rescaled correlation potential \(\hat{\Sigma}\).

We use equation (13) for all weak and electric dipole matrix elements in evaluating the SI and SD PNC amplitudes \([4]\) and \([6]\).

### IV. ACCURACY OF CALCULATIONS

The accuracy of the results obtained via direct summation over physical states with the use of expressions like \([5]\) is determined by the accuracy for the energies, electric dipole and weak matrix elements. We start from the notion that for the PNC amplitudes considered in present work the summation over intermediate \(p\)-states is strongly dominated by the \(6p_{1/2}\) and \(6p_{3/2}\) states for Ba\(^+\) and Yb\(^+\) and by \(7p_{1/2}\) and \(7p_{3/2}\) states for Ra\(^+\). Corresponding contributions constitute 70 to 90\% of the total PNC amplitude. Therefore, it is sufficient to compare with experiment energies and matrix elements involving these \(p\)-states. The energies and electric dipole matrix elements can be directly compared with experiment while standard practice of comparing experimental and theoretical hyperfine structure can be used to test the accuracy of the weak matrix elements.

To improve the accuracy for the amplitudes the energies of the \(6s\), \(6p_{1/2}\), \(6p_{3/2}\) and \(5d_{3/2}\) states (\(7s\), \(7p_{1/2}\), \(7p_{3/2}\) and \(6d_{3/2}\) for Ra\(^+\)) are fitted exactly in our calculations using rescaling of the correlation potential \(\hat{\Sigma}\) as it
In the end of section II we introduced the notations between theory and experiment for the hfs of the 6 states to remeasure the hfs of this state. The electric dipole transition data in Ba\(^+\), Yb\(^+\) and Ra\(^+\) can be found in Ref. [16] and [39].

The data in Table III shows good agreement between theory and experiment for most of the amplitudes, although the accuracy for the amplitudes involving the \(p_{3/2}\) states is lower than that for the \(p_{1/2}\) states.

Table V shows theoretical and experimental data on the hyperfine structure constants of the low states of Ba\(^+\), Yb\(^+\) and Ra\(^+\). Here again we only compare our calculations with the most accurate experimental data. A review of the available experimental and theoretical data for Ba\(^+\) can be found in Ref. [51]. The data in Table V shows several trends: (i) the accuracy is good for \(s_{1/2}\) and \(p_{1/2}\) states, especially in the cases of Ba\(^+\) and Ra\(^+\); (ii) the accuracy for Yb\(^+\) is lower than that for Ba\(^+\) and Ra\(^+\); (iii) the accuracy for \(p_{3/2}\) and \(d_{3/2}\) states is lower than that for the \(s_{1/2}\) and \(p_{1/2}\) states. The largest discrepancy is for the hfs of the \(6p_{3/2}\) state where theory and experiment differ almost three times. Note that the most complete calculations of Ref. [41] give the results which are close to our theoretical value rather than to the experiment. In principle, the discrepancy can be explained by configuration mixing involving configurations with excitations from the 4\(f\) subshell. Neither our present calculations nor those of Ref. [11] include this mixing explicitly. The configuration interaction calculations based on technique developed in Ref. [52, 53] which treats Yb\(^+\) as a system with fifteen valence electrons show that the hfs of the \(6p_{3/2}\) state is indeed very sensitive to the configuration mixing. One can find such mixing which reproduces the experimental hfs exactly while the accuracy for the energy and for the \(g\)-factor of the \(6p_{3/2}\) state is also good. However, the results are inconclusive due to strong instability of the hfs of the \(6p_{3/2}\) state. We can only say that the configuration mixing can explain current experimental value of the hfs of \(6p_{3/2}\) state but we cannot prove that this explanation is correct. Since the disagreement between theory and experiment for the hfs of the \(6p_{3/2}\) state of Yb\(^+\) is the main factor contributing to the uncertainty of the calculations for Yb\(^+\), it would be useful to remeasure the hfs of this state.

The fact that the accuracy for the \(p_{1/2}\) and \(p_{3/2}\) states is different complicates the analysis of the accuracy for the PNC amplitudes. There is cancelation between terms containing matrix elements with the \(p_{1/2}\) and \(p_{3/2}\) states. In the end of section III we introduced the notations \(S_1, S_2, S_3\) and \(S_4\) for these terms (see Eqs. [50, 51]). The terms involving the \(p_{1/2}\) states are \(S_1\) and \(S_3\), the terms with the \(p_{3/2}\) states are \(S_2\) and \(S_4\). Table V shows the \(S_1, S_2, S_3, S_4\) contributions to the reduced matrix elements of the nuclear-spin-dependent PNC interaction in some hfs components of the transitions in Ba\(^+\), of Yb\(^+\) and of Ra\(^+\). One can see that the \(S_2\) term is usually small while the \(S_1\) term is not small. For example, for Yb\(^+\) the contribution of the \(S_4\) term is more than half of the total sum. It is clear that the accuracy of the calculations in this case will be mostly determined by the accuracy of the \(S_4\) term.

To analyse the accuracy of the PNC calculations we need a procedure which takes into account the deviation of the experimental and theoretical data for the electric dipole matrix elements and for the hyperfine structure as well as the effect of partial cancelation between different contributions to the PNC amplitude. We do this by comparing the \(ab\) initio calculations with the calculations in which the electric dipole and weak matrix elements are rescaled to fit the experimental data. For example, assuming that the weak matrix elements between two states are proportional to the square root of the hfs constants for these states we rescale them as following

\[
\langle n|\hat{H}_{\text{PNC}}|m\rangle_{\text{rescaled}} = \sqrt{\frac{A_{n}^{\text{exp}} A_{m}^{\text{exp}}}{A_{n}^{\text{th}} A_{m}^{\text{th}}}} \langle n|\hat{H}_{\text{PNC}}|m\rangle. \tag{14}
\]

Here \(A_{n}^{\text{exp}}\) and \(A_{n}^{\text{th}}\) are experimental and theoretical values of the hfs constants from Table IV. This means that we perform accurate rescaling for matrix elements involving \(6p_{1/2}\) and \(6p_{3/2}\) states (\(7p_{1/2}\) and \(7p_{3/2}\) for Ra\(^+\)). As it was stated above, this corresponds to 70 to 90% of the total PNC amplitude. We use the same rescaling for all matrix elements involving higher \(p\) states. Electric dipole matrix elements are also rescaled to fit the experimental data for the transitions between lowest states. The difference between PNC amplitudes obtained in the \(ab\) initio calculations and calculations with rescaling serves as an estimation of the uncertainty of the calculations.

Note that the accuracy for the relative contribution of the nuclear-spin-dependent interaction can be higher that for each of the amplitudes (see also Ref. [54]). As we will see in the next section, this is usually the case when the \(S_2\) and \(S_1\) contributions are both small. This is because these terms are exactly zero for the spin-independent PNC amplitudes. Therefore, the spin-dependent PNC amplitudes in which the \(S_2\) and \(S_3\) terms are small, are similar to the spin-independent amplitudes. They both change under scaling at the same rate which cancels out in the ratio.
TABLE V: Contributions to the reduced matrix elements \( \langle 5d_{3/2} | H_{SDPNC} | 6s_{1/2}, F_2 \rangle \) of the spin-dependent parity-nonconserving s-d transitions. See text for explanation of notations. Units: \( 10^{-13} \text{zeVA} \).

| Ion     | \( F_1 \) | \( F_2 \) | \( S_1 \) | \( S_2 \) | \( S_3 \) | \( S_4 \) | \( \text{Sum} \) |
|---------|---------|---------|---------|---------|---------|---------|----------|
| \(^{133}\text{Ba}^+\) | 1       | 0       | 0.134   | 0.002   | 0.000   | -0.027  | 0.108    |
|         | 1       | -1      | -0.211  | -0.001  | 0.013   | 0.032   | -0.168   |
|         | 1       | -2      | -0.057  | 0.003   | 0.029   | -0.014  | -0.040   |
|         | 2       | 1       | 0.211   | -0.002  | -0.038  | -0.009  | 0.162    |
|         | 2       | 2       | 0.127   | -0.003  | 0.009   | 0.009   | 0.004    |
|         | 3       | 2       | -0.212  | -0.002  | 0.000   | 0.043   | -0.171   |
| \(^{141}\text{Yb}^+\) | 1       | 0       | 0.780   | 0.000   | -0.306  | -0.164  | 0.310    |
|         | 1       | 1       | 0.184   | -0.008  | -0.432  | 0.116   | -0.140   |
|         | 2       | 1       | -0.411  | -0.004  | 0.000   | 0.156   | -0.259   |
| \(^{226}\text{Ra}^+\) | 1       | 2       | -2.021  | 0.031   | 0.000   | -0.119  | 1.933    |
|         | 2       | 2       | -2.301  | -0.005  | 0.265   | 0.084   | -1.957   |
|         | 3       | 3       | -0.878  | 0.044   | 0.496   | -0.045  | -0.384   |
|         | 3       | 2       | 2.058   | -0.037  | -0.593  | -0.006  | 1.423    |
|         | 3       | 3       | 1.643   | -0.036  | -0.530  | 0.006   | 1.084    |
|         | 4       | 3       | -2.500  | -0.039  | 0.000   | 0.148   | -2.391   |

V. RESULTS

The results of the calculations for the spin-independent part of the PNC amplitudes (\( z \)-components) are

\[
\begin{align*}
\text{Ba}^+ & : E_1^{\text{PNC}}(5d_{3/2} - 6s) = 0.29(2) \times 10^{-12} Q_{\text{W}iea}, \\
\text{Yb}^+ & : E_1^{\text{PNC}}(5d_{3/2} - 6s) = 0.62(20) \times 10^{-12} Q_{\text{W}iea}, \\
\text{Ra}^+ & : E_1^{\text{PNC}}(6d_{3/2} - 7s) = 3.4(1) \times 10^{-12} Q_{\text{W}iea}.
\end{align*}
\]

The uncertainties are estimated by comparing \( ab \) \( initio \) calculations with the calculations in which matrix elements were rescaled as described in previous sections. The expressions (15, 16, 17) are valid for any isotopes. All dependence of nuclear number \( A \) is via weak nuclear charge \( Q_{\text{W}} \) (see, [2]) while dependence on nuclear radius is negligible. To be precise, the dependence of the PNC amplitudes on the nuclear radius can be included with the help of an additional factor

\[
E_1^{\text{PNC}}(A_2) = \left( \frac{A_2}{A_1} \right)^{2/3} E_1^{\text{PNC}}(A_1).
\]

For cases considered in this work the maximum value of the correction is 0.4% (between \(^{223}\text{Ra}^+ \) and \(^{229}\text{Ra}^+ \) ). For other cases the correction is even smaller. This is beyond the accuracy of present calculations.

It is convenient to present the total PNC amplitude (including the spin-dependent part) in a form

\[
E_1^{\text{PNC}} = P(1 + R \zeta),
\]

where \( P \) is the spin-independent part (including weak nuclear charge \( Q_{\text{W}} \) ) and \( R \) is the ratio of the spin-dependent to the spin-independent amplitudes. This has two important advantages: (i) extraction of the value of \( \zeta \) from experimental data can lead to no confusion over its sign, (ii) the uncertainty for the value of the ratio of the spin-dependent and spin-independent amplitudes \( R \) is usually lower than for each of the amplitudes. This is because the two amplitudes are very similar and numerical uncertainty cancels out in the ratio (see also Ref. [54]).

The total PNC amplitudes for different hfs transitions in \( \text{Ba}^+ \), \( \text{Yb}^+ \) and \( \text{Ra}^+ \) are presented in Table VI. The table includes all stable isotopes of Ba and Yb which have non-zero nuclear spin and the most stable isotopes of Ra with non-zero nuclear spin. The results for other isotopes can be obtained by rescaling appropriate PNC amplitudes (with required values of \( F_1, F_2 \) and \( I \)) using corresponding weak nuclear charges:

\[
\begin{align*}
E_1^{\text{PNC}}(A_2) & = P(A_1) F_1 F_2 I \left( \frac{Q_{\text{W}}(A_2)}{Q_{\text{W}}(A_1)} \right) \left[ 1 + R(A_1) F_1 F_2 I \frac{Q_{\text{W}}(A_1)}{Q_{\text{W}}(A_2)} \right],
\end{align*}
\]

where \( P(A_1) F_1 F_2 I \) and \( R(A_1) F_1 F_2 I \) are taken from Table VI and \( Q_{\text{W}}(A_1) \) and \( Q_{\text{W}}(A_2) \) are calculated using [2]. We stress ones more that the dependence of the amplitudes on the nuclear radius is much smaller than current theoretical uncertainty.

Numerical uncertainties for \( P \) and \( R \) are presented in parentheses in Table VI. One can see that for some hyperfine transitions the uncertainty for \( R \) is very low. Comparing the data in Tables VI and V reveals that low uncertainty in \( R \) corresponds to the cases when the spin-dependent PNC amplitude is strongly dominated by the sum \( S_1 + S_4 \) while the sum of two other terms \( S_2 \) and \( S_3 \) is small. This is because strong domination of \( S_1 + S_4 \) makes the spin-dependent PNC amplitude to be very similar to the spin-independent one where \( S_2 \equiv 0 \) and \( S_3 \equiv 0 \). In this case the rescaling changes both amplitudes at the same rate and the change cancels out in the ratio \( R \). The hfs transitions with low uncertainty in \( R \) are good candidates for the measurements when the aim is extraction of \( \zeta \).

A. Comparison with other calculations

Table VII summarizes present and past calculations of the spin-independent PNC s-d amplitudes in \( \text{Ba}^+ \) and \( \text{Ra}^+ \). We present the results in a form of the coefficients before weak nuclear charge \( Q_{\text{W}} \). These coefficients are practically isotope-independent. This is because the isotope-dependence of the PNC amplitudes is strongly dominated by weak nuclear charge while the dependence of the PNC amplitudes on the details of nuclear density is very weak and can be neglected on the present level of accuracy.

The technique used in the present work is very similar to the sum-over-states approach of our previous paper [13]. As expected, the results are very close...
TABLE VI: PNC amplitudes (z-components) for the $\{5d_{3/2}, F_1\} \rightarrow \{6s_{1/2}, F_2\}$ transitions in $^{135}$Ba$^+$, $^{137}$Ba$^+$, $^{171}$Yb$^+$ and $^{173}$Yb$^+$. and $\{6d_{3/2}, F_1\} \rightarrow \{7s_{1/2}, F_2\}$ transitions in $^{223}$Ra$^+$, $^{225}$Ra$^+$ and $^{229}$Ra$^+$. Units: $10^{-10} e\text{e}a_0$.

| Ion          | QW     | I   | F1  | F2  | PNC amplitude |
|--------------|--------|-----|-----|-----|--------------|
| Ba$^+$       | -74.11 | 1.5 | 0   | -0.152(9)$ \times [1 + 0.0049(2)]$ | |
|              |        |     | 1   | -0.170(11)$ \times [1 + 0.0040(2)]$ | |
|              |        |     | 2   | -0.059(4)$ \times [1 - 0.0021(2)]$ | |
| $^{137}$Ba$^+$| -76.09 | 1.5 | 0   | -0.156(10)$ \times [1 + 0.0038(2)]$ | |
|              |        |     | 1   | -0.175(11)$ \times [1 + 0.0039(2)]$ | |
|              |        |     | 2   | -0.061(4)$ \times [1 - 0.0021(2)]$ | |
| $^{171}$Yb$^+$| -94.86 | 0.5 | 1   | 0.59(19)$ \times [1 + 0.0030(6)]$ | |
|              |        |     | 1   | -0.29(9)$ \times [1 + 0.0019(2)]$ | |
| $^{173}$Yb$^+$| -96.84 | 2.5 | 1   | -0.41(13)$ \times [1 + 0.0027(9)]$ | |
|              |        |     | 2   | -0.56(17)$ \times [1 + 0.0015(8)]$ | |
| $^{223}$Ra$^+$| -127.2 | 1.5 | 1   | -3.04(9)$ \times [1 + 0.00252(1)]$ | |
|              |        |     | 1   | -3.40(10)$ \times [1 + 0.00233(3)]$ | |
| $^{225}$Ra$^+$| -129.2 | 0.5 | 1   | 4.37(13)$ \times [1 + 0.00389(3)]$ | |
|              |        |     | 1   | -2.19(6)$ \times [1 - 0.00033(6)]$ | |
| $^{229}$Ra$^+$| -133.1 | 2.5 | 1   | -3.02(9)$ \times [1 + 0.00220(1)]$ | |
|              |        |     | 2   | -3.97(12)$ \times [1 + 0.00180(1)]$ | |

TABLE VII: Spin-independent part of the parity-nonconserving s-d amplitudes in Ba$^+$, Yb$^+$ and Ra$^+$. Units: $10^{-12} Q_{W\text{e}a_0}$.

| Ion       | Transition | This work | Other |
|-----------|------------|-----------|-------|
| Ba$^+$    | $5d_{3/2} \rightarrow 6s_{1/2}$ | 0.29(2)  | 0.29, 0.304$^a$ |
| Yb$^+$    | $5d_{3/2} \rightarrow 6s_{1/2}$ | 0.62(20) | - |
| Ra$^+$    | $6d_{3/2} \rightarrow 7s_{1/2}$ | 3.4(1)   | 3.3, 3.36, 3.33$^d$ |

$^a$Ref. 14. $^b$Ref. 17. $^c$Ref. 18. $^d$Ref. 22.

too. There is also good agreement with Sahoo et al for Ba$^+$ [17] and with Wansbeek et al for Ra$^+$ [18] and with recent calculations by Pal et al [22] for Ra$^+$.

Table VIII compares our calculated reduced matrix elements of the spin-dependent PNC amplitudes with the results of the recent calculations by Sahoo et al [23]. To make the comparison easy we have multiplied all matrix elements from [23] by 2 and have changed their signs. The former is to take into account different definition of $\kappa$, the latter is due to the fact that we also have an opposite sign for the spin-independent PNC amplitude compared to what is presented in [18] and [23]. The total sign of an amplitude is not fixed and can be changed arbitrarily. Note however that the relative sign of the SI and SD PNC amplitudes is not arbitrary and the sign can only be changed for both parts of the amplitudes simultaneously.

Given that the accuracy of the present calculations is few per cents and similar accuracy should be expected for $\kappa$, the results presented in Table VIII are in a reasonable agreement with each other. Comparison of the data in Table VIII and Table VI shows that the difference between our results and those of Sahoo et al is larger for cases when there is strong cancelation between the $S_1, S_2, S_3$ and $S_4$ contributions to the reduced matrix element. For example, the largest difference is for the $F_1 = 2 \rightarrow F_2 = 3$ transition in $^{229}$Ra$^+$. The data in Table VI shows that the final value of the reduced matrix element for this case is just about 40% of the $S_1$ contribution. On the contrary, if the amplitude is dominated by the $S_1$ term the agreement between results of the two works is much better. This should be expected since the $S_1$ term is the most stable in the calculations.

VI. CONCLUSION

We present simultaneous calculation of the spin-independent and spin-dependent PNC amplitudes of the s-d transitions in Ba$^+$, Yb$^+$ and Ra$^+$. The results are to be used for accurate interpretation of future measurements in terms of the parameter of the spin-dependent PNC interaction $\kappa$. Both, sign and value of $\kappa$ can be determined. Theoretical uncertainty is at the level of 3 to 6% for Ba$^+$ and Ra$^+$ and 30 to 50% for Yb$^+$. Note that the uncertainty for the spin-independent PNC amplitude can be further reduced by including structure radiation and ladder diagrams for more accurate treatment of cor-
relations and by including other small corrections (Breit, QED, etc.). The uncertainty for the relative contribution of the nuclear-spin-dependent part of the PNC amplitude is already small being on the level of 1% in some cases. The ratio of the SD to SI PNC amplitude is to be measured to extract the value of $\kappa$. The results of the PNC calculations for Yb$^+$ are presented for the first time.

Acknowledgments

The authors are grateful to M. G. Kozlov and S. G. Porsev for useful discussions. The work was supported in part by the Australian Research Council.

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