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Calculation of nuclear-spin-dependent parity nonconservation in *s*–*d* transitions of Ba^+, Yb^+, and Ra^+ ions

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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^+ and Yb^+ and between the $7s_{1/2}$ ground state and the $6d_{3/2}$ excited state of Ra^+. The results are presented in a form convenient for the extracting of the constants of nuclear-spin-dependent interaction (such as, e.g., anapole moment) from the measurements.

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I. INTRODUCTION

The study of the parity nonconservation (PNC) in atoms is a low-energy relatively inexpensive alternative to the high-energy search for new physics beyond the standard model (see, e.g., Ref. [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 the review in Ref. [6]). It is also the only measurement of the nuclear *anapole moment* which is produced by the PNC nuclear forces [7]. The extraction of the weak nuclear charge from the PNC measurements relies on atomic calculations. The cesium atom has the simplest electron structure among all heavy atoms which were used or considered for the PNC measurements. Still it took the considerable efforts of several groups of theorists to bring the accuracy of the calculations in line with the accuracy of measurements and provide a reliable interpretation of the measurements in terms of the standard model and the possible new physics beyond it [3–5]. It is widely believed now that it would be hard to compete with the cesium experiment in terms of the accuracy of the interpretation of the PNC measurements. Therefore, the study of PNC in atoms is mostly focused 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 the contribution from the nuclear anapole moment (see, e.g., the reviews in Refs. [6,9]). 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 the standard model (see, e.g., Refs. [10–12]). The measurements of the anapole moment does require atomic calculations, but high accuracy is not critical here.

The Ba^+, Yb^+, and Ra^+ ions considered in the present paper are good candidates for both types of the experimental studies. Ba and Yb both have seven stable isotopes with the large difference in neutron numbers $\Delta N_{\max} = 8$. Radium has several long-living isotopes. There are two stable isotopes for each of the Ba and Yb atoms (^{135}Ba, ^{139}Ba, ^{171}Yb, and ^{173}Yb) which have a nonzero nuclear spin. There are also isotopes of Ra with a nonzero nuclear spin (^{223}Ra, ^{225}Ra, ^{229}Ra). In all cases nuclear spin is provided by the valence neutron. This is especially interesting since it allows one to measure the strength of the neutron-nucleus PNC potential [7] (the anapole moment has been measured only for the ^{133}Cs nucleus which has a valence proton).

Finally, Ba^+ and Ra^+ ions have an electron structure similar to those of the 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 [13].

The use of Ba^+ in the PNC measurements was first suggested by Fortson [14]. The work is in progress at Seattle (see, e.g., Refs. [15,16]) but no PNC results have been reported yet. A similar approach is now considered for the measurements of PNC in the Ra^+ ion at KVI (*Kernfysisch Versneller Instituut*) [17,18]. It is important that in Ra^+ the PNC effects are about 20 times larger than in Ba^+. There are plans to measure PNC in Yb^+ at Los Alamos [19]. Note that the PNC measurements for neutral ytterbium are in progress at Berkeley and first PNC results were recently reported [20]. The PNC measurements for the Yb^+ ion would provide an important consistency test for the measurements and their interpretation.

Calculations of the spin-independent PNC amplitude for Ba^+ and Ra^+ were performed in our early work [13] and in Ref. [21]. Calculations for Ra^+ were later performed in Refs. [17] and [22]. The only calculation of the spin-dependent PNC in Ra^+ was recently reported by Sahoo *et al.* [23]. To the best of our knowledge, no PNC calculations for Yb^+ have been published so far.

In the present paper we calculate both the 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 the 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 the 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 a high accuracy of the calculations is not needed, we do not include some small corrections, like some classes of diagrams for higher-order correlations, Breit and quantum electrodynamic (QED) corrections, and so on. 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 cancellation of the uncertainty in the ratio.

II. THEORY

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

$$H_{\rm PNC} = H_{\rm SI} + H_{\rm SD} = \frac{G_F}{\sqrt{2}}\left(-\frac{Q_W}{2}\gamma_5 + \frac{\varkappa}{I}\boldsymbol{\alpha}\boldsymbol{I}\right)\rho(\boldsymbol{r}), \qquad (1)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, Q_W is the nuclear weak charge, $\boldsymbol{\alpha} = \left(\begin{smallmatrix} 0 & \sigma \\ \sigma & 0 \end{smallmatrix}\right)$ and γ_5 are the Dirac matrices, $\boldsymbol{I}$ is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density normalized to 1. The strength of the SD PNC interaction is proportional to the dimensionless constant $\varkappa$ which is to be found from the measurements. There are three major contributions to $\varkappa$ arising from (i) the electromagnetic interaction of the atomic electrons with the nuclear *anapole moment* [24], (ii) the electron-nucleus SD weak interaction, and (iii) the combined effect of the SI weak interaction and magnetic hyperfine interaction [25] (see, also the review in Ref. [6]). In this work we do not distinguish between the different contributions to $\varkappa$ and present the results in terms of total $\varkappa$ which is the sum of all possible contributions.

Within the standard model the weak nuclear charge Q_W is given by [26]

$$Q_W \approx -0.9877N + 0.0716Z. \qquad (2)$$

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 $|i\rangle$ and $|f\rangle$ is equal to

$$E1^{\rm PNC}_{fi} = \sum_n \left[\frac{\langle f|\boldsymbol{d}|n\rangle\langle n|H_{\rm PNC}|i\rangle}{E_i - E_n} + \frac{\langle f|H_{\rm PNC}|n\rangle\langle n|d_q|i\rangle}{E_f - E_n}\right], \qquad (3)$$

where $\boldsymbol{d} = -e\sum_i \boldsymbol{r}_i$ is the electric dipole operator, $|a\rangle \equiv |J_a F_a M_a\rangle$, and $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{J}$ is the total angular momentum.

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

$$E1^{\rm PNC}_{fi} = (-1)^{F_f - M_f}\begin{pmatrix} F_f & 1 & F_i \\ -M_f & q & M_i \end{pmatrix}\langle J_f F_f||d_{\rm PNC}||J_i F_i\rangle. \qquad (4)$$

Detailed expressions for the reduced matrix elements of the SI and SD PNC amplitudes can be found in Refs. [27] and [28].

For the SI amplitude we have

$$\begin{aligned}&\langle J_f, F_f\|d_{\rm SI}\|J_i, F_i\rangle \\ &\quad = (-1)^{I+F_i+J_f+1}\sqrt{(2F_f+1)(2F_i+1)}\begin{Bmatrix} J_i & J_f & 1 \\ F_f & F_i & I \end{Bmatrix} \\ &\quad\times \sum_n \left[\frac{\langle J_f\|\boldsymbol{d}\|n, J_n\rangle\langle n, J_n\|H_{\rm SI}\|J_i\rangle}{E_i - E_n}\right. \\ &\quad\left. + \frac{\langle J_f\|H_{\rm SI}\|n, J_n\rangle\langle n, J_n\|\boldsymbol{d}\|J_i\rangle}{E_f - E_n}\right]. \end{aligned} \qquad (5)$$

For the SD PNC amplitude we have

$$\begin{aligned}&\langle J_f, F_f\|d_{\rm SD}\|J_i, F_i\rangle \\ &\quad = \frac{G_F}{\sqrt{2}}\varkappa\sqrt{(I+1)(2I+1)(2F_i+1)(2F_f+1)/I} \\ &\quad\times \sum_n \left[(-1)^{J_f - J_i}\begin{Bmatrix} J_n & J_i & 1 \\ I & I & F_i \end{Bmatrix}\begin{Bmatrix} J_n & J_f & 1 \\ F_f & F_i & I \end{Bmatrix}\right. \\ &\quad\times \frac{\langle J_f\|\boldsymbol{d}\|n, J_n\rangle\langle n, J_n\|\boldsymbol{\alpha}\rho\|J_i\rangle}{E_n - E_i} \\ &\quad + (-1)^{F_f - F_i}\begin{Bmatrix} J_n & J_f & 1 \\ I & I & F_f \end{Bmatrix}\begin{Bmatrix} J_n & J_i & 1 \\ F_i & F_f & I \end{Bmatrix} \\ &\quad\left.\times \frac{\langle J_f\|\boldsymbol{\alpha}\rho\|n, J_n\rangle\langle n, J_n\|\boldsymbol{d}\|J_i\rangle}{E_n - E_f}\right]. \end{aligned} \qquad (6)$$

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

$$\langle 5d_{3/2}, F_f\|d_{\rm SD}\|6s, F_i\rangle = S_1 + S_2 + S_3 + S_4, \qquad (7)$$

where

$$S_1 = c_1(F_f, F_i)\sum_n \frac{\langle 5d_{3/2}\|\boldsymbol{d}\|np_{1/2}\rangle\langle np_{1/2}\|\boldsymbol{\alpha}\rho\|6s\rangle}{E_{np_{1/2}} - E_{6s}}, \qquad (8)$$

$$S_2 = c_2(F_f, F_i)\sum_n \frac{\langle 5d_{3/2}\|\boldsymbol{d}\|np_{3/2}\rangle\langle np_{3/2}\|\boldsymbol{\alpha}\rho\|6s\rangle}{E_{np_{3/2}} - E_{6s}}, \qquad (9)$$

$$S_3 = c_3(F_f, F_i)\sum_n \frac{\langle 5d_{3/2}\|\boldsymbol{\alpha}\rho\|np_{1/2}\rangle\langle np_{1/2}\|\boldsymbol{d}\|6s\rangle}{E_{np_{1/2}} - E_{5d_{3/2}}}, \qquad (10)$$

$$S_4 = c_4(F_f, F_i)\sum_n \frac{\langle 5d_{3/2}\|\boldsymbol{\alpha}\rho\|np_{3/2}\rangle\langle np_{3/2}\|\boldsymbol{d}\|6s\rangle}{E_{np_{3/2}} - E_{5d_{3/2}}}. \qquad (11)$$

Here $c_m(F_f, F_i)$ $(m = 1,2,3,4)$ are coefficients which can be reconstructed using Eq. (6). The terms S_1, S_2, S_3, S_4 differ by the order of the operators $\boldsymbol{d}$ and $\boldsymbol{\alpha}\rho$ 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 *ab initio* approach which uses the correlation potential method [29] 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 Ba^+ and Ra^+ we use the all-order correlation potential $\hat{\Sigma}^{(\infty)}$ which includes two classes of the higher-order terms: screening of the Coulomb interaction and hole-particle interaction (see, e.g., Ref. [30] for details). For Yb^+ we use the second-order correlation potential $\hat{\Sigma}^{(2)}$. The reason for the use of a different approach for Yb^+ is its different electron structure. The all-order technique developed in Refs. [30–32] works very well for alkali-metal atoms and similar ions in which the valence electron is far from the atomic core and higher-order correlations are dominated by the screening of the core-valence residual Coulomb interaction by the core electrons. For atoms and ions similar to 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 *ladder diagrams* [33] becomes important. The applicability of the technique of Ref. [33] to Yb^+ needs further investigation. Meanwhile, the use of the second-order $\hat{\Sigma}^{(2)}$ leads to sufficiently good results. Note that an external electron in Ba^+ and Ra^+ ions is also closer to the atomic core than in neutral alkali-metal atoms Cs and Fr. This means that the 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 $\hat{\Sigma}$ [$\hat{\Sigma}^{(\infty)}$ or $\hat{\Sigma}^{(2)}$] 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 $40a_B$. The coefficients are chosen from the condition that the orbitals are the eigenstates of the RHF Hamiltonian $\hat{H}_0$ of the closed-shell core. The second-order operator $\hat{\Sigma}^{(2)}$ is calculated via direct summation over B-spline basis states. The all-order $\hat{\Sigma}^{(\infty)}$ is calculated with the technique which combines solving equations for the Green functions (for the direct diagram) with the summation over a complete set of states (exchange diagram) [30].

The correlation potential $\hat{\Sigma}$ 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 Eqs. (5) and (6). Here again we use the B-spline technique to build the basis. The procedure is very similar to the constructing of the RHF B-spline basis. The only difference is that new orbitals are now the eigenstates of the $\hat{H}_0 + \hat{\Sigma}$ 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 the experimental and theoretical energies. The energies of the lowest states of Ba^+, Yb^+, and Ra^+ in RHF and Brueckner approximations are presented in Table I. One can see that the inclusion of the correlations leads to the significant improvement of the accuracy in all cases. The deviation of the theory from the experiment is just a fraction of a percent in the case of Ba^+ and Ra^+ where an all-order $\hat{\Sigma}^{(\infty)}$ is used and does not exceed 1.3% for Yb^+ where the second-order $\hat{\Sigma}^{(2)}$ is used.

TABLE I. Ionization energies of lowest s,p, and d states of Ba^+, Yb^+, and Ra^+ in different approximations (cm^{-1}).

Ion	State	RHF	Brueckner	Experiment [35]
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
Yb^+	$6s_{1/2}$	90789	99477	98207
	$6p_{1/2}$	66087	70728	71145
	$6p_{3/2}$	63276	67101	67815
	$5d_{3/2}$	66517	75551	75246
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

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 $\hat{H}_0 + \hat{\Sigma}$ with the $\hat{H}_0 + \lambda\hat{\Sigma}$ Hamiltonian in which the rescaling parameter λ is chosen for each partial wave to fit the energy of the first valence state. The values of λ are presented in Table II. 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 [29,36] 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 ψ_0 is the unperturbed wave function. It is an eigenstate of the RHF Hamiltonian $\hat{H}_0$: $(\hat{H}_0 - \epsilon_0)\psi_0 = 0$. $\delta\psi$ is the correction due to the 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 the external field ($\delta\epsilon \equiv 0$ for all the 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.

TABLE II. Rescaling factors for the correlation potential $\hat{\Sigma}$.

Ion	$s_{1/2}$	$p_{1/2}$	$p_{3/2}$	$d_{3/2}$
Ba^+	0.978	0.960	0.964	0.941
Yb^+	0.862	1.081	1.170	0.968
Ra^+	0.970	0.946	0.960	0.959

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

$$\langle \psi_n | \hat{F} + \delta \hat{V}^{N-1} | \psi_m \rangle. \tag{13}$$

The best results are achieved when ψ_n and ψ_m are the Brueckner orbitals computed with the rescaled correlation potential $\hat{\Sigma}$.

We use Eq. (13) for all weak and electric dipole matrix elements in evaluating the SI and SD PNC amplitudes (5) and (6).

IV. ACCURACY OF CALCULATIONS

The accuracy of the results obtained via direct summation over physical states with the use of expressions like Eq. (3) 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 the 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 the experiment energies and matrix elements involving these p states. The energies and electric dipole matrix elements can be directly compared with the experiment while the standard practice of comparing the experimental and theoretical hyperfine structures 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 the rescaling of the correlation potential $\hat{\Sigma}$ as it has been described in the previous section.

The calculated and experimental $E1$-transition amplitudes are presented in Table III. Note that we need a comparison with the experiment only for the estimation of the accuracy of our calculations. Therefore, a comprehensive review of the experimental and theoretical data available for the ions goes beyond the scope of the present work. We only compare our results with the most accurate experimental data or with the most complete other calculations where the experimental data are not available. Good reviews of the electric dipole transition data in Ba$^+$ and Yb$^+$ can be found in Refs. [16] and [39].

TABLE III. Electric dipole matrix elements. Comparison of the present calculations with the experiment or most complete other calculations.

Ion	Transition	This work	Other
Ba$^+$	$6s_{1/2}$–$6p_{1/2}$	3.32	3.36(4)[a]
	$6s_{1/2}$–$6p_{3/2}$	4.69	4.55(10)[a]
	$5d_{3/2}$–$6p_{1/2}$	3.06	3.14(8)[b]
	$5d_{3/2}$–$6p_{3/2}$	1.34	1.54(19)[a]
Yb$^+$	$6s_{1/2}$–$6p_{1/2}$	2.72	2.471(3)[c]
	$6s_{1/2}$–$6p_{3/2}$	3.84	3.36(2)[d]
	$5d_{3/2}$–$6p_{1/2}$	3.09	2.97(4)[c]
	$5d_{3/2}$–$6p_{3/2}$	1.36	1.31[e]
Ra$^+$	$7s_{1/2}$–$7p_{1/2}$	3.24	3.254[f]
	$7s_{1/2}$–$7p_{3/2}$	4.49	4.511[f]
	$6d_{3/2}$–$7p_{1/2}$	3.56	3.566[f]
	$6d_{3/2}$–$7p_{3/2}$	1.51	1.512[f]

[a] Experiment, Ref. [37].
[b] Experiment, Ref. [16].
[c] Experiment, Refs. [38,39].
[d] Experiment, Ref. [40].
[e] Theory, Ref. [41].
[f] Theory, Ref. [22].

The data in Table III show good agreement between the 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 IV shows the 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 IV show 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$^+$, and (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 hyperfine structure (hfs) of the $6p_{3/2}$ state of Yb$^+$ where the theory and experiment differ almost three times. Note that the most complete calculations of Ref. [41] give the result which is 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 $4f$ subshell. Neither our present calculations nor those of Ref. [41] include this mixing explicitly. The configuration interaction calculations based on the technique developed in Refs. [52,53], which treats Yb$^+$ as a system with 15 valence electrons, show

TABLE IV. Magnetic dipole hyperfine constants A (MHz). A comparison of present calculations with the experiment.

Ion	State	This work	Experiment
^{135}Ba$^+$	$6s_{1/2}$	3671	3593.3(2.2)[a]
	$6p_{1/2}$	668	664.6(0.3)[b]
	$6p_{3/2}$	131	113.0(0.1)[b]
	$5d_{3/2}$	161	169.5892(9)[c]
^{171}Yb$^+$	$6s_{1/2}$	13217	12645(2)[d]
	$6p_{1/2}$	2533	2104.9(1.3)[d]
	$6p_{3/2}$	388	877(20)[e]
	$5d_{3/2}$	291	430(43)[f]
^{223}Ra$^+$	$7s_{1/2}$	3537	3404(2)[g]
	$7p_{1/2}$	679	667(2)[g]
	$7p_{3/2}$	69.8	56.5(8)[g]
	$6d_{3/2}$	57.8	77.6(8)[h]

[a] Ref. [42].
[b] Ref. [43].
[c] Ref. [44].
[d] Ref. [45].
[e] Ref. [46].
[f] Ref. [47].
[g] Refs. [48,49].
[h] Rescaled from ^{213}Ra [18] using magnetic moments from Ref. [50].

TABLE V. Contributions to the reduced matrix elements $\langle 5d_{3/2},F_1\|\hat{H}^{\rm eff}_{\rm SDPNC}\|6s_{1/2},F_2\rangle$ of the SD parity-nonconserving s–d transitions. See the text for an explanation of the notations. Units: $10^{-11}\varkappa iea_0$.

Ion	F_1	F_2	S_1	S_2	S_3	S_4	Sum
^{135}Ba$^+$	0	1	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	−0.038	0.009	0.094
	3	2	−0.212	−0.002	0.000	0.043	−0.171
^{171}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
^{229}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
	2	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

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 the strong instability of the hfs of the $6p_{3/2}$ state. We can only say that the configuration mixing can explain the current experimental value of the hfs of $6p_{3/2}$ state, but we cannot prove that this explanation is correct. Since the disagreement between the 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 cancellation between terms containing matrix elements with the $p_{1/2}$ and $p_{3/2}$ states. In the end of Sec. II we introduced the notations S_1,S_2,S_3, and S_4 for these terms [see Eqs. (8), (9), (10), and (11)]. 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_4 term is not small. For example, for Yb$^+$ the contribution of the S_4 term is more than a 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 analyze 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 hfs as well as the effect of the partial cancellation 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 in the following:

$$\langle n|H_{\rm PNC}|m\rangle_{\rm rescaled}=\sqrt{\frac{A_n^{\rm expt}A_m^{\rm expt}}{A_n^{\rm th}A_m^{\rm th}}}\,\langle n|H_{\rm PNC}|m\rangle. \tag{14}$$

Here $A_n^{\rm expt}$ and $A_n^{\rm th}$ are the 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 than 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_3 contributions are both small. This is because these terms are exactly zero for the SI PNC amplitudes. Therefore, the SD PNC amplitudes in which the S_2 and S_3 terms are small are similar to the SI amplitudes. They both change under scaling at the same rate which cancels out in the ratio.

V. RESULTS

The results of the calculations for the SI part of the PNC amplitudes (z components) are

$$\mathrm{Ba}^+ : E1^{\rm PNC}(5d_{3/2}-6s)=0.29(2)\times10^{-12}Q_W iea_0, \tag{15}$$

$$\mathrm{Yb}^+ : E1^{\rm PNC}(5d_{3/2}-6s)=0.62(20)\times10^{-12}Q_W iea_0, \tag{16}$$

$$\mathrm{Ra}^+ : E1^{\rm PNC}(6d_{3/2}-7s)=3.4(1)\times10^{-12}Q_W iea_0. \tag{17}$$

The uncertainties are estimated by comparing *ab initio* calculations with the calculations in which matrix elements were rescaled, as it was described in the previous section. The expressions (15), (16), and (17) are valid for any isotopes. All dependence on nuclear number A is via the weak nuclear charge Q_W [see Eq. (2)] while the 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

$$E1^{\rm PNC}(A_2)=\left(\frac{A_2}{A_1}\right)^{-\frac{Z^2\alpha^2}{3}}E1^{\rm PNC}(A_1). \tag{18}$$

For cases considered in this work the maximum value of the correction is 0.4% (between ^{223}Ra and ^{229}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 SD part) in a form

$$E1^{\rm PNC}=P(1+R\varkappa), \tag{19}$$

where P is the SI part (including weak nuclear charge Q_W) and R is the ratio of the SDt to the SI amplitudes. This has two important advantages [54]: (i) the extraction of the value of $\varkappa$ from the experimental data can lead to no confusion over its sign, (ii) the uncertainty for the value of the ratio of the SD and SI amplitudes R is usually lower than for each of the amplitudes. This is because the two amplitudes are very similar and the numerical uncertainty cancels out in the ratio (see also Ref. [54]).

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

$$E1^{\mathrm{PNC}}(A_2)_{F_1F_2I} = P(A_1)_{F_1F_2I}\frac{Q_W(A_2)}{Q_W(A_1)} \times \left[1 + R(A_1)_{F_1F_2I}\frac{Q_W(A_1)}{Q_W(A_2)}\varkappa\right], \quad (20)$$

where $P(A_1)_{F_1F_2I}$ and $R(A_1)_{F_1F_2I}$ are taken from Table VI and $Q_W(A_1)$ and $Q_W(A_2)$ are calculated using Eq. (2). We stress once more that the dependence of the amplitudes on the nuclear radius is much smaller than the current theoretical uncertainty.

TABLE VI. PNC amplitudes (z components) for the $|5d_{3/2},F_1\rangle \rightarrow |6s_{1/2},F_2\rangle$ transitions in $^{135}\mathrm{Ba}^+$, $^{137}\mathrm{Ba}^+$, $^{171}\mathrm{Yb}^+$, and $^{173}\mathrm{Yb}^+$ and $|6d_{3/2},F_1\rangle \rightarrow |7s_{1/2},F_2\rangle$ transitions in $^{223}\mathrm{Ra}^+$, $^{225}\mathrm{Ra}^+$, and $^{229}\mathrm{Ra}^+$. Units: $10^{-10}iea_0$. The uncertainties presented in parentheses reflect the effect of fitting of the energies and matrix elements as explained in the text.

Ion	Q_W	I	F_1	F_2	PNC amplitude
$^{135}\mathrm{Ba}^+$	−74.11	1.5	0	1	$-0.152(9) \times [1 + 0.0409(3)\varkappa]$
			1	1	$-0.169(11) \times [1 + 0.0401(3)\varkappa]$
			1	2	$-0.059(4) \times [1 - 0.021(2)\varkappa]$
			2	1	$0.132(9) \times [1 + 0.039(2)\varkappa]$
			2	2	$-0.152(9) \times [1 - 0.023(2)\varkappa]$
			3	2	$0.152(9) \times [1 - 0.0245(3)\varkappa]$
$^{137}\mathrm{Ba}^+$	−76.09	1.5	0	1	$-0.156(10) \times [1 + 0.0398(3)\varkappa]$
			1	1	$-0.175(11) \times [1 + 0.0392(4)\varkappa]$
			1	2	$-0.061(4) \times [1 - 0.021(2)\varkappa]$
			2	1	$0.135(8) \times [1 + 0.038(1)\varkappa]$
			2	2	$-0.156(10) \times [1 - 0.022(1)\varkappa]$
			3	2	$0.156(10) \times [1 - 0.0239(2)\varkappa]$
$^{171}\mathrm{Yb}^+$	−94.86	0.5	1	0	$0.59(19) \times [1 + 0.030(16)\varkappa]$
			1	1	$-0.29(9) \times [1 + 0.018(3)\varkappa]$
			2	1	$0.51(16) \times [1 - 0.016(6)\varkappa]$
$^{173}\mathrm{Yb}^+$	−96.84	2.5	1	2	$-0.41(13) \times [1 + 0.022(9)\varkappa]$
			2	2	$-0.53(17) \times [1 + 0.015(8)\varkappa]$
			2	3	$-0.17(6) \times [1 + 0.009(3)\varkappa]$
			3	2	$0.28(9) \times [1 + 0.003(5)\varkappa]$
			3	3	$-0.48(15) \times [1 - 0.001(3)\varkappa]$
			4	3	$0.37(12) \times [1 - 0.016(7)\varkappa]$
$^{223}\mathrm{Ra}^+$	−127.2	1.5	0	1	$-3.04(9) \times [1 + 0.0252(2)\varkappa]$
			1	1	$-3.40(10) \times [1 + 0.0233(3)\varkappa]$
			1	2	$-1.18(4) \times [1 - 0.0055(6)\varkappa]$
			2	1	$2.64(8) \times [1 + 0.0194(4)\varkappa]$
			2	2	$-3.04(9) \times [1 - 0.0093(4)\varkappa]$
			3	2	$3.04(9) \times [1 - 0.0151(2)\varkappa]$
$^{225}\mathrm{Ra}^+$	−129.2	0.5	1	0	$4.37(13) \times [1 + 0.0390(4)\varkappa]$
			1	1	$-2.19(6) \times [1 - 0.0034(8)\varkappa]$
			2	1	$3.79(11) \times [1 - 0.0149(2)\varkappa]$
$^{229}\mathrm{Ra}^+$	−133.1	2.5	1	2	$-3.02(9) \times [1 + 0.0202(2)\varkappa]$
			2	2	$-3.97(12) \times [1 + 0.0180(2)\varkappa]$
			2	3	$-1.27(4) \times [1 - 0.0068(4)\varkappa]$
			3	2	$2.12(6) \times [1 + 0.0147(4)\varkappa]$
			3	3	$-3.56(10) \times [1 - 0.0100(3)\varkappa]$
			4	3	$2.76(8) \times [1 - 0.0145(2)\varkappa]$

Numerical uncertainties for P and R are presented in parentheses in Table VI. These uncertainties are estimated as a difference between pure *ab initio* results and the results obtained with the fitting of the energies and rescaling of the matrix elements of weak and electric dipole interactions as explained in the previous section. Note that in some cases the calculated uncertainty for the ratio R is very low. Given that it might be an effect of some fortunate cancelations in the effects of rescaling of the matrix elements or the energy, we cannot exclude that the real error is larger. Comparing the data in Tables VI and V reveals that low uncertainty in R corresponds to the cases when the SD 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 SD PNC amplitude to be very similar to the SI 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 $\varkappa$.

A. Comparison with other calculations

Table VII summarizes the present and past calculations of the SI PNC s–d amplitudes in Ba^+ and Ra^+. We present the results in a form of the coefficients before the weak nuclear charge Q_W. These coefficients are practically isotope independent. This is because the isotope dependence of the PNC amplitudes is strongly dominated by a 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 as well. There is also good

TABLE VII. SI part of the parity-nonconserving s–d amplitudes in Ba^+, Yb^+, and Ra^+. Units: $10^{-12}Q_W iea_0$.

Ion	Transition	This work	Other
Ba^+	$5d_{3/2}$–$6s_{1/2}$	0.29(2)	0.29[a], 0.304[b]
Yb^+	$5d_{3/2}$–$6s_{1/2}$	0.62(20)	–
Ra^+	$6d_{3/2}$–$7s_{1/2}$	3.4(1)	3.3[a], 3.36[c], 3.33[d]

[a] Ref. [13].
[b] Ref. [21].
[c] Ref. [17].
[d] Ref. [22].

TABLE VIII. Reduced matrix of the SD parity-nonconserving s–d amplitudes in Ba^+ and Ra^+. Units: $10^{-12}\varkappa iea_0$.

Ion	Transition	I	F_1	F_2	This work	Ref. [23]
$^{135}\text{Ba}^+$	$6s_{1/2}$–$5d_{3/2}$	1.5	2	3	−1.70(10)	−1.94
			1	2	1.60(12)	1.79
$^{139}\text{Ba}^+$	$6s_{1/2}$–$5d_{3/2}$	3.5	3	3	−1.85(13)	−2.07
			3	2	1.85(12)	2.11
$^{225}\text{Ra}^+$	$7s_{1/2}$–$6d_{3/2}$	0.5	1	2	−17.8(5)	−19.8
$^{223}\text{Ra}^+$	$7s_{1/2}$–$6d_{3/2}$	1.5	2	3	−21.1(6)	−23.5
			1	2	16.1(5)	20.3
$^{229}\text{Ra}^+$	$7s_{1/2}$–$6d_{3/2}$	2.5	2	3	−3.8(3)	−6.5
			2	2	−19.6(6)	−22.9

agreement with Sahoo *et al.* for Ba^+ [21] and with Wansbeek *et al.* for Ra^+ [17] and with the recent calculations by Pal *et al.* [22] for Ra^+.

Table VIII compares our calculated reduced matrix elements of the SD 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 Ref. [23] by 2 and have changed their signs. The former is to take into account the different definition of $\varkappa$, the latter is due to the fact that we also have an opposite sign for the SI PNC amplitude compared to what is presented in Refs. [17] 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.

The results of this work and those of Ref. [23] presented in Table VIII are in a reasonable agreement with each other. Comparison of the data in Tables VIII and V shows that the difference between our results and those of Sahoo *et al.* is larger for cases when there is strong cancellation 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 $F_1 = 2$ to $F_2 = 3$ transition in $^{229}\text{Ra}^+$. The data in Table V show 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 the 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 the simultaneous calculation of the SI and SD PNC amplitudes of the s–d transitions in Ba^+, Yb^+, and Ra^+. The results are to be used for the accurate interpretation of future measurements in terms of the parameter of the SD PNC interaction $\varkappa$. Both the sign and value of $\varkappa$ 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 SI PNC amplitude can be further reduced by including structure radiation and ladder diagrams for a more accurate treatment of the correlations 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 calue of $\varkappa$.

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