

Calculation of parity-nonconserving amplitude and other properties of Ra^+

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We have calculated parity-nonconserving $7s-6d_{3/2}$ amplitude E_{PNC} in $^{223}\text{Ra}^+$ using high-precision relativistic all-order method where all single and double excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. Detailed study of the uncertainty of the parity-nonconserving amplitude is carried out; additional calculations are performed to estimate some of the missing correlation corrections. A systematic study of the parity-conserving atomic properties, including the calculation of the energies, transition matrix elements, lifetimes, hyperfine constants, and quadrupole moments of the $6d$ states, as well as dipole and quadrupole ground-state polarizabilities, is carried out. The results are compared with other theoretical calculations and available experimental values.

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I. INTRODUCTION

There are two separate reasons for parity violation studies in an atom: to search for new physics beyond the standard model of the electroweak interaction by precise evaluation of the weak charge Q_w , and to probe parity violation in the nucleus by evaluating the nuclear anapole moment. The atomic-physics tests of the standard model that are completed to date were carried out by comparing experimental weak charges of atoms Q_w , which depend on input from atomic theory, with predictions from the standard model [1]. The most precise experimental study to date, a 0.35% measurement in Cs was carried out by the Boulder group [2] using a Stark interference scheme for measuring the ratio of the parity-nonconserving (PNC) amplitude E_{PNC} and the vector part of the Stark-induced amplitude β for transitions between states of the same nominal parity. The value of the weak charge in Cs was ultimately found to be consistent with the theories of the standard model. However, such comparisons provide important constraints on its possible extensions. A recent analysis [3] of parity-violating electron-nucleus scattering measurements combined with atomic PNC measurements placed tight constraints on the weak neutral-current lepton-quark interactions at low energy, improving the lower bound on the scale of relevant new physics to ~ 1 TeV.

Experimental measurements of the spin-dependent contribution to the PNC $6s \rightarrow 7s$ transition in ^{133}Cs led to a value of the cesium anapole moment that is accurate to about 14% [2]. The analysis of this experiment, which required a calculation of the nuclear spin-dependent PNC amplitude, led to constraints on weak nucleon-nucleon coupling constants that are inconsistent with constraints from deep inelastic-scattering and other nuclear experiments, as pointed out in [4]. Therefore, new experiments (and associated theoretical analysis) are needed to resolve the issue. Currently, a microwave experiment to measure the spin-dependent PNC amplitude in the $7s$ state of Fr [5] and an isotopic chain experiment

in Yb [6] is underway. We note that when an experimental study is conducted in a single isotope, both theoretical and experimental determinations of PNC amplitude are required while the experiments conducted with isotopic chains should allow removing the dependence on the theory. However, accurate theoretical values for a number of atomic properties are useful for this type of experiments as well.

The present work is motivated by the project that was recently started at the Accelerator Institute (KVI) of the University of Groningen [7] to measure PNC amplitude in a single trapped radium ion. Ra^+ is a particularly good candidate for the PNC study, owing to high value of the nuclear charge Z and, correspondingly, large expected PNC effects. The $7s-6d_{3/2}$ transition in Ra^+ is of special interest owing to the long life of the $6d_{3/2}$ state and its sensitivity to both spin-independent PNC and spin-dependent PNC [8]. The $7s-6d_{3/2}$ transition in Ra^+ is also being considered for the development of optical frequency standards at the same laboratory [9]. The parity violation experiments are also accompanied by a number of measurements of parity-conserving quantities; as a result we have included a systematical study of such properties in this work.

In summary, we have calculated the PNC amplitude for the $7s-6d_{3/2}$ transition in $^{223}\text{Ra}^+$ together with the lifetimes of the $7p$ and $6d$ states, energy levels for ns , np , nd , and nf states, transition matrix elements for a number of the E1 and E2 transitions, quadrupole moments of the $6d$ states, ground-state dipole and quadrupole polarizabilities, and magnetic-dipole hyperfine constants A for the $7s$, $7p$, and $6d$ states using the relativistic all-order method. The all-order method has proved to be very reliable for calculating the properties of alkali-metal atoms and singly-ionized monovalent ions (see, for example, Refs. [10–16]). The effect of Breit interaction on the PNC amplitude is also evaluated. The sensitivity of the PNC amplitude to the nuclear radius and varying neutron distribution has been studied. Our results are compared with other theoretical values and available experimental data.

II. THEORY

In this section, we briefly discuss the all-order method which has been used to calculate the wave functions and the matrix elements necessary to evaluate the observed properties. The all-order method relies on including all single and double excitations of the core and valence electrons from the lowest-order wave function,

$$|\Psi_v\rangle = \left[1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v \right] |\Phi_v\rangle. \quad (1)$$

Here, $|\Phi_v\rangle$ is the lowest-order atomic wave function taken to be the frozen-core Dirac-Fock (DF) wave function of a state v ; a_i^\dagger, a_j are single-particle creation and annihilation operators, ρ_{ma} and ρ_{mv} are the single core and valence excitation coefficients, and ρ_{mnab} and ρ_{mnva} are double core and valence excitation coefficients, respectively. Indices at the beginning of the alphabet, a, b, \dots , refer to occupied core states, those in the middle of the alphabet m, n, \dots , refer to excited states, and index v designates the valence orbital.

To derive equations for the excitation coefficients, all-order wave function (1) is substituted into the many-body Schrödinger equation $H|\Psi_v\rangle = E|\Psi_v\rangle$, and terms on the left- and right-hand sides are matched, based on the number and type of operators they contain. Hamiltonian $H = H_0 + V_I$ is taken to be the relativistic *no-pair* Hamiltonian,

$$H_0 = \sum_{i=1}^N \varepsilon_i a_i^\dagger a_i, :$$

$$V_I = \frac{1}{2} \sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_l a_k, : \quad (2)$$

where ε_i are the single-particle energies, $::$ designate normal ordering of the operators with respect to closed core, and g_{ijkl} are the two-body Coulomb matrix elements. The all-order equations are solved numerically using a finite basis set of single-particle wave functions which are linear combinations of B splines. We have used 70 basis set B-spline orbitals of order 8 defined on a nonlinear grid with 500 points within a spherical cavity of radius 80 a.u. A large spherical cavity is needed to accommodate all the valence orbitals required for our calculation. A sufficiently large number of grid points were enclosed within the nucleus to accommodate the influence of the nucleus on certain atomic properties such as parity-violating matrix elements and hyperfine constants.

The resulting single-double (SD) excitation coefficients are used to calculate matrix elements of various one-body operators represented in the second quantization as $Z = \sum_{ij} z_{ij} a_i^\dagger a_j$,

$$Z_{wv} = \frac{\langle \Psi_w | Z | \Psi_v \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle \langle \Psi_w | \Psi_w \rangle}}. \quad (3)$$

Substituting the expression for the wave function from Eq. (1) in the above equation and simplifying, we get

$$Z_{wv} = \frac{z_{wv} + Z^{(a)} + \dots + Z^{(t)}}{\sqrt{(1 + N_v)(1 + N_w)}}, \quad (4)$$

where z_{wv} is the lowest-order DF matrix element and $Z^{(a)}, \dots, Z^{(t)}$ and normalization terms N_i are linear or quadratic functions of the single and double excitation coefficients [10,17]. The expression in Eq. (4) does not depend on the nature of the operator Z , only on its rank and parity. Therefore, all matrix elements calculated in this work (E1, M1, E2, hyperfine, and PNC matrix elements) are calculated using the same general code.

Corrections to the all-order equations from the dominant class of triple excitation terms are also evaluated where needed by including the term $\frac{1}{6} \sum_{mnrab} \rho_{mnrab} a_m^\dagger a_n^\dagger a_r^\dagger a_v a_b a_a |\Phi_v\rangle$ into SD wave function (1) and considering its effect on the energy and single valence excitation coefficient equations perturbatively (SDpT approach). Other classes of triple and higher excitations are included where needed using the scaling procedure by multiplying single excitation coefficients ρ_{mv} by the ratio of the “experimental” and corresponding (SD or SDpT) correlation energies [10]. The experimental correlation energies are determined as the difference of the total experimental energy and the DF lowest-order values. The calculation of the matrix elements is then repeated with the modified excitation coefficients. We refer the reader to the review [16] and references therein for the detailed description of the all-order method and its extensions. The various atomic properties calculated using the all-order method described above are discussed in detail in the following sections.

III. PROPERTIES OF Ra⁺

A. Energies

Results of our calculations of energies for a number of Ra⁺ levels are summarized in Table I. The first six columns of Table I give the lowest-order DF energies $E^{(0)}$, the all-order SD energies E^{SD} , the part of the third-order energies omitted in the SD calculation E^{extra} , first-order Breit contribution $B^{(1)}$, second-order Coulomb-Breit $B^{(2)}$ corrections, and Lamb shift contribution, E_{LS} (see Ref. [20] for detail). We take the sum of these six contributions to be our final all-order results, $E_{\text{tot}}^{\text{SD}}$ listed in the seventh column of Table I.

The column labeled δE^{SD} in Table I gives differences between our *ab initio* results and the experimental values [18,19]. The SD results are in good agreement with the experimental values taking into account very large size of the high-order correlation corrections. We predict the energies of the $9p_{1/2}$, $10p_{1/2}$, and $10p_{3/2}$ levels using our theoretical results and differences between our and experimental values for the known np levels. The predicted values are listed in Table I and are expected to be accurate to a few cm^{-1} .

We compare our results for the excitation energies important to the calculation of the $7s-6d_{3/2}$ PNC amplitude with other theoretical calculations and experiment [19] in Table II. The calculations in both Refs. [21,22] use high-precision all-order methods, but represent very different approaches. The calculations in Ref. [21] are performed using the correlation potential method. The results of Ref. [22] are obtained using

TABLE I. Contributions to the energies of Ra II: lowest-order (DF) $E^{(0)}$, single-double Coulomb all-order correlation energy E^{SD} , third-order terms not included in the SD value $E_{\text{extra}}^{(3)}$, first-order Breit and second-order Coulomb-Breit corrections $B^{(n)}$, and Lamb shift E_{LS} . The total energies $E_{\text{tot}}^{\text{SD}}$ are compared with experimental energies $E_{\text{expt.}}$ [18,19], $\delta E = E_{\text{tot}}^{\text{SD}} - E_{\text{expt.}}$. Our predicted energy values are listed for the $9p_{1/2}$ and $10p_j$ energy levels. Units: cm^{-1} .

nlj	$E^{(0)}$	E^{SD}	$E_{\text{extra}}^{(3)}$	$B^{(1)}$	$B^{(2)}$	E_{LS}	$E_{\text{tot}}^{\text{SD}}$	$E_{\text{expt.}}$	δE^{SD}
$7s_{1/2}$	-75898	-6692	1152	147	-250	33	-81508	-81842	334
$6d_{3/2}$	-62356	-8042	1152	155	-398	0	-69488	-69758	270
$6d_{5/2}$	-61592	-7034	926	114	-360	0	-67947	-68099	152
$7p_{1/2}$	-56878	-4027	587	102	-109	0	-60326	-60491	165
$7p_{3/2}$	-52906	-3020	433	63	-90	0	-55519	-55633	114
$8s_{1/2}$	-36860	-1745	316	46	-74	7	-38311	-38437	126
$7d_{3/2}$	-31575	-1590	245	39	-92	0	-32973	-33098	125
$7d_{5/2}$	-31204	-1456	204	29	-84	0	-32509	-32602	93
$5f_{5/2}$	-28660	-4438	371	11	-63	0	-32780	-32854	74
$5f_{7/2}$	-28705	-4159	353	8	-61	0	-32564	-32570	6
$8p_{1/2}$	-30053	-1298	201	39	-42	0	-31152	-31236	84
$8p_{3/2}$	-28502	-1034	156	25	-36	0	-29391	-29450	59
$9s_{1/2}$	-22004	-741	136	21	-33	2	-22618	-22677	59
$9p_{1/2}$	-18748	-605	96	20	-21	0	-19259, -19305 ^a		
$9p_{3/2}$	-17975	-495	76	13	-18	0	-18399	-18432	33
$8d_{3/2}$	-19451	-683	105	18	-40	0	-20051	-20107	56
$8d_{5/2}$	-19261	-634	90	13	-37	0	-19829	-19868	39
$10s_{1/2}$	-14651	-388	72	11	-18	1	-14972	-15004	32
$10p_{1/2}$	-12838	-335	53	11	-11	0	-13120, -13144 ^a		
$10p_{3/2}$	-12397	-278	43	7	-10	0	-12635, -12653 ^a		
$9d_{3/2}$	-13226	-366	56	10	-22	0	-13548	-13578	30
$9d_{5/2}$	-13118	-342	49	7	-20	0	-13424	-13447	23
$10d_{3/2}$	-9587	-221	34	6	-13	0	-9780		
$10d_{5/2}$	-9519	-207	30	4	-12	0	-9704		

^aOur predicted values.

coupled-cluster method including single, double, and partial triple excitations. The results of Ref. [21] are in better agreement with experiment for the $7s-7p$ transitions and the results from the present work are in better agreement with experiment for the $6d_{3/2}-7p$ transitions. Large discrepancies of the coupled-cluster results from Ref. [22] for the $6d-7p$ transitions with experiment are somewhat surprising and may indicate insufficient number of higher partial wave functions in the basis set. In our calculations, all partial wave up to $l_{\text{max}}=6$ are explicitly included in all calculations and

TABLE II. Comparison of the excitation energies important to the calculation of the $7s-6d_{3/2}$ PNC amplitude. All results are in cm^{-1} .

Transition	Present	Ref. [21]	Ref. [22]	Expt.
$7s-7p_{1/2}$	21182	21279	21509	21351
$7s-7p_{3/2}$	25989	26226	26440	26209
$6d_{3/2}-7p_{1/2}$	9162	9468	9734	9267
$6d_{3/2}-7p_{3/2}$	13969	14415	14665	14125

extrapolation for higher number of partial waves is carried out for the dominant second-order correlation energy contribution.

B. Electric-dipole matrix elements

We calculate all allowed reduced electric-dipole matrix elements between ns , np , and n_1d states, where $n=7-10$ and $n_1=6-10$ using the method described above. The subset of these matrix elements is compared with the correlation potential calculations of Ref. [21] and coupled-cluster calculations of Refs. [9,22] in Table III. Absolute values of the reduced matrix elements in atomic units are listed in the table. All present values with the exception of the $7p_{1/2}-8s$, $7p_{3/2}-8s$, $8p_{1/2}-7s$, and $8p_{3/2}-7s$ transitions are *ab initio* SD values. For these four transitions, we used scaling procedure described above to provide recommended values as we expect the scaled values to be more accurate based on Cs “best set” data [23]. The calculations of Ref. [21] are carried out using fitted Brueckner orbitals (i.e., include semiempirical correction to the correlation operator) and include core polarization, structure radiation, and normalization corrections. We note that Ref. [21] quotes radial integrals rather

TABLE III. Comparison of the present results for the absolute values of the electric-dipole reduced matrix elements in Ra II with other theoretical calculations. All results are in atomic units. The lowest-order DF values are listed in the column labeled “DF” to illustrate the size of the correlation correction. Negative sign of the DF value for the $8p_{1/2}-7s_{1/2}$ transition indicates that the lowest-order value is of the opposite sign with the final result.

Transition	DF	Present	Ref. [21]	Ref. [9]	Ref. [22]
$7p_{1/2}-7s_{1/2}$	3.877	3.254	3.224	3.28	3.31
$7p_{1/2}-8s_{1/2}$	2.637	2.517	2.534		
$7p_{1/2}-9s_{1/2}$	0.716	0.702	0.708		
$7p_{1/2}-6d_{3/2}$	4.446	3.566	3.550	3.64	3.68
$7p_{1/2}-7d_{3/2}$	4.527	4.290	4.358		
$7p_{1/2}-8d_{3/2}$	1.584	1.445	1.432		
$7p_{3/2}-7s_{1/2}$	5.339	4.511	4.477	4.54	4.58
$7p_{3/2}-8s_{1/2}$	4.810	4.644	4.663		
$7p_{3/2}-9s_{1/2}$	1.078	1.035	1.036		
$7p_{3/2}-6d_{3/2}$	1.881	1.512	1.504	1.54	1.56
$7p_{3/2}-7d_{3/2}$	2.488	2.384	2.407		
$7p_{3/2}-8d_{3/2}$	0.733	0.652	0.641		
$7p_{3/2}-6d_{5/2}$	5.862	4.823	4.816	4.92	
$7p_{3/2}-7d_{5/2}$	7.249	6.921	6.995		
$7p_{3/2}-8d_{5/2}$	2.227	2.011	1.954		
$8p_{1/2}-7s_{1/2}$	-0.125	0.047	0.088	0.04	
$8p_{1/2}-8s_{1/2}$	7.371	6.949	6.959		
$8p_{1/2}-9s_{1/2}$	5.227	5.012	5.035		
$8p_{1/2}-6d_{3/2}$	0.105	0.049	0.013	0.07	
$8p_{1/2}-7d_{3/2}$	10.21	9.553	9.540		
$8p_{1/2}-8d_{3/2}$	7.184	7.010	7.104		
$8p_{3/2}-7s_{1/2}$	0.625	0.395	0.339	0.50	
$8p_{3/2}-8s_{1/2}$	9.880	9.294	9.320		
$8p_{3/2}-9s_{1/2}$	9.244	9.022	9.036		
$8p_{3/2}-6d_{3/2}$	0.168	0.144	0.127	0.15	
$8p_{3/2}-7d_{3/2}$	4.331	4.035	4.028		
$8p_{3/2}-8d_{3/2}$	4.047	4.002	4.034		
$8p_{3/2}-6d_{5/2}$	0.462	0.378	0.347	0.40	
$8p_{3/2}-7d_{5/2}$	13.37	12.55	12.53		
$8p_{3/2}-8d_{5/2}$	11.68	11.49	11.58		

than reduced matrix elements, so we have multiplied their results by the appropriate angular factors for the purpose of comparison. The calculations of the Refs. [9,22] are carried out using the coupled-cluster method.

We have also listed the lowest-order DF values in the first column of the table to illustrate the size of the correlation corrections for various transitions. Negative sign of the DF value for the $8p_{1/2}-7s_{1/2}$ transition indicates that the lowest-order value is of the opposite sign with the final result. The correlation corrections for the primary $7s-7p$ and $7p-6d$ transitions are quite large, 18–25 %. The correlation corrections for the remaining strong transitions are generally smaller, 2–10 %. All theoretical values are in good agreement for these transitions. Our values for $7s-7p$ and $7p-6d$ are in better agreement with results of Ref. [21] than

those of Refs. [9,22]. The agreement is generally poorer for the transitions with small values of the matrix elements as expected, owing to very large size of the correlation corrections. Since different methods omit or include somewhat different classes of the high-order corrections, discrepancies are expected when such corrections are large. The issue of the very small matrix elements, such as $8p-7s$, is also discussed in Ref. [21].

C. Polarizabilities

We calculate the static dipole and quadrupole polarizabilities of the Ra^+ ion in its ground $7s$ state. The static polarizability is calculated as the sum of three terms representing contributions from the ionic core α_c , a small counteracting term to compensate for the excitations from the core states to the valence state α_{vc} , and valence polarizability α_v ,

$$\alpha = \alpha_c + \alpha_{vc} + \alpha_v. \quad (5)$$

1. Dipole polarizability

The valence polarizability contributes over 90% of the total value of the electric-dipole polarizability and is calculated using sum-over-states approach,

$$\alpha_v(E1) = \frac{1}{3} \sum_n \left(\frac{|\langle 7s || D || np_{1/2} \rangle|^2}{E_{np_{1/2}} - E_{7s}} + \frac{|\langle 7s || D || np_{3/2} \rangle|^2}{E_{np_{3/2}} - E_{7s}} \right). \quad (6)$$

The sum over n in Eq. (6) converges extremely fast. In fact, the first term with $n=7$ contributes 99.8% of the total value. As a result, we calculate the first few terms (with $n=7-10$) using our all-order matrix elements from Table III and experimental energies [18,19] where available. The remainder α_v^{tail} is calculated in the DF approximation without loss of accuracy. The ionic core contribution α_c and term α_{vc} are calculated in the random-phase approximation (RPA). The RPA core value is expected to be accurate to better than 5% (see Ref. [24] and references therein). All contributions to the dipole polarizability are listed in Table IV. The contributions from $n=7-10$ are given together as α_v^{main} .

The value of the ground-state Ba^+ polarizability calculated by the same approach [24] is in near perfect agreement with the experiment [25] (to 0.2%). Moreover, the theoretical SD $6p$ lifetimes in Ba^+ are also in excellent agreement with experimental values [24]. We note that lifetime experiments are conducted entirely differently from the polarizability measurement of [25]. There are two differences between the Ba^+ and Ra^+ dipole polarizability calculations: increased ionic core contribution and increased size of the correlation corrections. The core contribution increases from 8% in Ba^+ to 13% in Ra^+ , and the correlation correction contribution to the $7s-7p$ matrix elements increases by about 3% (from 16.6% to 19.1% for the $7s-7p_{1/2}$ transition). Neither of these changes is expected to significantly decrease the accuracy of the Ra^+ ground-state dipole polarizability in comparison with the Ba^+ one. Therefore, we expect our value to be accurate to better than 1%. Our result is in agreement with the coupled-cluster calculation of Ref. [9].

TABLE IV. Contributions to the ground-state dipole polarizability of Ra^+ . The contributions from the $(7-10)p$ states are given separately. Our result is compared with calculation from Ref. [9]. All results are in a.u.

Contribution	α_{E1}
$7p_{1/2}-7s$	36.29
$7p_{3/2}-7s$	56.79
$8p_{1/2}-7s$	0.00
$8p_{3/2}-7s$	0.23
$(9-10)p-7s$	0.04
α_v^{main}	93.35
α_c	13.74
α_v^{tail}	0.11
α_{vc}	-0.98
Total	106.22
Theory ^a	106.12

^aReference [9].

2. Quadrupole polarizability

The valence part of the quadrupole polarizability is calculated using the sum-over-states approach as

$$\alpha_v(E2) = \frac{1}{5} \sum_n \left(\frac{|\langle 7s||Q||nd_{3/2}\rangle|^2}{E_{nd_{3/2}} - E_{7s}} + \frac{|\langle 7s||Q||nd_{5/2}\rangle|^2}{E_{nd_{5/2}} - E_{7s}} \right). \quad (7)$$

All contributions to the quadrupole polarizability are listed in Table V. The correlation correction to the E2 matrix elements is dominated by a single term among twenty terms in the numerator of Eq. (4). As described in detail in Ref.

TABLE V. Contributions to the ground-state quadrupole polarizability and the E2 reduced matrix elements of Ra^+ in a.u. The comparison of our result with other theoretical calculation [9] is also presented.

Contribution	E2	α_{E2}
$6d_{3/2}-7s$	14.74(15)	789(13)
$6d_{5/2}-7s$	18.86(17)	1136(16)
$7d_{3/2}-7s$	14.21(30)	182(3)
$7d_{5/2}-7s$	16.49(38)	243(4)
$8d_{3/2}-7s$	5.63(4)	22.6(2)
$8d_{5/2}-7s$	6.79(6)	32.6(2)
$9d_{3/2}-7s$	3.30(3)	7.0(1)
$9d_{5/2}-7s$	4.03(3)	10.4(1)
$10d_{3/2}-7s$	2.27(3)	3.1
$10d_{5/2}-7s$	2.79(3)	4.7
α_v^{main}		2430(21)
α_v^{tail}		35(10)
α_c		68(12)
Total		2533(26)
Theory ^a		2547.5

^aReference [9].

[24], additional omitted correlation correction to this term may be estimated by the scaling procedure described above. The scaling modifies the SD results by 0.7 to 2.3% depending on the transition. We have also carried out the *ab initio* all-order calculation with inclusion of the triple valence excitation coefficients as described in the Sec. II (SDpT approach). The scaling procedure was repeated starting from the SDpT approximation for the dominant $7s-6d_{3/2}$ and $7s-6d_{5/2}$ transitions. These additional calculations allow us to directly evaluate the uncertainty in our calculations since they produce different evaluations of the omitted correlation correction. We take the uncertainty in the calculation of the $7s-6d_{3/2}$ and $7s-6d_{5/2}$ matrix elements to be the maximum of the difference of final SD scaled results with *ab initio* and scaled SDpT data. We note that SD approach generally underestimates the correlation energy and SDpT approach generally overestimates the correlation energy used in the scaling procedure. The scaled SD and SDpT results are rather close, further confirming the validity of this procedure and of our uncertainty estimate. Therefore, we take the uncertainty of the remaining transitions to be the difference of the final SD scaled and *ab initio* SDpT values. The resulting final matrix elements and their uncertainties are listed in Table V in column labeled “E2.” The relative uncertainty of the corresponding polarizability values is twice the relative uncertainty of the matrix elements since we assume the experimental energies be accurate to all figures quoted. The sum over n converges far slower than in the case of the dipole polarizability so calculating a first few terms to high precision is essential to obtain an accurate final value. The tail contribution, while small, is significant and has to be treated with care. We estimated that DF value for the main ($n=6-10$) term is larger than our final all-order result by 22%. Therefore, we decrease the DF tail of 45 a.u. by 22% and take the difference of the DF tail and the final adjusted value to be its uncertainty. The core contribution is calculated in the RPA approximation; we take the difference between DF and RPA core values to be the uncertainty of the core contribution. Our final value is in agreement with the result of Ref. [9].

D. Lifetimes of the $7p$ and $6d$ states

The lifetimes τ of the $7p$ and $6d$ states in Ra^+ are calculated as the inverse of the sum of the transition probabilities A . The $7p$ states decay via strong electric-dipole transitions. Total of five E1 transitions contribute to the lifetimes of these two states: $7p_{1/2}-7s$, $7p_{1/2}-6d_{3/2}$, $7p_{3/2}-7s$, $7p_{3/2}-6d_{3/2}$, and $7p_{3/2}-6d_{5/2}$. The electric-dipole transition rates are calculated using formula

$$A_{if}^{E1} = \frac{2.026 \times 10^{18}}{\lambda^3} \frac{|\langle i||D||f\rangle|^2}{2j_i + 1} s^{-1}, \quad (8)$$

where λ is the wavelength of the transition in Å and $\langle i||D||f\rangle$ is the electric-dipole reduced matrix element in atomic units. We use the experimental wavelength [18,19] and our all-order matrix elements listed in Table III when evaluating the transition rates. The results are summarized in Table VI. We find that while the contributions of the $7s-7p$ transitions to

TABLE VI. Contributions to the lifetimes of the $7p_{1/2}$ and $7p_{3/2}$ states. The transitions rates A are given in 10^6 s^{-1} and the lifetimes are given in ns.

	$7p_{1/2}$		$7p_{3/2}$
$A(7p_{1/2}-7s)$	104.4	$A(7p_{3/2}-7s)$	185.5
$A(7p_{1/2}-6d_{3/2})$	10.3	$A(7p_{3/2}-6d_{3/2})$	3.3
ΣA	114.7	$A(7p_{3/2}-6d_{5/2})$	22.8
$\tau(7p_{1/2})$	8.72 ns	ΣA	211.6
		$\tau(7p_{3/2})$	4.73 ns
Ref. [26]	8.57(12)		4.67(5)

the $7p$ lifetimes are dominant, the contributions of the $7p-6d$ transitions are significant (over 10%). Our values are in agreement with the results of Ref. [26] within the uncertainties quoted in [26] but are about 1% larger.

Only one transition, $6d_{3/2}-7s$, has to be considered for the calculation of the $6d_{3/2}$ lifetime. The corresponding transition rate is calculated as

$$A_{if}^{E2} = \frac{1.119\,95 \times 10^{18}}{\lambda^5} \frac{|\langle i||Q||f \rangle|^2}{2j_i + 1} \text{s}^{-1}, \quad (9)$$

where λ is the wavelength of the transition in Å and $\langle i||Q||f \rangle$ is the electric-quadrupole reduced matrix element in atomic units.

Two transitions have to be considered in the calculation of the $6d_{5/2}$ lifetime: E2 $6d_{5/2}-7s$ transition and M1 $6d_{5/2}-6d_{3/2}$ transition. The M1 transition rate is calculated as

$$A_{if}^{M1} = \frac{2.697\,35 \times 10^{13}}{\lambda^3} \frac{|\langle i||M1||f \rangle|^2}{2j_i + 1} \text{s}^{-1}. \quad (10)$$

We use the experimental wavelengths [18,19] and our all-order matrix elements listed in Table V when evaluating the E2 transition rates. Our result for the reduced M1 $6d_{5/2}-6d_{3/2}$ matrix element is 1.55 a.u. The E2 and M1 transition rates contributing to the $6d_{5/2}$ lifetime are 3.255 s^{-1} and 0.049 s^{-1} . We verified that the contribution of the $6d_{5/2}-6d_{3/2}$ E2 transition is negligible.

Our results for the $6d_{3/2}$ and $6d_{5/2}$ lifetimes are presented in Table VII together with other theoretical values. Our values for the lifetimes of the $6d$ states are in better agreement with those published by Dzuba *et al.* [21] than with the results of Sahoo *et al.* [9]; however, the discrepancies with Ref. [9] are small. We also list the uncertainties of our values in

TABLE VII. Lifetimes of the $6d_{3/2}$ and $6d_{5/2}$ states of Ra^+ in seconds. Comparison of our results with other theoretical calculations is presented.

Term	$\tau(6d_{3/2})$	$\tau(6d_{5/2})$
Present	0.638(10)	0.303(4)
Theory ^a	0.627(4)	0.297(4)
Theory ^b	0.641	0.302

^aReference [9].

^bReference [21].

TABLE VIII. Quadrupole moments of the $6d_{3/2}$ and $6d_{5/2}$ states in Ra^+ in a.u.

State	SD	SDpT	SD _{sc}	SDpT _{sc}	Final	Ref. [9]
$6d_{3/2}$	2.814	2.868	2.839	2.829	2.84(3)	2.90(2)
$6d_{5/2}$	4.311	4.380	4.342	4.329	4.34(4)	4.45(9)

Table VII. The relative uncertainties in our values of the $6d$ lifetimes are twice the relative uncertainties in the values of the E2 matrix elements listed in Table V. We note that the estimated uncertainties quoted in Ref. [9] are obtained by carrying out calculations with different bases; i.e., they are numerical uncertainties resulting from the particular choice of the basis set and do not include estimation of the missing correlation effects. In our calculations, the basis set is complete (70 splines for each partial wave) and increasing its size does not change the result. Our uncertainties include estimation of the terms beyond triple contributions as described above as well as uncertainty owing to truncation of the partial waves above $l > 6$. Therefore, while our uncertainty is higher for $6d_{3/2}$ state than the one quoted in Ref. [9], it represents an attempt to provide an actual boundary for the recommended value of this lifetime.

E. Quadrupole moments of the $6d$ states

We also calculated the values of the quadrupole moments of the $6d_{3/2}$ and $6d_{5/2}$ states since these properties are of interest to the investigation of possible use of Ra^+ for the development of optical frequency standard [9]. The quadrupole moment $\Theta(\gamma J)$ can be expressed via the reduced matrix element of the quadrupole operator Q as

$$\Theta(\gamma J) = \frac{(2J)!}{\sqrt{(2J-2)!(2J+3)!}} \langle \Psi(\gamma J) || Q || \Psi(\gamma J) \rangle. \quad (11)$$

The calculation follows that of the E2 matrix elements. As in the case of the E2 $7s-nd$ matrix elements, a single correlation correction term is dominant, and the omitted correlation contributions may be estimated via the scaling procedure. We have conducted four different calculations: *ab initio* SD and SDpT, and scaled SD and SDpT ones to evaluate the uncertainty in the final values. The results are summarized in Table VIII. The correlation correction to the quadrupole moments is on the order of 20%. Our values are compared with coupled-cluster calculation of Ref. [9]. Our results are lower than that of Ref. [9]. This issue has been discussed in detail in Ref. [27], where we have demonstrated that CCSD(T) method may overestimate quadrupole moments by a few percent owing to the cancellation of various terms. Omission of orbitals with $l > 4$ from the basis set may also lead to higher values.

F. Magnetic-dipole hyperfine constants

Our results for the magnetic-dipole hyperfine constants $A(\text{MHz})$ in $^{223}\text{Ra}^+$ are compared with theory [9,22] and experiment [28,29] in Table IX. The gyromagnetic ratio g_I for

TABLE IX. Magnetic-dipole hyperfine constants A (MHz) for the $7s$, $7p_{1/2}$, $7p_{3/2}$, $6d_{3/2}$, and $6d_{5/2}$ states in $^{223}\text{Ra}^+$ calculated using SD and SDpT all-order approaches. Lowest-order (DF) values are also listed to illustrate the size of the correlation corrections. The present values are compared with other theoretical [9,22] and experimental values from Refs. [28,29].

State	DF	SD	SDpT	Ref. [22]	Ref. [9]	Expt.
$7s$	2614	3577	3450	3557	3567	3404(2)
$6d_{3/2}$	52.92	81.51	79.56	79.80	77.08	
$6d_{5/2}$	19.24	-23.98	-24.08		-23.90	
$7p_{1/2}$	444.5	699.5	671.5	671.0	666.9	667(2)
$7p_{3/2}$	33.91	56.62	54.40	56.53	56.75	56.5(8)

^{223}Ra is taken to be $g_I=0.1803$ and corresponds to the value $\mu_I=0.2705(19)\mu_N$ from Ref. [30]. We note that the magnetic moment of ^{223}Ra have not been directly measured but recalculated from measurements of ^{213}Ra and ^{225}Ra nuclear magnetic moments in Ref. [30]. The magnetization distribution is modeled by a Fermi distribution with the same parameters as our charge distribution ($c=6.862$ fm and 10–90 % thickness parameter is taken to be $t=2.3$ fm). The lowest-order values are also listed to demonstrate the size of the correlation corrections for various states. The triple contributions are important for the hyperfine constants and are partially included as described in Sec. II. These values are listed in column labeled “SDpT.” The SD values are also listed for comparison in column labeled “SD.”

The value $g_I=0.18067$ that corresponds to the rounded off value $\mu_I=0.271(2)\mu_N$ from [30] was used in Ref. [9]. The values for A/g_I were quoted in Ref. [22], so we multiplied their values by 0.18067 for comparison. The differences between our results and experimental values are 1.3%, 0.7%, and 4% for $7s$, $7p_{1/2}$, and $7p_{3/2}$ states, respectively. We note that the uncertainty in the value of the nuclear magnetic moment is 0.7%. Larger difference of the $A(7p_{3/2})$ SDpT value with the experiment is similar to that one in Cs [11], where the difference of the SDpT value for the $6p_{3/2}$ magnetic-dipole hyperfine constant with experiment is 3.5%. Interestingly, the Cs SDpT values are below the experimental ones while the Ra^+ SDpT results are above the experimental values. This can be explained by the uncertainty in the treatment of the finite-size correction, uncertainty in the value of Ra nuclear magnetic moment, and the difference in the size and distribution of the correlation corrections in Cs and Ra^+ .

IV. PARITY NONCONSERVATION

Nuclear-spin-independent PNC effects in atoms are caused by the exchange of a virtual Z_0 boson between an electron of the atom and a quark in the nucleus, or between two atomic electrons [31]. The second effect is extremely small and will not be considered in this work. The dominant PNC interaction between an atomic electron and the nucleus is described by a Hamiltonian $A_e V_N$, which is the product of axial-vector electron current A_e and vector nucleon current V_N . The PNC interaction leads to a nonzero amplitude for

transitions otherwise forbidden by the parity selection rule, such as the $6d_{3/2}-7s$ transition in singly ionized radium. Combining experimental measurements and theoretical calculations of the PNC amplitude permits one to infer the value of the weak charge Q_W for precise atomic-physics tests of the standard model.

The $7s-6d_{3/2}$ PNC amplitude in Ra^+ can be evaluated as a sum over states,

$$E_{\text{PNC}} = \sum_{n=2}^{\infty} \frac{\langle 6d_{3/2}|D|np_{1/2}\rangle\langle np_{1/2}|H_{\text{PNC}}|7s\rangle}{E_{7s} - E_{np_{1/2}}} + \sum_{n=2}^{\infty} \frac{\langle 6d_{3/2}|H_{\text{PNC}}|np_{3/2}\rangle\langle np_{3/2}|D|7s\rangle}{E_{6d_{3/2}} - E_{np_{3/2}}}, \quad (12)$$

where D is the dipole transition operator. The values of m_j are customary taken to be $m_j=1/2$ for all states. The PNC Hamiltonian H_{PNC} is given by

$$H_{\text{PNC}} = \frac{G_F}{2\sqrt{2}} Q_W \gamma_5 \rho(r), \quad (13)$$

where G_F is the universal Fermi coupling constant, Q_W is the weak charge, and γ_5 is the Dirac matrix associated with pseudoscalars. The quantity $\rho(r)$ is a nuclear density function, which is approximately the neutron density. In our calculations, we model $\rho(r)$ by the charge form factor, which is taken to be a Fermi distribution with 50% radius $c_{\text{PNC}}=c_{\text{charge}}=6.8617$ fm [32] and 10–90 % thickness parameter $t=2.3$ fm for $^{223}\text{Ra}^+$, i.e., we take $\rho(r)$ to be the same distribution as the charge distribution used our entire all-order calculation of the Ra^+ wave functions and corresponding properties. We also investigate how the PNC amplitude vary with changes in both c_{PNC} and c_{charge} .

The sum over n in Eq. (12) converges very fast in our case, and only first few terms need to be calculated accurately. Therefore, we divide our calculation of E_{PNC} into three parts: a main term $E_{\text{PNC}}^{\text{main}}$ that consists of the sum over states with $n=7-10$, a tail $E_{\text{PNC}}^{\text{tail}}$ which is the sum over states with $n=11, \dots, \infty$, and the contribution $E_{\text{PNC}}^{\text{auto}}$ from autoionizing states given by the terms with $n=2-6$. The calculation of the main term is illustrated in Table X, where we list the best set of the dipole and PNC matrix elements used in our calculation as well as relevant energy differences. The final electric-dipole matrix elements are taken to be *ab initio* single-double all-order results (following the comparison of the similar Cs and Ba^+ results with experiment [11,24]). Reduced electric-dipole matrix elements are listed for consistency with previous tables; they need to be multiplied by $1/\sqrt{6}$ to obtain relevant values of $\langle i|D|j\rangle$ ($m_j=1/2$ for all states). The final PNC matrix elements for the $6d_{3/2}-7p_{1/2}$ and $6d_{3/2}-8p_{1/2}$ transitions are taken to be SD all-order scaled values since the contribution that can be accounted for by scaling is the dominant one for these cases; remaining PNC matrix elements are taken to be *ab initio* SD values. Experimental energies are used where they are available; our predicted energy values from Table I are used for the $9p_{1/2}$, $10p_{1/2}$, and $10p_{3/2}$ levels. Our results are compared with results of Ref. [21] calculated using the correlation potential

TABLE X. Contributions to the $E_{\text{PNC}}^{\text{main}}$ in $^{223}\text{Ra}^+$ in units of $10^{-11}|e|a_0(-Q_W/N)$. D and H_{PNC} are dipole and PNC matrix elements, respectively. Reduced electric-dipole matrix elements are listed for consistency with previous tables; they need to be multiplied by $1/\sqrt{6}$ to obtain relevant values of $\langle i|D|j\rangle$ ($m_j=1/2$ for all states). All values are in a.u. Our results are compared with calculations of Ref. [21].

n	$\langle 6d_{3/2} D np_{1/2}\rangle$	$\langle np_{1/2} H_{\text{PNC}} 7s\rangle$	$E_{7s}-E_{np_{1/2}}$	E_{PNC}	Ref. [21]
7	3.566	-2.665	-0.0973	39.882	40.69
8	0.049	-1.590	-0.2306	0.137	0.11
9	0.017	-1.124	-0.2849	0.027	0.02
10	0.008	-0.841	-0.3130	0.009	
n	$\langle 6d_{3/2} H_{\text{PNC}} np_{3/2}\rangle$	$\langle np_{3/2} D 7s\rangle$	$E_{6d_{3/2}}-E_{np_{3/2}}$	E_{PNC}	Ref. [21]
7	-0.047	-4.551	-0.0644	-1.348	-2.33
8	-0.040	-0.405	-0.1837	-0.036	-0.05
9	-0.032	-0.140	-0.2339	-0.008	-0.01
10	-0.026	-0.069	-0.2602	-0.003	

method. The main part of the PNC amplitude is overwhelmingly dominated by a single term listed in the first row of Table X. Our result for this term slightly differs from the calculation in Ref. [21] (by 2.2%). However, the Ref. [21] does not list the Ra^+ isotope for which the calculation has been conducted. Since the value of the PNC amplitude is multiplied by the neutron number in the present commonly accepted units of $10^{-11}|e|a_0(-Q_W/N)$, the difference between values for the PNC amplitudes for $^{223}\text{Ra}^+$ and $^{226}\text{Ra}^+$ is 2% just owing to 138/135 neutron number ratio. Therefore, the difference may be either explained by the simple isotope rescaling, difference in the choice of the nuclear density function parameters, or differences in the treatment of the correlation correction. The only significant discrepancy between our calculation and that of Ref. [21] is in the other term with $n=7$ (-1.35 vs -2.33). This difference has to result from the differences in the treatment of the correlation correction since this entire value comes from the correlation effects. Taking into account that the DF value for this term is consistent with zero and RPA result, -4.08, is larger than the all-order value by nearly a factor of 3, such discrepancy is not very surprising.

To provide some estimate of the uncertainty in the calculation of the main term, we conduct the “scatter” analysis of the data following the calculation of the Cs PNC amplitude [33]. In such analysis, sets of data for dipole matrix elements, PNC matrix elements, and energies are varied (i.e., taken to be SD, SDpT, expt.) and the scatter in the final PNC values is analyzed. The results are summarized in Table XI. Our final value (corresponding to data in Table X) is listed in the last row of Table XI. We note that essentially the entire difference in the results comes from the dominant term (first row of Table X) and the variation in all other terms is insignificant. Therefore, the possible uncertainty in the next term (-1.35), which is bound to be substantial, cannot be evaluated by this approach. While we have included the values with SDpT dipole matrix elements, there is no reason to expect these data to be more accurate than SD values. This conclusion is based on the breakdown of the correlation correction contributions and comparisons of the similar calcula-

tions in other monovalent systems that demonstrate cancellation of some missing effects in SD approximation but not in SDpT one. As a result, we conclude that the uncertainty in the dominant term owing to the Coulomb correlation correction is probably on the order of 2%. We note that completely *ab initio* SD value is in good agreement with our final value. Measurement of the $6d_{3/2}-7p_{1/2}$ oscillator strength would help to reduce this uncertainty.

We calculate remaining terms $E_{\text{PNC}}^{\text{tail}}$ and $E_{\text{PNC}}^{\text{auto}}$ in both DF and RPA approximations. The RPA results are listed in Table XII together with our total value for the PNC amplitude. The corresponding DF results are $E_{\text{PNC}}^{\text{auto}}=4.8$ and $E_{\text{PNC}}^{\text{tail}}=1.2$. The relative correction due to Breit interaction is taken from sophisticated all-order calculation of Ref. [34] (-1.27%) and rescaled for the present calculation. Our final value is compared with other calculations from Refs. [21,22]. Our result for the terms with $n<7$ and $n>9$ (6.8) is in reasonably good agreement with the value from Ref. [21] (7.5). The notable feature of Table XII is an excellent agreement of all rather different high-precision calculations (with the exception of the mixed-states result [21]) despite relatively large possible

TABLE XI. “Scatter” analysis of the main part of the PNC amplitude ($n=7-10$) in $^{223}\text{Ra}^+$. Lowest-order DF and random-phase RPA values are listed for reference. SD labels single-double all-order values, SDpT values include partial triple contributions.

Energies	$\langle i D j\rangle$	$\langle i H_{\text{PNC}} j\rangle$	$E_{\text{PNC}}^{\text{main}}$
DF	DF	DF	38.95
DF	RPA	RPA	37.10
SD	SD	SD	39.05
Expt.	SD	SD	39.65
Expt.	SDpT	SD	40.22
Expt.	SD	SDpT	38.09
Expt.	SDpT	SDpT	38.65
Expt.	SD	SD _{sc} ^a	38.66

^aScaled values are used for the $7p_{1/2}-7s$ and $8p_{1/2}-7s$ matrix elements only, remaining data are taken to be SD.

TABLE XII. Contribution to the E_{PNC} in $^{223}\text{Ra}^+$ and comparison with other theory. Our value for $^{226}\text{Ra}^+$ is obtained by reducing our 223 value by 0.2%, owing to the correction for the different nuclear parameters and multiplying by 138/135 neutron number ratio. All results are in units of $10^{-11}|e|a_0(-Q_W/N)$. The Breit contribution is taken from Ref. [34] and rescaled for the present calculation.

Isotope	Term	Value
223	$E_{\text{PNC}}^{\text{main}}$	38.66
223	$E_{\text{PNC}}^{\text{tail}}$	-0.02
223	$E_{\text{PNC}}^{\text{auto}}$	6.83
223	Breit	-0.58
223	Total	44.89
226	Total	45.89
	Mixed states ^a	42.9
	Sum over states ^a	45.9
226	CCSD ^b	46.1
226	CCSD(T) ^b	46.4

^aReference [21].

^bReference [22].

uncertainties in various terms and inclusion of different high-order terms by different methods. We note, however, that Ref. [21] does not specify the isotope for which the calculation was carried out, leading to intrinsic 2% uncertainty in the comparison. The calculation of Ref. [21] also omits structure radiation and normalization corrections that are included in the present work. Our calculation of PNC amplitude includes some triple excitations and estimates of higher-order effects that were not included by previous coupled-cluster calculations of Ref. [22]. We omit some nonlinear terms present in calculation of [22]. However, it has been demonstrated [35] that inclusion of the nonlinear terms without the inclusion of the higher-order triples omitted in the CCSD(T) method of Ref. [22] may lead to less accurate values for electric-dipole matrix elements than linearized SD values. We also include contributions from higher partial waves and Breit interaction. The latter contribution was omitted in both Refs. [21,22] and is quite substantial (-1.3%). Moreover, our implementation of coupled-cluster method is very different from that of Ref. [22] (for example, we use complete basis set of orbitals that are generated using B splines, leading to essentially zero numerical basis set error, and carry out sum over states). Further calculations as well as experimental measurements will be necessary to achieve 1% accuracy in the PNC amplitude.

We also investigated the dependence of the PNC amplitude on the values of the nuclear distribution parameters c_{charge} and c_{PNC} . As we described in the beginning of this section, the parameter c_{charge} is used in the charge distribution in the all-order wave-function calculations. The parameter c_{PNC} is used in the modeling of the nuclear density function $\rho(r)$ in the PNC Hamiltonian given by Eq. (13). Both are modeled by the Fermi distributions; the all-order calculation is carried with both half-density parameters being equal to 6.8617 fm [32]. Since the DF result is rather close to the final value owing to various cancellations, it is sufficient to carry

TABLE XIII. Dependence of the lowest-order Ra^+ PNC amplitude on the parameters of the nuclear distributions $c_{\text{charge}}(\text{fm})$ and $c_{\text{PNC}}(\text{fm})$. The parameter c_{charge} is used in the charge distribution in the all-order wave-function calculations. The parameter c_{PNC} is used in the modeling the nuclear density function in the PNC Hamiltonian. The variation in the given parameter is listed in % for convenience. The units for the PNC amplitude is $10^{-11}|e|a_0(-Q_W/N)$.

c_{charge}	δc_{charge} (%)	c_{PNC}	δc_{PNC} (%)	$E_{\text{PNC}}^{\text{DF}}$	$\delta E_{\text{PNC}}^{\text{DF}}$ (%)
6.8617	0	6.8617		44.913	
6.8960	0.5	6.8617		44.853	-0.13
6.9303	1	6.8617		44.792	-0.27
6.9989	2	6.8617		44.671	-0.54
7.2048	5	6.8617		44.310	-1.34
6.8617		6.8960	0.5	44.875	-0.08
6.8617		6.9303	1	44.837	-0.17
6.8617		6.9989	2	44.761	-0.34
6.8617		7.2048	5	44.531	-0.85
6.8960	0.5	6.8960	0.5	44.815	-0.22
6.9303	1	6.9303	1	44.717	-0.44
6.9989	2	6.9989	2	44.523	-0.87
7.2048	5	7.2048	5	43.954	-2.14

out this study using DF data. The results are summarized in Table XIII, where we list $E_{\text{PNC}}^{\text{DF}}$ calculated with varying values or either one or both parameters. The variation in the given parameter is listed in % for convenience. The results show that possible uncertainty in the PNC amplitude owing to the uncertainty in the value of the charge radius (that is unlikely to be large) is negligible in comparison with the uncertainty in the correlation correction. For example, difference in the rms radii for $A=223$ and $A=226$ isotopes corresponds to the change in c_{charge} that is on the order of 0.5% resulting in only 0.2% change in the PNC amplitude. Possible variance in the density $\rho(r)$ in Eq. (13) which is approximately neutron density is higher, but even 5% change in c_{PNC} with the fixed value of the c_{charge} leads to 0.85% change in the PNC amplitude value. Table XIII may be used to recalculate the values of the PNC amplitude between different isotopes since the change in E_{PNC} with the nuclear parameters is essentially linear.

V. CONCLUSION

We have calculated the energies, transition matrix elements, lifetimes, hyperfine constants, and quadrupole moments of the $6d$ states, as well as dipole and quadrupole ground-state polarizabilities and PNC amplitude in $^{223}\text{Ra}^+$ using high-precision all-order method. The energies of the $9p_{1/2}$, $10p_{1/2}$, and $10p_{3/2}$ levels are predicted. The results for atomic properties are compared with available theoretical and experimental data. The PNC amplitude for the $7s - 6d_{3/2}$ transition is found to be $44.9 \times 10^{-11}|e|a_0(-Q_W/N)$. The dependence of the PNC amplitude on the choice of

nuclear parameters c_{charge} and c_{PNC} is studied. The parameter c_{charge} is used in the charge distribution in the all-order wavefunction calculations. The parameter c_{PNC} is used in the modeling of the nuclear density function in the PNC Hamiltonian. Our study establishes the dependence of the PNC amplitude on the choice of isotope which is particularly important in the case of Ra^+ where the availability of various isotopes may allow conducting the experimental PNC study with isotopic chains. Our calculation also established pos-

sible uncertainty in the PNC amplitude that may be caused by the uncertainty in the nuclear parameters. This work also provides a number of recommended values for yet unmeasured properties of Ra^+ .

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