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

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We have calculated parity-nonconserving $7s\rightarrow6d_{3/2}$ amplitude $E_{\text{PNC}}$ 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 $E_{\text{PNC}}$ and the vector part of the Stark-induced amplitude $\beta$ 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 $\sim 1$ TeV.

Experimental measurements of the spin-dependent contribution to the PNC $6s\rightarrow7s$ 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 $7s\rightarrow6d_{3/2}$ 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 $7s\rightarrow6d_{3/2}$ 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 $7s\rightarrow6d_{3/2}$ 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,

\[ \Psi_v = \left[ 1 + \sum_{ma} \rho_{ma} \hat{a}^\dagger_m \hat{a}_a + \frac{1}{2} \sum_{mnab} \rho_{mnab} \hat{a}^\dagger_m \hat{a}^\dagger_n \hat{a}_b \hat{a}_a + \sum_{m\neq v} \rho_{ma} \hat{a}^\dagger_m + \sum_{mna} \rho_{mna} \hat{a}^\dagger_m \hat{a}_n \right] \Psi_v. \] (1)

Here, \( \Psi_v \) is the lowest-order atomic wave function taken to be the frozen-core Dirac-Fock (DF) wave function of a state \( v \), \( a^\dagger, \hat{a} \) are single-particle creation and annihilation operators, \( \rho_{ma} \) and \( \rho_{mna} \) are the single core and valence excitation coefficients, and \( \rho_{mnab} \) and \( \rho_{mna} \) are double core and valence excitation coefficients, respectively. Indices at the beginning of the alphabet, \( a, b, \ldots \), refer to occupied core states, those in the middle of the alphabet \( m, n, \ldots \) refer to excited states, and index \( v \) designates the valence orbital.

To derive equations for the excitation coefficients, the wave function (1) is substituted into the many-body Schrödinger equation \( H[\Psi_v]=E[\Psi_v] \), 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,

\[ H_0 = \sum_{i=1}^N \epsilon_i \hat{c}_i^\dagger \hat{c}_i, \]

\[ V_I = \frac{1}{2} \sum_{ijkl} \tilde{g}_{ijkl} \hat{c}_i^\dagger \hat{c}_k^\dagger \hat{c}_j \hat{c}_l. \] (2)

where \( \epsilon_i \) are the single-particle energies, \( \hat{c}_i \) designate normal ordering of the operators with respect to closed core, and \( \tilde{g}_{ijkl} \) 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 \( Z = \sum_{ijkl} \tilde{g}_{ijkl} \hat{c}_i^\dagger \hat{c}_k \hat{c}_j \hat{c}_l \),

\[ Z_{uv} = \frac{\langle \Psi_v | Z | \Psi_u \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle \langle \Psi_u | \Psi_u \rangle}}. \] (3)

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

\[ Z_{uv} = \frac{z_{uv} + Z^{(1)} + \cdots + Z^{(l)}}{\sqrt{(1+N_u)(1+N_v)}}, \] (4)

where \( z_{uv} \) is the lowest-order DF matrix element and \( Z^{(1)}, \ldots, Z^{(l)} \) and normalization terms \( N_u \) 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 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 \( \frac{1}{4} \sum_{mnab} \rho_{mnab} \hat{a}^\dagger_m \hat{a}^\dagger_n \hat{a}_b \hat{a}_a \) 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 \( \rho_{mn} \) 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 \( E^{(3)}_{\text{extra}} \), first-order Breit contribution \( B^{(1)} \), second-order Coulomb-Breit \( B^{(2)} \) corrections, and Lamb shift contribution, \( E_{\text{LS}} \) (see Ref. [20] for detail). We take the sum of these six contributions to be our final all-order results, \( E^{\text{tot}} \) listed in the seventh column of Table I.

The column labeled \( \Delta E^{SD} \) in Table I gives differences between our \( ab \text{ initio} \) 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 9p1/2, 10p1/2, and 11p3/2 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–6d1/2 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 $E^{(3)}_{\text{extra}}$, first-order Breit and second-order Coulomb-Breit corrections $B^{(2)}$, and Lamb shift $E_{LS}$. The total energies $E^{SD}_{\text{tot}}$ are compared with experimental energies $E_{\text{expt.}}$ [18,19]. $\delta E = E^{SD}_{\text{tot}} - E_{\text{expt.}}$. Our predicted energy values are listed for the $9p_{1/2}$ and $10p_{3/2}$ energy levels. Units: cm$^{-1}$.

| nlj     | $E^{(0)}$ | $E^{SD}$ | $E^{(3)}_{\text{extra}}$ | $B^{(1)}$ | $B^{(2)}$ | $E_{LS}$ | $E^{SD}_{\text{tot}}$ | $E_{\text{expt.}}$ | $\delta E^{SD}$ |
|---------|----------|----------|--------------------------|-----------|-----------|---------|----------------------|-------------------|-----------------|
| $7s_{1/2}$ | -75898   | -66992  | 1152                     | 147       | -250      | 33       | -81508              | -81842           | 334             |
| $6d_{3/2}$ | -62356   | -8042   | 1152                     | 155       | -398      | 33       | -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             |
| $7d_{3/2}$ | -36860   | -1745   | 316                      | 46        | -74       | 7        | -38311              | -38437           | 126             |
| $7d_{5/2}$ | -31575   | -1590   | 245                      | 39        | -92       | 0        | -32973              | -33098           | 125             |
| $7d_{7/2}$ | -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        | -32654              | -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.

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 |

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 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 $n,d$ 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 |       |       |
| $7p_{1/2} - 8d_{3/2}$ | 0.716 | 0.702 | 0.708 |       |       |
| $7p_{1/2} - 6d_{5/2}$ | 4.446 | 3.566 | 3.550 | 3.64 | 3.68 |
| $7p_{1/2} - 7d_{5/2}$ | 4.527 | 4.290 | 4.358 |       |       |
| $7p_{1/2} - 8d_{5/2}$ | 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 |       |       |
| $8p_{1/2} - 7s_{1/2}$ | 0.625 | 0.395 | 0.339 | 0.50 |       |
| $8p_{1/2} - 8s_{1/2}$ | 9.880 | 9.294 | 9.320 |       |       |
| $8p_{1/2} - 9s_{1/2}$ | 9.244 | 9.022 | 9.036 |       |       |
| $8p_{1/2} - 6d_{5/2}$ | 0.168 | 0.144 | 0.127 | 0.15 |       |
| $8p_{1/2} - 7d_{5/2}$ | 4.331 | 4.035 | 4.038 | 4.028 |       |
| $8p_{1/2} - 8d_{5/2}$ | 4.047 | 4.002 | 4.034 |       |       |
| $8p_{1/2} - 6d_{5/2}$ | 0.462 | 0.378 | 0.347 | 0.40 |       |
| $8p_{1/2} - 7d_{5/2}$ | 13.37 | 12.55 | 12.53 |       |       |
| $8p_{1/2} - 8d_{5/2}$ | 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 $\alpha_c$, a small counteracting term to compensate for the excitations from the core states to the valence state $\alpha_{vc}$, and valence polarizability $\alpha_v$.

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

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 $\alpha_{vtail}$ is calculated in the DF approximation without loss of accuracy. The ionic core contribution $\alpha_c$ and term $\alpha_{vc}$ 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 $\alpha_{vmin}$. 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 polarization 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        | \(\alpha_{E1}\) |
|---------------------|-----------------|
| \(7p_{1/2} - 7s\)   | 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            |
| \(\alpha_{\text{c}}\) | 93.35           |
| \(\alpha_{\text{v}}\) | 13.74           |
| \(\alpha_{\text{sc}}\) | 0.11            |
| \(\alpha_{\text{sv}}\) | -0.98           |
| Total               | 106.22          |

Theory\(^3\) 106.12

\(^3\)Reference [9].

2. Quadrupole polarizability

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

\[
\alpha_{q}(E2) = \frac{1}{5} \sum_{n}^{n} \left( \frac{|\langle 7s | Q | nd_{s/2} \rangle|^2}{E_{nd_{s/2}} - E_{7s}} + \frac{|\langle 7s | Q | nd_{d/2} \rangle|^2}{E_{nd_{d/2}} - E_{7s}} \right).
\]  

(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. [9].

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           | \(\alpha_{E2}\) |
|---------------------|--------------|-----------------|
| \(6d_{3/2} - 7s\)   | 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             |
| \(\alpha_{\text{c}}\) | 2430(21)     |
| \(\alpha_{\text{v}}\) | 35(10)       |
| Total               | 2533(26)     |

Theory\(^3\) 2547.5

\(^3\)Reference [9].

D. Lifetimes of the \(7p\) and \(6d\) states

The lifetimes \(\tau\) 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

\[
A_{E1} = \frac{2.026 \times 10^{18} |\langle i | D | f \rangle|^2}{\lambda^3 2j_i + 1} s^{-1},
\]

(8)

where \(\lambda\) is the wavelength of the transition in Å and \(|\langle i | D | f \rangle|^2\) 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
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

$$A_{ij}^{E2} = \frac{1.1199 \times 10^{18}}{\lambda^5} \left| \langle i|Q|f\rangle \right|^2 \frac{2j_i + 1}{2j_f + 1},$$

(9)

where $\lambda$ 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

$$A_{ij}^{M1} = \frac{2.6973 \times 10^{13}}{\lambda^5} \left| \langle i|M1|f\rangle \right|^2 \frac{2j_i + 1}{2j_f + 1},$$

(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 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.

### Table VII. Lifetimes of the 6d_{3/2} and 6d_{5/2} states of Ra⁺ in a.u.

| 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            |

$^a$Reference [9].

$^b$Reference [21].

### Table VIII. Quadrupole moments of the 6d_{3/2} and 6d_{5/2} states in a.u.

| State | SD  | SDpT | SD_{ac} | SDpT_{ac} | 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 $\Theta(\gamma f)$ can be expressed via the reduced matrix element of the quadrupole operator $Q$ as

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

(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 $A(MHz)$ in $^{223}$Ra⁺ are compared with theory [9,22] and experiment [28,29] in Table IX. The gyromagnetic ratio $g_f$ 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 $^{223}$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 $^{210}$Ra and $^{229}$Ra nuclear magnetic moments in Ref. [30]. The magnetization distribution is modeled by a Fermi distribution with the same parameters as our charge distribution ($\sigma=6.862$ 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 $g_I=0.1807$ that corresponds to the rounded off value $\mu_I=0.2711(2)\mu_N$ from [30] was used in Ref. [9]. The values for $A/g_I$ were quoted in Ref. [22], so we multiplied their values by 0.1807 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 $A_{i}V_{NP}$, which is the product of axial-vector electron current $A_{i}$ and vector nucleon current $V_{NP}$. 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,

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

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 $H_{\text{PNC}}$ is given by

$$H_{\text{PNC}} = \frac{G_{F}}{2\sqrt{2}} Q_{W} \gamma_{5} \rho(r),$$

where $G_{F}$ is the universal Fermi coupling constant, $Q_{W}$ is the weak charge, and $\gamma_{5}$ 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 $^{223}$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 $c_{\text{PNC}}$ and $c_{\text{charge}}$.

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 $E_{\text{PNC}}$ 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 $n=11,\ldots,\infty$, 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 $ab\text{ initio}$ 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 $ab\text{ initio}$ 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

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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 $10^{-11} |\langle \alpha | Q_W | \alpha \rangle / N|$, 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 to provide some estimate of the uncertainty in the calculation 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 $ab\text{ initio}$ SD value is in good agreement with our final value.

We calculate remaining terms $E_{\text{PPNC}}^\text{tail}$ 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 $E_{\text{PPNC}}^\text{tail} = 1.2$. 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 differences 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 $ab\text{ initio}$ SD value is in good agreement with our final value.

Measurement of the 6$d_{3/2}^{-7}p_{1/2}$ oscillator strength would help to reduce this uncertainty.

We calculate remaining terms $E_{\text{PPNC}}^\text{tail}$ 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 $E_{\text{PPNC}}^\text{tail} = 1.2$. 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

| $n$ | $\langle 6d_{3/2}|D|np_{1/2}\rangle$ | $\langle np_{1/2}|H_{\text{PNC}}|7s\rangle$ | $E_{7s}-E_{np_{1/2}}$ | $E_{\text{PNC}}$ | 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 | |

| $n$ | $\langle 6d_{3/2}|H_{\text{PNC}}|np_{3/2}\rangle$ | $\langle np_{3/2}|D|7s\rangle$ | $E_{6d_{3/2}}-E_{np_{3/2}}$ | $E_{\text{PNC}}$ | Ref. [21] |
|---|---|---|---|---|---|
| 7 | −0.047 | −4.551 | −0.0644 | −1.348 | −2.33 |
| 8 | −0.040 | −4.045 | −0.1837 | −0.036 | −0.05 |
| 9 | −0.032 | −1.40 | −0.2339 | −0.008 | −0.01 |
| 10 | −0.026 | −0.069 | −0.2602 | −0.003 | |

TABLE XII. “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 | $\langle i|D(j)\rangle$ | $\langle i|H_{\text{PNC}}(j)\rangle$ | $E_{\text{PNC}}^\text{min}$ |
|---|---|---|---|
| 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 | 38.66 |

Scaled values are used for the $7p_{1/2}^{-7}s$ and $8p_{1/2}^{-7}s$ matrix elements only, remaining data are taken to be SD.
TABLE XII. Contribution to the $E_{\text{PNC}}$ in $^{226}\text{Ra}^+$ 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 $10^{-11}|e|a_0/\langle Q_W\rangle N$. The Breit contribution is taken from Ref. [34] and rescaled for the present calculation.

| Isotope | Term          | Value  |
|---------|---------------|--------|
| 223     | $E_{\text{main}}^\text{PNC}$ | 38.66  |
| 223     | $E_{\text{tail}}^\text{PNC}$  | −0.02  |
| 223     | $E_{\text{auto}}^\text{PNC}$  | 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   |

$^a$Reference [21].
$^b$Reference [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 $c_{\text{charge}}$ and $c_{\text{PNC}}$. As we described in the beginning of this section, the parameter $c_{\text{charge}}$ is used in the charge distribution in the all-order wave-function calculations. The parameter $c_{\text{PNC}}$ 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 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 of either one or both parameters. The variation in the given parameter is listed in % for convenience. The units for the PNC amplitude is $10^{-11}|e|a_0/\langle Q_W\rangle N$.

TABLE XIII. Dependence of the lowest-order Ra$^+$ PNC amplitude on the parameters of the nuclear distributions $c_{\text{charge}}$ (fm) and $c_{\text{PNC}}$ (fm). The parameter $c_{\text{charge}}$ is used in the charge distribution in the all-order wave-function calculations. The parameter $c_{\text{PNC}}$ 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 $10^{-11}|e|a_0/\langle Q_W\rangle N$.

| $c_{\text{charge}}$ | $\delta c_{\text{charge}}$ (%) | $c_{\text{PNC}}$ | $\delta c_{\text{PNC}}$ (%) | $E_{\text{PNC}}^{\text{DF}}$ | $\delta E_{\text{PNC}}^{\text{DF}}$ (%) |
|---------------------|-----------------------------|-----------------|-----------------------------|--------------------------|----------------------------------|
| 6.8617              | 0                           | 6.8617          | 0                           | 44.913                   | −0.13                            |
| 6.8960              | 0.5                         | 6.8617          | 0.5                         | 44.853                   | −0.03                            |
| 6.9303              | 1                           | 6.8617          | 1                           | 44.792                   | −0.27                            |
| 6.9989              | 2                           | 6.8617          | 2                           | 44.671                   | −0.54                            |
| 7.2048              | 5                           | 6.8617          | 5                           | 44.310                   | −1.34                            |
| 6.8617              | 0                           | 6.8960          | 0.5                         | 44.875                   | −0.08                            |
| 6.8617              | 1                           | 6.9303          | 1                           | 44.837                   | −0.17                            |
| 6.8617              | 2                           | 6.9989          | 2                           | 44.761                   | −0.34                            |
| 6.8617              | 3                           | 7.2048          | 4.5                         | 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          | 4.5                         | 43.954                   | −2.14                            |

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 $^{226}\text{Ra}^+$ 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 $44.9 \times 10^{-11}|e|a_0/\langle Q_W\rangle N$. The dependence of the PNC amplitude on the choice of...
nuclear parameters $c_{\text{charge}}$ and $c_{\text{PNC}}$ is studied. The parameter $c_{\text{charge}}$ is used in the charge distribution in the all-order wave-function calculations. The parameter $c_{\text{PNC}}$ 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 possible 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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