Excitation energies, E1, M1, and E2 transition rates, and lifetimes in Ca\(^+\), Sr\(^+\), Cd\(^+\), Ba\(^+\), and Hg\(^+\)

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Abstract

Excitation energies of \(ns_{1/2}\), \(np_j\) and \(nd_j\) states in Cd\(^+\) \((n = 5)\), Hg\(^+\) \((n = 6)\) and \(ns_{1/2}\), \(np_j\) and \((n - 1)d_j\) states in Ca\(^+\) \((n = 4)\), Sr\(^+\) \((n = 5)\), and Ba\(^+\) \((n = 6)\) are evaluated using the linearised coupled-cluster (all-order) method. Reduced matrix elements, oscillator strengths, and transition rates are determined for the \(ns - np_j - nd_j\) (or \(ns - np_j - (n - 1)d_j\)) possible electric-dipole transitions in Ca\(^+\), Sr\(^+\), Ba\(^+\), Cd\(^+\), and Hg\(^+\). Electric-quadrupole matrix elements are evaluated to obtain \(ns_{1/2} - (n - 1)d_j\) transition rates in Ca\(^+\) \((n = 5)\), Sr\(^+\) \((n = 5)\), and Ba\(^+\) \((n = 6)\).

The matrix elements are calculated using both relativistic many-body perturbation theory, complete through third order, and the relativistic all-order method restricted to single and double (SD) excitations. The SD lifetime results for the \(np\) and \(nd\) states in Ca\(^+\), Sr\(^+\), Ba\(^+\), Cd\(^+\), and Hg\(^+\), are compared with the latest available experimental measurements. The contribution of the magnetic-dipole \(nd_{3/2} - nd_{5/2}\) transition to the lifetimes of the lowest \(nd_{5/2}\) level in Ca\(^+\), Sr\(^+\), and Ba\(^+\) ions is discussed. These calculations provide a theoretical benchmark for comparison with experiment and theory as well as data needed for various applications.

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I. INTRODUCTION

High-precision measurements of the atomic lifetimes for the low-lying states were recently carried out for various atomic systems [1–4]. The lifetime of the $1s^22s^22p^2P_{3/2}$ metastable level of boronlike $\text{Ar}^{13+}$ was determined at the Heidelberg Electron Beam Ion Trap by Lapierre et al. in Ref. [1]. The measurement of the $6s$ level lifetime in neutral rubidium using time-correlated single-photon counting technique was reported by Gomez et al. in Ref. [2]. The measurement of the $3d^2D_j$ metastable state lifetime of a single laser-cooled $^{40}\text{Ca}^+$ ion in a linear Paul trap was presented in Ref. [3]. The precision measurements of the $5p^2P_J$ level lifetimes of a single trapped $\text{Cd}^+$ ion were reported in Ref. [4]. These measurements are important for various fields such as optical frequency standards, quantum information, and astronomy [3]. The comparison of high-precision measurements with theoretical predictions tests the quality of the approximation method used to account for correlation and relativistic effects in high-precision atomic calculations.

In the present paper, we calculate the lifetimes of the $np_j$ and $nd_j$ states in $\text{Cd}^+ (n = 5)$, $\text{Hg}^+ (n = 6)$ and $np_j$ and $(n - 1)d_j$ states in $\text{Ca}^+ (n = 4)$, $\text{Sr}^+ (n = 5)$, and $\text{Ba}^+ (n = 6)$. Electric-dipole, electric-quadrupole, and magnetic-dipole matrix elements are evaluated to calculate the lifetimes of above mentioned states. The matrix elements are calculated using both relativistic many-body perturbation theory, complete through third order, and the relativistic all-order method restricted to single and double (SD) excitations.

Recently, relativistic many-body calculation of energies, lifetimes, hyperfine constants, and multipole polarizabilities in $^{137}\text{Ba}^+$ and $^{87}\text{Sr}^+$ were presented by Safronova [5, 6]. The $6s - np_j (n = 6–9)$ electric-dipole matrix elements and the $6s - nd_j (n = 5–7)$ electric-quadrupole matrix elements in $\text{Ba}^+$ were calculated by Iskrenova-Tchoukova and Safronova [7] using the relativistic all-order linearized coupled-cluster method. This set of matrix elements was used in Ref. [7] for accurate calculation of the ground-state dipole and quadrupole polarizabilities and lifetimes of the $6p_j$ and $5d_j$ levels. Previously, the $n_1s - n_2p_j$ and $n_3d_{j'} - n_2p_j \ (n_1 = 6–8, \ n_2 = 6–8, \ \text{and} \ n_3 = 5–7)$ electric-dipole matrix elements were evaluated by Dzuba et al. [8] to determine the parity-nonconserving $6s - 5d$ amplitudes in $\text{Ba}^+$. Correlation corrections to the electron orbitals were calculated using the correlation potential method. Dzuba et al. [9] carried out accurate ab initio nonperturbative calculations of the Breit correction to the parity nonconserving (PNC) amplitudes of the $6s - 5d_{3/2}$ transi-
Electric dipole and quadrupole transition amplitudes in \( \text{Ba}^+ \) were calculated by Gopakumar et al. [10] using the relativistic coupled-cluster method. Numerical values for the \( n_1s - n_2p_j \) and \( 5d_j - n_2p_j \) (\( n_1 = 6-8 \) and \( n_2 = 6-8 \)) electric-dipole matrix elements were calculated in [10] using the relativistic third-order many-body perturbation theory (MBPT). A description of this method and explicit formulas for the associated diagrams were given in the paper by Blundell et al. [11].

Recently [12], the calculation of the \( 4d^2 D_J - 4s^2 S_{1/2} \) electric-quadrupole matrix elements in \( \text{Sr}^+ \) was performed using an \textit{ab initio} relativistic all-order method which sums infinite sets of many-body perturbation theory terms. These matrix elements were used to evaluate the \( 4d \) radiative lifetimes and their ratio [12]. In Ref. [13], the relativistic coupled-cluster theory was used to perform accurate calculations of the lifetimes of the lowest excited \( 4d^2 D_J \) states in singly ionized strontium. The lifetimes of the \( 4d^2 D_J \) levels and other \( \text{Sr}^+ \) properties were recently evaluated by Mitroy et al. [14] by diagonalizing a semiempirical Hamiltonian in a large dimension single-electron basis.

Recently, relativistic configuration-interaction oscillator strengths for lowest E1 transitions in gold isoelectronic sequence were presented by Glowacki and Migdalek in Ref. [15]. Numerical results for Hg II ion were listed only for the \( 6s - 6p_j \) transitions. Relativistic corrections to the transition frequencies of Ag I, Dy I, Ho I, Yb II, Yb III, Au I, and Hg II ions were investigated recently by Dzuba and Flambaum [16] owing to the search for variation of the fine-structure constant. Relativistic many-body perturbation theory was used by Safronova and Johnson [17] to evaluate excitation energies, oscillator strengths, and lifetimes of ions along the gold isoelectronic sequence. Numerical results for Hg II ion were presented for the \( ns_{1/2} \) (\( n = 6-9 \)), \( np_j \) (\( n = 6-8 \)), \( nd_j \) (\( n = 6-7 \)), and \( 5f_j \) states for excitation energies and oscillator strengths between those states.

In this paper, we conduct both RMBPT and SD all-order calculations of the \( \text{Ca}^+ \), \( \text{Sr}^+ \), \( \text{Cd}^+ \), \( \text{Ba}^+ \), and \( \text{Hg}^+ \) properties. Such calculations permit one to investigate the convergence of the perturbation theory and estimate the theoretical error of predicted data. In the present paper, we evaluate reduced matrix elements, transition rates, and lifetimes for the low-lying levels in \( \text{Ca}^+ \), \( \text{Sr}^+ \), \( \text{Cd}^+ \), \( \text{Ba}^+ \), and \( \text{Hg}^+ \) ions. Our results are compared with theoretical results from Refs. [18–27].
II. ENERGIES OF HG+, BA+, CD+, SR+, AND CA+

We start from the “no-pair” Hamiltonian [28]

\[ H = H_0 + V_I, \]

(1)

where \( H_0 \) and \( V_I \) can be written in a second-quantized form as

\[ H_0 = \sum_i \varepsilon_i a_i^+ a_i, \]

(2)

\[ V_I = \frac{1}{2} \sum_{ijkl} g_{ijkl} a_i^+ a_j^+ a_l a_k, \]

(3)

and the negative energy (positron) states are excluded from the sums. The quantities \( \varepsilon_i \) are eigenvalues of the one-electron Dirac-Fock (DF) equations with a frozen core, the two-particle matrix element \( g_{ijkl} \) is the Coulomb matrix element, and \( a_i^+ \), \( a_i \) are creation and annihilation operators, respectively.

We carry out our calculations starting from a \( V_{N-1} \) DF potential [Ar], [Kr], [Kr]4d10, [Kr]4d10s25p6, and [Kr]4d104f14s25p65d10 in the cases of Ca+, Sr+, Cd+, Ba+, and Hg+, respectively. There is a number of advantages associated with this potential, including greatly reduced number of the Goldstone diagrams [29], a clean separation of the core and valence states, and one set of single-particle states, leading to important simplifications in the calculation of excitation energies and transition matrix elements. Thus, the total energy of different valence states of a one-electron atom, can be written as

\[ E = E_v + E_{\text{core}}, \]

(4)

where \( E_{\text{core}} \) is the same for all valence states \( v \). Because the first-order correlation correction to valence removal energies vanishes for a \( V_{N-1} \) DF potential, the first nonvanishing corrections are found in second order.

Despite the elimination of a large set of Goldstone diagrams owing to the use of the \( V_{N-1} \) DF potential, third-order energy expression still contains 52 terms, given by Blundell et al. in Ref. [30]. The third-order expression for the energy includes terms with one-, two-, three-, and four-particle sums over virtual states and sums over core states.

The all-order single-double method was discussed previously in Refs. [31–37]. Briefly, we represent the wave function \( \Psi_v \) of an atom with one valence electron atom as \( \Psi_v \cong \Psi_v^{\text{SD}} \).
with

\[ \Psi_{SD}^{v} = \left[ 1 + \sum_{ma} \rho_{ma} a_{m}^{+} a_{a} + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_{m}^{+} a_{n}^{+} a_{b} a_{a} + \sum_{m \neq v} \rho_{me} a_{m}^{+} a_{v} + \sum_{mna} \rho_{mnva} a_{m}^{+} a_{n}^{+} a_{a} a_{v} \right] \Phi_{v}, \]  

where \( \Phi_{v} \) is the lowest-order atomic wave function, which is taken to be the frozen-core DF wave function of a state \( v \). We note that we again start from the \( V^{N-1} \) DF potential. Substituting the wave function \( \Psi_{SD}^{v} \) into the many-body Schrödinger equation, with Hamiltonian given by the Eqs. (1–3), one obtains the coupled equations for the single- and double-excitation coefficients \( \rho_{mv}, \rho_{ma}, \rho_{mnva}, \) and \( \rho_{mnab} \). The coupled equations for the excitation coefficients are solved iteratively. The resulting excitation coefficients are used to evaluate multipole matrix elements. This method allows to include the contribution of certain classes of RMBPT terms to all orders.

The valence \( E_{SD}^{v} \) energy given by

\[ E_{SD}^{v} = \sum_{ma} \tilde{g}_{vam} \rho_{ma} + \sum_{mab} \tilde{g}_{abvm} \tilde{\rho}_{mvab} + \sum_{mna} \tilde{g}_{vamn} \tilde{\rho}_{mnva} \]  

does not include a certain part of the third-order contribution associated with triple excitation. This part of the third-order contribution, \( E_{extra}^{(3)} \), is given in Ref. [34] and needs to be calculated separately. We use our third-order energy code to separate out \( E_{extra}^{(3)} \) and add it to the \( E_{SD}^{v} \). We drop the index \( v \) in the designations in the text and tables below.

We use B-splines [38] to generate a complete set of basis DF wave functions for use in the evaluation of MBPT and all-order expressions. For \( \text{Ca}^{+}, \text{Sr}^{+}, \text{Cd}^{+}, \text{Ba}^{+}, \) and \( \text{Hg}^{+} \), we use 50 splines of order \( k = 8 \) for each angular momentum. The basis orbitals are constrained to a spherical cavity. The cavity radius \( R = 65 \) a.u. is chosen large enough to accommodate all \( ns_{1/2} \) and \( nd_{j} \) orbitals considered here and small enough that 50 splines can approximate inner-shell DF wave functions with good precision (\( 10^{-4}\% – 10^{-5}\% \) for \( \text{Ba}^{+} \) ion and \( 10^{-6}\% – 10^{-7}\% \) for \( \text{Sr}^{+} \) ion).

Results of our calculations of energies for the lowest states of \( \text{Hg}^{+}, \text{Ba}^{+}, \text{Cd}^{+}, \text{Sr}^{+}, \) and \( \text{Ca}^{+} \) ions are summarized in Table I. The first six columns of Table I give the lowest-order DF energies \( E^{(0)} \), second- and third-order Coulomb correlation energies, \( E^{(2)} \) and \( E^{(3)} \), first-order Breit contribution \( B^{(1)} \), second-order Coulomb-Breit \( B^{(2)} \) corrections, and Lamb shift contribution, \( E_{LS} \). We take the sum of these six contributions to be our final third-order
RMBPT results, $E_{\text{tot}}^{(3)}$, listed in the seventh column of Table I. We list the all-order SD energies in the column labeled $E^{\text{SD}}$ and the part of the third-order energies omitted in the SD calculation in column $E_{\text{extra}}^{(3)}$. We note that $E^{\text{SD}}$ contains $E^{(2)}$ contribution. We take the sum of the six terms $E^{(0)}, E^{\text{SD}}, E_{\text{extra}}^{(3)}, B^{(1)}, B^{(2)}$, and $E_{\text{LS}}$ to be our final all-order results $E_{\text{tot}}^{\text{SD}}$ listed in the ninth column of Table I. The recommended values from the National Institute of Standards and Technology (NIST) database [39] are given in column labeled $E_{\text{NIST}}$. The differences between our calculations and the NIST data, $\delta E^{(3)} = E_{\text{tot}}^{(3)} - E_{\text{NIST}}$ and $\delta E^{\text{SD}} = E_{\text{tot}}^{\text{SD}} - E_{\text{NIST}}$, are given in the last two columns of Table I, respectively.

As expected, the largest correlation contribution to the valence energy comes from the second-order term, $E^{(2)}$. This term is simple to calculate in comparison with the $E^{(3)}$ and $E^{\text{SD}}$ terms. Thus, we calculate the $E^{(2)}$ term with better numerical accuracy than $E^{(3)}$ and $E^{\text{SD}}$ terms.

The second-order energy $E^{(2)}$ includes partial waves up to $l_{\text{max}} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [40, 41]). As an example of the convergence of $E^{(2)}$ with the number of partial waves $l$, we consider the $6s_{1/2}$ state in Hg$^+$ ion. Calculations of $E^{(2)}$ with $l_{\text{max}} = 6$ and 8 yield $E^{(2)}(6s_{1/2}) = -18158.0$ and -18351.4 cm$^{-1}$, respectively. Extrapolation of these calculations yields -18387.3 and -18381.3 cm$^{-1}$, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(6s_{1/2})$ of 6.0 cm$^{-1}$. It should be noted that the 193.3 cm$^{-1}$ contribution from partial waves with $l > 6$ for the 6s state is the largest among all Hg$^+$ states considered in Table I; smaller (about 16-17 cm$^{-1}$) contributions are obtained for the 6d$3/2$ and 6d$5/2$ states and much smaller contributions (2-3 cm$^{-1}$) are obtained for $n=7$ states. Similar convergence patterns are found for all other ions considered.

Owing to the computational complexity, we restrict $l \leq l_{\text{max}} = 6$ in the $E^{\text{SD}}$ calculation. As noted above, the second-order contribution dominates $E^{\text{SD}}$; therefore, we can use the extrapolated value of the $E^{(2)}$ described above to account for the contributions of the higher partial waves. Six partial waves are also used in the calculation of $E^{(3)}$. Since the asymptotic $l$-dependence of the second- and third-order energies are similar (both fall off as $l^{-4}$), we use the second-order remainder as a guide to estimate the remainder in the third-order contribution. The term $E_{\text{extra}}^{(3)}$ in Table I, which accounts for that part of the third-order MBPT energy missing from the SD energy, is smaller than $E^{(3)}$ by a factor of 2–3 for the states considered here.
The first-order Breit energies (column $B^{(1)}$ of Table I) include retardation, whereas the second-order Coulomb-Breit energies (column $B^{(2)}$ of Table I) are evaluated using the unretarded Breit operator. The Lamb shift $E_{\text{LS}}$ is approximated as the sum of the one-electron self energy and the first-order vacuum-polarization energy. The vacuum-polarization contribution is calculated from the Uehling potential using the results of Fullerton and Rinker [42]. The self-energy contribution is estimated for the $s$, $p_{1/2}$ and $p_{3/2}$ orbitals by interpolating among the values obtained by Mohr [43, 44, 45] using Coulomb wave functions. For this purpose, an effective nuclear charge $Z_{\text{eff}}$ is obtained by finding the value of $Z_{\text{eff}}$ required to give a Coulomb orbital with the same average $\langle r \rangle$ as the DF orbital. It should be noted that the values of $E_{\text{LS}}$ are very small ($E_{\text{LS}} \leq 79 \text{ cm}^{-1}$ for Hg II and $E_{\text{LS}} \leq 8 \text{ cm}^{-1}$ for Ba II).

We find that the correlation corrections to energies for the ions considered in this work large, especially for the $nd$ states in Ba II, Sr II, and Ca II and for the $ns$ states in Hg II and Cd II. For example, $E^{(2)}$ is about 13% of $E^{(0)}$ and $E^{(3)}$ is about 30% of $E^{(2)}$ for the $5d_j$ states of Ba II. Despite the evident slow convergence of the perturbation theory expansion, the $6s$ energy in Hg II from the third-order MBPT calculation is within 1.3% of the measured energy.

As expected, the SD results agree better with the recommended values than the third-order MBPT results, owing to more complete inclusion of the correlation correction. The difference of the all-order values with experiment, $\delta E^{\text{SD}}$, are smaller than the corresponding third-order differences, $\delta E^{(3)}$, by a factor of 3–5 as illustrated by two last columns of Table I. Better agreement of the all-order values with experiment demonstrates the importance of the higher-order correlation contributions.

### III. ELECTRIC-DIPOLE MATRIX ELEMENTS, TRANSITION RATES, AND LIFETIMES IN SR$^+$, CD$^+$, BA$^+$, HG$^+$, AND RA$^+$

**A. Electric-dipole matrix elements**

The one-body matrix element of the operator $Z$ is given by [31]

$$Z_{wv} = \frac{\langle \Psi_w | Z | \Psi_v \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle \langle \Psi_w | \Psi_w \rangle}},$$ (7)
where $\Psi_v$ is the exact wave function for the many-body “no-pair” Hamiltonian $H$

$$H |\Psi_v\rangle = E |\Psi_v\rangle .$$

(8)

In MBPT, we expand the many-electron wave function $\Psi_v$ in powers of $V_I$ as

$$|\Psi_v\rangle = |\Psi_v^{(0)}\rangle + |\Psi_v^{(1)}\rangle + |\Psi_v^{(2)}\rangle + |\Psi_v^{(3)}\rangle + \cdots .$$

(9)

The denominator in Eq. (7) arises from the normalization condition that contributes starting from the third order of RMBPT [46]. In the lowest order, we find

$$Z_{wv}^{(1)} = \langle \Psi_w^{(0)} | Z | \Psi_v^{(0)} \rangle = z_{wv},$$

(10)

where $z_{wv}$ is the corresponding one-electron matrix element [47]. Since $\Psi_w^{(0)}$ is a DF function we use $Z^{(\text{DF})}$ designation instead of $Z^{(1)}$ below.

The second-order Coulomb correction to the transition matrix element in the DF case with $V^{N-1}$ potential is given by [48]

$$Z_{wv}^{(2)} = \sum_{na} \frac{z_{an}(g_{wvna} - g_{wavn})}{\varepsilon_a + \varepsilon_v - \varepsilon_n - \varepsilon_w} + \sum_{na} \frac{(g_{wavn} - g_{wanv})z_{na}}{\varepsilon_a + \varepsilon_w - \varepsilon_n - \varepsilon_v}. $$

(11)

The second-order Breit corrections are obtained from Eq. (11) by changing $g_{ijkl}$ to Breit matrix element $b_{ijkl}$ [49].

In the all-order SD calculation, we substitute the all-order SD $\Psi_v^{\text{SD}}$ wave function into the matrix element expression given by Eq. (7) and obtain the expression [31]

$$Z_{wv}^{(\text{SD})} = \frac{z_{wv} + Z^{(a)} + \cdots + Z^{(t)}}{\sqrt{(1 + N_w)(1 + N_v)}} ,$$

(12)

where $Z_{wv}$ is the lowest-order (DF) matrix element given by Eq. (10) and the terms $Z^{(k)}$, $k = a \cdots t$ are linear or quadratic functions of the excitation coefficients introduced in Eq. (5). The normalization terms $N_w$ are quadratic functions of the excitation coefficients. As a result, certain sets of many-body perturbation theory terms are summed to all orders in this method. Unlike the energy, the SD all-order matrix elements contain the entire third-order RMBPT contribution.

The calculation of the transition matrix elements provides another test of the quality of atomic-structure calculations and another measure of the size of correlation corrections. Reduced electric-dipole matrix elements between low-lying states of Hg II. Ba II, Cd II Sr II,
and Ca II calculated in the third order RMBPT and in the all-order SD approximation are presented in Table II.

Our calculations of reduced matrix elements in the lowest-, second-, and third-orders $Z^{(n)}$ in Hg II, Ba II, Cd II, Ca II, and Sr II ions are carried out following the method described above. The lowest order DF value is obtained from Eq. (10). The values of $Z^{(DF+2)}$ are the sum of the second-order correlation correction $Z^{(2)}$ given by Eq. (11) and the DF matrix elements $Z^{(DF)}$. It should be noted that the second-order Breit corrections $B^{(2)}$ is rather small in comparison with the the second-order Coulomb correction $Z^{(2)}$ (the ratio of $B^{(2)}$ and $Z^{(2)}$ is about 0.2\%–2\%).

The third-order matrix elements $Z^{(DF+2+3)}$ include the DF values, the second-order $Z^{(2)}$ results, and the third-order $Z^{(3)}$ correlation correction, which includes random-phase-approximation terms (RPA) iterated to all orders, Brueckner orbitals (BO) corrections, the structural radiation $Z^{(SR)}$, and normalization $Z^{(NORM)}$ terms (see [50] for detailed expressions for these terms).

The terms $Z^{(RPA)}$ and $Z^{(BO)}$ give the largest contributions to $Z^{(3)}$. The sum of terms $Z^{(RPA)}$ and $Z^{(BO)}$ is about 15 – 25% of the $Z^{(DF)}$ term and has different sign. The smallest contributions (about 1\%) come from the structural radiation, $Z^{(SR)}$, and normalization $Z^{(NORM)}$ terms. The basis set used here is the same as in the calculation of the energy contributions. We find correlation corrections $Z^{(2+3)}$ to be very large, 10–25\% for many cases. All results given Table II are obtained using the length form of the matrix elements. Length-form and velocity-form matrix elements differ typically by 5–20\% for the DF matrix elements and 2–5\% for the second-order matrix elements in this calculations.

Electric-dipole matrix elements evaluated in the all-order SD approximation (Eq. (12)) are given in columns labeled $Z^{(SD)}$ of Table II. The SD matrix elements $Z^{(SD)}$ include $Z^{(3)}$ completely, along with important fourth- and higher-order corrections. The fourth-order corrections omitted from the SD matrix elements were discussed recently by Derevianko and Emmons [51]. The $Z^{(SD)}$ values are smaller than the $Z^{(DF+2)}$ values and larger than the $Z^{(DF+2+3)}$ values for all transitions given in Table II.
B. Transition rates and lifetimes in Ca$^+$, Sr$^+$, Cd$^+$, Ba$^+$, and Hg$^+$

Transition rates $A$ and lifetimes in Ca$^+$, Sr$^+$, Cd$^+$, Ba$^+$, and Hg$^+$ calculated in SD approximation are summarized in Tables III and IV, respectively.

In Table III, we compare transition rates $A$ ($10^7$ cm$^{-1}$) with available theoretical and experimental measurements given in Refs. [52] for Ba II. The SD data are used for dipole matrix elements and energies in columns with headings $A_{SD}$. In the column with headings $A_{NIST}^{SD}$, the NIST data are used for energies and SD data are used for the matrix elements. We include these values since the NIST data also were used in the theoretical results by Gopakumar et al. in Ref. [52]. Experimental results given in the last column of Table III are taken from Ref. [52]. The accuracy of experimental results is not very high and does not allow us to make decision which theoretical data in Table III are in better agreement with experimental values.

We calculate lifetimes of the $np$ and $nd$ states in Cd$^+$ ($n = 5$), Hg$^+$ ($n = 6$) and $np_j$ states in Ca$^+$ ($n = 4$), Sr$^+$ ($n = 5$), and Ba$^+$ ($n = 6$) using SD results for dipole matrix elements and experimental energies. The lifetimes of the $(n-1)d_j$ states in Sr$^+$ ($n = 5$), Ba$^+$ ($n = 6$) and Ra$^+$ ($n = 7$) are discussed in the next section. We compare the lifetimes $\tau^{(SD)}$ with available experimental measurements in Table IV. Our SD results are in a good agreement with experimental measurements when we take into account the experimental uncertainties. The largest disagreement (about 1%) between the SD results and measurements by Pinnigton et al. in Ref. [23] is observed for the 5$d_j$ states in Cd II. We list two SD numbers for the lifetime of 5$d_{3/2}$ level in Cd II 1.51(1.79): the first number comes from two decay channels, 5$p_{1/2} - 5d_{3/2}$ and 5$p_{3/2} - 5d_{3/2}$. The second number includes only the 5$p_{1/2} - 5d_{3/2}$ transition. We note that the second result agrees very well with experimental measurements given in Ref. [23].

IV. ELECTRIC-QUADRUPOLE AND MAGNETIC-DIPOLE TRANSITIONS IN CA II, SR II AND BA II

Reduced matrix elements of the electric-quadrupole (E2) and magnetic-dipole (M1) operators in lowest, second, third, and all orders of perturbation theory are given in Table V for Ca II, Sr II, and Ba II. Detailed descriptions of the calculations of the reduced matrix
elements of the E2 and M1 operators in lowest and second orders of perturbation theory were given by Safronova et al. [53]. Third-order and all-order calculations are done in the same way as the calculations of E1 matrix elements.

As additional test of accuracy of our ab initio SD values, we compare our results for the lifetimes of the nd levels for Ba II, Sr II, and Ca II with recommended theoretical values and experimental measurements from Refs. [3, 7, 12, 20, 25] in Table VI. Recommended theoretical values Refs. [3, 7, 12] are from a similar all-order calculation but include semiempirical scaling that estimates dominant class of missing correlation effects. The ratio of the M1 5d_{3/2} → 5d_{5/2} and the E2 6s_{1/2} → 5d_{5/2} transition is equal to 0.206 that decreases the lifetime of the 5d_{5/2} level by 17 %. It is smaller the ratio of the M1 4d_{3/2} → 4d_{5/2} and the E2 5s_{1/2} → 4d_{5/2} transition in Sr II (about 0.01 %).

V. CONCLUSION

In summary, a systematic relativistic MBPT study of the energies of ns, np and nd states in Ca⁺, Sr⁺, Ba⁺, Cd⁺, and Hg⁺ is presented. The energy values are in good agreement with existing experimental data. A systematic all-order SD study of the reduced matrix elements and transition rates for the ns_{1/2} → np_{j} → nd_{j} and ns_{1/2} → np_{j} → (n−1)d_{j} allowed electric-dipole transitions in Cd⁺ (n = 5), Hg⁺ (n = 6) and in Ca⁺ (n = 4), Sr⁺ (n = 5), and Ba⁺ (n = 6) is conducted. The SD lifetime results for np and nd states in Ca⁺, Sr⁺, Ba⁺, Cd⁺, and Hg⁺ are compared with the latest available experimental measurements. The contribution of the magnetic-dipole nd_{3/2} → nd_{5/2} transition to the lifetimes of the nd_{5/2} level in Ca⁺ (n = 4), Sr⁺ (n = 5), and Ba⁺ (n = 6) ions are included. Our work provide data for analyzing existing experimental data and for planning future measurements.

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TABLE I: Zeroth-order (DF), second-, and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb $E_{SD}^{(3)}$, first-order Breit and second-order Coulomb-Breit corrections $B^{(n)}$ to the energies of Hg II, Ba II, Cd II, Sr II, and Ca II. The total energies ($E^{(3)}_{\text{tot}} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)} + E_{LS}$, $E^{SD}_{\text{tot}} = E^{(0)} + E^{SD} + E^{(3)}_{\text{extra}} + B^{(1)} + B^{(2)} + E_{LS}$) are compared with experimental energies $E_{\text{NIST}}$ [39], $\delta E = E_{\text{tot}} - E_{\text{NIST}}$. Units: cm$^{-1}$.

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<th>$nlj$</th>
<th>$E^{(0)}$</th>
<th>$E^{(2)}$</th>
<th>$E^{(3)}$</th>
<th>$B^{(1)}$</th>
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<td>4p_{1/2}</td>
<td>4s_{1/2}</td>
<td>3.2012</td>
<td>3.0045</td>
<td>2.8826</td>
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<tr>
<td>4p_{3/2}</td>
<td>4s_{1/2}</td>
<td>4.5269</td>
<td>4.2499</td>
<td>4.0773</td>
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18
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<tr>
<td>$4p_{1/2}$</td>
<td>$3d_{3/2}$</td>
<td>3.0825</td>
<td>2.9296</td>
<td>2.2998</td>
<td>2.4173</td>
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<td>$4p_{3/2}$</td>
<td>$3d_{3/2}$</td>
<td>1.3764</td>
<td>1.3088</td>
<td>1.0260</td>
<td>1.0788</td>
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<tr>
<td>$4p_{3/2}$</td>
<td>$3d_{5/2}$</td>
<td>4.1348</td>
<td>3.9311</td>
<td>3.0882</td>
<td>3.2452</td>
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</table>
TABLE III: The E1 transition rates $A \ (10^7 \text{ s}^{-1})$ for transitions in Ba II calculated in the SD $A_{SD}$ approximation (i.e. SD data are used for both energies and matrix elements). Data in the column $A_{SD}$ are obtained by using NIST data for wavelengths and SD matrix elements. Our results are compared with theoretical $A^{(\text{theor})}$ and experimental $A^{(\text{expt})}$ data given in Ref. [52] and references therein.

<table>
<thead>
<tr>
<th>Transition $\rightarrow$</th>
<th>$A_{SD}$</th>
<th>$A_{NIST}$</th>
<th>$A^{(\text{theor})}$</th>
<th>$A^{(\text{expt})}$</th>
</tr>
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<tbody>
<tr>
<td>$6s_{1/2} \rightarrow 6p_{1/2}$</td>
<td>9.115</td>
<td>9.390</td>
<td>9.368</td>
<td>9.5±0.9</td>
</tr>
<tr>
<td>$6s_{1/2} \rightarrow 6p_{3/2}$</td>
<td>11.54</td>
<td>11.89</td>
<td>11.94</td>
<td>10.6±0.9</td>
</tr>
<tr>
<td>$5d_{3/2} \rightarrow 6p_{1/2}$</td>
<td>3.323</td>
<td>3.443</td>
<td>3.493</td>
<td>3.77±0.24</td>
</tr>
<tr>
<td>$5d_{3/2} \rightarrow 6p_{3/2}$</td>
<td>0.433</td>
<td>0.449</td>
<td>0.425</td>
<td>0.469±0.029</td>
</tr>
<tr>
<td>$5d_{5/2} \rightarrow 6p_{3/2}$</td>
<td>3.587</td>
<td>3.691</td>
<td>3.261</td>
<td>3.38±0.19</td>
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</table>
TABLE IV: Lifetimes $\tau$ of the $nl$ levels in Ca II, Sr II, Ba II, Cd II, and Hg II. The SD data are compared with other theoretical results and experimental measurements for Ba II from Ref. [54] and references therein - (a), for Sr II from Ref. [55] and references therein - (b), for Ca II from Ref. [27] - (b1), for Hg II from Ref. [22] and references therein (c), and for Cd II from Ref. [26] - (d), Ref. [4] - (f), Ref. [23] -(f1).

<table>
<thead>
<tr>
<th>Level</th>
<th>$\tau^{(SD)}$</th>
<th>$\tau^{\text{theor}}$</th>
<th>$\tau^{\text{expt}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba II, $Z=56$</td>
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<tr>
<td>6p$_{1/2}$</td>
<td>7.798</td>
<td>7.89$^a$</td>
<td>7.90±0.10$^a$</td>
</tr>
<tr>
<td>6p$_{3/2}$</td>
<td>6.245</td>
<td>6.30$^a$</td>
<td>6.32±0.10$^a$</td>
</tr>
<tr>
<td>Sr II, $Z=38$</td>
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<td></td>
</tr>
<tr>
<td>5p$_{1/2}$</td>
<td>7.383</td>
<td>7.48$^b$</td>
<td>7.39±0.07$^b$</td>
</tr>
<tr>
<td>5p$_{3/2}$</td>
<td>6.660</td>
<td>6.74$^b$</td>
<td>6.63±0.07$^b$</td>
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<tr>
<td>Ca II, $Z=20$</td>
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<tr>
<td>4p$_{1/2}$</td>
<td>6.892</td>
<td>6.931$^{b1}$</td>
<td>6.978±0.056$^{b1}$</td>
</tr>
<tr>
<td>4p$_{3/2}$</td>
<td>6.702</td>
<td>6.881$^{b1}$</td>
<td>6.926±0.036$^{b1}$</td>
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<tr>
<td>Hg II, $Z=80$</td>
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<tr>
<td>6p$_{1/2}$</td>
<td>2.64</td>
<td>2.91$^c$</td>
<td>2.91±0.11$^c$</td>
</tr>
<tr>
<td>6p$_{3/2}$</td>
<td>1.61</td>
<td>1.80±0.06$^c$</td>
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</tr>
<tr>
<td>6d$_{3/2}$</td>
<td>1.29</td>
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<tr>
<td>6d$_{5/2}$</td>
<td>1.60</td>
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<td>Cd II, $Z=48$</td>
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<tr>
<td>5p$_{1/2}$</td>
<td>3.102</td>
<td>3.09$^d$</td>
<td>3.148±0.011$^f$</td>
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<td>5p$_{3/2}$</td>
<td>2.612</td>
<td>2.60$^d$</td>
<td>2.647±0.010$^f$</td>
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<td>5d$_{3/2}$</td>
<td>1.51(1.79)</td>
<td>1.86$^d$</td>
<td>1.79±0.11$^{f1}$</td>
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<tr>
<td>5d$_{5/2}$</td>
<td>1.61</td>
<td>1.67$^d$</td>
<td>1.85±0.15$^{f1}$</td>
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<tr>
<td>Transition</td>
<td>Z^{(DF)}</td>
<td>Z^{(DF+2)}</td>
<td>Z^{(DF+2+3)}</td>
</tr>
<tr>
<td>--------------</td>
<td>----------</td>
<td>------------</td>
<td>--------------</td>
</tr>
<tr>
<td><strong>Ba II</strong></td>
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</tr>
<tr>
<td>6s_{1/2}</td>
<td>14.7633</td>
<td>15.6749</td>
<td>11.8208</td>
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<tr>
<td>6s_{1/2}</td>
<td>18.3840</td>
<td>19.5789</td>
<td>14.8623</td>
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<tr>
<td><strong>Sr II</strong></td>
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<tr>
<td>5s_{1/2}</td>
<td>12.9681</td>
<td>13.2533</td>
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<td>5s_{1/2}</td>
<td>15.9721</td>
<td>16.3366</td>
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<td>4d_{3/2}</td>
<td>7.2603</td>
<td>8.5432</td>
<td>5.5821</td>
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<tr>
<td><strong>Ca II</strong></td>
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<tr>
<td>4s_{1/2}</td>
<td>9.7673</td>
<td>9.7272</td>
<td>7.4009</td>
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<tr>
<td>4s_{1/2}</td>
<td>11.9782</td>
<td>11.9265</td>
<td>9.0914</td>
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<tr>
<td>3d_{3/2}</td>
<td>5.0183</td>
<td>4.9554</td>
<td>3.3275</td>
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TABLE V: Reduced matrix elements of the electric-quadrupole and magnetic-dipole operator in first, second, third, and all orders of perturbation theory in Ba II, Sr II, and Ca II.
TABLE VI: Lifetimes $\tau$ of the $nd$ levels in Ba$^+$, Sr$^+$ and Ca$^+$ in sec. The SD data are compared with theoretical recommended values and experimental measurements for Ba II from Ref. [7]–(a) and Ref. [20]–(a1), for Sr II from Ref. [12]–(b) and Ref. [25]–(c), and for Ca II from Ref. [3]–(d).

<table>
<thead>
<tr>
<th>Level</th>
<th>$\tau$ SD</th>
<th>$\tau$ theor</th>
<th>$\tau$ expt</th>
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<tr>
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<tr>
<td>Ba II, Z=56</td>
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<tr>
<td>$5d_{3/2}$</td>
<td>83.26</td>
<td>81.5(1.2)$^a$</td>
<td>89.4±15.6$^{a1}$</td>
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<tr>
<td>$5d_{5/2}$</td>
<td>30.88</td>
<td>30.3(4)$^a$</td>
<td>31.6±4.6$^{a1}$</td>
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<tr>
<td>Sr II, Z=38</td>
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<tr>
<td>$4d_{3/2}$</td>
<td>0.4509</td>
<td>0.441(3)$^b$</td>
<td>0.435±0.004$^c$</td>
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<tr>
<td>$4d_{5/2}$</td>
<td>0.4029</td>
<td>0.394(3)$^b$</td>
<td>0.408±0.022$^c$</td>
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<td>Ca II, Z=20</td>
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<tr>
<td>$3d_{3/2}$</td>
<td>1.243</td>
<td>1.196(11)$^d$</td>
<td>1.176(11)$^d$</td>
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<tr>
<td>$3d_{5/2}$</td>
<td>1.209</td>
<td>1.165(11)$^d$</td>
<td>1.168(7)$^d$</td>
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