# All-order perturbation calculation of energies, hyperfine constants, multipole polarizabilities, and blackbody radiation shift in $^{87}Sr^+$

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Excitation energies of the [Kr]$ns_{1/2}$, [Kr]$np_j$, [Kr]$nd_j$, and [Kr]$nf_j$ ($n \leqslant 9$ and [Kr] = ($1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$) in Sr II are evaluated. First-order, second-order, third-order, and all-order Coulomb energies and first-order and second-order Coulomb-Breit energies are calculated. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes are determined for the levels up to $n = 7$. Electric-dipole ($5s_{1/2}$-$np_j$, $n = 5$–26), electric-quadrupole ($5s_{1/2}$-$nd_j$, $n = 4$–26), and electric-octupole ($5s_{1/2}$-$nf_j$, $n = 4$–26) matrix elements are calculated to obtain the ground-state $E1$, $E2$, and $E3$ static polarizabilities. Scalar and tensor polarizabilities for the $5p_j$-$9p_j$ and $4d_j$-$8d_j$ excited states in Sr II are also calculated. All the above-mentioned matrix elements are determined using the all-order method. We also investigate the hyperfine structure in $^{87}Sr^+$. The hyperfine $A$ values and $B$ values are determined for the first low-lying levels up to $n = 7$. The quadratic Stark effect on hyperfine-structure levels of the $^{87}Sr^+$ ground state is investigated. The calculated shift for the $(F = 5, M = 0) \leftrightarrow (F = 4, M = 0)$ transition is found to be 0.120(1) Hz/(kV/cm)$^2$. These calculations provide a theoretical benchmark for comparison with the experiment and theory. A careful study of uncertainty of our calculations is carried out for the transition-matrix elements, line strengths, transition rates, lifetimes, polarizabilities, and the Stark shift coefficient.

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## I. INTRODUCTION

The lifetimes of the metastable $4d\ ^2D_{3/2}$ and $4d\ ^2D_{5/2}$ levels in $Sr^+$ have been the subjects of theoretical and experimental studies. The properties of $Sr^+$ are of present interest of many applications in various fields such as optical frequency standards, quantum information, and astronomy. Recently, precision lifetime measurement of the $4d\ ^2D_{5/2}$ level in $Sr^+$ was presented by Letchumanan *et al.* in Ref. [1]. The measurement was performed using a single laser-cooled ion in a radio-frequency trap. Precision measurements and calculations of the $4d\ ^2D_J$ lifetimes were presented by Biémont *et al.* [2]. The experiment was performed at an ion storage ring utilizing collinear laser excitation. The calculation was carried out using the Hartree-Fock method including relativistic effects and core polarization [2]. Recently [3], the calculation of the $4d\ ^2D_J$-$4s\ ^2S_{1/2}$ electric-quadrupole matrix elements in $Sr^+$ was performed using an *ab initio* relativistic all-order method, which sums infinite sets of many-body perturbation theory terms. These matrix elements were used to evaluate the $4d$-level radiative lifetimes and their ratio [3]. In Ref. [4], the relativistic coupled-cluster theory was used to perform accurate calculations of the lifetimes of the lowest-excited $4d\ ^2D_J$ states in singly ionized strontium. The lifetimes of the $4d\ ^2D_J$ levels and other $Sr^+$ properties were recently evaluated by Mitroy *et al.* [5] by diagonalizing a semiempirical Hamiltonian in a large-dimension single-electron basis. Early theoretical calculations and measurements of the $4d\ ^2D_{3/2}$ and $4d\ ^2D_{5/2}$ lifetimes in $Sr^+$ were presented in Refs. [6–11].

Early theoretical calculations of the polarizabilities of the low-lying states presented in Refs. [12–14] used the simplest nonrelativistic approximations. Indirect spin-orbit $K$ splittings in strontium were used recently by Nunkaew *et al.* [15] to determine the $Sr^+$ dipole and quadrupole polarizabilities. The polarizabilities of the low-lying states ($5s$,$6s$,$5p$,$6p$,$4d$,$5d$) of the $Sr^+$ ions were recently evaluated by Mitroy *et al.* [5]. The nonrelativistic semiempiriacal Hamiltonians in a large-dimension single-electron basis were used to evaluate polarizabilities and oscillator strengths [5]. The blackbody radiation (BBR) shift of the $5s$-$4d_{5/2}$ clock transition in $^{88}Sr$ II was calculated in Ref. [3] using the relativistic all-order method where all single and double excitations of the Dirac-Fock wave function are included to all orders of perturbation theory. The scalar polarizabilities of the $5s$ and $4d_{5/2}$ levels, as well as the tensor polarizability of the $4d_{5/2}$ level, were presented together with the evaluation of their uncertainties.

The first lifetime measurements of the $5p\ ^2P_{1/2}$ and $5p\ ^2P_{3/2}$ levels in $Sr^+$ were performed by Gallagher [16] using the Hanle-effect method with optical excitation from the $5s\ ^2S_{1/2}$ ground state. The same technique was used later in Refs. [17–19] to measure the $5p\ ^2P_{3/2}$ lifetime. A pulsed dye laser was used to determine the lifetime of the resonance levels of Sr II [19] via the beam-laser method. Lifetime measurements of using frequency-doubled laser-induced fluorescence were used by Pinnington *et al.* [20] to determine the lifetimes of the $5p\ ^2P_{1/2,3/2}$ and $4f\ ^2F_{5/2,7/2}$ levels in Sr II.

Experimental values of a few $Sr^+$ oscillator strengths derived from lifetime measurements were presented by Penkin [21], Gallagher [16], and Pinnington *et al.* [20]. Warner reported [6] theoretical oscillator strengths for the $ns$-$n'p$, $np$-$n'd$, and $nd$-$n'f$ transitions with $ns = 5s$-$9s$, $np = 5p$-$9p$, $nd = 4d$-$7d$, and $nf = 4f$-$7f$ calculated using scaled Thomas-Fermi-Dirac wave functions, including the spin-orbit interaction. Dipole transition rates, oscillator strengths lifetimes, and branching ratios derived from a numerical Coulomb approximation were presented by Lindgård and Nielsen [22] for the Sr II and other ions of the rubidium isoelectronic sequence. Relativistic Hartree-Fock oscillator strengths for the lowest $5s\ ^2S_{1/2}$-$5p\ ^2P_{1/2,3/2}$ transitions in Sr II, with an

 

allowance for core polarization, were presented by Migdalek and Baylis [23]. The SUPERSTRUCTURE code was used by Bautista *et al.* [24] to evaluate oscillator strengths, transition rates, and electron-impact excitation-rate coefficients for Sr II. The authors underlined that the purpose of their work was to study the nature of the peculiar Sr II emission filament found in the ejecta of Eta Carinae. The oscillator strengths of the resonance transitions in Sr II calculated by the Dirac-Fock method were recently presented by Zilitis in Ref. [25].

High-precision measurement of the ground-state hyperfine splitting of $^{87}Sr^{+}$ was presented by Shinozuka *et al.* [26]. The magnetic-dipole hyperfine constant was determined to be $A = 1000.473\,673(11)$ kHz. Early measurements of the $A$ constant for the $5s\ ^2S_{1/2}$ state were presented in Refs. [27–30]. The magnetic-dipole $A$ and electric quadrupole $B$ hyperfine constants for the $5p\ ^2P_{3/2}$ state were measured by collinear fast-beam laser spectroscopy [29,30]. The hyperfine structure of the $^2S_{1/2}$-$^2D_{5/2}$ quadrupole transition at 674 nm in $^{87}Sr^{+}$ was observed by Barwood *et al.* [31]. The $^2D_{5/2}$ state hyperfine-structure constants were determined to be $A = 2.174\,3(14)$ MHz and $B = 49.11(6)$ MHz [31].

The hyperfine interactions in Sr II were investigated using the relativistic linked-cluster many-body perturbation theory (RLCMBPT) [32]. The theoretical value of hyperfine magnetic-dipole constant $A$ for the ground-state $5s\ ^2S_{1/2}$ was found to be $-987$ MHz [32]. Relativistic coupled-cluster calculations for the magnetic and quardupole hyperfine constants were presented by Mårtensson-Pendrill [33] for the low-lying states of the ion $^{87}Sr^{+}$. The author underlined that those properties are of interest as a possible frequency standard. The calculated $B/Q$ value for the $5p\ ^2P_{3/2}$ state was combined with experimental $B$ factors for the isotope sequence $^{79-93}$Sr, giving revised values for the nuclear quadrupole moments $Q$ [33]. A relativistic many-body calculation was performed in Ref. [34] for the low-lying states of $^{87}Sr^{+}$. The zeroth-order hyperfine-structure constants were evaluated with Dirac-Fock wave functions, and the finite basis sets of the Dirac-Fock equation were constructed by B splines. Numerical results were given for the $A$ ($5s\ ^2S_{1/2}$, $5p\ ^2P_J$, and $4d\ ^2D_J$ states) and $B$ ($5p\ ^2P_{3/2}$ and $4d\ ^2D_J$ states) hyperfine constants [34].

In the present paper, the relativistic all-order method is used to calculate atomic properties of singly ionized strontium for the $ns$, $np_j$, $nd_j$, and $nf_j$ ($n \leqslant 9$) states. We evaluated a large number of transition-matrix elements to calculate the $E1$, $E2$, and $E3$ ground-state polarizabilities, scalar polarizabilities of the $ns_{1/2}$, $np_j$ and $nd_j$ states, and tensor polarizabilities of the $np_{3/2}$ and $nd_j$ excited states of $Sr^{+}$. Excitation energies are calculated for the 37 first excited states. The hyperfine $A$ and $B$ values are determined for the first low-lying levels up to $n = 7$. The quadratic Stark effect on hyperfine-structure levels of the $^{87}Sr^{+}$ ground state is investigated.

The main motivation for this work is to provide recommended values for a number of atomic properties via a systematic high-precision study for use in the planning and analysis of various experiments as well as theoretical modeling. We evaluated the uncertainties of the recommended values for the transition-matrix elements, line strengths, transition rates, lifetimes, polarizabilities, and the Stark shift coefficient. The calculation of uncertainties involved the estimation of missing high-order effects and *ab initio* calculations in different approximations to establish the size of the higher-order corrections and approximate missing contributions. Another motivation is to study the methods to accelerate the convergence of the all-order iterative scheme for the $nd$ states. We have tested an approach that significantly reduced the time required for the calculation of the all-order excitation coefficients without loss of accuracy. Moreover, our tests demonstrate the improvement of the accuracy over the original scheme. Such a method is of importance for evaluating properties of the $nd$ states in heavy systems where the calculation time is significant or for the combination of the all-order and configuration interaction methods where the calculations have to be carried out for a large number of states [35].

## II. THIRD-ORDER AND ALL-ORDER CALCULATIONS OF ENERGIES

The energies of $nl_j$ states in Sr II are evaluated for $n \leqslant 10$ and $l \leqslant 3$ using both third-order relativistic many-body perturbation theory (RMBPT) and the single-double (SD) all-order method discussed in Ref. [36], in which single and double excitations of Dirac-Fock (DF) wave functions are iterated to all orders. The results of our energy calculations are summarized in Table I. Columns 2 through 8 of Table I give the lowest-order DF energies $E^{(0)}$, second-order and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, first-order and second-order Breit corrections $B^{(1)}$ and $B^{(2)}$, and an estimated Lamb-shift contribution $E^{(\mathrm{LS})}$. The Lamb shift $E^{(\mathrm{LS})}$ is calculated 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 [38]. The self-energy contribution is estimated for the $s$, $p_{1/2}$, and $p_{3/2}$ orbitals by interpolating among the values obtained by [39–41] using Coulomb wave functions. For this purpose, an effective nuclear charge $Z_{\mathrm{eff}}$ is obtained by finding the value of $Z_{\mathrm{eff}}$ 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 $E^{(\mathrm{LS})}$ are very small. For states with $l > 0$, the Lamb shift is estimated to be smaller than 0.1 cm$^{-1}$ using scaled Coulomb values and is ignored. We list the all-order SD energies in the column labeled $E^{\mathrm{SD}}$ and list that part of the third-order energies missing from $E^{\mathrm{SD}}$ in the column labeled $E^{(3)}_{\mathrm{extra}}$. The sum of the seven terms $E^{(0)}$, $E^{\mathrm{SD}}$, $E^{(3)}_{\mathrm{extra}}$, $B^{(1)}$, $B^{(2)}$, and $E^{(\mathrm{LS})}$ is our final all-order result $E^{\mathrm{SD}}_{\mathrm{tot}}$, listed in the 11th column of Table I. Recommended energies from the National Institute of Standards and Technology (NIST) database [37] are given in the column labeled $E_{\mathrm{NIST}}$. The differences between our third-order and all-order calculations the and experimental data, $\delta E^{(3)} = E^{(3)}_{\mathrm{tot}} - E_{\mathrm{NIST}}$ and $\delta E^{\mathrm{SD}} = E^{\mathrm{SD}}_{\mathrm{tot}} - E_{\mathrm{NIST}}$, are given in the two final columns of Table I, respectively.

As expected, the largest correlation contribution to the valence energy comes from the second-order term $E^{(2)}$. Therefore, we calculate $E^{(2)}$ with higher numerical accuracy. The second-order energy includes partial waves up to $l_{\max} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [42,43] for details of the extrapolation procedure). As an example of the convergence of $E^{(2)}$ with the number of partial waves $l$, consider the $5s_{1/2}$ state.

TABLE I. Zeroth-order (DF), second-order, and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies $E^{\rm SD}$, $E^{(3)}_{\rm extra}$, first-order Breit and second-order Coulomb-Breit corrections $B^{(n)}$ to the energies of Sr II. The total energies [$E^{(3)}_{\rm tot} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)}$, $E^{\rm SD}_{\rm tot} = E^{(0)} + E^{\rm SD} + E^{(3)}_{\rm extra} + B^{(1)} + B^{(2)}$] for Sr II are compared with experimental energies $E_{\rm NIST}$ [37], $\delta E = E_{\rm tot} - E_{\rm NIST}$. Units are given in cm$^{-1}$.

| $nlj$ | $E^{(0)}$ | $E^{(2)}$ | $E^{(3)}$ | $B^{(1)}$ | $B^{(2)}$ | $E^{(LS)}$ | $E^{(3)}_{\rm tot}$ | $E^{\rm SD}$ | $E^{(3)}_{\rm extra}$ | $E^{\rm SD}_{\rm tot}$ | $E_{\rm NIST}$ | $\delta E^{(3)}$ | $\delta E^{\rm SD}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $5s_{1/2}$ | −84042 | −5610.2 | 1236.9 | 48.8 | −63.7 | 5.9 | −88425 | −5386.3 | 618.2 | −88819 | −88964 | 539 | 145 |
| $4d_{3/2}$ | −67385 | −7907.6 | 1643.5 | 61.3 | −161.5 | 0.0 | −73750 | −7718.7 | 758.3 | −74446 | −74408 | 659 | −38 |
| $4d_{5/2}$ | −67242 | −7727.6 | 1592.7 | 44.5 | −157.4 | 0.0 | −73490 | −7546.1 | 732.8 | −74169 | −74128 | 638 | −41 |
| $5p_{1/2}$ | −62512 | −2982.0 | 572.4 | 37.8 | −30.7 | −0.1 | −64915 | −3000.4 | 309.5 | −65196 | −65249 | 334 | 53 |
| $5p_{3/2}$ | −61828 | −2844.0 | 544.3 | 27.9 | −31.3 | 0.1 | −64131 | −2860.7 | 294.4 | −64397 | −64447 | 317 | 50 |
| $5d_{3/2}$ | −34247 | −1689.5 | 334.5 | 15.6 | −37.5 | 0.0 | −35624 | −1489.2 | 159.7 | −35599 | −35678 | 54 | 79 |
| $5d_{5/2}$ | −34177 | −1660.5 | 326.5 | 11.5 | −37.0 | 0.0 | −35537 | −1467.9 | 155.4 | −35515 | −35591 | 54 | 76 |
| $4f_{5/2}$ | −27545 | −430.5 | 62.0 | 0.0 | −0.5 | 0.0 | −27914 | −460.6 | 46.4 | −27960 | −27972 | 58 | 13 |
| $4f_{7/2}$ | −27547 | −430.2 | 61.9 | 0.0 | −0.5 | 0.0 | −27915 | −460.1 | 46.3 | −27961 | −27972 | 57 | 11 |
| $5f_{5/2}$ | −17647 | −252.2 | 37.9 | 0.0 | −0.4 | 0.0 | −17862 | −270.9 | 27.0 | −17892 | −17898 | 36 | 7 |
| $5f_{7/2}$ | −17649 | −251.9 | 37.8 | 0.0 | −0.4 | 0.0 | −17863 | −270.4 | 26.9 | −17893 | −17898 | 35 | 6 |
| $6s_{1/2}$ | −39906 | −1552.4 | 351.6 | 15.5 | −19.5 | 0.6 | −41111 | −1427.7 | 172.4 | −41165 | −41227 | 117 | 63 |
| $6p_{1/2}$ | −32302 | −995.5 | 93.8 | 14.4 | −11.6 | 0.0 | −33201 | −968.6 | 48.9 | −33219 | −33194 | −6 | −24 |
| $6p_{3/2}$ | −32044 | −957.2 | 190.2 | 10.6 | −11.9 | 0.0 | −32812 | −931.7 | 99.8 | −32877 | −32906 | 94 | 29 |
| $6d_{3/2}$ | −20835 | −711.1 | 138.0 | 6.9 | −16.0 | 0.0 | −21417 | −630.0 | 67.0 | −21407 | −21441 | 24 | 34 |
| $6d_{5/2}$ | −20800 | −700.8 | 135.2 | 5.0 | −15.8 | 0.0 | −21376 | −622.5 | 65.4 | −21368 | −21401 | 24 | 33 |
| $6f_{5/2}$ | −12256 | −155.9 | 23.8 | 0.0 | −0.3 | 0.0 | −12388 | −167.7 | 16.7 | −12407 | −12411 | 22 | 3 |
| $6f_{7/2}$ | −12257 | −155.6 | 23.7 | 0.0 | −0.3 | 0.0 | −12389 | −167.3 | 16.6 | −12408 | −12411 | 22 | 3 |
| $7s_{1/2}$ | −23442 | −663.5 | 152.0 | 7.0 | −8.7 | 0.1 | −23955 | −601.0 | 73.8 | −23971 | −24000 | 45 | 29 |
| $7p_{1/2}$ | −19870 | −465.7 | 93.8 | 7.0 | −5.7 | 0.0 | −20241 | −448.0 | 48.9 | −20268 | −20319 | 78 | 51 |
| $7p_{3/2}$ | −19745 | −449.5 | 90.4 | 5.2 | −5.8 | 0.0 | −20105 | −432.6 | 47.0 | −20131 | −20170 | 66 | 39 |
| $7d_{3/2}$ | −14023 | −374.6 | 72.0 | 3.7 | −8.4 | 0.0 | −14331 | −333.1 | 35.3 | −14326 | −14343 | 12 | 17 |
| $7d_{5/2}$ | −14004 | −369.7 | 70.6 | 2.7 | −8.4 | 0.0 | −14308 | −329.5 | 34.5 | −14304 | −14321 | 12 | 16 |
| $7f_{5/2}$ | −9002 | −101.9 | 15.7 | 0.0 | −0.2 | 0.0 | −9089 | −109.8 | 10.9 | −9101 | −9103 | 14 | 1 |
| $7f_{7/2}$ | −9003 | −101.7 | 15.6 | 0.0 | −0.2 | 0.0 | −9089 | −109.5 | 10.8 | −9102 | −9103 | 14 | 1 |
| $8s_{1/2}$ | −15438 | −346.7 | 79.9 | 3.7 | −4.6 | 0.0 | −15706 | −312.0 | 38.6 | −15712 | −15727 | 21 | 15 |
| $8p_{1/2}$ | −13478 | −257.0 | 52.0 | 4.0 | −3.2 | 0.0 | −13682 | −245.8 | 27.0 | −13696 | | | |
| $8p_{3/2}$ | −13407 | −248.8 | 50.2 | 2.9 | −3.3 | 0.0 | −13606 | −237.9 | 26.0 | −13620 | −13652 | 46 | 33 |
| $8d_{3/2}$ | −10085 | −223.2 | 42.6 | 2.2 | −5.0 | 0.0 | −10268 | −198.8 | 21.0 | −10265 | −10275 | 7 | 10 |
| $8d_{5/2}$ | −10073 | −220.4 | 41.9 | 1.6 | −5.0 | 0.0 | −10255 | −196.8 | 20.6 | −10252 | −10262 | 7 | 9 |
| $8f_{5/2}$ | −6890 | −69.9 | 11.0 | 0.0 | −0.1 | 0.0 | −6949 | −75.3 | 7.6 | −6958 | −6958 | 9 | 0 |
| $8f_{7/2}$ | −6890 | −69.7 | 11.0 | 0.0 | −0.1 | 0.0 | −6949 | −75.1 | 7.6 | −6958 | −6958 | 9 | 0 |
| $9s_{1/2}$ | −10937 | −203.6 | 47.2 | 2.2 | −2.7 | 0.0 | −11094 | −183.2 | 22.8 | −11098 | −11107 | 12 | 8 |
| $9p_{1/2}$ | −9747 | −157.7 | 31.8 | 2.4 | −2.0 | 0.0 | −9872 | −149.8 | 16.5 | −9880 | | | |
| $9p_{3/2}$ | −9704 | −153.1 | 30.8 | 1.8 | −2.0 | 0.0 | −9826 | −145.2 | 15.9 | −9833 | | | |
| $9d_{3/2}$ | −7601 | −144.1 | 27.6 | 1.4 | −3.2 | 0.0 | −7720 | −128.5 | 13.7 | −7718 | −7724 | 4 | 6 |
| $9d_{5/2}$ | −7593 | −142.4 | 27.1 | 1.1 | −3.2 | 0.0 | −7711 | −127.3 | 13.4 | −7709 | −7715 | 4 | 6 |

Calculations of $E^{(2)}$ with $l_{\rm max} = 6$ and 8 yield $E^{(2)}(5s_{1/2}) = -5567.9$ and $-5595.3$ cm$^{-1}$, respectively. An extrapolation of these calculations yields $-5610.2$ and $-5611.2$ cm$^{-1}$, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(5s_{1/2})$ of 1.0 cm$^{-1}$. It should be noted that the 27.4 cm$^{-1}$ contribution from partial waves with $l > 6$ for the $5s$ state is the largest among all the states considered in Table I; smaller (about 4–6 cm$^{-1}$) contributions are obtained for the $4d$, $5p$, and $5d$ states and much smaller contributions (0.5–1.5 cm$^{-1}$) are obtained for the $n = 6$ states.

Owing to numerical complexity, we restrict $l \leqslant l_{\rm max} = 6$ in the $E^{\rm SD}$ calculation. As noted previously, the second-order contribution dominates $E^{\rm SD}$; therefore, we can use the extrapolated value of the $E^{(2)}$ described previously 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-order 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 $E^{(3)}_{\rm extra}$ in Table I, which accounts for that part of the third-order many-body perturbation theory (MBPT) energy missing from the SD expression for the energy, is smaller than $E^{(3)}$ by an order of magnitude for the states considered here.

The column labeled $\delta E^{\rm SD}$ in Table I gives the differences between our *ab initio* results and the available experimental values [37]. The SD results agree better with the recommended values than do the third-order MBPT results (the ratio of $\delta E^{(3)}/\delta E^{\rm SD}$ is about 10 for some of the cases), illustrating the importance of fourth and higher-order correlation corrections.

## III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN Sr II

### A. Electric-dipole matrix elements

The calculation of the transition-matrix elements provides another test of the quality of atomic-structure calculations and another measure of the size of the correlation corrections. Reduced electric-dipole matrix elements between low-lying states of Sr II calculated in the third-order RMBPT and in the all-order SD approximation are presented in Table II. We include only a limited number of transitions in this table to illustrate our results.

Our calculations of reduced matrix elements in the lowest, second, and third orders are carried out following the method described in Refs. [44,45]. The lowest-order DF values labeled $Z^{(\mathrm{DF})}$ are given in the third column of Table II. The values $Z^{(\mathrm{DF+2})}$ are obtained as the sum of the second-order correlation correction $Z^{(2)}$ and the DF matrix elements $Z^{(\mathrm{DF})}$. It should be noted that the second-order Breit corrections $B^{(2)}$ included in the $Z^{(\mathrm{DF+2})}$ terms are rather small in comparison with the second-order Coulomb corrections $Z^{(2)}$ [the ratio of $B^{(2)}$ to $Z^{(2)}$ is about 1–2%].

The third-order matrix elements $Z^{(\mathrm{DF+2+3})}$ include the DF values, the second-order $Z^{(2)}$ results, and the third-order $Z^{(3)}$ correlation correction. $Z^{(3)}$ includes random-phase-approximation (RPA) terms iterated to all orders, Brueckner orbitals (BO) corrections, the structural radiation $Z^{(\mathrm{SR})}$, and normalization $Z^{(\mathrm{NORM})}$ terms (see [46] for the definition of these terms).

The terms $Z^{(\mathrm{RPA})}$ and $Z^{(\mathrm{BO})}$ give the largest contributions to $Z^{(3)}$. The sum of the terms $Z^{(\mathrm{RPA})}$ and $Z^{(\mathrm{BO})}$ is about 10–20% of the $Z^{(\mathrm{DF})}$ term and they have a different sign for the $5s$-$5p$ and $4d$-$5p$ transitions. As a result, the values of $Z^{(\mathrm{DF+2+3})}$ became smaller than the $Z^{(\mathrm{DF})}$ value by 15–25%. The values of $Z^{(\mathrm{BO})}$ are larger than the values of $Z^{(\mathrm{RPA})}$ and have a different sign for the $5p$-$5d$ transitions. The structural radiation $Z^{(\mathrm{SR})}$ and normalization $Z^{(\mathrm{NORM})}$ terms are small. All results given in Table II are obtained using the length form of the matrix elements. The 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 these calculations.

The electric-dipole matrix elements evaluated in the all-order SD and single-double all-order method including partial triple excitations (SDpT [45]) approximations are given in the columns labeled $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ of Table II. The SD and SDpT matrix elements $Z^{(\mathrm{SD})}$ include $Z^{(3)}$ completely, along with the important fourth-order and higher-order corrections. The fourth-order corrections omitted from the SD matrix elements were discussed recently by [47]. The $Z^{(\mathrm{SD})}$ values are smaller than the $Z^{(\mathrm{DF+2})}$ values and larger than the $Z^{(\mathrm{DF+2+3})}$ values for some of the transitions given in Table II. The difference between the $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ values is about 0.1–0.2%.

To evaluate the uncertainties of our matrix-element values and to provide the recommended values, we carry out a semiempiriacal evaluation of the missing correlation corrections using the scaling procedure described in Ref. [48]. The correlation terms that are adjusted by this procedure are dominant for most of the transitions listed in Table II. We note that it is a rather complicated procedure that involves the scaling of valence excitation coefficients and a complete recalculation of the matrix elements. The scaling factors depend on the correlation energy given by the particular calculation. Therefore, the scaling factors are different for the SD and SDpT calculations, and these values have to be scaled separately. Generally, scaled SD and SDpT values are close together, as expected. The corresponding results are listed in Table II with the subscript "sc" [3,49]. We chose the SD scaled values as final (see Ref. [48] and references therein for a discussion of the selection of the final values). We estimate the uncertainty of these values as the maximum difference between the $Z_{\mathrm{sc}}^{(\mathrm{SD})}$ result and the other three results obtained in the SD, SDpT, and $\mathrm{SDpT_{sc}}$ approximations. The last column of Table II gives the uncertainties in percent relative to the final values $Z^{(\mathrm{final})}$. We find that the uncertainties are 0.2–0.5% for most of the transitions. Larger uncertainties (1.2–1.5%) occur for the $4d_j$-$5p_{j'}$ and $4d_j$-$4f_{j'}$ transitions. Our final results and their uncertainties are used to calculate the recommended values for lifetimes and polarizabilities and evaluate the uncertainties of these results.

### B. Transition rates, oscillator strengths, and line strengths in Sr II

Transition rates $A_r(s^{-1})$, oscillator strengths ($f$), and line strengths $S$ (a.u.) for the $ns$-$n_1p_j$, $n_1p_j$-$n_2d_{j'}$, and $n_2d_j$-$n_3f_{j'}$ ($n = 5$–9, $n_1 = 5$–8, $n_2 = 4$–7, and $n_3 = 4$–5) transitions in Sr II calculated in the SD scaled approximation are summarized in Table III. We use the available, recommended NIST energies [37] or SD energies given in Table I in the calculation of the transition rates $A_r$ and oscillator strengths $f$. In Table III, we divide the transitions into groups according to the initial state for a better presentation. The relative uncertainties of the transition rates, oscillator strengths, and line strengths are double those of the corresponding matrix elements as all these properties depend on the square of the matrix elements. The uncertainties in percent are listed in the column labeled "Unc."

We present the $ns$-$n_1p_j$, $n_1p_j$-$n_2d_{j'}$, and $n_2d_j$-$n_3f_{j'}$ transitions with $n = 5$–9, $n_1 = 5$–8, $n_2 = 4$–7, and $n_3 = 4$–5. In all these cases, we check the quality of our functions created in the $R = 220$ a.u. cavity with $N = 70$ splines by comparing the $nl_j$-$nl'_{j'}$ dipole matrix elements evaluated using the B-spline basis set orbitals and directly obtained DF values.

Using transition rates $A$ given in Table III, we calculate the values of the branching ratios of the $5p\ ^2P_{3/2}$ and $5p\ ^2P_{1/2}$ decays of $Sr^+$. Our value of branching ratios $A(P_{3/2}\text{-}S_{1/2})/\sum_J A(P_{3/2}\text{-}D_J)$ and $A(P_{1/2}\text{-}S_{1/2})/\sum_J A(P_{1/2}\text{-}D_J)$ are equal to 15.96 and 17.30, respectively. The results of branching ratios $A(P_{3/2}\text{-}S_{1/2})/\sum_J A(P_{3/2}\text{-}D_J)$ and $A(P_{1/2}\text{-}S_{1/2})/\sum_J A(P_{1/2}\text{-}D_J)$ from measurements given by Gallagher [16] are $14.8 \pm 2.5$ and $13.4 \pm 2$. Our SD value for the $A(P_{3/2}\text{-}S_{1/2})/\sum_J A(P_{3/2}\text{-}D_J)$ agree with the results from Ref. [16] when uncertainties are taken into account, while our SD value for the $A(P_{1/2}\text{-}S_{1/2})/\sum_J A(P_{1/2}\text{-}D_J)$ branching ratios rather disagree with the measurements [16].

In Table IV, the SD and SDpT oscillator strengths ($f$) are compared with the available experimental [16,50] and theoretical [23–25] results. Relativistic single-configuration

TABLE II. Reduced electric-dipole matrix elements calculated to first-order, second-order, third-order, SD, and SDpT methods; the label "sc" indicates the scaled values. Final results and their uncertainties are given in the [$Z^{(\mathrm{final})}$] column. The last column gives uncertainties in percent relative to the final values.

| Transition | | $Z^{(\mathrm{DF})}$ | $Z^{(\mathrm{DF+2})}$ | $Z^{(\mathrm{DF+2+3})}$ | $Z^{(\mathrm{SD})}$ | $Z^{(\mathrm{SDpT})}$ | $Z_{\mathrm{sc}}^{(\mathrm{SD})}$ | $Z_{\mathrm{sc}}^{(\mathrm{SDpT})}$ | $Z^{(\mathrm{final})}$ | Unc. (%) |
|---|---|---|---|---|---|---|---|---|---|---|
| $6s_{1/2}$ | $5p_{1/2}$ | 2.375 1 | 2.419 9 | 2.342 2 | 2.321 1 | 2.327 5 | 2.331 0 | 2.328 4 | 2.331(10) | 0.43 |
| $6s_{1/2}$ | $5p_{3/2}$ | 3.497 2 | 3.553 4 | 3.457 0 | 3.425 5 | 3.433 5 | 3.437 2 | 3.433 6 | 3.437(12) | 0.34 |
| $6s_{1/2}$ | $6p_{1/2}$ | 6.810 3 | 6.715 8 | 6.475 0 | 6.517 1 | 6.539 3 | 6.530 2 | 6.528 0 | 6.530(22) | 0.34 |
| $6s_{1/2}$ | $6p_{3/2}$ | 9.577 5 | 9.447 9 | 9.100 5 | 9.161 9 | 9.193 9 | 9.181 5 | 9.178 3 | 9.181(32) | 0.35 |
| $7s_{1/2}$ | $5p_{1/2}$ | 0.640 4 | 0.663 8 | 0.642 8 | 0.640 0 | 0.641 1 | 0.640 0 | 0.641 3 | 0.640(1) | 0.17 |
| $7s_{1/2}$ | $5p_{3/2}$ | 0.920 2 | 0.950 0 | 0.921 6 | 0.918 0 | 0.919 5 | 0.917 8 | 0.919 7 | 0.918(1) | 0.16 |
| $7s_{1/2}$ | $6p_{1/2}$ | 4.859 8 | 4.889 9 | 4.787 5 | 4.758 3 | 4.769 1 | 4.772 3 | 4.767 7 | 4.772(14) | 0.29 |
| $7s_{1/2}$ | $6p_{3/2}$ | 7.119 7 | 7.156 5 | 7.033 2 | 6.989 5 | 7.002 9 | 7.004 6 | 6.998 5 | 7.005(15) | 0.22 |
| $7s_{1/2}$ | $7p_{1/2}$ | 11.152 6 | 11.110 0 | 10.794 7 | 10.852 9 | 10.881 3 | 10.889 1 | 10.885 3 | 10.889(36) | 0.33 |
| $7s_{1/2}$ | $7p_{3/2}$ | 15.652 4 | 15.595 3 | 15.136 6 | 15.222 1 | 15.263 2 | 15.268 3 | 15.262 9 | 15.268(46) | 0.30 |
| $8s_{1/2}$ | $6p_{1/2}$ | 1.193 1 | 1.210 5 | 1.177 9 | 1.178 4 | 1.180 9 | 1.178 5 | 1.180 8 | 1.178(2) | 0.21 |
| $8s_{1/2}$ | $6p_{3/2}$ | 1.699 0 | 1.721 8 | 1.675 7 | 1.677 3 | 1.680 8 | 1.677 4 | 1.680 7 | 1.677(4) | 0.21 |
| $8s_{1/2}$ | $7p_{1/2}$ | 8.078 2 | 8.103 1 | 7.981 7 | 7.935 5 | 7.949 7 | 7.880 5 | 7.873 2 | 7.880(55) | 0.69 |
| $8s_{1/2}$ | $7p_{3/2}$ | 11.806 1 | 11.836 5 | 11.693 6 | 11.627 2 | 11.644 6 | 11.572 2 | 11.562 5 | 11.572(55) | 0.47 |
| $9s_{1/2}$ | $6p_{1/2}$ | 0.622 3 | 0.636 8 | 0.617 5 | 0.618 3 | 0.619 4 | 0.618 1 | 0.619 4 | 0.618(1) | 0.02 |
| $9s_{1/2}$ | $6p_{3/2}$ | 0.881 0 | 0.900 5 | 0.872 5 | 0.874 2 | 0.875 8 | 0.874 1 | 0.875 9 | 0.874(2) | 0.01 |
| $9s_{1/2}$ | $7p_{1/2}$ | 1.885 8 | 1.903 6 | 1.855 3 | 1.858 4 | 1.862 0 | 1.858 6 | 1.862 4 | 1.859(4) | 0.20 |
| $9s_{1/2}$ | $7p_{3/2}$ | 2.673 4 | 2.698 9 | 2.627 9 | 2.633 7 | 2.638 9 | 2.635 3 | 2.640 7 | 2.635(5) | 0.20 |
| $4d_{3/2}$ | $5p_{1/2}$ | 3.729 2 | 3.477 9 | 2.978 5 | 3.083 0 | 3.119 3 | 3.111 9 | 3.101 7 | 3.112(36) | 1.18 |
| $4d_{3/2}$ | $5p_{3/2}$ | 1.657 2 | 1.549 3 | 1.321 7 | 1.369 4 | 1.385 8 | 1.382 5 | 1.377 9 | 1.382(16) | 1.20 |
| $4d_{5/2}$ | $5p_{3/2}$ | 5.002 5 | 4.677 6 | 4.011 5 | 4.149 7 | 4.197 7 | 4.186 8 | 4.173 2 | 4.187(48) | 1.16 |
| $5d_{3/2}$ | $6p_{1/2}$ | 9.087 2 | 9.022 6 | 8.446 1 | 8.559 3 | 8.596 5 | 8.555 9 | 8.549 3 | 8.556(37) | 0.43 |
| $5d_{3/2}$ | $6p_{3/2}$ | 4.036 8 | 4.010 2 | 3.746 2 | 3.798 5 | 3.815 4 | 3.797 1 | 3.794 1 | 3.797(17) | 0.45 |
| $5d_{5/2}$ | $6p_{3/2}$ | 12.163 8 | 12.080 5 | 11.306 6 | 11.457 3 | 11.507 0 | 11.451 0 | 11.442 1 | 11.451(50) | 0.43 |
| $6d_{3/2}$ | $6p_{1/2}$ | 7.125 9 | 7.117 1 | 7.270 8 | 7.155 9 | 7.163 0 | 7.202 9 | 7.197 4 | 7.203(47) | 0.66 |
| $6d_{3/2}$ | $6p_{3/2}$ | 3.297 2 | 3.290 5 | 3.367 7 | 3.315 9 | 3.318 3 | 3.334 8 | 3.332 5 | 3.335(19) | 0.57 |
| $6d_{5/2}$ | $6p_{3/2}$ | 9.821 6 | 9.806 0 | 10.019 3 | 9.870 2 | 9.878 8 | 9.930 5 | 9.923 4 | 9.930(60) | 0.61 |
| $6d_{3/2}$ | $7p_{1/2}$ | 16.063 1 | 16.038 4 | 15.335 0 | 15.457 9 | 15.504 8 | 15.474 5 | 15.466 4 | 15.474(47) | 0.30 |
| $6d_{3/2}$ | $7p_{3/2}$ | 7.138 7 | 7.129 3 | 6.805 5 | 6.862 6 | 6.884 1 | 6.867 5 | 6.863 9 | 6.867(22) | 0.31 |
| $6d_{5/2}$ | $7p_{3/2}$ | 21.493 4 | 21.461 0 | 20.512 4 | 20.676 7 | 20.739 7 | 20.687 7 | 20.677 0 | 20.688(63) | 0.30 |
| $7d_{3/2}$ | $6p_{1/2}$ | 2.421 3 | 2.406 9 | 2.372 2 | 2.363 5 | 2.368 4 | 2.365 1 | 2.369 6 | 2.365(5) | 0.21 |
| $7d_{3/2}$ | $6p_{3/2}$ | 1.093 2 | 1.085 8 | 1.068 3 | 1.065 0 | 1.067 3 | 1.065 4 | 1.067 4 | 1.065(2) | 0.21 |
| $7d_{5/2}$ | $6p_{3/2}$ | 3.277 3 | 3.255 8 | 3.205 4 | 3.195 3 | 3.202 0 | 3.196 7 | 3.202 7 | 3.197(7) | 0.21 |
| $7d_{3/2}$ | $7p_{1/2}$ | 10.450 3 | 10.456 0 | 10.697 3 | 10.551 8 | 10.559 5 | 10.515 2 | 10.504 7 | 10.515(37) | 0.35 |
| $7d_{3/2}$ | $7p_{3/2}$ | 4.847 1 | 4.847 1 | 4.970 0 | 4.902 5 | 4.904 7 | 4.896 4 | 4.892 0 | 4.896(6) | 0.12 |
| $7d_{5/2}$ | $7p_{3/2}$ | 14.423 9 | 14.430 0 | 14.771 3 | 14.577 8 | 14.586 5 | 14.566 2 | 14.553 1 | 14.566(12) | 0.08 |
| $7d_{3/2}$ | $8p_{1/2}$ | 24.719 1 | 24.709 4 | 23.856 3 | 23.999 4 | 24.057 1 | 24.024 9 | 24.014 4 | 24.025(58) | 0.24 |
| $7d_{3/2}$ | $8p_{3/2}$ | 10.988 8 | 10.985 9 | 10.591 6 | 10.658 2 | 10.684 8 | 10.677 3 | 10.672 5 | 10.677(27) | 0.25 |
| $7d_{5/2}$ | $8p_{3/2}$ | 33.070 4 | 33.057 2 | 31.902 3 | 32.094 1 | 32.171 8 | 32.144 0 | 32.129 9 | 32.144(78) | 0.24 |
| $4d_{3/2}$ | $4f_{5/2}$ | 3.579 3 | 3.403 4 | 2.716 2 | 2.878 5 | 2.921 6 | 2.916 5 | 2.900 6 | 2.916(43) | 1.50 |
| $4d_{5/2}$ | $4f_{5/2}$ | 0.964 1 | 0.916 7 | 0.737 3 | 0.779 2 | 0.790 4 | 0.788 7 | 0.784 6 | 0.789(11) | 1.44 |
| $4d_{5/2}$ | $4f_{7/2}$ | 4.312 9 | 4.100 5 | 3.298 3 | 3.485 8 | 3.536 0 | 3.527 8 | 3.509 2 | 3.528(50) | 1.44 |
| $5d_{3/2}$ | $4f_{5/2}$ | 12.730 0 | 12.619 7 | 12.211 4 | 12.194 3 | 12.237 7 | 12.209 6 | 12.205 5 | 12.210(43) | 0.36 |
| $5d_{5/2}$ | $4f_{5/2}$ | 3.406 3 | 3.376 7 | 3.269 0 | 3.264 3 | 3.275 8 | 3.268 2 | 3.267 1 | 3.268(11) | 0.35 |
| $5d_{5/2}$ | $4f_{7/2}$ | 15.231 9 | 15.100 0 | 14.618 9 | 14.597 6 | 14.648 8 | 14.615 7 | 14.610 8 | 14.616(51) | 0.35 |
| $6d_{3/2}$ | $4f_{5/2}$ | 5.917 8 | 5.937 7 | 6.376 8 | 6.198 3 | 6.187 0 | 6.227 3 | 6.222 0 | 6.227(29) | 0.47 |
| $6d_{5/2}$ | $4f_{5/2}$ | 1.568 4 | 1.574 5 | 1.688 1 | 1.641 6 | 1.638 9 | 1.650 0 | 1.648 6 | 1.650(8) | 0.51 |
| $6d_{5/2}$ | $4f_{7/2}$ | 7.011 1 | 7.038 1 | 7.546 8 | 7.339 5 | 7.326 8 | 7.378 6 | 7.372 4 | 7.379(39) | 0.53 |
| $7d_{3/2}$ | $4f_{5/2}$ | 1.249 0 | 1.267 0 | 1.251 5 | 1.238 6 | 1.242 0 | 1.240 2 | 1.242 5 | 1.240(3) | 0.28 |
| $7d_{5/2}$ | $4f_{5/2}$ | 0.333 3 | 0.338 1 | 0.334 4 | 0.330 9 | 0.331 8 | 0.331 4 | 0.332 0 | 0.331(1) | 0.27 |
| $7d_{5/2}$ | $4f_{7/2}$ | 1.490 1 | 1.511 7 | 1.495 1 | 1.479 4 | 1.483 4 | 1.481 7 | 1.484 4 | 1.482(4) | 0.27 |

TABLE III. Wavelengths λ (Å), transition rates $A_r$ ($s^{-1}$), oscillator strengths ($f$), and line strengths $S$ (a.u.) for transitions in Sr II calculated using our "final" values of reduced electric-dipole matrix elements [$Z^{(\mathrm{final})}$] and their uncertainties. The uncertainties in column "Unc." are given in percent. Numbers in brackets represent powers of 10 here and in the following tables.

| Transition | | λ | $A_r$ | $f$ | $S$ | Unc. | Transition | | λ | $A_r$ | $f$ | $S$ | Unc. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $5p_{1/2}$ | $6s_{1/2}$ | 4163.0 | 7.63[7] | 1.98[−1] | 5.43[ 0] | 0.85 | $5p_{3/2}$ | $5d_{3/2}$ | 3475.9 | 4.72[7] | 8.54[−2] | 3.91[ 0] | 1.09 |
| $5p_{3/2}$ | $6s_{1/2}$ | 4306.6 | 1.50[8] | 2.08[−1] | 1.18[ 1] | 0.68 | $5p_{3/2}$ | $5d_{5/2}$ | 3465.4 | 2.82[8] | 7.63[−1] | 3.48[ 1] | 1.15 |
| $5p_{1/2}$ | $7s_{1/2}$ | 2424.3 | 2.91[7] | 2.57[−2] | 4.10[−1] | 0.40 | $5p_{1/2}$ | $5d_{3/2}$ | 3381.7 | 2.41[8] | 8.26[−1] | 1.84[ 1] | 1.23 |
| $5p_{3/2}$ | $7s_{1/2}$ | 2472.3 | 5.65[7] | 2.59[−2] | 8.42[−1] | 0.41 | $5p_{3/2}$ | $6d_{3/2}$ | 2325.2 | 1.50[7] | 1.22[−2] | 3.72[−1] | 1.06 |
| $5p_{1/2}$ | $8s_{1/2}$ | 2019.3 | 1.50[7] | 9.14[−3] | 1.22[−1] | 0.44 | $5p_{3/2}$ | $6d_{5/2}$ | 2323.1 | 9.08[7] | 1.10[−1] | 3.37[ 0] | 1.04 |
| $5p_{3/2}$ | $8s_{1/2}$ | 2052.5 | 2.89[7] | 9.13[−3] | 2.47[−1] | 0.45 | $5p_{1/2}$ | $6d_{3/2}$ | 2282.7 | 7.90[7] | 1.23[−1] | 1.86[ 0] | 0.98 |
| $5p_{1/2}$ | $9s_{1/2}$ | 1847.0 | 8.76[6] | 4.48[−3] | 5.45[−2] | 0.45 | $5p_{3/2}$ | $7d_{3/2}$ | 1995.8 | 6.93[6] | 4.14[−3] | 1.09[−1] | 1.57 |
| $5p_{3/2}$ | $9s_{1/2}$ | 1874.7 | 1.69[7] | 4.46[−3] | 1.10[−1] | 0.45 | $5p_{3/2}$ | $7d_{5/2}$ | 1995.0 | 4.21[7] | 3.77[−2] | 9.90[−1] | 1.57 |
| $6p_{1/2}$ | $7s_{1/2}$ | 10876.2 | 1.79[7] | 3.18[−1] | 2.28[ 1] | 0.58 | $5p_{1/2}$ | $7d_{3/2}$ | 1964.4 | 3.70[7] | 4.28[−2] | 5.53[−1] | 1.49 |
| $6p_{3/2}$ | $7s_{1/2}$ | 11228.1 | 3.51[7] | 3.32[−1] | 4.91[ 1] | 0.43 | $6p_{3/2}$ | $6d_{3/2}$ | 8722.2 | 8.49[6] | 9.68[−2] | 1.11[ 1] | 1.13 |
| $6p_{1/2}$ | $8s_{1/2}$ | 5725.0 | 7.50[6] | 3.68[−2] | 1.39[ 0] | 0.40 | $6p_{3/2}$ | $6d_{5/2}$ | 8691.7 | 5.07[7] | 8.62[−1] | 9.86[ 1] | 1.21 |
| $6p_{3/2}$ | $8s_{1/2}$ | 5821.0 | 1.45[7] | 3.67[−2] | 2.81[ 0] | 0.41 | $6p_{1/2}$ | $6d_{3/2}$ | 8508.3 | 4.27[7] | 9.26[−1] | 5.19[ 1] | 1.30 |
| $6p_{1/2}$ | $9s_{1/2}$ | 4527.4 | 4.17[6] | 1.28[−2] | 3.82[−1] | 0.42 | $6p_{3/2}$ | $7d_{3/2}$ | 5386.9 | 3.68[6] | 1.60[−2] | 1.14[ 0] | 0.36 |
| $6p_{3/2}$ | $9s_{1/2}$ | 4587.2 | 8.02[6] | 1.26[−2] | 7.64[−1] | 0.42 | $6p_{3/2}$ | $7d_{5/2}$ | 5380.6 | 2.22[7] | 1.44[−1] | 1.02[ 1] | 0.33 |
| $7p_{1/2}$ | $8s_{1/2}$ | 21777.5 | 6.09[6] | 4.33[−1] | 6.21[ 1] | 1.40 | $6p_{1/2}$ | $7d_{3/2}$ | 5304.6 | 1.90[7] | 1.60[−1] | 5.59[ 0] | 0.28 |
| $7p_{3/2}$ | $8s_{1/2}$ | 22504.8 | 1.19[7] | 4.52[−1] | 1.34[ 2] | 0.95 | $7p_{3/2}$ | $7d_{3/2}$ | 17159.4 | 2.40[6] | 1.06[−1] | 2.40[ 1] | 0.34 |
| $7p_{1/2}$ | $9s_{1/2}$ | 10855.1 | 2.74[6] | 4.83[−2] | 3.45[ 0] | 0.37 | $7p_{3/2}$ | $7d_{5/2}$ | 17095.5 | 1.43[7] | 9.42[−1] | 2.12[ 2] | 0.28 |
| $7p_{3/2}$ | $9s_{1/2}$ | 11032.8 | 5.24[6] | 4.78[−2] | 6.94[ 0] | 0.28 | $7p_{1/2}$ | $7d_{3/2}$ | 16733.3 | 1.20[7] | 1.00[ 0] | 1.11[ 2] | 0.85 |
| $8p_{1/2}$ | $9s_{1/2}$ | 38619.4 | 2.44[6] | 5.46[−1] | 1.39[ 2] | 1.34 | | | | | | | |
| $8p_{3/2}$ | $9s_{1/2}$ | 39281.9 | 4.94[6] | 5.71[−1] | 2.95[ 2] | 1.97 | $5s_{1/2}$ | $5p_{1/2}$ | 4216.7 | 1.29[8] | 3.44[−1] | 9.55[ 0] | 0.80 |
| | | | | | | | $5s_{1/2}$ | $5p_{3/2}$ | 4078.9 | 1.42[8] | 7.11[−1] | 1.91[ 1] | 0.81 |
| $4d_{3/2}$ | $5p_{1/2}$ | 10917.9 | 7.54[6] | 6.74[−2] | 9.68[ 0] | 1.84 | $6s_{1/2}$ | $6p_{1/2}$ | 12448.4 | 2.24[7] | 5.20[−1] | 4.26[ 1] | 0.40 |
| $4d_{5/2}$ | $5p_{3/2}$ | 10330.2 | 8.05[6] | 8.59[−2] | 1.75[ 1] | 1.76 | $6s_{1/2}$ | $6p_{3/2}$ | 12017.3 | 2.46[7] | 1.07[ 0] | 8.43[ 1] | 0.43 |
| $4d_{3/2}$ | $5p_{3/2}$ | 10039.5 | 9.57[5] | 1.45[−2] | 1.91[ 0] | 1.89 | $7s_{1/2}$ | $7p_{1/2}$ | 27165.8 | 5.99[6] | 6.63[−1] | 1.19[ 2] | 0.66 |
| $5d_{3/2}$ | $6p_{1/2}$ | 40267.5 | 1.14[6] | 1.38[−1] | 7.32[ 1] | 0.95 | $7s_{1/2}$ | $7p_{3/2}$ | 26113.1 | 6.63[6] | 1.36[ 0] | 2.33[ 2] | 0.60 |
| $5d_{5/2}$ | $6p_{3/2}$ | 37244.9 | 1.29[6] | 1.78[−1] | 1.31[ 2] | 0.98 | $8s_{1/2}$ | $8p_{1/2}$ | 49236.1 | 2.24[6] | 8.14[−1] | 2.64[ 2] | 0.67 |
| $5d_{3/2}$ | $6p_{3/2}$ | 36080.4 | 1.55[5] | 3.03[−2] | 1.44[ 1] | 0.97 | $8s_{1/2}$ | $8p_{3/2}$ | 48199.7 | 2.35[6] | 1.63[ 0] | 5.19[ 2] | 0.88 |
| $6d_{3/2}$ | $7p_{1/2}$ | 89100.4 | 3.43[5] | 2.04[−1] | 2.39[ 2] | 0.39 | | | | | | | |
| $6d_{5/2}$ | $7p_{3/2}$ | 81271.1 | 4.04[5] | 2.67[−1] | 4.28[ 2] | 0.50 | $4f_{5/2}$ | $6d_{3/2}$ | 15311.2 | 5.47[6] | 1.28[−1] | 3.88[ 1] | 0.93 |
| $6d_{3/2}$ | $7p_{3/2}$ | 78694.9 | 4.90[4] | 4.55[−2] | 4.72[ 1] | 0.48 | $4f_{7/2}$ | $6d_{5/2}$ | 15217.3 | 5.22[6] | 1.36[−1] | 5.44[ 1] | 1.06 |
| $7d_{3/2}$ | $8p_{1/2}$ | 154600.1 | 1.58[5] | 2.84[−1] | 5.77[ 2] | 0.21 | $4f_{5/2}$ | $6d_{5/2}$ | 15217.3 | 2.61[5] | 9.06[−3] | 2.72[ 0] | 1.01 |
| $7d_{5/2}$ | $8p_{3/2}$ | 149543.9 | 1.56[5] | 3.50[−1] | 1.03[ 3] | 0.31 | $4f_{5/2}$ | $7d_{3/2}$ | 7337.0 | 1.97[6] | 1.06[−2] | 1.54[ 0] | 0.27 |
| $7d_{3/2}$ | $8p_{3/2}$ | 144822.6 | 1.90[4] | 5.98[−2] | 1.14[ 2] | 0.36 | $4f_{7/2}$ | $7d_{5/2}$ | 7325.3 | 1.89[6] | 1.14[−2] | 2.20[ 0] | 0.31 |
| | | | | | | | $4f_{5/2}$ | $7d_{5/2}$ | 7325.3 | 9.43[4] | 7.59[−4] | 1.10[−1] | 0.30 |
| $4d_{3/2}$ | $4f_{5/2}$ | 2153.5 | 2.88[8] | 3.00[−1] | 8.51[ 0] | 2.59 | $5f_{5/2}$ | $7d_{3/2}$ | 28125.4 | 3.37[6] | 2.66[−1] | 1.48[ 2] | 0.89 |
| $4d_{5/2}$ | $4f_{5/2}$ | 2166.6 | 2.07[7] | 1.45[−2] | 6.22[−1] | 2.39 | $5f_{5/2}$ | $7d_{5/2}$ | 27954.0 | 1.60[5] | 1.88[−2] | 1.04[ 1] | 0.99 |
| $4d_{5/2}$ | $4f_{7/2}$ | 2166.6 | 3.10[8] | 2.91[−1] | 1.24[ 1] | 2.37 | $5f_{7/2}$ | $7d_{5/2}$ | 27954.0 | 3.21[6] | 2.82[−1] | 2.08[ 2] | 1.05 |

Hartree-Fock oscillator strengths were presented by Migdalek and Baylis [23]. The effect of polarization of the ion core by the valence electron was included by introducing a polarization potential in the one-electron Hamiltonian and by employing the corresponding correction for the dipole-moment operator in the transition-matrix elements [23]. The radiative transition probabilities and ion wave functions were obtained with the atomic structure code SUPERSTRUCTURE [24]. The configuration interaction (CI) expansion employed includes the electron configurations $4s^24p^6nl$, $4s^24p^5nln'l'$, and $4s4p^6nln'l'$ with $n = 4-6$, $n' = 4-6$ [24]. The oscillator strengths of the resonance transitions in Sr II calculated by the DF method were recently presented by Zilitis in Ref. [25]. The author underlined that the core polarization in [25] was neglected because the corresponding values are unavailable in the literature. It can be seen from the comparison of the results listed in Table IV that our $f^{(\mathrm{SD})}$ and $f^{(\mathrm{SDpT})}$ values agree with $f^{(\mathrm{theor})}$ results from Refs. [23,24] and disagree with the result from Ref. [25]. This disagreement is explained by the large contribution of correlation effects that were omitted in [25]. Our results are in good agrement with the experimental values presented by Volz and Schmoranzer [50]. Measurements of the $4d$-$5p$ oscillator strengths given in [16] have large uncertainties.

Averaged-over-$j$ oscillator strengths evaluated by the SD method in the Sr II ion are listed in Table V for the $5s$-$np$, $6s$-$np$, $5p$-$ns$, $5p$-$nd$, $6p$-$ns$, $6p$-$nd$, $4d$-$np$, $4d$-$nf$, $5d$-$np$, and $5d$-$nf$ with a large number of $n$ up to $n = 10$.

Our averaged-over-$j$ oscillator strengths evaluated by the SD and SDpT methods are compared with the theoretical results from Ref. [5] in Table VI. It should be noted that the nonrelativisic approach was used in Ref. [5] to evaluate oscillator strengths. The wave functions and transition-matrix elements by Mitroy *et al.* were obtained by diagonalizing the semiempiriacal Hamiltonian in a large, mixed Laguerre-type

TABLE IV. The SD and SDpT oscillator strengths ($f$) are compared with experimental (expt) and theoretical (theor) results.

| Transitions | | $f^{(SD)}$ | $f^{(SDpT)}$ | $f^{(expt)}$ | $f^{(theor)}$ |
|---|---|---|---|---|---|
| $5s_{1/2}$ | $5p_{1/2}$ | 0.3413 | 0.3454 | 0.342 [50] | 0.344 [23] |
| $5s_{1/2}$ | $5p_{3/2}$ | 0.704 8 | 0.713 3 | 0.696 [50] | 0.696 [23] |
| $4d_{5/2}$ | $5p_{3/2}$ | 0.084 4 | 0.086 4 | 0.096(0.02) [16] | 0.084 [24] |
| $4d_{3/2}$ | $5p_{3/2}$ | 0.014 2 | 0.014 5 | 0.016(0.03) [16] | 0.015 [24] |
| $4d_{3/2}$ | $5p_{1/2}$ | 0.066 1 | 0.067 7 | 0.084(0.015) [16] | 0.062 [24] |
| $4d_{3/2}$ | $4f_{5/2}$ | 0.292 2 | 0.301 0 | | 0.384 [25] |

orbital (LTO) and Slater-type orbital (STO) basis set. The difference between our SD and SDpT oscillator strengths and the results from Ref. [5] is about 1–3% except for two transitions ($5s$-$6p$ and $4d$-$6p$) with very small values of oscillator strengths. The difference in oscillator strengths calculated by different methods is due to the large contribution of correlation effects.

### C. Lifetimes in Sr II

We calculate the lifetimes of the $ns_{1/2}$ ($n = 6$–7), $np_j$ ($n = 5$–6), $nd_j$ ($n = 4$–5), and $nf_j$ ($n = 4$) states in Sr II using the SD, SDpT, and corresponding scaled values for the dipole matrix elements and NIST energies [37] that were available or SD energies otherwise. We list lifetimes from these four different calculations, SD, SDpT, $SD_{sc}$, and $SDpT_{sc}$, in columns with corresponding labels in Table VII. As in the case of the electric-dipole matrix elements, scaled SD values are taken as final. We estimate the uncertainty of our final values as the maximum difference between the final result and the other three results obtained in SD, SDpT, and $SDpT_{sc}$ approximations. The final values, $\tau^{\text{final}}$ are compared with the available experimental [20] and theoretical [2] results. The calculation in Ref. [2] was performed by the Hartree-Fock method including relativistic effects and core polarization. It should be seen from Table VII that the largest difference between our SD and SDpT results and the results from [2] is for the $6p_{1/2}$ and $6p_{3/2}$ lifetimes. However, the lifetimes from [2] for these levels coincide with our $\tau^{(DF)}$ values given in the second column of Table VII. This agreement underlines the importance of correlation correction since the difference between $\tau^{(DF)}$ and $\tau^{(SD)}$ is about 10%.

TABLE VI. Averaged-over-$j$ oscillator strengths evaluated by SD and SDpT methods are compared with theoretical results from Ref. [5] in Sr II ion.

| Transitions | $f^{(SD)}$ | $f^{(SDpT)}$ | $f^{(theor)}$ |
|---|---|---|---|
| $5s$-$5p$ | 1.046 1 | 1.058 7 | 1.026 2 |
| $5s$-$6p$ | 1.507[−4] | 1.476[−4] | 4.02[−5] |
| $6s$-$6p$ | 1.579 2 | 1.589 7 | |
| $5p$-$6s$ | 0.203 4 | 0.204 5 | 0.207 5 |
| $5p$-$5d$ | 0.830 9 | 0.833 1 | 0.833 9 |
| $5p$-$6d$ | 0.123 2 | 0.124 1 | |
| $4d$-$5p$ | 0.082 0 | 0.084 7 | 0.0823 3 |
| $4d$-$6p$ | 3.621[−4] | 2.995[−4] | 8.45[−5] |
| $5d$-$6p$ | 0.174 5 | 0.176 0 | |
| $4d$-$4f$ | 0.295 8 | 0.304 5 | 0.303 8 |
| $5d$-$4f$ | 0.866 6 | 0.872 7 | 0.851 9 |

In Table VIII, we list lifetimes of the $4d_j$ states in Sr II. The SD [$\tau^{(SD)}$], SDpT [$\tau^{(SDpT)}$], SD-scaled [$\tau^{(SD_{sc})}$], and SDpT-scaled [$\tau^{(SDpT_{sc})}$] values are compared with the theoretical [3,4] values and experimental results given by Biémont *et al.* [2]. There are some small contributions to the lifetime values given in Table VIII, such as the Breit interaction and the contribution from high partial waves. The effect of the Breit interaction to the values of the electric-quadrupole matrix elements in the Ca II ion was investigated in Ref. [51]. The Breit interaction arises from the exchange of a virtual photon between atomic electrons. Following the procedure described in [51], we find that the second-order electric-quadrupole matrix elements in Sr II increase by 0.024 608 and 0.023 920 a.u. for the $5s_{1/2}$-$4d_{3/2}$ and $5s_{1/2}$-$4d_{5/2}$ matrix elements, respectively. Those contributions lead to the decreasing of the $4d_{3/2}$ and $4d_{5/2}$ lifetimes by 0.001 229 and 0.000 875 s, respectively.

The magnetic-dipole $4d_{3/2}$-$4d_{5/2}$ transition gives an additional contribution (0.000 238 s) to the $4d_{5/2}$ lifetime [9]. Recently, Safronova *et al.* [52] considered two-photon $5s$-$np$-$4d$ transitions. It was found that contributions of these transitions to the $4d_{3/2}$ and $4d_{5/2}$ lifetimes are equal to 0.000 705 and 0.000 761 s, respectively. As a result, we find additional contributions from the previously mentioned effects are equal to −0.000 52 and 0.000 12 s for the $4d_{3/2}$ and $4d_{5/2}$ lifetimes, respectively. Following the procedure described in Ref. [3], we estimate the uncertainties using the $\tau^{(SD)}$, $\tau^{(SDpT)}$, $\tau^{(SD_{sc})}$, and $\tau^{(SDpT_{sc})}$ values. Final values for the $4d_{3/2}$ and $4d_{5/2}$ lifetimes

TABLE V. Averaged-over-$j$ oscillator strengths evaluated by SD method in Sr II ion.

| Transitions | $n = 4$ | $n = 5$ | $n = 6$ | $n = 7$ | $n = 8$ | $n = 9$ | $n = 10$ |
|---|---|---|---|---|---|---|---|
| $5s$-$np$ | | 1.046[0] | 1.507[−4] | 6.981[−4] | 6.642[−4] | 4.994[−4] | 3.636[−4] |
| $6s$-$np$ | | | 1.579[0] | 5.823[−3] | 2.121[−4] | 2.697[−5] | 3.149[−5] |
| $5p$-$ns$ | | | 2.034[−1] | 2.575[−2] | 9.156[−3] | 4.478[−3] | 2.572[−3] |
| $6p$-$ns$ | | | | 3.220[−1] | 3.678[−2] | 1.272[−2] | 6.194[−3] |
| $5p$-$nd$ | | 8.309[−1] | 1.232[−1] | 4.245[−2] | 2.017[−2] | 1.136[−2] | 7.098[−3] |
| $6p$-$nd$ | | | 9.386[−1] | 1.602[−1] | 5.900[−2] | 2.922[−2] | 1.694[−2] |
| $4d$-$np$ | | 8.275[−2] | 3.621[−4] | 1.458[−4] | 7.629[−5] | 4.515[−5] | 2.905[−5] |
| $5d$-$np$ | | | 1.745[−1] | 5.782[−4] | 9.325[−5] | 2.584[−5] | 9.764[−6] |
| $4d$-$nf$ | 2.958[−1] | 1.164[−1] | 5.765[−2] | 3.298[−2] | 2.075[−2] | 1.394[−2] | 9.851[−3] |
| $5d$-$nf$ | 8.666[−1] | 5.807[−2] | 4.177[−2] | 2.565[−2] | 1.649[−2] | 1.117[−2] | 7.921[−3] |

TABLE VII. Lifetimes (in ns) of $nl_j$ states calculated using DHF, SD, and SDpT methods; the label "sc" indicates the scaled values. Final results together with their uncertainties given in the "$\tau^{\text{final}}$" column are compared with theoretical [2] and experimental data [20].

| Level | $\tau^{(\text{DF})}$ | $\tau^{(\text{SD})}$ | $\tau^{(\text{SDpT})}$ | $\tau_{\text{sc}}^{(\text{SD})}$ | $\tau_{\text{sc}}^{(\text{SDpT})}$ | $\tau^{\text{final}}$ | $\tau^{\text{theor}}$ [2] | $\tau^{\text{expt}}$ [20] |
|---|---|---|---|---|---|---|---|---|
| $6s_{1/2}$ | 4.267 | 4.455 | 4.433 | 4.422 | 4.432 | 4.42(3) | 4.97 | |
| $7s_{1/2}$ | 7.102 | 7.225 | 7.199 | 7.213 | 7.200 | 7.21(1) | 7.32 | |
| $5p_{1/2}$ | 5.717 | 7.383 | 7.291 | 7.320 | 7.326 | 7.32(6) | 7.71 | $7.39 \pm 0.07$ |
| $5p_{3/2}$ | 5.164 | 6.660 | 6.577 | 6.603 | 6.608 | 6.60(6) | 6.96 | $6.63 \pm 0.05$ |
| $6p_{1/2}$ | 37.79 | 41.69 | 41.58 | 41.69 | 41.62 | 41.69(11) | 37.50 | |
| $6p_{3/2}$ | 32.33 | 37.24 | 37.17 | 37.34 | 37.17 | 37.34(17) | 33.80 | |
| $5d_{3/2}$ | 3.404 | 3.513 | 3.503 | 3.471 | 3.472 | 3.47(4) | 3.62 | |
| $5d_{5/2}$ | 3.474 | 3.583 | 3.573 | 3.541 | 3.542 | 3.54(4) | 3.85 | |
| $6d_{3/2}$ | 6.094 | 6.657 | 6.623 | 6.637 | 6.617 | 6.64(2) | 6.60 | |
| $6d_{5/2}$ | 6.244 | 6.822 | 6.788 | 6.803 | 6.784 | 6.80(2) | 6.90 | |
| $4f_{5/2}$ | 2.037 | 3.078 | 2.993 | 3.004 | 3.035 | 3.00(7) | 3.08 | $3.09 \pm 0.06$ |
| $4f_{7/2}$ | 2.042 | 3.063 | 2.982 | 2.995 | 3.025 | 2.99(7) | 3.21 | $2.97 \pm 0.05$ |

are equal to 0.441(3) and 0.394(2) s and are presented in the column labeled "Final" of Table VIII.

## IV. STATIC MULTIPOLE POLARIZABILITIES OF THE 5*S* GROUND STATE OF Sr II

The static valence multipole polarizability $\alpha^{Ek}$ of Sr II in its $5s$ ground state can be separated into two terms: a dominant first term from the intermediate valence-excited states and a smaller second term from the intermediate core-excited states. The latter term is smaller than the former one by several orders of magnitude and is evaluated here in the RPA [53]. The dominant valence contribution is calculated using the sum-over-state approach

$$\alpha_v^{Ek} = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j \| r^k C_{kq} \| 4s \rangle|^2}{E_{nlj} - E_{4s}}, \tag{1}$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic and where $nl_j$ is $np_j$, $nd_j$, and $nf_j$ for $k = 1$, 2, and 3, respectively [54]. The reduced matrix elements in the above sum are evaluated using the SD approximation for basis states with $n \leqslant 26$ and in the DF approximation for the remaining states, scaling is included into the $E2$ and $E3$ matrix elements.

The contributions to dipole, quadrupole, and octupole polarizabilities of the $5s$ ground state are presented in Table IX. The first two terms in the sum-over-states for $\alpha^{E1}$, $\alpha^{E2}$, and $\alpha^{E3}$ contribute 99.4%, 94.18%, and 48.2%, respectively, of the totals. The rapid convergence of the sum-over-states for $\alpha^{E1}$ has been emphasized in many publications (for example, Refs. [55,56]). We use the available, recommended NIST energies [37] for $nl = 5s$-$13s$,$5p$-$7p$,$4d$-$14d$,$4f$-$12f$ and theoretical SD energies for other states up to $n = 26$. The remaining contributions to $\alpha^{Ek}$ from basis functions with $27 \leqslant n \leqslant 70$ are evaluated in the DF approximation. As one can see from Table IX, sums over $n$ for $n \leqslant 26$ in $\alpha^{E2}$ and $\alpha^{E3}$ essentially reproduce the final results since the contributions from $27 \leqslant n \leqslant 70$ are smaller than 0.01% in all cases.

As in the lifetimes calculations, we carried out four different calculations for the main terms with lower $n$, using SD, SDpT, $\text{SD}_{\text{sc}}$, and $\text{SDpT}_{\text{sc}}$ $E_k$ matrix elements. Only the results of the calculation with SD-scaled data are given. We estimate the uncertainty of our final values as the maximum difference between the final result and the other three results obtained in the SD, SDpT, and $\text{SDpT}_{\text{sc}}$ approximations. The final results for the multipole polarizabilities of the ground state of Sr II are compared in Table IX with the high-precision calculations given in Refs. [3,5] and the experimental measurements presented in Ref. [15]. Our results agree with the values given by [5] for the multipole polarizability. The best agreement is found for the $\alpha^{E2}$ value (0.3%), while the differences for the $\alpha^{E1}$ and $\alpha^{E3}$ values are equal to 1.7% and 1.3%, respectively. The uncertainty in the experimental measurements [15] of the dipole polarizability is too large (13%) to reflect on the accuracy of the present calculations.

## V. SCALAR POLARIZABILITIES OF THE $ns_{1/2}$, $np_j$, AND $nd_j$ STATES AND TENSOR POLARIZABILITIES OF THE $np_{3/2}$ AND $nd_j$ EXCITED STATES OF Sr II

The valence part of the scalar $\alpha_0(v)$ and tensor $\alpha_2(v)$ polarizabilities of an excited state $v$ of Sr II are given by

$$\alpha_0(v) = \frac{2}{3(2j_v+1)} \sum_{nlj} I_v(nlj),\ I_v(nlj) = \frac{|\langle v||rC_1||nlj\rangle|^2}{E_{nlj} - E_v}, \tag{2}$$

TABLE VIII. Lifetimes (in s) of $4d_j$ states in Sr II. The SD [$\tau^{(\text{SD})}$] and SD scaled [$\tau^{(\text{SD}_{\text{sc}})}$] values are compared with theoretical and experimental data.

| State | SD | SDpT | $\text{SD}_{\text{sc}}$ | $\text{SDpT}_{\text{sc}}$ | Final | Theor. [3] | Theor. [4] | Expt. [2] |
|---|---|---|---|---|---|---|---|---|
| $4d_{3/2}$ | 0.4509 | 0.4379 | 0.4410 | 0.4437 | 0.441(3) | 0.441(3) | 0.426(8) | 0.435(4) |
| $4d_{5/2}$ | 0.4029 | 0.3915 | 0.3944 | 0.3967 | 0.394(2) | 0.394(3) | 0.357(12) | 0.408(22) |

TABLE IX. Contributions to multipole polarizabilities (a.u.) of the $5s$ state of Sr II. The two leading terms and those terms with $n \leqslant 26$ in the expression for $\alpha_v^{Ek}$ [Eq. (1)] are evaluated using "final" values of reduced electric-multipole matrix elements [$Z^{(\mathrm{final})}$] together with uncertainties. The remainders ($n > 26$), labeled "tail" below, are evaluated in the Dirac-Hartree-Fock (DHF) approximation. Contributions from core-excited states $\alpha_c^{Ek}$ are evaluated in the RPA. Our final SD $\alpha^{E1}$, $\alpha^{E2}$, and $\alpha^{E3}$ of the $5s$ ground state of Sr II are compared with other calculations and with the experiment.

| | | | | | |
|---|---|---|---|---|---|
| $nlj = 5p_{1/2}$ | 29.470 | $nlj = 4d_{3/2}$ | 373.76 | $nlj = 4f_{5/2}$ | 5680.8 |
| $nlj = 5p_{3/2}$ | 56.945 | $nlj = 4d_{5/2}$ | 559.11 | $nlj = 4f_{7/2}$ | 7574.3 |
| $nl = [6p\text{–}26p]$ | 0.214 | $nl = [5d\text{–}26d]$ | 418.76 | $nl = [5f\text{–}26f]$ | 2159.7 |
| $nl = [2p\text{–}4p]$ | −0.263 | $nl = [3d]$ | 0.0 | | |
| tail | 0.008 | tail | 1.23 | tail | 32.8 |
| $\alpha_v^{E1}$ | 86.374 | $\alpha_v^{E2}$ | 1352.86 | $\alpha_v^{E3}$ | 15447.5 |
| $\alpha_c^{E1}$ | 5.812 | $\alpha_c^{E2}$ | 17.14 | $\alpha_c^{E3}$ | 113.4 |
| $\alpha^{E1}$ | 92.2(7) | $\alpha^{E2}$ | 1370.0(28) | $\alpha^{E3}$ | 15560.0(330) |
| $\alpha^{E1}_{\mathrm{theor}}$ [5] | 89.88 | $\alpha^{E2}_{\mathrm{theor}}$ [5] | 1346 | $\alpha^{E3}_{\mathrm{theor}}$ [5] | 15430.0 |
| $\alpha^{E1}_{\mathrm{theor}}$ [3] | 91.30 | | | | |
| $\alpha^{E1}_{\mathrm{expt}}$ [15] | 86(11) | $\alpha^{E2}_{\mathrm{expt}}$ [15] | $1.1(10) \times 10^3$ | | |

$$\alpha_2(v) = (-1)^{j_v}\sqrt{\frac{40j_v(2j_v-1)}{3(j_v+1)(2j_v+1)(2j_v+3)}} \times \sum_{nlj}(-1)^j \begin{Bmatrix} j_v & 1 & j \\ 1 & j_v & 2 \end{Bmatrix} I_v(nlj). \quad (3)$$

Our calculation of the sums is divided into three parts. The first part contains the sum over valence states with $n \leqslant 26$, which is carried out using SD wave functions. For lower $n$ transitions, we carried out four different calculations for the main term, using SD, SDpT, $\mathrm{SD_{sc}}$, and $\mathrm{SDpT_{sc}}$ electric-dipole matrix elements. Only the results of the calculation with SD-scaled data are included. We estimate the uncertainty of our final values as the maximum difference between the final result and the other three results obtained in the SD, SDpT, and $\mathrm{SDpT_{sc}}$ approximations.

The second part includes the sum over basis states with $n > 26$, which is carried out in the RPA. The third part contains the contribution from core-excited states, which is carried out also in the RPA. A breakdown of the contributions to the scalar dipole polarizability for the excited $ns_{1/2}$ ($n = 6$–$10$), $np_j$ ($n = 5$–$9$), and $nd_j$ ($n = 4$–$8$) states is presented in Table X.

We evaluate the contribution from ionic core $\alpha_{\mathrm{core}}$ in the RPA and find $\alpha_{\mathrm{core}} = 5.812a_0^3$.

Contributions from the excited $np_j$ states with $n > 26$ in the case of the excited $ns_{1/2}$ states is too small (0.001–0.005) in comparison with the main contribution. Therefore, we put zero in the line for $\alpha_{\mathrm{tail}}^{(\mathrm{RPA})}$. Contributions from the excited $ns$ and $nd$ states with $n > 26$ in the case of the excited $np_j$ states are very small $\alpha_{n>26}(5p_{1/2}) = 0.090a_0^3$, $\alpha_{n>26}(5p_{3/2}) = 0.071a_0^3$ and are calculated in the RPA approximation.

A counter term $\alpha_{\mathrm{vc}}(n_j)$ compensating for the excitation from the core to the valence shell, which violates the Pauli principle, is also evaluated in the RPA and found to be very small. The largest contribution of this term $\alpha_{\mathrm{vc}}(nl_j)$ is for the $nl_j = 4d_j$ [$\alpha_{\mathrm{vc}}(4d_{3/2}) = -0.363a_0^3$ and $\alpha_{\mathrm{vc}}(4d_{5/2}) = -0.401a_0^3$].

The above values were combined to obtain our final result for the scalar polarizabilities $\alpha^{(\mathrm{SD})}(nlj)$ for the five $ns_j$ ($n = 6$–$10$), $np_j$ ($n = 5$–$9$), and $nd_j$ ($n = 4$–$8$) excited states in Sr II.

The final results for the scalar dipole polarizabilities of $\alpha^{(\mathrm{SD})}(nlj)$ in Sr II are compared in Table X with the nonrelativistic values evaluated by Mitroy *et al.* [5]. The largest disagreement between our SD values and the semiempirical values from [5] is observed for the $\alpha^{(\mathrm{SD})}(5p_j)$ states where relativistic effects are very important.

A breakdown of contributions to the tensor dipole polarizability for the excited $np_{3/2}$ ($n = 5$–$9$), and $nd_j$ ($n = 4$–$9$) states is presented in Table XI. Evaluation of the tensor polarizability follows the same pattern as the scalar polarizability [compare Eqs. (2) and (3)]. The difference in evaluations of the $\alpha_0^{(\mathrm{SD})}(nlj)$ and $\alpha_2^{(\mathrm{SD})}(nlj)$ values is in the angular part only. As one sees from a comparison of the results given in Tables X and XI, we obtain a different distribution from the $\sum_{n'=5}^{26} I_{np_j}^{(\mathrm{SD})}(n's_{1/2})$, $\sum_{n'=4}^{26} I_{np_j}^{(\mathrm{SD})}(n'd_{3/2})$, and $\sum_{n'=4}^{26} I_{np_j}^{(\mathrm{SD})}(n'd_{5/2})$ terms (in the case of $np_j$ excited states) and from the $\sum_{n'=5}^{26} I_{nd_j}^{(\mathrm{SD})}(n'p_{1/2})$, $\sum_{n'=5}^{26} I_{nd_j}^{(\mathrm{SD})}(n'p_{3/2})$, and $\sum_{n'=4}^{26} I_{nd_j}^{(\mathrm{SD})}(n'f_{5/2})$ terms ($nd_j$ excited states) in the scalar and tensor polarizabilities. As a result, the values of $\alpha_2^{(\mathrm{SD})}(nlj)$ are smaller than the values of $\alpha_0^{(\mathrm{SD})}(nlj)$ and have a different sign.

States with $n > 19$ in our basis have positive energies and provide a discrete representation of the continuum. We find that the continuous part of the spectra is responsible for 2% of the $\alpha_2(np_{3/2})$ and $\alpha_2(nd_j)$ states. Those contributions appear from the $np$-$n'd$ transitions for the $\alpha_2(np_{3/2})$ values and from the $nd$-$n'f$ transitions for the $\alpha_2(nd_j)$ values. Contributions from states with $n > 26$ are negligible (about $10^{-4}$%). Our final results $\alpha_2^{(\mathrm{SD})}(nlj)$ are given in Table XI. The final results for the tensor polarizabilities of $\alpha^{(\mathrm{SD})}(nlj)$ in Sr II are compared in Table XI with semiempiriacal nonrelativistic values evaluated by Mitroy *et al.* [5]. The best agreement between our SD results and the semiempiriacal results from Ref. [5] is for the $5p_{3/2}$ and $4d_{5/2}$ states (less than 1% disagreement). For all other states ($6p_{3/2}$, $4d_{3/2}$, $5d_{3/2}$, and $5d_{5/2}$) the difference is about 10%.

TABLE X. Contributions to scalar polarizabilities of Sr II in the excited $ns_{1/2}$ states ($n = 6$–10), $np_{1/2}$, $np_{3/2}$ states ($n = 5$–9) and $nd_{3/2}$, $nd_{5/2}$ states ($n = 4$–8) calculated using "final" values of reduced electric-dipole matrix elements [$Z^{(\mathrm{final})}$] together with uncertainties. $\alpha_0(ns_{1/2}) = \sum_{n'=2}^{70} I_{ns_{1/2}}(n'p_j)$. $\alpha_0(np_{1/2}) = \sum_{n'=3}^{70} I_{np_{1/2}}(n'd_{3/2}) + \sum_{n'=1}^{70} I_{np_{1/2}}(n's_{1/2})$, $\alpha_0(np_{3/2}) = \sum_{n'=3}^{70} I_{np_{3/2}}(n'd_j) + \sum_{n'=1}^{70} I_{np_{3/2}}(n's_{1/2})$. $\alpha_0(nd_{3/2}) = \sum_{n'=4}^{70} I_{nd_{3/2}}(n'f_{5/2}) + \sum_{n'=2}^{70} I_{nd_{3/2}}(n'p_j)$, $\alpha_0(nd_{5/2}) = \sum_{n'=4}^{70} I_{nd_{5/2}}(n'f_j) + \sum_{n'=2}^{70} I_{nd_{5/2}}(n'p_{3/2})$. $\alpha_{\mathrm{core}} = 5.8125$ a.u.

| Contribution | $6s_{1/2}$ | $7s_{1/2}$ | $8s_{1/2}$ | $9s_{1/2}$ | $10s_{1/2}$ |
|---|---|---|---|---|---|
| $\sum_{n'=5}^{26} I_{ns_j}^{(\mathrm{SD})}(n'p_{1/2})$ | 371.97 | 2175.9 | 8472.4 | 26374.4 | 70807.2 |
| $\sum_{n'=5}^{26} I_{ns_j}^{(\mathrm{SD})}(n'p_{3/2})$ | 704.45 | 4053.3 | 15984.5 | 48681.2 | 129289.9 |
| $\alpha_{\mathrm{main}}^{(\mathrm{SD})}(ns_j)$ | 1076.42 | 6229.2 | 24456.8 | 75055.6 | 200097.1 |
| $\alpha_{\mathrm{vc}}(ns_j)$ | −0.041 | −0.015 | −0.007 | −0.004 | −0.002 |
| $\alpha^{(\mathrm{SD})}(ns_j)$ | 1082(4) | 6235(39) | 24463(148) | 75062(220) | 200100(1000) |
| Ref. [5] | 1089.0 | | | | |
| Contribution | $5p_{1/2}$ | $6p_{1/2}$ | $7p_{1/2}$ | $8p_{1/2}$ | $9p_{1/2}$ |
| $\sum_{n'=5}^{26} I_{np_j}^{(\mathrm{SD})}(n's_{1/2})$ | −11.611 | −198.10 | −1327.5 | −5443.6 | −17553.7 |
| $\sum_{n'=4}^{26} I_{np_j}^{(\mathrm{SD})}(n'd_{3/2})$ | −26.520 | −1797.91 | −14116.1 | −60353.7 | −203337.5 |
| $\alpha_{\mathrm{main}}^{(\mathrm{SD})}(np_j)$ | −38.132 | −1996.01 | −15443.6 | −65797.2 | −220891.2 |
| $\alpha_{\mathrm{vc}}(np_j)$ | −0.002 | −0.001 | 0.000 | 0.000 | 0.000 |
| $\alpha_{\mathrm{tail}}^{(\mathrm{RPA})}(np_j)$ | 0.090 | 0.131 | 0.127 | 0.107 | 0.084 |
| $\alpha^{(\mathrm{SD})}(np_j)$ | −32.2(9) | −1990(5) | −15438(72) | −65792(255) | −220880(880) |
| Ref. [5] | −23.13 | −2056.0 | | | |
| Contribution | $5p_{3/2}$ | $6p_{3/2}$ | $7p_{3/2}$ | $8p_{3/2}$ | $9p_{3/2}$ |
| $\sum_{n'=5}^{26} I_{np_j}^{(\mathrm{SD})}(n's_{1/2})$ | −8.505 | −159.82 | −1084.39 | −4766.0 | −14595.9 |
| $\sum_{n'=4}^{26} I_{np_j}^{(\mathrm{SD})}(n'd_{3/2})$ | −1.515 | −151.20 | −1192.87 | −5501.4 | −17636.1 |
| $\sum_{n'=4}^{26} I_{np_j}^{(\mathrm{SD})}(n'd_{5/2})$ | −17.279 | −1440.28 | −112 67.91 | −517 82.0 | −165 681.0 |
| $\alpha_{\mathrm{main}}^{(\mathrm{SD})}(np_j)$ | −27.299 | −1751.30 | −135 45.16 | −620 49.4 | −197 913.0 |
| $\alpha_{\mathrm{vc}}(np_j)$ | −0.001 | 0.000 | 0.000 | 0.000 | 0.000 |
| $\alpha_{\mathrm{tail}}^{(\mathrm{RPA})}(np_j)$ | 0.071 | 0.098 | 0.093 | 0.077 | 0.060 |
| $\alpha^{(\mathrm{SD})}(np_j)$ | −21.4(8) | −1745(5) | −13539(42) | −620 44(330) | −197 910(990) |
| Ref. [5] | −23.13 | −2056.0 | | | |
| Contribution | $4d_{3/2}$ | $5d_{3/2}$ | $6d_{3/2}$ | $7d_{3/2}$ | $8d_{3/2}$ |
| $\sum_{n'=5}^{26} I_{nd_j}^{(\mathrm{SD})}(n'p_{1/2})$ | 38.687 | 1055.67 | 7644.3 | 319 70.6 | 106 139.2 |
| $\sum_{n'=5}^{26} I_{nd_j}^{(\mathrm{SD})}(n'p_{3/2})$ | 7.025 | 185.33 | 1322.2 | 5888.6 | 18621.6 |
| $\sum_{n'=4}^{26} I_{nd_j}^{(\mathrm{SD})}(n'f_{5/2})$ | 11.929 | 728.45 | 4705.7 | 19169.5 | 60133.3 |
| $\alpha_{\mathrm{main}}^{(\mathrm{SD})}(nd_j)$ | 57.642 | 1969.45 | 13672.3 | 57028.7 | 184894.1 |
| $\alpha_{\mathrm{vc}}(nd_j)$ | −0.365 | −0.040 | −0.013 | −0.006 | −0.003 |
| $\alpha_{\mathrm{tail}}^{(\mathrm{RPA})}(nd_j)$ | 0.228 | 0.175 | 0.129 | 0.092 | 0.066 |
| $\alpha^{(\mathrm{SD})}(nd_j)$ | 63.3(9) | 1975(2) | 136 78(38) | 570 35(100) | 184 900(900) |
| Ref. [5] | 61.77 | 2099. | | | |
| Contribution | $4d_{5/2}$ | $5d_{5/2}$ | $6d_{5/2}$ | $7d_{5/2}$ | $8d_{5/2}$ |
| $\sum_{n'=5}^{26} I_{nd_j}^{(\mathrm{SD})}(n'p_{3/2})$ | 44.186 | 1161.64 | 8273.5 | 367 96.1 | 116 242.3 |
| $\sum_{n'=4}^{26} I_{nd_j}^{(\mathrm{SD})}(n'f_{5/2})$ | 0.582 | 35.22 | 228.2 | 931.1 | 2927.4 |
| $\sum_{n'=4}^{26} I_{nd_j}^{(\mathrm{SD})}(n'f_{7/2})$ | 11.663 | 704.47 | 4563.7 | 186 22.3 | 585 58.3 |
| $\alpha_{\mathrm{main}}^{(\mathrm{SD})}(nd_j)$ | 56.431 | 1901.34 | 13065.4 | 563 49.5 | 177 728.0 |
| $\alpha_{\mathrm{vc}}(nd_j)$ | −0.401 | −0.043 | −0.013 | −0.006 | −0.003 |
| $\alpha_{\mathrm{tail}}^{(\mathrm{RPA})}(nd_j)$ | 0.187 | 0.138 | 0.100 | 0.070 | 0.050 |
| $\alpha^{(\mathrm{SD})}(nd_j)$ | 62.0(9) | 1907(2) | 130 71(45) | 563 56(99) | 177 730(880) |
| Ref. [5] | 61.77 | 2099.0 | | | |
| Ref. [3] | 62.0(5) | | | | |

TABLE XI. Contributions to tensor polarizabilities of Sr II in the excited $np_{3/2}$ states ($n = 5$–9) and $nd_{3/2}$, $nd_{5/2}$ states ($n = 4$–9) calculated using "final" values of reduced electric-dipole matrix elements [$Z^{(\mathrm{final})}$] together with uncertainties; $\alpha_0(np_{3/2}) = \sum_{n'=3}^{70} I_{np_{3/2}}(n'd_j) + \sum_{n'=1}^{70} I_{np_{3/2}}(n's_{1/2})$. $\alpha_0(nd_{3/2}) = \sum_{n'=4}^{70} I_{nd_{3/2}}(n'f_{5/2}) + \sum_{n'=2}^{70} I_{nd_{3/2}}(n'p_j)$, $\alpha_0(nd_{5/2}) = \sum_{n'=4}^{70} I_{nd_{5/2}}(n'f_j) + \sum_{n'=2}^{70} I_{nd_{5/2}}(n'p_{3/2})$.

| Contribution | $5p_{3/2}$ | $6p_{3/2}$ | $7p_{3/2}$ | $8p_{3/2}$ | $9p_{3/2}$ | |
|---|---|---|---|---|---|---|
| $\sum_{n'=5}^{26} I^{(\mathrm{SD})}_{np_j}(n's_{1/2})$ | 8.505 | 159.82 | 1068.99 | 4632.6 | 14595.9 | |
| $\sum_{n'=4}^{26} I^{(\mathrm{SD})}_{np_j}(n'd_{3/2})$ | −1.212 | −120.96 | −959.12 | −4407.9 | −14108.9 | |
| $\sum_{n'=4}^{26} I^{(\mathrm{SD})}_{np_j}(n'd_{5/2})$ | 3.456 | 288.06 | 2265.67 | 10376.0 | 33136.2 | |
| $\alpha^{(\mathrm{SD})}_{\mathrm{main}}(np_j)$ | 10.749 | 326.92 | 2375.53 | 10600.7 | 33623.2 | |
| $\alpha^{(\mathrm{RPA})}_{\mathrm{tail}}(np_j)$ | −0.011 | −0.011 | −0.009 | −0.007 | −0.006 | |
| $\alpha^{(\mathrm{SD})}(np_j)$ | 10.74(23) | 326.9(3.5) | 2376(17) | 10600(120) | 33620(300) | |
| Ref. [5] | 10.58 | 363.5 | | | | |
| Contribution | $4d_{3/2}$ | $5d_{3/2}$ | $6d_{3/2}$ | $7d_{3/2}$ | $8d_{5/2}$ | $9d_{3/2}$ |
| $\sum_{n'=5}^{26} I^{(\mathrm{SD})}_{nd_j}(n'p_{1/2})$ | −38.687 | −1055.67 | −7644.35 | −31970.6 | −106139.2 | −307157.0 |
| $\sum_{n'=5}^{26} I^{(\mathrm{SD})}_{nd_j}(n'p_{3/2})$ | 5.620 | 148.26 | 1057.73 | 4710.9 | 14897.3 | 42825.3 |
| $\sum_{n'=4}^{26} I^{(\mathrm{SD})}_{nd_j}(n'f_{5/2})$ | −2.386 | −145.69 | −941.15 | −3833.9 | −12026.7 | −31672.8 |
| $\alpha^{(\mathrm{SD})}_{\mathrm{main}}(nd_j)$ | −35.453 | −1053.09 | −7527.77 | −31093.6 | −103268.6 | −296004.5 |
| $\alpha^{(\mathrm{RPA})}_{\mathrm{tail}}(nd_j)$ | −0.046 | −0.035 | −0.026 | −0.02 | −0.01 | −0.01 |
| $\alpha^{(\mathrm{SD})}(nd_j)$ | −35.5(6) | −1053(10) | −7528(27) | −31094(78) | −103270(300) | −296000(900) |
| Ref. [5] | −47.20 | −1543 | | | | |
| Contribution | $4d_{5/2}$ | $5d_{5/2}$ | $6d_{5/2}$ | $7d_{5/2}$ | $8d_{5/2}$ | $9d_{5/2}$ |
| $\sum_{n'=5}^{26} I^{(\mathrm{SD})}_{nd_j}(n'p_{3/2})$ | −44.186 | −1161.64 | −8273.53 | −36796.1 | −116242.3 | −334211.7 |
| $\sum_{n'=4}^{26} I^{(\mathrm{SD})}_{nd_j}(n'f_{5/2})$ | 0.665 | 40.25 | 260.78 | 1064.1 | 3345.6 | 8821.1 |
| $\sum_{n'=4}^{26} I^{(\mathrm{SD})}_{nd_j}(n'f_{7/2})$ | −4.165 | −251.60 | −1629.88 | −6650.8 | −20913.7 | −55144.1 |
| $\alpha^{(\mathrm{SD})}_{\mathrm{main}}(nd_j)$ | −47.686 | −1372.99 | −9642.63 | −42382.8 | −133810.4 | −380534.7 |
| $\alpha^{(\mathrm{RPA})}_{\mathrm{tail}}(nd_j)$ | −0.051 | −0.037 | −0.026 | −0.02 | −0.01 | −0.01 |
| $\alpha^{(\mathrm{SD})}(nd_j)$ | −47.7(8) | −1373(13) | −9643(45) | −42383(112) | −133800(400) | −380500(1100) |
| Ref. [5] | −47.20 | −1543 | | | | |
| Ref. [3] | −47.7(3) | | | | | |

## VI. HYPERFINE CONSTANTS FOR $^{87}$Sr II

Calculations of hyperfine constants follow the pattern described earlier for calculations of transition-matrix elements. In Table XII, we list hyperfine constants $A$ for $^{87}$Sr II and compare our values with the available theoretical [33] results and experimental measurements of Refs. [26,30,31].

In this table, we present the lowest-order $A^{(\mathrm{DF})}$, the all-order $A^{(\mathrm{SD})}$, and $A^{(\mathrm{SDpT})}$ values for the $ns$, $np$, and $nd$ levels up to $n = 9$. It should be noted that the values of $A^{(\mathrm{SDpT})}$ are obtained by using the single-double all-order method including partial triple excitations. The difference between $A^{(\mathrm{SD})}$ and $A^{(\mathrm{SDpT})}$ is about 0.1–0.4%, while the ratios $A^{(\mathrm{DF})}$ and $A^{(\mathrm{SD})}$ are equal to 0.5–10 for some cases. For the ground $5s\,^2S_{1/2}$ state, our SDpT result is in better agreement with a very precision measurement [26] than the SD result. On the opposite side, the $A^{(\mathrm{SD})}$ value is in better agreement with the experimental measurements [30] than the $A^{(\mathrm{SDpT})}$ value for the $5p\,^2P_{3/2}$ state. Both $A^{(\mathrm{SD})}$ and $A^{(\mathrm{SDpT})}$ values are in disagreement with recent precision experimental measurements [31] for the $4d\,^2D_{5/2}$ state. For this state, the correlation contribution is larger than the $A^{(\mathrm{DF})}$ value by a factor of 10. We present theoretical results given by Mårtensson-Pendrill [33] in the column of Table XII labeled $A^{\mathrm{theor}}$. A relativistic coupled-cluster was used in [33] to evaluate the $A$ constant for the $5s_{1/2}$, $5p_j$, and $4d_j$ states. The $A$ values from [33] are in excellent agreement with our $A^{(\mathrm{SDpT})}$ values except for the result for the $4d\,^2D_{5/2}$ state, where disagreement is about 50% owing to the very large correlation contributions to the $A$ value for this state.

Hyperfine constants $B$ (in MHz) in $^{87}$Sr$^+$ are given in Table XIII. The nuclear quadrupole moment $Q$ is equal to 0.327(24) in barns (1 b = $10^{-24}$cm$^2$) [33]. The SD and SDpT data are compared with the theoretical [33] and experimental data from Refs. [30,31]. Three columns of Table XIII list the $B^{(\mathrm{DF})}$, $B^{(\mathrm{SD})}$, and $B^{(\mathrm{SDpT})}$ values divided by nuclear quadrupole moment $Q$. Those values are compared with the theoretical results given by Mårtensson-Pendrill [33]. For the $5p\,^2P_{3/2}$ state, the $B^{(\mathrm{SDpT})}/Q$ value is in better agreement with the result from [33] than the $B^{(\mathrm{SD})}/Q$ value. On the opposite side, the $B^{(\mathrm{SD})}/Q$ values are in better agreement with the results from [33] than the $B^{(\mathrm{SDpT})}/Q$ values for the $4d\,^2D_J$ states. Three other columns of Table XIII list the $B^{(\mathrm{DF})}$, $B^{(\mathrm{SD})}$, and $B^{(\mathrm{SDpT})}$

TABLE XII. Hyperfine constants $A$ (in MHz) in $^{87}Sr^{+}$ ($I = 9/2$, $\mu = -1.092\,83$ [57]). The SD and SDpT data are compared with other theoretical values and experimental results.

| Level | $A^{(DF)}$ | $A^{(SD)}$ | $A^{(SDpT)}$ | $A^{(theor)}$ | $A^{(expt)}$ |
|---|---|---|---|---|---|
| $5s\ ^2S_{1/2}$ | −731.59 | −1021.27 | −997.85 | −1000 [33] | −1000.473 673(11) [26] |
| $6s\ ^2S_{1/2}$ | −233.28 | −299.47 | −296.04 | | |
| $7s\ ^2S_{1/2}$ | −104.70 | −130.98 | −129.91 | | |
| $8s\ ^2S_{1/2}$ | −55.94 | −69.11 | −68.65 | | |
| $9s\ ^2S_{1/2}$ | −33.36 | −40.91 | −40.68 | | |
| $5p\ ^2P_{1/2}$ | −121.51 | −181.73 | −177.33 | −177 [33] | |
| $6p\ ^2P_{1/2}$ | −46.21 | −64.43 | −63.40 | | |
| $7p\ ^2P_{1/2}$ | −22.54 | −30.67 | −30.26 | | |
| $8p\ ^2P_{1/2}$ | −12.67 | −17.02 | −16.82 | | |
| $9p\ ^2P_{1/2}$ | −7.82 | −10.43 | | | |
| $5p\ ^2P_{3/2}$ | −21.33 | −36.13 | −35.26 | −35.3 [33] | −36.0(0.4) [30] |
| $6p\ ^2P_{3/2}$ | −8.15 | −12.86 | −12.65 | | |
| $7p\ ^2P_{3/2}$ | −3.99 | −6.14 | −6.06 | | |
| $8p\ ^2P_{3/2}$ | −2.24 | −3.41 | −3.37 | | |
| $9p\ ^2P_{3/2}$ | −1.39 | −2.09 | | | |
| $4d\ ^2D_{3/2}$ | −31.12 | −47.51 | −46.70 | −46.7 [33] | |
| $5d\ ^2D_{3/2}$ | −8.03 | −10.72 | −10.73 | | |
| $6d\ ^2D_{3/2}$ | −3.54 | −4.68 | −4.69 | | |
| $7d\ ^2D_{3/2}$ | −1.90 | −2.49 | −2.50 | | |
| $8d\ ^2D_{3/2}$ | −1.14 | −1.49 | | | |
| $9d\ ^2D_{3/2}$ | −0.74 | −0.96 | | | |
| $4d\ ^2D_{5/2}$ | −12.97 | 1.41 | 1.63 | 1.07 [33] | 2.1743(14) [31] |
| $5d\ ^2D_{5/2}$ | −3.36 | −1.99 | −1.93 | | |
| $6d\ ^2D_{5/2}$ | −1.48 | −1.13 | −1.10 | | |
| $7d\ ^2D_{5/2}$ | −0.79 | −0.66 | −0.65 | | |
| $8d\ ^2D_{5/2}$ | −0.48 | −0.41 | | | |
| $9d\ ^2D_{5/2}$ | −0.31 | −0.28 | | | |

TABLE XIII. Hyperfine constants $B$ (in MHz) in $^{87}Sr^{+}$. Nuclear quadrupole moment $Q$ is equal to 0.327(24)b in barns (1 b = $10^{-24}$ cm$^2$) [33]. The SD and SDpT data are compared with experimental results.

| Level | $\frac{B^{(DF)}}{Q}$ | $\frac{B^{(SD)}}{Q}$ | $\frac{B^{(SDpT)}}{Q}$ | $B^{(DF)}$ | $B^{(SD)}$ | $B^{(SDpT)}$ | $\frac{B^{(theor)}}{Q}$ | $B^{(expt)}$ |
|---|---|---|---|---|---|---|---|---|
| $5p\ ^2P_{3/2}$ | 165.61 | 278.09 | 271.98 | 54.15 | 90.93 | 88.94 | 271 [33] | 88.5(5.4) [30] |
| $6p\ ^2P_{3/2}$ | 63.20 | 97.66 | 96.20 | 20.67 | 31.93 | 31.46 | | |
| $7p\ ^2P_{3/2}$ | 30.84 | 46.16 | 45.59 | 10.09 | 15.10 | 14.91 | | |
| $8p\ ^2P_{3/2}$ | 17.30 | 25.49 | 25.20 | 5.66 | 8.34 | 8.24 | | |
| $9p\ ^2P_{3/2}$ | 10.64 | 15.54 | | 3.48 | 5.08 | | | |
| $4d\ ^2D_{3/2}$ | 80.21 | 115.23 | 113.26 | 26.23 | 37.68 | 37.04 | 115 [33] | |
| $5d\ ^2D_{3/2}$ | 20.59 | 32.93 | 32.75 | 6.73 | 10.77 | 10.71 | | |
| $6d\ ^2D_{3/2}$ | 9.00 | 14.52 | 14.46 | 2.94 | 4.75 | 4.73 | | |
| $7d\ ^2D_{3/2}$ | 4.76 | 7.69 | 7.66 | 1.56 | 2.51 | 2.51 | | |
| $8d\ ^2D_{3/2}$ | 2.81 | 4.54 | | 0.92 | 1.48 | | | |
| $9d\ ^2D_{3/2}$ | 1.77 | 2.89 | | 0.58 | 0.94 | | | |
| $4d\ ^2D_{5/2}$ | 109.85 | 160.24 | 157.58 | 35.92 | 52.40 | 51.53 | 160 [33] | 49.11(6) [31] |
| $5d\ ^2D_{5/2}$ | 28.27 | 45.98 | 45.71 | 9.25 | 15.03 | 14.95 | | |
| $6d\ ^2D_{5/2}$ | 12.37 | 20.27 | 20.19 | 4.05 | 6.63 | 6.60 | | |
| $7d\ ^2D_{5/2}$ | 6.55 | 10.74 | 10.70 | 2.14 | 3.51 | 3.50 | | |
| $8d\ ^2D_{5/2}$ | 3.86 | 6.34 | | 1.26 | 2.07 | | | |
| $9d\ ^2D_{5/2}$ | 2.44 | 4.03 | | 0.80 | 1.32 | | | |

values. In the last column of Table XIII we show two available experimental measurements of $B$ constant for the $5p\,^2P_{3/2}$ and $4d\,^2D_{5/2}$ states. Experimental values for the $5p\,^2P_{3/2}$ state [30] are given with 6% uncertainty. The difference between our $B^{(\mathrm{SD})}$ and $B^{(\mathrm{SDpT})}$ values is 2%. In this case, we can use the experimental value to judge our approximation for the $5p\,^2P_{3/2}$ state. The uncertainty in the $B$ constant for the $4d\,^2D_{5/2}$ given in Ref. [31] is too small to compare with the difference between the experimental value and our $B^{(\mathrm{SD})}$ and $B^{(\mathrm{SDptT})}$ values.

## VII. HYPERFINE-INDUCED TRANSITION POLARIZABILITY OF THE $^{87}$Sr II GROUND STATE

We now turn to the calculation of the quadratic Stark shift of the ground-state hyperfine interval ($F = 5 - F = 4$) in $^{87}$Sr II. The quadratic Stark shift is closely related to the BBR shift discussed, for example, in Refs. [36,49,58,59] and our calculation follows the procedure outlined in [36].

The dominant second-order contribution to the polarizability cancels between the two hyperfine components of the $5s$ state so the Stark shift of the hyperfine interval is governed by the the third-order $F$-dependent polarizability $\alpha_F^{(3)}(0)$. The expression for the $\alpha_F^{(3)}(0)$ is [36]

$$\alpha_F^{(3)}(0) = \frac{1}{3}\sqrt{(2I)(2I+1)(2I+2)}\begin{Bmatrix} j_v & I & F \\ I & j_v & 1 \end{Bmatrix} \times g_I \mu_n (-1)^{F+I+j_v}(2T + C + R), \tag{4}$$

where $g_I$ is the nuclear gyromagnetic ratio, $\mu_n$ is the nuclear magneton, $I = 9/2$ is the nuclear spin, and $j_v = 1/2$ is the total angular momentum of the atomic ground state in Sr II. The $F$-independent sums are ($|v\rangle \equiv |5s_{1/2}\rangle$) given by Eqs. (5) through (7) by [36].

We note first that in the DHF approximation the values of $T$, $C$, and $R$ in atomic units are

$$2T^{\mathrm{DF}} = 5.639\,2 \times 10^{-4}, \quad C^{\mathrm{DF}} = 3.831\,4 \times 10^{-6}, \quad R^{\mathrm{DF}} = 1.016\,9 \times 10^{-3}. \tag{5}$$

Since the value of $C^{\mathrm{DF}}$ is smaller than the $T^{\mathrm{DF}}$ and $R^{\mathrm{DF}}$ by three orders of magnitude, we do not recalculate the $C$ term in the SD approximation.

The expression for $R$ is similar to that for $\alpha^{E1}(0)$ [compare Eqs. (1) and (7) [36]]. The difference is an additional factor of the diagonal hyperfine matrix element

$$\langle 5s_{1/2}\|\mathcal{T}\|5s_{1/2}\rangle^{(\mathrm{SD})} = 7.668\,42 \times 10^{-7}\ \text{a.u.}$$

We evaluate the reduced electric-dipole matrix elements $\langle v\|rC_1\|n\rangle$ in the SD, SDpT, $\mathrm{SD_{sc}}$, and $\mathrm{SDpT_{sc}}$ approximations. We use the available, recommended NIST energies [37] for $nl = 5s$–$13s$,$5p$–$7p$ and SD energies for other states up to $n = 26$. The sum of terms for $n \leqslant 26$ is equal to

$$R^{\mathrm{SD}} = 8.932\,5 \times 10^{-4}, \quad R^{\mathrm{SDpT}} = 9.039\,7 \times 10^{-4}, \quad R^{\mathrm{SD_{sc}}} = 9.005\,3 \times 10^{-4}, \quad R^{\mathrm{SDpT_{sc}}} = 9.000\,9 \times 10^{-4}. \tag{6}$$

Following the procedure described previously, we find $R^{\mathrm{final}} = 9.005(73) \times 10^{-4}$. The remainder of the sum, evaluated in the DHF approximation $R_{n>26} = 3.9 \times 10^{-9}$ is less than 0.001%.

The expression for $T$ includes sums over two indices $m$ and $n$. To calculate the dominant part of $T$, we limit sum over $m$ to four states ($m = 5p_{1/2}$, $5p_{3/2}$, $6p_{1/2}$, $6p_{3/2}$, $7p_{1/2}$, and $7p_{3/2}$) and sum over $n$ up to $n = 26$

$$2T_{\substack{m\leqslant 3\\ n\leqslant 26}} = -\sum_{ns=6s}^{26s}\frac{\langle ns\|\mathcal{T}^{(1)}\|5s\rangle}{(E_{ns}-E_{5s})}\left[\frac{\langle 5s\|rC_1\|5p_{1/2}\rangle\langle 5p_{1/2}\|rC_1\|ns\rangle}{(E_{5p_{1/2}}-E_{5s})} - \frac{\langle 5s\|rC_1\|5p_{3/2}\rangle\langle 5p_{3/2}\|rC_1\|ns\rangle}{(E_{5p_{3/2}}-E_{5s})} + \frac{\langle 5s\|rC_1\|6p_{1/2}\rangle\langle 6p_{1/2}\|rC_1\|ns\rangle}{(E_{6p_{1/2}}-E_{5s})} - \frac{\langle 5s\|rC_1\|6p_{3/2}\rangle\langle 6p_{3/2}\|rC_1\|ns\rangle}{(E_{6p_{3/2}}-E_{5s})} + \frac{\langle 5s\|rC_1\|7p_{1/2}\rangle\langle 7p_{1/2}\|rC_1\|ns\rangle}{(E_{7p_{1/2}}-E_{5s})} - \frac{\langle 5s\|rC_1\|7p_{3/2}\rangle\langle 7p_{3/2}\|rC_1\|ns\rangle}{(E_{7p_{3/2}}-E_{5s})}\right]. \tag{7}$$

The sum of the six contributions from Eq. (7) is $5.491\,9 \times 10^{-4}$, $5.535\,7 \times 10^{-4}$, $5.528\,6 \times 10^{-4}$, and $5.524\,2 \times 10^{-4}$ in the SD, SDpT, $\mathrm{SD_{sc}}$, and $\mathrm{SDpT_{sc}}$ approximations, respectively. The ratio of contributions to the sum from the $6p$ and $7p$ to $5p$ states is surprisingly very small (about $10^{-3}$). The relatively small remainder $T - T_{\substack{m>7\\ n>26}} = 0.010\,5 \times 10^{-4}$ is evaluated in the DHF approximation, leading to a final value $2T^{(\mathrm{final})} = 5.539(37) \times 10^{-4}$. Combining these contributions, we obtain

$$2T^{\mathrm{final}} + C^{\mathrm{DF}} + R^{\mathrm{final}} = 1.458(11) \times 10^{-3}\ \text{a.u.} \tag{8}$$

The $F$-dependent factor [see Eq. (4)]

$$A(F) = \frac{g_I\mu_n}{3I}\sqrt{(2I)(2I+1)(2I+2)} \times \begin{Bmatrix} j_v & I & F \\ I & j_v & 1 \end{Bmatrix}(-1)^{F+I+j_v},$$

is equal to 0.363526 for $F = 4$ and $-0.297431$ for $F = 5$.

Using these values and the result from Eq. (8), we obtain

$$\alpha_{F=5}^{(3)}(0) - \alpha_{F=4}^{(3)}(0) = -9.638(72) \times 10^{-4}\ \text{a.u.}$$

The Stark shift coefficient $k$ defined as $\Delta\nu = kE^2$ is $k = -\frac{1}{2}[\alpha^{(3)}_{F=5}(0) - \alpha^{(3)}_{F=4}(0)]$. Converting from atomic units, we obtain

$$k^{(\mathrm{final})} = 4.819(36) \times 10^{-4}\,\mathrm{a.u.} = 1.199(9) \times 10^{-11}\ \mathrm{Hz/(V/m)^2}.$$

In the DHF approximation [Eq. (5)], we find $k^{(\mathrm{DF})} = 1.303\,1 \times 10^{-11}\mathrm{Hz/(V/m)^2}$.

The relative blackbody radiative shift $\beta$ is defined as

$$\beta = -\frac{2}{15}\frac{1}{\nu_{\mathrm{hf}}}(\alpha\pi)^3 T^4 \alpha_{\mathrm{hf}}(5s_{1/2}), \tag{9}$$

where $\nu_{\mathrm{hf}}$ is the $^{87}$Sr II hyperfine ($F = 5$ and $F = 4$) splitting equal to 5002.368 365 MHz and $T$ is a temperature equal to 300 K. Using those factors, we can rewrite Eq. (9)

$$\beta = -1.721\,42 \times 10^{-12}\,\alpha_{\mathrm{hf}}(5s_{1/2}). \tag{10}$$

Using the SD value for $\alpha_{\mathrm{hf}}(5s_{1/2}) = -9.638(72) \times 10^{-4}$ a.u., we obtain finally

$$\beta^{(\mathrm{SD})} = 1.66(1) \times 10^{-15}. \tag{11}$$

## VIII. CONCLUSION

In summary, a systematic RMBPT study of the energies of the $ns_{1/2}$, $np_j$, $nd_j$, and $nf_j$ ($n \leqslant 9$) states in singly ionized strontium is presented. The energy values are in excellent agreement with the existing experimental data. Electric-dipole ($5s_{1/2}$-$np_j$, $n = 5$–26), electric-quadrupole ($5s_{1/2}$-$nd_j$, $n = 4$–26), and electric-octupole ($5s_{1/2}$-$nf_j$, $n = 4$–26) matrix elements are calculated to obtain the ground-state $E1$, $E2$, and $E3$ static polarizabilities. Scalar polarizabilities of the $ns_{1/2}$, $np_j$, and $nd_j$ states and tensor polarizabilities of the $np_{3/2}$ and $nd_j$ excited states of Sr II are evaluated by including matrix elements with high $n$ up to $n = 26$. All of the previously mentioned matrix elements are determined using the all-order method. Hyperfine $A$ and B values are presented for the first low-lying levels up to $n = 7$. The quadratic Stark shift of the ground-state hyperfine interval in $^{87}$Sr II is also evaluated. These calculations provide a theoretical benchmark for comparison with the experiment and theory.

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