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Relativistic many-body calculation of energies, lifetimes, hyperfine constants, multipole polarizabilities, and blackbody radiation shift in ^{137}Ba II

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Excitation energies of the [Xe]$ns_{1/2}$, [Xe]np_j, and [Xe]nd_j ($n \leqslant 12$ and [Xe] = $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^6$) in Ba II are evaluated. First-, second-, third-, and all-order Coulomb energies and first- and second-order Coulomb-Breit energies are calculated. Electric-dipole ($6s_{1/2}$-np_j, $n = 6$–26), electric-quadrupole ($6s_{1/2}$-nd_j, $n = 5$–26), and electric-octupole ($6s_{1/2}$-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 Ba$^+$ are evaluated. All aforementioned matrix elements are determined using the relativistic all-order method. The hyperfine structure in ^{137}Ba II is also investigated. The hyperfine A and B values are determined for the first low-lying levels up to $n = 9$. The quadratic Stark effect on hyperfine structure levels of ^{137}Ba II ground state is investigated. The calculated shift for the ($F = 2$, $M = 0$) ↔ ($F = 1$, $M = 0$) transition is -0.2931 Hz/(kV/cm)^2, in agreement with a previous theoretical result, $-0.284(3)$). These calculations provide a theoretical benchmark for comparison with experiment and theory.

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I. INTRODUCTION

Recently, the $6s$-np_j ($n = 6$–9) electric-dipole matrix elements and $6s$-nd_j ($n = 5$–7) electric-quadrupole matrix elements in Ba$^+$ were calculated by Iskrenova-Tchoukova and Safronova [1] using the relativistic all-order linearized coupled-cluster method. This set of matrix elements was needed in Ref. [1] for accurate calculation of 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, and $n_3 = 5$–7) electric-dipole matrix elements were evaluated by Dzuba *et al.* [2] to determine the parity-nonconserving $6s$-$5d$ amplitudes in Ba$^+$. Correlation corrections to the electron orbitals were calculated using the correlation potential method. Dzuba *et al.* [3] carried out accurate *ab initio* nonperturbative calculations of the Breit correction to the parity nonconserving (PNC) amplitudes of the $6s$-$5d_{3/2}$ transition in Ba$^+$. Electric dipole and quadrupole transition amplitudes in Ba$^+$ were calculated by Gopakumar *et al.* [4] using the RCC 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 [4] using relativistic third-order many-body perturbation theory (MBPT). It was mentioned in Ref. [4] that a very elaborate description of the preceding types of corrections with the associated diagrams were given in the article by Blundell *et al.* [5].

Sherman *et al.* [6] compared values of the dipole matrix elements for the $6s$-np_j and $5d_{3/2}$-np_j transitions with $n =$ 6–8 given in Refs. [1,2,4]. Excellent agreement (less than 1% disagreement) was found only for the $6s$-$6p_j$ dipole matrix elements. Results in Refs. [2,4] for the $5d_{3/2}$-$6p_j$, $5d_{3/2}$-$7p_j$, and $5d_{3/2}$-$8p_j$ dipole matrix elements disagree by 3.6%, 17%, 5.8% (for $j = 1/2$) and by 3.8%, 12%, 7.1% (for $j = 13/2$), respectively. The largest disagreement (by factor of 2–10) was found between results for the $6s$-$7p_j$ and $6s$-$8p_j$ dipole matrix elements. Sherman *et al.* [6] presented also recently published recommended National Institute of Standards and Technology (NIST) values [7] for the aforementioned transitions. It is difficult to comment about the accuracy of those recommended NIST values since they were based on theoretical values [8] rather than measurements. The nonrelativistic Coulomb approximation was used by Lindgård and Nielsen in Ref. [8] to evaluate transition rates for the alkali-metal isoelectronic sequences.

Recently, the relativistic coupled-cluster (RCC) method was used by Sahoo *et al.* [9] to calculate electric dipole matrix elements in Ba$^+$. Authors underlined that accurate determination of the electric dipole matrix elements is essential in achieving sub-1% PNC amplitudes. Tabulated values for the dipole matrix elements differs by 1–5% from results previously published in [4], where the RCC method was also used. The difference in results was explained by the use of a mix of numerical orbitals from the GRASP code and Gaussian-type analytical orbitals (GTOs). In contrast, the purely analytical GTOs were used in Ref. [9]. It should be noted that the largest difference (factor of 2–5) in the [4] and [9] results happens for the $6s$-$7p_{3/2}$ and $6s$-$8p_j$ dipole matrix elements.

In present article, electric-dipole matrix elements are evaluated in the all-order SD and SDpT approximations (single-double all-order method including partial triple excitations [10]). This approach differs from Ref. [1] by the treatments of the Breit interaction. In Ref. [1], Breit contributions to the Dirac-Fock potential was omitted and Breit corrections were included perturbatively in second-order MBPT. In the approach used in the present article, I include both Coulomb and Breit contributions to the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. B splines [11] are used to generate a complete set of Dirac-Fock (DF) basis orbitals for use in the evaluation of all atomic properties.

Dipole matrix elements were used to calculate oscillator strengths, transition rates, and lifetimes in Ba$^+$ ion. More than 40 years ago, Warner [12] reported oscillator strengths for the ns-$n'p$, np-$n'd$, and nd-$n'f$ transitions with $ns = 6s$-$11s$,

$np = 6p$-$8p$, $nd = 5d$-$10d$, and $nf = 4f$-$7f$. The radial wave functions were taken to be scaled Thomas-Fermi-Dirac wave functions with including spin-orbit interaction [12]. The relativistic pseudopotential approach was applied by Hafner and Schwarz [13] to the calculation of electric-dipole transition probabilities in Ba^+ for the ns-$n'p$ and $(n-1)s$-$n'p$ transitions with $n = 6$–9 and $n' = 6$–8. Relativistic Hartree-Fock oscillator strengths for the lowest $6s\,^2S_{1/2}$–$6p\,^2P_{1/2,3/2}$ transitions in Ba II, with allowance for core polarization, were presented by Migdalek and Baylis [14]. Model potential calculations were performed by Migdalek and Wyrozumska [15] to investigate the influence of valence-core electron exchange on Ba II oscillator strength. Tabulated values of oscillator strengths were given for the $6s$-$6p$, $6p$-$5d$, $6p$-$6d$, $6p$-$7d$, $5d$-$4f$, $5d$-$5f$, and $5d$-$6f$ transitions [15]. A relativistic Hartree-Fock method, being a slight modification of the conventional formulation and closely related to the approach of Cowan and Griffin [16], was examined by Karwowski and Szulkin [17] to calculate oscillator strengths for the Cs isoelectronic series. Numerical results for Ba II were given for the $6s$-$7p$ transition. A quasirelativistic local spin density functional with correlation energy was used in conjunction with the concept of a Slater transition state to calculate the (ns-np) dipole oscillator strength in Ba II ($n = 6$) and other alkali-metal atomic systems [18]. Relativistic MBPT was applied by Guet and Johnson [19] to determine the $6s$-$6p$ and $6p$-$5d$ dipole matrix elements and the lifetimes of the $6p_{1/2}$ and $6p_{3/2}$ states.

Experimental measurements of oscillator strengths, branching ratios, and lifetimes were performed in Refs. [20–39]. High-precision measurement of the branching ratios from the $6p\,^2P_{3/2}$ state of Ba II into all dipole-allowed decay channels, $6s\,^2S_{1/2}$, $5d\,^2D_{3/2}$, and $5d\,^2D_{5/2}$, was presented by Kurz *et al.* [39]. Relative strengths normalized to unity were found to be 0.756 ± 0.046, 0.0290 ± 0.0015, and 0.215 ± 0.0064 for the $6s\,^2S_{1/2}$, $5d\,^2D_{3/2}$, and $5d\,^2D_{5/2}$ channels, respectively. Those results were compared in [39] with other measurements [21, 36] and theoretical calculations [2,4,19]. I mentioned earlier that critically evaluated transition rates, oscillator strengths, and line strengths were given by Klose *et al.* [7]. Energy levels, wavelengths, and transition probabilities for the second spectra of barium, Ba II, were compiled by Curry [40]. Wavelengths of observed transitions and energy levels derived from those wavelengths were critically evaluated using the available literature. Measured and calculated transition probabilities for some of the observed transitions were obtained from the recent compilation of Klose *et al.* [7].

The lifetimes of the metastable $5d\,^2D_{3/2}$ and $5d\,^2D_{5/2}$ levels in Ba^+ is a subject of theoretical and experimental studies owing to their application in various fields such as optical frequency standards, quantum information, and astronomy. Therefore, a separate overview of the recent status of these values is presented. Recently, precision lifetime measurements of the $5d\,^2D_{5/2}$ level in Ba^+ was given by Royen *et al.* in Ref. [41]. Precision measurements and calculations of the $5d\,^2D_J$ lifetimes were presented by Gurell *et al.* [42]. The experiment utilized a laser probing technique (LPT) together with a beam of Ba^+ ions stored in the ion storage ring CRYRING at the Manne Siegbahn Laboratory in Stockholm, Sweden. Three different theoretical models were considered within the framework of the pseudorelativistic Hartree-Fock (HFR) method described by Cowan [43]. In a first calculation [HFR(A)], only valence correlation was considered in the physical model including the $5s^25p^6ns$ ($n = 6$–8) and $5s^25p^6nd$ ($n = 5$–8) configurations. In a second calculation [HFR(B)], some core-valence correlations were included by means of additional configurations with one hole in the $5s$ or $5p$ subshell. In the third calculation [HFR(C)], the [HFR(B)] model was extended with configurations characterized by two holes in the $5s$ or $5p$ subshell. Recently [1], the calculation of the $5d\,^2D_J$–$6s\,^2S_{1/2}$ electric-quadrupole matrix elements in Ba^+ was carried out using an *ab initio* relativistic all-order method which sums infinite sets of MBPT terms. These matrix elements were used to evaluate the $5d$-level radiative lifetimes and their ratio [1]. In Ref. [44], the RCC theory was used to perform accurate calculations of the lifetimes of the lowest excited $5d\,^2D_J$ states in singly ionized barium. The calculations of the $5d\,^2D_J$ lifetimes in Ref. [2] were performed with fitted Brueckner orbitals; core polarization, structural radiation, and normalization contributions were included in the $E2$ transition amplitudes. The $M1$ contribution to lifetime of the lowest excited (metastable) $5d_{5/2}$ state arising from transitions to $5d_{3/2}$ state in Ba II was evaluated by Guet and Johnson in errata [45]. It was emphasized that this contribution should be added to transition rates given previously in Ref. [19] to obtain the correct value of the lifetime of the $5d_{5/2}$ state. Early theoretical calculations and measurements of the $5d\,^2D_{3/2}$ and $5d\,^2D_{5/2}$ lifetimes in Ba^+ were presented in Refs. [46–51].

One of the first measurements of the dipole (α_0) and quadrupole (α_2) polarizabilities in Ba II was performed by Gallagher *et al.* in Ref. [52]. The values of α_0 and α_2 were found to be equal to $125.5 \pm 10\ a_0^3$ and $2050 \pm 100\ a_0^5$. More than 20 years later, Snow *et al.* in Ref. [53] reported determination of dipole and quadrupole polarizabilities of Ba^+ by measuring the fine structure of high-L $n = 9$ and 10 Rydberg states of barium. Their values of α_0 and α_2 were in good agreement with previous results, taking into account uncertainties in both measurements ($\alpha_0 = 124.30 \pm 0.16\ a_0^3$ and $\alpha_0 = 2462 \pm 361\ a_0^5$). A few years later, Snow and Lundin in Ref. [54] determined the dipole and quadrupole polarizabilities of Ba^+ using fine-structure measurements in high-L $n = 17$ and 20 Rydberg states of barium. The reported value of dipole polarizability only slightly changed ($123.88 \pm 5\ a_0^3$); however, the value of quadrupole polarizability dramatically changed ($4420 \pm 250\ a_0^5$) in comparison with result in [53], owing to including contributions from higher-excited levels as described in [55]. This last experimental value of quadrupole polarizability was in a good agreement with the theoretical result published by Iskrenova-Tchoukova and Safronova [1]. Patil and Tang [56] gave a 10% larger number for quadrupole polarizability ($4821\ a_0^5$) using simple wave functions based on the asymptotic behavior and on the binding energies of the valence electron. Dipole polarizability in Ba II was evaluated by Lim and Schwerdtfeger in Ref. [57]. Static dipole polarizabilities were calculated by RCC calculations using finite field techniques together with carefully optimized Gaussian-type basis sets [57].

High-precision measurement of the ground-state hyperfine splitting of $^{137}Ba^+$ was presented by Blatt and Werth [58].

The magnetic dipole hyperfine constant was determined to be $A = 4018.870\,833\,85(18)$ mHz. Early measurements of the A constant for the $6s^2S_{1/2}$ state were presented in Refs. [59,60]. Ground-state magnetic-dipole hyperfine coupling constants A for different Ba$^+$ isotopes (^{135}Ba$^+$, ^{133}Ba$^+$, and ^{131}Ba$^+$) measured in a Paul ion trap were presented by Trapp *et al.* in Ref. [61]. The magnetic dipole A and electric quadrupole B hyperfine constants for the $6p^2P_{3/2}$ state were measured by collinear fast-beam laser spectroscopy [62]. The hyperfine structure of the $5d^2D_{5/2}$ states in ^{135,137}Ba$^+$ was studied by Silverans *et al.* [63] using fast-ion-beam laser-rf spectroscopy.

The RCC method was applied by Sahoo *et al.* [64] to calculate the magnetic dipole hyperfine constant A of the $6s_{1/2}$, $6p_{1/2}$, $6p_{3/2}$, and $5d_{3/2}$ states of singly ionized barium, ^{137}Ba$^+$. After the inclusion of two-body correlation effects into the computation of the hyperfine matrix elements, the accuracy of the resulting values was significantly increased compared to earlier computations [65]. The RCC method was used later in Ref. [66] to determine the hyperfine constants A for the $7s_{1/2}$, $7p_{1/2}$, $7p_{3/2}$, and $5d_{5/2}$ states and the hyperfine constants B for the $6p_{3/2}$, $7p_{3/2}$, and $5d_j$ states. A slightly different value of the hyperfine constants A for the ground $6s_{1/2}$ state was given by Sur *et al.* [67]. The relativistic MBPT method was used by Dzuba *et al.* [68] to determine the magnetic dipole hyperfine constant A of the $6s_{1/2}$ state in ^{137}Ba$^+$.

In the present article, relativistic all-order SD and SDpT approximations (single-double all-order method including partial triple excitation) methods are used to calculate atomic properties of singly ionized barium for the ns, np_j, nd_j, and nf_j ($n \leqslant 10$) states. I evaluate a large number of transition matrix elements to calculate $E1$, $E2$, 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 Ba$^+$. 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 $n = 8$. The quadratic Stark effect on hyperfine structure levels of ^{137}Ba II ground state is investigated.

In the present work, the relativistic single-double method is also used; however, the number of the basis-set orbitals is increased to 70 instead of 50 used in [1] to increase the number of states considered. B splines [11] are used to generate a complete set of DF basis orbitals for use in the evaluation of all atomic properties. The present calculation of the polarizabilities required accurate representation of rather highly excited states, such as $6l_j$-$13l_j$, leading to the use of the large $R = 220$ a.u. cavity for the generation of the finite basis set and higher number of splines to produce high-accuracy single-particle orbitals.

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

Energies of nl_j states in Ba II are evaluated for $n \leqslant 12$ and $l \leqslant 2$ using both third-order relativistic many-body perturbation theory (RMBPT) and the single-double (SD) all-order method discussed in Refs. [69,70], in which single and double excitations of DF wave functions are iterated to all orders. Results of my energy calculations are summarized in Table I. Columns 2–6 of Table I give the lowest-order DF energies $E^{(0)}$, second-order and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, second-order Breit corrections $B^{(2)}$, 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 [71]. 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 [72–74] using Coulomb wave functions. For this purpose, an effective nuclear charge Z_{eff} is obtained by finding the value of Z_{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. I list the all-order SD energies in the column labeled E^{SD} and list that part of the third-order energies missing from E^{SD} in the column labeled $E^{(3)}_{\mathrm{extra}}$. The sum of the five terms $E^{(0)}$, E^{SD}, $E^{(3)}_{\mathrm{extra}}$, $B^{(2)}$, and $E^{(\mathrm{LS})}$ give the final all-order result $E^{\mathrm{SD}}_{\mathrm{tot}}$, listed in the 10th column of Table I. Recommended energies from the NIST database [75] are given in the column labeled E_{NIST}. Differences between my third-order and all-order calculations 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 rightmost columns of Table I, respectively. As mentioned earlier, I include both Coulomb and Breit contributions to the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. As a result, the first-order Breit correction $B^{(1)}$ was already included in the lowest-order DF energies $E^{(0)}$ and omitted from Table I.

As expected, the largest correlation contribution to the valence energy comes from the second-order term $E^{(2)}$. Therefore, $E^{(2)}$ is calculated 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. [76,77] for details of the extrapolation procedure). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, consider the $6s_{1/2}$ state. Calculations of $E^{(2)}$ with $l_{\max} = 6$ and 8 yield $E^{(2)}(5d_{3/2}) = -8911.0$ and -9079.3 cm^{-1}, respectively. Extrapolation of these calculations yields -9148.4 and -9137.3 cm^{-1}, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(5d_{3/2})$ of 10.1 cm^{-1}. It should be noted that the 168.3 cm^{-1} contribution from partial waves with $l > 6$ for the $6s$ state is the largest among all states considered in Table I. For example, we find $E^{(2)}(6s_{1/2}) = -6520.5$ and -6558.6 cm^{-1} with $l_{\max} = 6$ and 8; that gives the 38.1 cm^{-1} contribution from partial waves with $l > 6$. Extrapolation of these calculations yields -6577.3 and -6577.2 cm^{-1}, respectively. That gives a numerical uncertainty in $E^{(2)}(6s_{1/2})$ of only 0.1 cm^{-1}.

Owing to the computational complexity, $l \leqslant l_{\max} = 6$ is restricted in the E^{SD} calculation. As noted previously, the second-order contribution dominates E^{SD}; therefore, we can use the extrapolated value of the $E^{(2)}$ described previously to account for the contributions of the higher partial waves.

TABLE I. Zeroth-order (DF), second- and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies E^{SD}, $E^{(3)}_{\mathrm{extra}}$, second-order Coulomb-Breit corrections $B^{(2)}$ to the energies of Ba II. The total energies [$E^{(3)}_{\mathrm{tot}} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(2)}$, $E^{\mathrm{SD}}_{\mathrm{tot}} = E^{(0)} + E^{\mathrm{SD}} + E^{(3)}_{\mathrm{extra}} + B^{(1)} + B^{(2)}$] for Ba II are compared with experimental energies E_{NIST} [75], $\delta E = E_{\mathrm{tot}} - E_{\mathrm{NIST}}$. Units: cm^{-1}.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(2)}$	$E^{(LS)}$	$E^{(3)}_{\mathrm{tot}}$	E^{SD}	$E^{(3)}_{\mathrm{extra}}$	$E^{\mathrm{SD}}_{\mathrm{tot}}$	E_{NIST}	$\delta E^{(3)}$	δE^{SD}
$6s_{1/2}$	−75 326	−6577.3	2332.8	−102.4	8.0	−79 665	−5975.7	1012.5	−80 383	−80 686	1022	303
$6p_{1/2}$	−57 237	−3631.9	1122.1	−48.4	−0.2	−59 795	−3517.4	516.4	−60 287	−60 425	629	138
$6p_{3/2}$	−55 861	−3281.0	1011.0	−46.7	0.1	−58 177	−3175.2	465.0	−58 618	−58 734	556	116
$5d_{3/2}$	−68 183	−9148.4	2738.7	−257.4	0.0	−74 850	−8401.4	1220.9	−75 621	−75 812	962	191
$5d_{5/2}$	−67 727	−8699.5	2548.1	−246.3	0.0	−74 125	−8024.4	1136.0	−74 862	−75 011	886	149
$7s_{1/2}$	−36 846	−1884.4	687.2	−32.2	0.8	−38 075	−1625.1	294.8	−38 208	−38 331	256	123
$7p_{1/2}$	−30 229	−1247.5	400.1	−18.9	−0.1	−31 095	−1158.0	181.1	−31 225	−31 296	201	72
$7p_{3/2}$	−29 694	−1147.4	367.7	−18.4	0.0	−30 492	−1066.5	165.9	−30 613	−30 675	183	62
$6d_{3/2}$	−33 272	−1758.8	501.6	−49.4	0.0	−34 579	−1542.6	235.1	−34 629	−34 737	158	108
$6d_{5/2}$	−33 104	−1704.9	479.2	−48.2	0.0	−34 378	−1505.4	224.1	−34 434	−34 531	153	98
$7d_{3/2}$	−20 254	−753.0	213.0	−21.2	0.0	−20 815	−663.2	100.8	−20 837	−20 886	71	49
$7d_{5/2}$	−20 172	−734.0	205.3	−20.8	0.0	−20 722	−650.4	96.8	−20 746	−20 791	70	45
$8s_{1/2}$	−22 021	−823.1	303.6	−14.6	0.0	−22 555	−696.5	129.4	−22 602	−22 661	106	59
$8p_{1/2}$	−18 842	−593.8	192.8	−9.4	0.0	−19 253	−543.2	86.8	−19 308	−19 347	94	38
$8p_{3/2}$	−18 577	−550.7	178.8	−9.2	0.0	−18 958	−504.6	80.2	−19 011	−19 044	86	34
$8d_{3/2}$	−13 673	−402.0	113.3	−11.3	0.0	−13 973	−354.9	53.9	−13 986	−14 013	39	27
$8d_{5/2}$	−13 628	−393.0	109.7	−11.1	0.0	−13 922	−348.9	52.0	−13 936	−13 961	38	25
$9s_{1/2}$	−14 665	−436.8	161.9	−7.9	−0.1	−14 948	−366.2	68.8	−14 970	−15 003	55	32
$9p_{1/2}$	−12 894	−331.7	108.2	−5.3	0.0	−13 123	−301.3	48.6	−13 152	−13 175	52	23
$9p_{3/2}$	−12 743	−309.1	100.9	−5.3	0.0	−12 957	−281.2	45.2	−12 984	−13 005	48	20
$9d_{3/2}$	−9862	−241.8	68.0	−6.8	0.0	−10 042	−213.7	32.4	−10 050	−10 066	24	16
$9d_{5/2}$	−9833	−236.8	66.0	−6.7	0.0	−10 011	−210.4	31.4	−10 019	−10 034	23	15
$10s_{1/2}$	−10 471	−260.2	96.7	−4.7	−0.1	−10 640	−217.1	41.0	−10 652	−10 672	32	20
$10p_{1/2}$	−9384	−204.6	66.9	−3.3	0.0	−9525	−185.1	30.1	−9543	−9556	31	14
$10p_{3/2}$	−9290	−191.3	62.6	−3.3	0.0	−9422	−173.3	28.0	−9439	−9451	29	12
$10d_{3/2}$	−7451	−157.2	44.1	−4.4	0.0	−7569	−139.0	21.1	−7574	−7585	16	11
$10d_{5/2}$	−7433	−154.1	42.9	−4.3	0.0	−7548	−136.9	20.4	−7554	−7564	16	10
$11s_{1/2}$	−7852	−167.8	62.4	−3.1	0.0	−7961	−139.5	26.5	−7968	−7981	20	13
$11p_{1/2}$	−7137	−135.2	44.3	−2.2	0.0	−7231	−122.0	19.9	−7242	−7250	20	8
$11p_{3/2}$	−7075	−126.7	41.5	−2.2	0.0	−7162	−114.5	18.6	−7173	−7180	17	7
$11d_{3/2}$	−5829	−109.0	30.3	−3.0	0.0	−5911	−95.6	14.5	−5913	−5921	10	7
$11d_{5/2}$	−5816	−107.0	29.5	−3.0	0.0	−5897	−94.2	14.1	−5900	−5906	9	7
$12s_{1/2}$	−6107	−115.1	42.6	−2.1	0.0	−6181	−95.0	18.1	−6186	−6195	13	9
$12p_{1/2}$	−5612	−96.0	30.9	−1.6	0.0	−5679	−84.7	13.9	−5684	−5689	10	5
$12p_{3/2}$	−5568	−90.4	29.0	−1.6	0.0	−5631	−79.7	13.0	−5636			
$12d_{3/2}$	−4685	−77.5	21.7	−2.6	0.0	−4744	−68.6	10.4	−4746			
$12d_{5/2}$	−4676	−76.1	21.2	−2.6	0.0	−4734	−67.7	10.1	−4736	−4740	7	4

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}), the second-order remainder is used as a guide to estimate the remainder in the third-order contribution. The term $E^{(3)}_{\mathrm{extra}}$ 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 an order of magnitude for the states considered here.

The column labeled δE^{SD} in Table I gives differences between my *ab initio* results and the available experimental values [75]. The SD results agree better with recommended values than do the third-order MBPT results (the ratio of $\delta E^{(3)}/\delta E^{\mathrm{SD}}$ is about three for some of cases), illustrating the importance of fourth- and higher-order correlation corrections.

It should be noted that the nf states are not included in Table I. Unfortunately, calculations of the nf states present convergence problems in the present implementation of the all-order method.

III. REDUCED MULTIPLE MATRIX ELEMENTS IN BA 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 correlation corrections. Reduced electric-dipole matrix elements between low-lying states of Ba II calculated with the third-order RMBPT and with the all-order SD approximation are presented in Table II. Only a limited number of transitions are included in this table to illustrate the results and compare with other high-precision results given in Refs. [2,4,9].

TABLE II. Reduced electric-dipole matrix elements calculated with first-order, second-order, third-order MBPT, SD, and SDpT methods (SD all-order method including partial triple excitations) in Ba II are compared with theoretical results given by Dzuba *et al.* [2], Gopakumar *et al.* [4], and Sahoo *et al.* [9].

Transition		$Z^{(\mathrm{DF})}$	$Z^{(\mathrm{DF+2})}$	$Z^{(\mathrm{DF+2+3})}$	$Z^{(\mathrm{SD})}$	$Z^{(\mathrm{SDpT})}$	Ref. [2]	Ref. [4]	Ref. [9]
$6p_{1/2}$	$6s_{1/2}$	3.8915	3.5276	3.2754	3.3380	3.3710	3.310	3.3266	3.36
$6p_{1/2}$	$7s_{1/2}$	2.5524	2.5981	2.5003	2.4652	2.4770	2.493	2.3220	2.44
$6p_{1/2}$	$8s_{1/2}$	0.7021	0.7256	0.7026	0.6973	0.6993	0.705	0.7283	0.66
$6p_{1/2}$	$5d_{3/2}$	3.7405	3.4183	2.9023	3.0503	3.0957	3.055	2.9449	3.11
$6p_{1/2}$	$6d_{3/2}$	5.1500	5.0117	4.9278	4.8531	4.8793	4.889		4.89
$6p_{1/2}$	$7d_{3/2}$	1.5506	1.4524	1.3952	1.3925	1.4008	1.373		1.50
$7p_{1/2}$	$6s_{1/2}$	0.0671	−0.0881	−0.0455	−0.0605	−0.0607	−0.099	0.1193	0.10
$7p_{1/2}$	$7s_{1/2}$	7.3916	7.2600	6.9128	6.9984	7.0361	7.008	7.3300	
$7p_{1/2}$	$8s_{1/2}$	5.0940	5.1262	4.9884	4.9411	4.9609	4.964	2.0804	
$7p_{1/2}$	$5d_{3/2}$	0.3543	0.2148	0.3155	0.2792	0.2775	0.261	0.3050	0.28
$7p_{1/2}$	$6d_{3/2}$	9.1821	9.0956	8.5168	8.6411	8.6894	8.646		
$7p_{1/2}$	$7d_{3/2}$	8.3760	8.3438	8.2169	8.1702	8.2038	8.238		
$8p_{1/2}$	$6s_{1/2}$	0.0062	0.1043	0.0816	0.0868	0.0866	0.115	0.4896	0.11
$8p_{1/2}$	$7s_{1/2}$	0.2018	0.1277	0.1698	0.1368	0.1354	0.113	−0.6021	
$8p_{1/2}$	$8s_{1/2}$	11.9154	11.8537	11.4129	11.5286	11.5753	11.556	8.2315	
$8p_{1/2}$	$5d_{3/2}$	0.1971	0.1087	0.1481	0.1346	0.1349	0.119	0.1121	0.13
$8p_{1/2}$	$6d_{3/2}$	0.0941	0.0489	0.1483	0.1108	0.1090	0.117		
$8p_{1/2}$	$7d_{3/2}$	16.1846	16.1466	15.4495	15.5780	15.6387	15.582		
$6p_{3/2}$	$6s_{1/2}$	5.4785	4.9820	4.6177	4.7097	4.7569	4.6746	4.6982	4.73
$6p_{3/2}$	$7s_{1/2}$	3.9583	4.0078	3.9028	3.8451	3.8587	3.8826	3.6482	3.80
$6p_{3/2}$	$8s_{1/2}$	1.0297	1.0545	1.0231	1.0172	1.0201	1.0256	1.0518	0.97
$6p_{3/2}$	$5d_{3/2}$	1.6335	1.5003	1.2635	1.3324	1.3532	1.3346	1.2836	1.34
$6p_{3/2}$	$5d_{5/2}$	4.9927	4.6074	3.9108	4.1032	4.1631	4.1186	3.9876	4.02
$6p_{3/2}$	$6d_{3/2}$	2.4482	2.3811	2.3537	2.3182	2.3287	2.3346		2.33
$6p_{3/2}$	$6d_{5/2}$	7.2633	7.0679	6.9734	6.8768	6.9095	6.9236		6.91
$6p_{3/2}$	$7d_{3/2}$	0.6900	0.6439	0.6136	0.6139	0.6180	0.6046		0.67
$6p_{3/2}$	$7d_{5/2}$	2.0869	1.9519	1.8678	1.8667	1.8782	1.8386		2.01
$7p_{3/2}$	$6s_{1/2}$	0.2615	0.0414	0.1101	0.0870	0.0858	0.035	0.3610	0.17
$7p_{3/2}$	$7s_{1/2}$	10.3131	10.1371	9.6276	9.7571	9.8122	9.773	10.2645	
$7p_{3/2}$	$8s_{1/2}$	7.8123	7.8495	7.7073	7.6301	7.6527	7.660	3.0172	
$7p_{3/2}$	$5d_{3/2}$	0.1872	0.1283	0.1703	0.1555	0.1548	0.147	0.1645	0.16
$7p_{3/2}$	$5d_{5/2}$	0.5461	0.3764	0.4918	0.4513	0.4500	0.432	0.4788	0.46
$7p_{3/2}$	$6d_{3/2}$	4.0174	3.9845	3.7140	3.7736	3.7961	3.775		
$7p_{3/2}$	$6d_{5/2}$	12.2054	12.1044	11.3195	11.4837	11.5489	11.492		
$7p_{3/2}$	$7d_{3/2}$	4.0133	3.9949	3.9598	3.9341	3.9468	3.963		
$7p_{3/2}$	$7d_{5/2}$	11.8661	11.8141	11.6869	11.6228	11.6633	11.707		
$8p_{3/2}$	$6s_{1/2}$	0.0789	−0.0618	−0.0236	−0.0331	−0.0334	−0.073	−0.5710	0.11
$8p_{3/2}$	$7s_{1/2}$	0.5683	0.4664	0.5414	0.4950	0.4912	0.463	−0.5514	
$8p_{3/2}$	$8s_{1/2}$	16.5521	16.4706	15.8128	15.9899	16.0592	16.032	12.6033	
$8p_{3/2}$	$5d_{3/2}$	0.1023	0.0647	0.0825	0.0768	0.0769	0.070	0.0650	0.07
$8p_{3/2}$	$5d_{5/2}$	0.2993	0.1924	0.2384	0.2232	0.2239	0.206	0.1926	0.21
$8p_{3/2}$	$6d_{3/2}$	0.1313	0.1138	0.1599	0.1436	0.1422	0.146		
$8p_{3/2}$	$6d_{5/2}$	0.3254	0.2725	0.4017	0.3578	0.3548	0.364		
$8p_{3/2}$	$7d_{3/2}$	7.0929	7.0791	6.7499	6.8117	6.8403	6.814		
$8p_{3/2}$	$7d_{5/2}$	21.5026	21.4593	20.5055	20.6744	20.7570	20.685		

My calculations of reduced matrix elements in the lowest, second, and third orders are carried out following the method described in Refs. [10,78]. 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 correction $B^{(2)}$ is rather small in comparison with the second-order Coulomb correction $Z^{(2)}$ [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 orbital (BO) corrections, the structural radiation $Z^{(\mathrm{SR})}$, and normalization $Z^{(\mathrm{NORM})}$ terms (see [79] for definition of these terms).

The smallest differences (5–15%) between $Z^{(\mathrm{DF+2+3})}$ and $Z^{(\mathrm{DF})}$ are for the transitions involving $6p_j$ states ($6p_j$-$ns_{1/2}$

TABLE III. Reduced electric-dipole matrix elements in first, second, and third orders of perturbation theory, calculated in length (L) and velocity (V) forms for Ba II, are compared with results given by Sahoo *et al.* [9].

Transitions		$Z^{(\mathrm{DF})}_{vw}$		$Z^{(\mathrm{DF+2})}_{vw}$		$Z^{(\mathrm{DF+2+3})}_{vw}$		
v	w	L	V	L	V	L	V	Ref. [9]
$5d_{3/2}$	$4f_{5/2}$	4.2074	4.0258	3.7976	3.7976	3.6216	3.6189	3.75
$5d_{3/2}$	$5f_{5/2}$	2.3333	2.1921	1.9677	1.9678	1.8513	1.8490	1.59
$5d_{3/2}$	$6f_{5/2}$	1.5159	1.4049	1.2074	1.2074	0.9208	0.9189	0.17
$5d_{5/2}$	$4f_{5/2}$	1.1454	1.0922	1.0384	1.0384	0.9951	0.9943	1.08
$5d_{5/2}$	$5f_{5/2}$	0.6290	0.5881	0.5344	0.5344	0.5005	0.4998	0.45
$5d_{5/2}$	$6f_{5/2}$	0.4064	0.3743	0.3268	0.3268	0.2449	0.2443	0.15
$5d_{5/2}$	$4f_{7/2}$	5.1277	4.8978	4.6507	4.6507	4.4504	4.4486	4.84
$5d_{5/2}$	$5f_{7/2}$	2.8125	2.6359	2.3930	2.3930	2.2445	2.2429	2.47
$5d_{5/2}$	$6f_{7/2}$	1.8155	1.6778	1.4649	1.4649	1.1160	1.1147	1.04

and $6p_j$-$nd_{j'}$ transitions). The largest differences (30–50%) between $Z^{(\mathrm{DF+2+3})}$ and $Z^{(\mathrm{DF})}$ are for the for transitions with $8p_j$ states ($8p_j$-$6s_{1/2}$, $8p_j$-$5d_{j'}$, and $8p_j$-$6d_{j'}$ transitions). The largest ratio (by a factor of 13) of the $Z^{(\mathrm{DF+2+3})}$ and $Z^{(\mathrm{DF})}$ is for the $8p_{1/2}$-$6s_{1/2}$ transition. The terms $Z^{(\mathrm{RPA})}$ and $Z^{(\mathrm{BO})}$ give the largest contributions to $Z^{(3)}$. The ratios of $Z^{(\mathrm{RPA})}/Z^{(\mathrm{DF})}$ are equal to 2.3, 15.9, and 1.8 for the $7p_{1/2}$-$6s_{1/2}$, $8p_{1/2}$-$6s_{1/2}$, and $8p_{3/2}$-$6s_{1/2}$ transitions, respectively. The values of the $Z^{(\mathrm{BO})}$ term are smaller than the value of the $Z^{(\mathrm{RPA})}$ term for these three transitions and have different signs since they partly cancel each other.

It should be noted that the largest disagreement (by a factor of 2–5) between the $Z^{(\mathrm{DF+2+3})}$ values and the reduced electric-dipole matrix elements calculated with the RCC method [4] was found for aforementioned transitions with $8p_j$ states. One sees from comparison of the results given in the columns labeled $Z^{(\mathrm{DF+2+3})}$ and Ref. [4] in Table II that the values of the $7p_{1/2}$-$6s_{1/2}$, $8p_{1/2}$-$6s_{1/2}$, $8p_{1/2}$-$7s_{1/2}$, $8p_{3/2}$-$6s_{1/2}$, and $8p_{3/2}$-$7s_{1/2}$ transitions disagree by a factor of 2–5. In rightmost column of Table II, recent results of the reduced electric-dipole matrix elements calculated by improved the RCC method are listed [9]. The largest difference (by a factor of 2–10) in the results of Refs. [4] and [9] happens for the $7p_{3/2}$-$6s_{1/2}$, $7p_{3/2}$-$8s_{1/2}$, $8p_{1/2}$-$6s_{1/2}$, and $8p_{3/2}$-$6s_{1/2}$ electric-dipole matrix elements. Sahoo *et al.* [9] explained that a mix of numerical orbitals from the GRASP code and GTOs was used in [4], while in [9] the purely analytical GTOs were used.

Electric-dipole matrix elements evaluated in the all-order SD and SDpT approximations (SD all-order method including partial triple excitations [10]) are given in the columns labeled $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ in Table II. The difference between the $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ values is very small (about 0.1%–1.2%). The SD and SDpT matrix elements $Z^{(\mathrm{SD})}$ 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 [80]. The $Z^{(\mathrm{SD})}$ values differ from the $Z^{(\mathrm{DF+2+3})}$ values by 1–5% for most of the cases except cases when the term $Z^{(\mathrm{RPA})}$ gives the largest contribution in the value of $Z^{(\mathrm{DF+2})}$ that was discussed previously. It should be noted that the electric-dipole matrix elements evaluated by Dzuba *et al.* [2] (column labeled Ref. [2] in Table II) are in better agreement with the $Z^{(\mathrm{SD})}$ values than with the $Z^{(\mathrm{DF+2+3})}$ values.

B. Form-independent third-order transition amplitudes

I mentioned earlier that the all-order method did not converge for nf_j states in Ba II. The form-independent third-order perturbation theory approach developed by Savukov and Johnson in Ref. [81] was used to evaluate the multipole reduced matrix elements that include the nf_j states. Previously, good precision of this method has been demonstrated for alkali-metal atoms. In this method, form-dependent "bare" amplitudes are replaced with form-independent RPA ("dressed") amplitudes to obtain form-independent third-order amplitudes to some degree of accuracy. As in the case of the third-order energy calculation, a limited number of partial waves with $l_{\max} < 7$ is included. This restriction is not very important for Ba$^+$ $E1$ matrix elements because third-order energy correction is smaller than the second-order energy correction, but it gives rise to some loss of gauge invariance. The gauge independence serves as an additional check that no numerical problems occurred. Recently, this method was used in Ref. [82] to evaluate the electric-dipole reduced matrix elements in Yb II.

Length and velocity-form matrix elements from DF, second-order (RPA), and third-order calculations are given in Table III for the $5d_j$-$4f_{j'}$, $5d_j$-$5f_{j'}$, and $5d_j$-$6f_{j'}$ transitions in Ba II. These transitions are chosen to compare with values calculated by the RCC method in Ref. [9]. The $Z^{(\mathrm{DF})}$ values in L and V forms differ by 4–8%. The second-order RPA contribution completely removes this difference in $L-V$ values, and the L and V columns with the $Z^{(\mathrm{DF+2})}$ headings are almost identical. There are, however, small $L-V$ differences (0.04%–0.24%) in the third-order matrix elements. These remaining small differences can be explained by limitation in the number of partial waves taken into account in the evaluations of the third-order matrix elements.

The best agreement (about 3.5%) between my $Z^{(\mathrm{DF+2+3})}$ values and values from Ref. [9] is for the $5d_{3/2}$-$4f_{5/2}$ transition. The largest disagreement (by a factor of 5) is for the $5d_{3/2}$-$6f_{5/2}$ transition.

C. Electric-qudrupole and magnetic-dipole matrix elements

Reduced electric-qudrupole and magnetic-dipole matrix elements calculated with first-order, second-order, third-order MBPT and SD and SDpT all-order method

TABLE IV. Reduced electric-qudrupole and magnetic-dipole matrix elements calculated with first-order, second-order, third-order, SD, and SDpT methods (SD all-order method including partial triple excitations) in Ba II are compared with theoretical results given by Iskrenova-Tchoukova and Safronova [1] and by Gopakumar *et al.* [4].

Transition			$Z^{(\mathrm{DF})}$	$Z^{(\mathrm{DF+2})}$	$Z^{(\mathrm{DF+2+3})}$	$Z^{(\mathrm{SD})}$	$Z^{(\mathrm{SDpT})}$	$Z^{(\mathrm{SD})}_{\mathrm{sc}}$	$Z^{(\mathrm{SDpT})}_{\mathrm{sc}}$	$Z^{(\mathrm{final})}$	Ref. [1]	Ref. [4]
$E2$	$6s_{1/2}$	$5d_{3/2}$	14.753	14.528	11.811	12.489	12.732	12.626	12.589	12.63(11)	12.63(9)	12.6251
$E2$	$6s_{1/2}$	$5d_{5/2}$	18.362	18.119	14.841	15.632	15.924	15.800	15.755	15.80(12)	15.80(11)	15.7832
$E2$	$7s_{1/2}$	$5d_{3/2}$	6.177	6.254	4.038	4.641	4.789	4.743	4.653	4.74(9)		3.9021
$E2$	$7s_{1/2}$	$5d_{5/2}$	7.896	7.972	5.372	6.043	6.216	6.166	6.059	6.17(11)		5.2072
$M1$	$5d_{3/2}$	$5d_{5/2}$	1.549	1.549	1.531	1.549	1.549	1.549	1.549	1.549		

(SD all-order method including partial triple excitations) in Ba II are compared in Table IV with theoretical results given by Iskrenova-Tchoukova and Safronova [1] and by Gopakumar *et al.* [4]. I mentioned earlier that here I use a different approach than that used in Ref. [1]. The major difference is in treatments of the Breit interaction. In the approach used in [1], Breit contributions were treated perturbatively through the second-order MBPT. Here, I include both Coulomb and Breit contributions to the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. B splines are used to generate a complete set of DF basis orbitals for use in the evaluation of all atomic properties. Also, the number of basis-set orbitals is increased to 70 instead of the 50 used in [1]. Results in Ref. [1] also include semiemperical scaling in some cases.

The $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ values given in Table IV for the $6s_{1/2}$-$5d_j$ transitions differ from those in [1] by about 1%. A similar difference (about 1%) is found between the $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ values and results in Ref. [4] for the $6s_{1/2}$-$5d_j$ transitions; however, there is a large difference (about 20%) in results for the $7s_{1/2}$-$5d_j$ transitions. It looks that treatment in [4] was different for the $6s_{1/2}$-$5d_j$ and $7s_{1/2}$-$5d_j$ transitions. One can see from Table IV that values in [4] for the $6s_{1/2}$-$5d_j$ transitions are in better agreement with the $Z^{(\mathrm{SD})}$ and $Z^{(\mathrm{SDpT})}$ values, but those for the $7s_{1/2}$-$5d_j$ transitions are in better agreement with my $Z^{(\mathrm{DF+2+3})}$ values. Included in Table IV are results for the $5d_{3/2}$-$5d_{5/2}$ reduced magnetic-dipole matrix element. The importance of this transition for lifetime value of the $5d_{5/2}$ state was recently shown by Guet and Johnson in [45].

I have estimated uncertainties of my results on the examples of the electric-qudrupole matrix elements and $5d_j$ state lifetimes. Table IV lists results for electric-quadrupole matrix elements calculated in different approximations: lowest-order DF, second-order RMBPT, third-order RMBPT, and all-order method with and without the triple excitations. These results allow us to estimate the size of the correlation corrections and study the convergence of the perturbation theory. We find that the correlation correction, estimated as the relative difference between the lowest order and the final results, contributed about 16% for the $6s$-$5d_j$ transitions and 30% for $7s$-$5d_j$ transitions. Moreover, fourth- and higher-order corrections beyond RPA, estimated as the difference between the final and the third-order results, contribute 7% and 14% for the $6s$-$5d_j$ and $7s$-$5d_j$ transitions, respectively. Such large contributions of higher-order corrections beyond RPA indicate poor convergence of low-order perturbation theory. To make a more accurate estimate of the uncertainty of my calculations, I carry out semiempirical scaling that accounts for the effect of dominant missing contributions starting from both SD and SDpT approximations. The corresponding results are listed in Table IV with subscript sc [1]. I estimate the uncertainty of these values as max($[Z^{(\mathrm{SD})}_{\mathrm{sc}}$-$Z^{(\mathrm{SDpT})}]$, $[Z^{(\mathrm{SD})}_{\mathrm{sc}}$-$Z^{(\mathrm{SDpT})}_{\mathrm{sc}}]$). The $Z^{(\mathrm{SD})}_{\mathrm{sc}}$ results are taken as final. We find that the uncertainties of the $6s$-$5d_j$ and $7s$-$5d_j$ transitions are on the order of 1% and 2%, respectively. Larger uncertainties of the $7s$-$5d_j$ transitions in comparison with $6s$-$5d_j$ ones are consistent with the larger size (by a factor of 2) of the correlation corrections to these properties. These final results and their uncertainties are used to evaluate the uncertainties of the $5d_j$ state lifetimes given in Table V.

In this section, only a limited set of multipole matrix elements are considered. I choose transitions to compare with available precision calculations to compare various approaches. In what follows, results for different properties of Ba II are presented.

IV. LIFETIMES IN BA II

I calculate lifetimes of the $ns_{1/2}$ ($n = 7$–8), np_j ($n = 6$–8), nd_j ($n = 5$–6), and nf_j ($n = 4$) states in Ba II using the SD and SDpT results for dipole matrix elements and NIST data [75] for energies. I list lifetimes $\tau^{(\mathrm{SD})}$ obtained with the SD

TABLE V. Lifetimes (in s) of $5d_j$ states in Ba II. The SD [$\tau^{(\mathrm{SD})}$], SDpT [$\tau^{(\mathrm{SDpT})}$], SD scaled [$\tau^{(\mathrm{SD_{sc}})}$], and SDpT scaled [$\tau^{(\mathrm{SDpT_{sc}})}$] values are compared with theoretical and experimental data.

State	SD	SDpT	SD$_{\mathrm{sc}}$	SDpT$_{\mathrm{sc}}$	Final	Th [1]	Th [44]	Expt. [42]
$5d_{3/2}$	83.26	80.12	81.46	81.94	81.5(1.3)	81.5(1.2)	80.1(7)	89.4(15.6)
$5d_{5/2}$	30.88	29.94	30.33	30.48	30.3(4)	30.3(4)	29.9(3)	31.6(4.6)

TABLE VI. Lifetimes (in ns) of nl_j states in Ba II. The SD [$\tau^{(\mathrm{SD})}$] and SDpT [$\tau^{(\mathrm{SDpT})}$] values are compared with theoretical [9] and experimental data [28,37].

Level	$\tau^{(\mathrm{DF})}$	$\tau^{(\mathrm{SD})}$	$\tau^{(\mathrm{SDpT})}$	$\tau^{\mathrm{th.}}$	τ^{expt}
$6p_{1/2}$	5.579	7.798	7.626	7.92(10) [9]	7.90(10) [37]
$6p_{3/2}$	4.504	6.245	6.107	6.30(17) [9]	6.32(10) [37]
$7p_{1/2}$	28.98	36.02	35.84		31.8(1.3) [37]
$7p_{3/2}$	20.75	27.36	27.19		24.5(8) [37]
$8p_{1/2}$	73.47	90.60	90.18		
$8p_{3/2}$	52.51	73.00	72.58		
$7s_{1/2}$	4.855	5.165	5.124		7.91(56) [28]
$8s_{1/2}$	7.933	8.196	8.146		
$6d_{3/2}$	3.708	4.169	4.126		5.56(34) [28]
$6d_{5/2}$	3.959	4.417	4.375		4.99(33) [28]
$4f_{5/2}$	1.912	2.577			2.75(6) [37]
$4f_{7/2}$	1.912	2.538			2.75(8) [37]

method and $\tau^{(\mathrm{SDpT})}$ obtained with the SDpT method in Table VI and compare my values with available experimental [28,37] and latest recent theoretical [9] results. The calculation in Ref. [9] was performed with the RCC method for the $6p_j$ states only. It should be noted that I did not find any precision calculation for other states. The only available calculations for these states include the scaled Thomas-Fermi-Dirac wave function with including spin-orbit interaction results [12] and the nonrelativistic Coulomb approximation values [8]. I noted large contributions of correlation effects in the electric-dipole matrix elements in the previous section. One can see from Table VI that $\tau^{(\mathrm{DF})}$ values differ from the $\tau^{(\mathrm{SD})}$ and $\tau^{(\mathrm{SDpT})}$ values by 20–30%. The difference between $\tau^{(\mathrm{SD})}$ and $\tau^{(\mathrm{SDpT})}$ values is about 1–2%. The $\tau^{(\mathrm{SD})}$ values for the $6p_j$ states agree with experimental measurements performed by Pinnington *et al.* [37] when experimental uncertainties are taken into account. Good agreement is found between my third-order RMBPT values and measurements in [37] for the lifetimes of the $4f_j$ levels, even that the correlation contribution to DF value is about 26%. Experimental lifetime values for the $7p_j$ states are between my DF and SD values [the difference between $\tau^{(\mathrm{expt})}$ and $\tau^{(\mathrm{DF})}$ is equal to 8.8% and 15% for $j = 1/2$ and 3/2, respectively, while the difference between $\tau^{(\mathrm{expt})}$ and $\tau^{(\mathrm{SD})}$ is equal -13% and -12% for $j = 1/2$ and 3/2, respectively]. Disagreement between my results and the measurements in [28] can be explained by considering only one channel for decay in [28]. For example, there are two channels for decay from the $7s_{1/2}$ level ($7s_{1/2} \rightarrow 6p_{1/2}$ and $7s_{1/2} \rightarrow 6p_{3/2}$). Taken into account only the $7s_{1/2} \rightarrow 6p_{3/2}$ channel with largest transition rate, we find $\tau^{(\mathrm{DF})} = 7.418$ ns, $\tau^{(\mathrm{SD})} = 7.862$ ns, and $\tau^{(\mathrm{SDpT})} = 7.806$ ns. Experimental lifetime values of the $7s_{1/2}$ (7.91 ± 0.56 ns; see Table VI) are in perfect agreement with those values.

Recently, precision measurements of the branching ratio in the $6p_{3/2}$ decay of Ba II was performed by Kurz *et al.* [39] using a single trapped ion. Relative strengths normalized to unity were found to be 0.756 ± 0.046, 0.0290 ± 0.0015, and 0.215 ± 0.0064 for $6s_{1/2}$, $5d_{3/2}$, and $5d_{5/2}$, respectively [39]. The SD results (0.743, 0.0280, and 0.230) and SDpT results (0.741, 0.0282, and 0.231) are in a good agreement with measurements, taking into account uncertainties in [39].

Table V lists lifetimes of $5d_j$ states in Ba II. The SD [$\tau^{(\mathrm{SD})}$], SDpT [$\tau^{(\mathrm{SDpT})}$], SD scaled [$\tau^{(\mathrm{SD_{sc}})}$], and SDpT scaled [$\tau^{(\mathrm{SDpT_{sc}})}$] values are compared with theoretical [1,44] values and experimental results given by Gurell *et al.* [42]. Reduced electric-qudrupole matrix elements for the $6s_{1/2}$-$5d_j$ transitions and magnetic-dipole matrix elements for the $5d_{3/2}$-$5d_{5/2}$ transition calculated in SD and SDpT approximations are given in Table IV. I use NIST energies [75] to evaluate the electric-qudrupole and magnetic-dipole transition rates and finally, the lifetime of $5d_j$ calculated with the SD [$\tau^{(\mathrm{SD})}$] and SDpT [$\tau^{(\mathrm{SDpT})}$] approximations. I also added the SD scaled [$\tau^{(\mathrm{SD_{sc}})}$] and SDpT scaled [$\tau^{(\mathrm{SDpT_{sc}})}$] values in Table V. The scaled values of lifetimes [$\tau^{(\mathrm{SD_{sc}})}$ and $\tau^{(\mathrm{SDpT_{sc}})}$] are in better agreement with each other than the $\tau^{(\mathrm{SD})}$ and SDpT $\tau^{(\mathrm{SDpT})}$ values, as expected. As a result, I use scaled values as final result and list them under "Final" in Table V. There is a small difference between my results and results given by Iskrenova-Tchoukova and Safronova [1], owing to different treatment of the Breit interaction.

V. STATIC MULTIPOLE POLARIZABILITIES OF THE 6*S* GROUND STATE OF BA II

The static multipole polarizability α^{Ek} of Ba II in its $6s$ ground state can be separated into two terms: a dominant first term from intermediate valence-excited states, and a smaller second term from intermediate core-excited states. The later term is smaller than the former one by several orders of magnitude and is evaluated here in the RPA [83]. The dominant valence contribution is calculated using the sum-over-state approach,

$$\alpha_v^{Ek} = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j \| r^k C_{kq} \| 6s \rangle|^2}{E_{nlj} - E_{6s}}, \tag{1}$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic and nl_j is np_j, nd_j, and nf_j for $k = 1$, 2, and 3, respectively [84]. The reduced matrix elements in the preceding 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 $E2$ and $E3$ matrix elements.

Contributions to dipole, quadrupole, and octupole polarizabilities of the $6s$ ground state are presented in Table VII. The first two terms in the sum-over-states for α^{E1}, α^{E2}, and α^{E3} contribute 99.8%, 81.5%, and 77.1%, respectively, of the totals. The rapid convergence of the sum over states for α^{E1} has been emphasized in many publications (for example, Refs. [69,70,85]). I use available recommended NIST energies [75] for $nl = 6s$-$12s$,$6p$-$11p$,$5d$-$11d$,$4f$-$12f$ and theoretical SD energies for other states up to $n = 26$. The sums over n for $n \leqslant 26$ in α^{E2} and α^{E3} essentially reproduce the final results, since the contributions from $27 \leqslant n \leqslant 70$ are smaller than 0.01% in all cases.

The final results for the multipole polarizabilities of the ground-state Ba II are compared in Table VII with calculations given in Refs. [1,56] and experimental measurements presented in Ref. [54]. I mentioned earlier that dipole polarizability α^{E1} was studied theoretically [1,56,57,86] and experimentally [52–55] in a number of works. The difference between all of the results are within 0.3%–1.5%. Theoretical

TABLE VII. Contributions to multipole polarizabilities (in a.u.) of the $6s$ state of Ba II. The two leading terms and those terms with $n \leqslant 26$ in the expression for α_v^{Ek} [Eq. (1)] are evaluated using SD wave functions. The remainders ($n > 26$), labeled "tail," are evaluated in the DHF approximation. Contributions from core-excited states α_c^{Ek} are evaluated in the RPA. My final SD α^{E1}, α^{E2}, and α^{E3} polarizabilities of the $6s$ ground state of Ba II are compared with other calculations and with experiment.

$nlj = 6p_{1/2}$	40.231	$nlj = 5d_{3/2}$	1404.72	$nlj = 4f_{5/2}$	11 924
$nlj = 6p_{3/2}$	73.920	$nlj = 5d_{5/2}$	1890.06	$nlj = 4f_{7/2}$	15 846
$nl = [7p\text{-}26p]$	0.225	$nl = [6d\text{-}26d]$	747.09	$nl = [5f\text{-}26f]$	8274
$nl = [2p\text{-}5p]$	−0.511	$nl = [3d\text{-}4d]$	0.0		
tail	0.014	tail	3.64	tail	24
α_v^{E1}	113.879	α_v^{E2}	4045.51	α_v^{E3}	36 067
α_c^{E1}	10.630	α_c^{E2}	45.99	α_c^{E3}	401
α^{E1}	124.51	α^{E2}	4091.5	α^{E3}	36 468
$\alpha_{\text{th.}}^{E1}$ [1]	124.15	$\alpha_{\text{th.}}^{E2}$ [1]	4182(34)	$\alpha_{\text{th.}}^{E3}$ [56]	26 510
$\alpha_{\text{th.}}^{E1}$ [56]	124.7	$\alpha_{\text{th.}}^{E2}$ [56]	4821		
$\alpha_{\text{expt}}^{E1}$ [54]	123.88(5)	$\alpha_{\text{expt}}^{E2}$ [54]	4420(250)		

results for quadrupole polarizability α^{E2} given in Refs. [1,56] differ by 20%. I mentioned previously that experimental results for α^{E2} given in Refs. [52,53] and in Refs. [54,55] differ almost by a factor of two; these differences have been addressed in Ref. [55]. It was noted in [55] the importance of contributions from higher-excited levels, the core, and a valence-core counterterm. There is only one publication [56] concerning the octupole polarizability in Ba II. I mentioned earlier that the α^{E3} polarizabilities in [56] were calculated using simple wave functions based on the asymptotic behavior and on the binding energies of the valence electron. One can see from the rightmost column of Table VII that the difference between the SD α^{E3} values and the α_{th}^{E3} values from Ref. [56] is equal to contributions from all states ($nl = [5f\text{-}26f]$) except the $nl = 4f$ state.

VI. 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 BA II

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

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

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

As before, the calculation of the sums is divided into three parts. The first part is the sum over valence states with $n \leqslant 26$, which is carried out using SD wave functions. The second part is the sum over basis states with $n > 26$, which is carried out in the RPA. The third part is the contribution from core-excited states, which is carried out also in the RPA.

A breakdown of contributions to the scalar dipole polarizability for the excited $ns_{1/2}$ (n = 7–10), np_j ($n = 6$ and 7), and nd_j ($n = 5$ and 6) states is presented in Table VIII. I evaluate contribution from ionic core α_{core} in the RPA and find $\alpha_{\text{core}} = 10.630\,3\ a_0^3$.

Contributions from the excited np_j states with $n > 26$ in the case of the excited $9s_{1/2}$ and $10s_{1/2}$ are below 0.1 a_0^3. Contributions from excited ns and nd states with $n > 26$ are very small in the case of the excited np_j [$\alpha_{n>26}(6p_{1/2}) = -0.002\,7\ a_0^3$ and $\alpha_{n>26}(6p_{3/2}) = -0.0006\ a_0^3$] and are calculated in the RPA approximation. Contributions from the excited np_j and nf_j states with $n > 26$ are the largest in the case of the excited $5d_j$ states [$\alpha_{n>26}(5d_{3/2}) = -0.674\,8\ a_0^3$, $\alpha_{n>26}(5d_{5/2}) = -0.820\,9\ a_0^3$].

A counterterm $\alpha_{\text{vc}}(nl_j)$ compensating for excitation from the core to the valence shell which violates the Pauli principle is also evaluated in the RPA and found to be larger than the $\alpha_{\text{tail}}^{(\text{RPA})}(nl_j)$ for the $6p_j$ and $7p_j$ states. The largest contribution of the $\alpha_{\text{vc}}(n_j)$ term is for the $5d_j$ state [$\alpha_{\text{vc}}(5d_{3/2}) = 0.465\,4\ a_0^3$ and $\alpha_{\text{vc}}(5d_{5/2}) = 0.418\,3\ a_0^3$]. It should be noted that the terms $\alpha_{\text{tail}}^{(\text{RPA})}(nl_j)$ and $\alpha_{\text{vc}}(nl_j)$ have different signs and partly cancel each other.

The above values were combined to obtain the final results for the scalar polarizabilities $\alpha^{(\text{SD})}(nlj)$ for the four ns_j (n = 7, 8, 9, and 10), two np_j ($n = 6$ and 7), and two nd_j ($n = 5$ and 6) excited states in Ba II.

It should be noted that I have very different $np_{1/2}$, $np_{3/2}$, $nf_{5/2}$, and $nf_{7/2}$ contributions for the $\alpha^{(\text{SD})}(5dj)$ with $j = 3/2$ and $5/2$. In the case of $j = 5/2$, the contribution from the $np_{1/2}$ [$\sum_{n=6}^{26} I_{5d_{5/2}}^{(\text{SD})}(np_{1/2})$] is equal to zero owing to $E1$ selection rules. This term gives the largest contribution in the value of $\alpha^{(\text{SD})}(5d_{3/2})$. However, the resulting values of $\alpha^{(\text{SD})}(5dj)$ with $j = 3/2$ and $5/2$ differ by 0.2% only. The larger difference (3%) is found between values of $\alpha^{(\text{SD})}(6dj)$ with $j = 3/2$ and $5/2$. The largest difference (factor of 2.2) is between values of $\alpha^{(\text{SD})}(6pj)$ with $j = 1/2$ and $3/2$. In the case of $j = 1/2$, the contribution from the $nd_{5/2}$ [$\sum_{n=5}^{26} I_{6p_j}^{(\text{SD})}(nd_{5/2})$] is equal to zero owing to $E1$ selection rules, while this term gives the largest contribution in the value of $\alpha^{(\text{SD})}(6pj)$ with $j = 3/2$. Final results for the scalar dipole polarizabilities of $\alpha^{(\text{SD})}(nlj)$ in Ba II are given in Table VIII.

A breakdown of contributions to the tensor dipole polarizability for the excited $np_{3/2}$ (n = 6–9) and nd_j ($n = 5$ and 6) states is presented in Table IX. Evaluation of the tensor

TABLE VIII. Contributions to scalar polarizability of Ba II in the excited $ns_{1/2}$ states ($n = 7 - 10$), $np_{1/2}$, $np_{3/2}$ states ($n = 6$, 7), and $nd_{3/2}$, $nd_{5/2}$ states ($n = 5$, 6) calculated with SD wave functions: $\alpha_0(ns_{1/2}) = \sum_{n'=2}^{70} I_{ns_{1/2}}(n'p_j)$; $\alpha_0(np_{1/2}) = \sum_{n'=3}^{70} I_{np_{1/2}}(n'd_{3/2}) + \sum_{n'=1}^{70} I_{np_{1/2}}(n's_{1/2})$,$\alpha_0(np_{3/2}) = \sum_{n'=3}^{70} I_{np_{3/2}}(n'd_j) + \sum_{n'=1}^{70} I_{np_{3/2}}(n's_{1/2})$; $\alpha_0(nd_{3/2}) = \sum_{n'=4}^{70} I_{nd_{3/2}}(n'f_{5/2}) + \sum_{n'=2}^{70} I_{nd_{3/2}}(n'p_j)$, $\alpha_0(nd_{5/2}) = \sum_{n'=4}^{70} I_{nd_{5/2}}(n'f_j) + \sum_{n'=2}^{70} I_{nd_{5/2}}(n'p_{3/2})$.

Contribution	$7s_{1/2}$	$8s_{1/2}$	$9s_{1/2}$	$10s_{1/2}$
$\sum_{n'=6}^{26} I_{ns_j}^{(SD)}(n'p_{1/2})$	489.42	2727.19	10 528.7	32 300.7
$\sum_{n'=6}^{26} I_{ns_j}^{(SD)}(n'p_{3/2})$	857.73	4645.99	17 560.7	52 967.9
$\alpha_{\text{main}}^{(SD)}(ns_j)$	1347.15	7373.18	28 089.4	85 268.5
$\alpha_{\text{tail}}^{(RPA)}(ns_j)$	0.01	0.01	0.0	0.0
α_{core}	10.63	10.63	10.6	10.6
$\alpha_{\text{vc}}(ns_j)$	−0.08	−0.03	−0.0	−0.0
$\alpha^{(SD)}(ns_j)$	1357.7	7383.8	28 100.0	85 279.0
	$6p_{1/2}$	$6p_{3/2}$	$7p_{1/2}$	$7p_{3/2}$
$\sum_{n'=6}^{26} I_{np_j}^{(SD)}(n's_{1/2})$	−18.359	−8.575	−291.22	−177.30
$\sum_{n'=5}^{26} I_{np_j}^{(SD)}(n'd_{3/2})$	28.581	4.948	−1078.59	−66.39
$\sum_{n'=5}^{26} I_{np_j}^{(SD)}(n'd_{5/2})$	0	38.892	0	−713.98
$\alpha_{\text{main}}^{(SD)}(np_j)$	10.222	35.265	−1369.81	−957.67
$\alpha_{\text{tail}}^{(RPA)}(np_j)$	−0.003	−0.001	−0.00	−0.00
α_{core}	10.630	10.630	10.63	10.63
$\alpha_{\text{vc}}(np_j)$	0.189	0.135	0.35	0.24
$\alpha^{(SD)}(np_j)$	21.04	46.03	−1358.8	−946.8
	$5d_{3/2}$	$5d_{5/2}$	$6d_{3/2}$	$6d_{5/2}$
$\sum_{n'=6}^{26} I_{nd_j}^{(SD)}(n'p_{1/2})$	22.211	0	760.42	0
$\sum_{n'=6}^{26} I_{nd_j}^{(SD)}(n'p_{3/2})$	3.833	25.400	120.12	786.56
$\sum_{n'=4}^{26} I_{nd_j}^{(SD)}(n'f_{5/2})$	19.224	0.980	1963.34	101.87
$\sum_{n'=4}^{26} I_{nd_j}^{(SD)}(n'f_{7/2})$	0	19.226	0	1863.32
$\alpha_{\text{main}}^{(SD)}(nd_j)$	45.268	45.605	2843.88	2751.75
$\alpha_{\text{tail}}^{(RPA)}(nd_j)$	−0.675	−0.821	−0.05	−0.06
α_{core}	10.630	10.630	10.63	10.63
$\alpha_{\text{vc}}(nd_j)$	0.465	0.418	0.33	0.29
$\alpha^{(SD)}(nd_j)$	55.69	55.83	2854.8	2762.6

polarizability follows the same patterns as evaluation of the scalar polarizability [compare Eqs. (2) and (3)]. The difference in the evaluations of the $\alpha_0^{(SD)}(nlj)$ and $\alpha_2^{(SD)}(nlj)$ values is in the angular part only. As one can see from comparison results given in Tables VIII and IX, we obtain different distribution from the $\sum_{n'=6}^{26} I_{np_j}^{(SD)}(n's_{1/2})$, $\sum_{n'=5}^{26} I_{np_j}^{(SD)}(n'd_{3/2})$, and $\sum_{n'=5}^{26} I_{np_j}^{(SD)}(n'd_{5/2})$ terms (in the case of np_j excited states) and from the $\sum_{n'=6}^{26} I_{nd_j}^{(SD)}(n'p_{1/2})$, $\sum_{n'=6}^{26} I_{nd_j}^{(SD)}(n'p_{3/2})$, and $\sum_{n'=4}^{26} I_{nd_j}^{(SD)}(n'f_{5/2})$ terms (nd_j excited states) in scalar and tensor polarizabilities. As a result, the values of $\alpha_2^{(SD)}(nlj)$ are smaller than those of $\alpha_0^{(SD)}(nlj)$ and have different sign.

TABLE IX. Contributions to tensor polarizability of Ba II in the excited $np_{3/2}$ states ($n = 6$–9) and $nd_{3/2}$, $nd_{5/2}$ states ($n = 5$, 6) calculated with SD wave functions: $\alpha_2(np_{3/2}) = \sum_{n'=3}^{70} I_{np_{3/2}}(n'd_j) + \sum_{n'=1}^{70} I_{np_{3/2}}(n's_{1/2})$; $\alpha_2(nd_{3/2}) = \sum_{n'=4}^{70} I_{nd_{3/2}}(n'f_{5/2}) + \sum_{n'=2}^{70} I_{nd_{3/2}}(n'p_j)$, $\alpha_2(nd_{5/2}) = \sum_{n'=4}^{70} I_{nd_{5/2}}(n'f_j) + \sum_{n'=2}^{70} I_{nd_{5/2}}(n'p_{3/2})$.

Contribution	$6p_{3/2}$	$7p_{3/2}$	$8p_{3/2}$	$9p_{3/2}$
$\sum_{n'=6}^{26} I_{np_j}^{(SD)}(n's_{1/2})$	8.575	177.30	1124.55	4685.47
$\sum_{n'=5}^{26} I_{np_j}^{(SD)}(n'd_{3/2})$	3.959	−53.11	−527.23	−2554.84
$\sum_{n'=5}^{26} I_{np_j}^{(SD)}(n'd_{5/2})$	−7.778	142.80	1336.62	6370.67
$\alpha_{\text{main}}^{(SD)}(np_j)$	4.755	266.99	1933.95	8501.30
$\alpha_{\text{tail}}^{(RPA)}(np_j)$	−0.029	−0.035	−0.033	−0.028
$\alpha^{(SD)}(np_j)$	4.726	266.95	1933.9	8501.3
	$5d_{3/2}$	$5d_{5/2}$	$6d_{3/2}$	$6d_{5/2}$
$\sum_{n'=6}^{26} I_{nd_j}^{(SD)}(n'p_{1/2})$	−22.211	0	−760.42	0
$\sum_{n'=6}^{26} I_{nd_j}^{(SD)}(n'p_{3/2})$	3.067	−25.400	96.09	−786.56
$\sum_{n'=4}^{26} I_{nd_j}^{(SD)}(n'f_{5/2})$	−3.845	1.119	−392.67	116.42
$\sum_{n'=4}^{26} I_{nd_j}^{(SD)}(n'f_{7/2})$	0	−6.867	0	−665.47
$\alpha_{\text{main}}^{(SD)}(nd_j)$	−22.989	−31.147	−1056.99	−1335.61
$\alpha_{\text{tail}}^{(RPA)}(nd_j)$	−0.095	−0.119	−0.07	−0.08
$\alpha^{(SD)}(nd_j)$	−23.08	−31.27	−1057.1	−1335.7

States with $n > 20$ in my basis have positive energies and provide a discrete representation of the continuum. One can see that the continuous part of spectra is responsible for about 1% of $\alpha_2(6p_{3/2})$. I decided to evaluate the continuum contributions and near continuum contribution in the range $11 < n \leqslant 26$ using SD wave functions for both dipole matrix elements and energies. For $n \leqslant 11$, I use SD matrix elements and NIST energies [75] in the sums. The resulting contribution to $\alpha_2(nlj)$ comes from states with $n \leqslant 26$. Contributions from states with $n > 26$ is negligible (about 10^{-4}%). The final results for $\alpha_2^{(SD)}(nlj)$ are given in Table IX.

VII. HYPERFINE CONSTANTS FOR ^{137}BA II

Calculations of hyperfine constants follow the pattern described earlier for calculations of transition matrix elements. Table X lists hyperfine constants A for ^{137}Ba II and compares my values with available theoretical [66] results and experimental measurements from Refs. [58,62,63].

This table presents the lowest-order $A^{(DF)}$, the all-order $A^{(SD)}$, and $A^{(SDpT)}$ values for the ns, np, and nd levels up to $n = 8$. It should be noted that the values of $A^{(SDpT)}$ are obtained by using the SD all-order method including partial triple excitations. The difference between $A^{(SD)}$ and $A^{(SDpT)}$ is about 0.1–4%, while the ratios of $A^{(SD)}$ and $A^{(DF)}$ are equal to 0.6–1.6 for some cases. The largest difference between $A^{(SD)}$ and $A^{(SDpT)}$ (15%) is for the $5d^2D_{5/2}$ level. Even the sign of $A^{(DF)}$ and $A^{(SD)}$ is different and the ratio $A^{(DF)}$ and $A^{(SD)}$ is

TABLE X. Hyperfine constants A (in MHz) in ^{137}Ba$^+$ ($I = 3/2$, $\mu = 0.937\,365$ [87]). The SD and SDpT (SD all-order method including partial triple excitations) data are compared with other theoretical values and experimental results.

Level	$A^{(\mathrm{DF})}$	$A^{(\mathrm{SD})}$	$A^{(\mathrm{SDpT})}$	$A^{(\mathrm{th.})}$ [66]	$A^{(\mathrm{expt.})}$
$6s\,^2S_{1/2}$	2912.73	4162.52	3997.39	4078.20	4018.870 833 85(18) [58]
$7s\,^2S_{1/2}$	957.35	1237.83	1211.73	1196.30	
$8s\,^2S_{1/2}$	439.39	551.14	542.50		
$6p\,^2P_{1/2}$	490.97	765.75	733.98	740.77	743.79(3) [62]
$7p\,^2P_{1/2}$	192.25	274.72	267.00	264.92	
$8p\,^2P_{1/2}$	95.56	132.44	129.35	109.93	
$6p\,^2P_{3/2}$	71.77	126.62	121.35	128.27	127.29(2) [62]
$7p\,^2P_{3/2}$	28.43	46.23	44.87	45.77	
$8p\,^2P_{3/2}$	14.22	22.48	21.91		
$5d\,^2D_{3/2}$	128.43	195.90	191.53	189.22	189.728 8(6) [63]
$6d\,^2D_{3/2}$	27.75	38.50	38.39		
$7d\,^2D_{3/2}$	12.30	16.85	16.83		
$5d\,^2D_{5/2}$	51.59	−8.70	−9.99	−11.67	−12.028 (11) [63]
$6d\,^2D_{5/2}$	11.27	7.26	6.90		
$7d\,^2D_{5/2}$	5.01	4.05	3.91		

equal to 7.1. The largest difference (about 16%) between my $A^{(\mathrm{SD})}$ and $A^{(\mathrm{SDpT})}$ values and the $A^{(\mathrm{th.})}$ value from Ref. [66] is for the $8p\,^2P_{1/2}$ level. The difference between $A^{(\mathrm{SD})}$ and $A^{(\mathrm{SDpT})}$ values and available experimental measurements is about 0.5–1.5%, except for the results for the $5d\,^2D_{5/2}$ level, where the difference is about 20%.

Hyperfine constants B (in MHz) in ^{137}Ba$^+$ are given in Table XI. The nuclear quadrupole moment Q is equal to 0.246(2) in barns (1 b $= 10^{-24}$ cm^2) [63]. The SD and SDpT data are compared with theoretical [66] and experimental data from Refs. [62,63] in the same table. Three columns of Table XI list the $B^{(\mathrm{DF})}$, $B^{(\mathrm{SD})}$, and $B^{(\mathrm{SDpT})}$ values divided by nuclear quadrupole moment Q. Three other columns of Table XI list the $B^{(\mathrm{DF})}$, $B^{(\mathrm{SD})}$, and $B^{(\mathrm{SDpT})}$ values. The difference between $B^{(\mathrm{SD})}$ and $B^{(\mathrm{SDpT})}$ is about 0.9–3.7%, while the ratios $B^{(\mathrm{SD})}$ and $B^{(\mathrm{DF})}$ are equal to 1.4–1.68 for some cases. In the two last columns of Table XI show few available theoretical and experimental values of the B constant. The $B^{(\mathrm{SDpT})}$ value for the $6p^2P_{3/2}$ level is in better agreement with both results than the $B^{(\mathrm{SD})}$. For the $5d^2D_{3/2}$ and $5d^2D_{5/2}$ states, one can see that the $B^{(\mathrm{SD})}$ values are in an excellent agreement (0.1–0.9%) with theoretical results from Ref. [66], while experimental values [63] are in a better agreement (2%) with the $B^{(\mathrm{SDpT})}$ values.

VIII. HYPERFINE-INDUCED TRANSITION POLARIZABILITY OF THE ^{137}BA II GROUND STATE

I now turn to the calculation of the quadratic Stark shift of the ground-state hyperfine interval ($F = 2$ to $F = 1$) in ^{137}Ba II. The quadratic Stark shift is closely related to the blackbody radiation shift discussed, for example, in Refs. [69,70,88] and my calculation follows the procedure outlined in [69].

The dominant second-order contribution to the polarizability cancels between the two hyperfine components of the $6s$ 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 [69]:

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

where g_I is the nuclear gyromagnetic ratio, μ_n is the nuclear magneton, $I = 3/2$ is the nuclear spin, and $j_v = 1/2$ is the total angular momentum of the ground state in Ba II. The F-independent sums ($|v\rangle \equiv |6s_{1/2}\rangle$) are given by Eqs. (5)–(7) by Johnson *et al.* [69].

TABLE XI. Hyperfine constants B (in MHz) in ^{137}Ba$^+$. Nuclear quadrupole moment Q equal to 0.246(2)b in barns (1 b $= 10^{-24}$ cm^2) [63]. The SD and SDpT (SD all-order method including partial triple excitations) data are compared with experimental results.

Level	$\frac{B^{(\mathrm{DF})}}{Q}$	$\frac{B^{(\mathrm{SD})}}{Q}$	$\frac{B^{(\mathrm{SDpT})}}{Q}$	$B^{(\mathrm{DF})}$	$B^{(\mathrm{SD})}$	$B^{(\mathrm{SDpT})}$	$B^{(\mathrm{th})}$	$B^{(\mathrm{expt})}$
$6p\,^2P_{3/2}$	223.20	393.11	378.57	54.91	96.71	93.13	92.87 [66]	92.5(2) [62]
$7p\,^2P_{3/2}$	88.41	141.58	137.89	21.75	34.83	33.92	32.98 [66]	
$8p\,^2P_{3/2}$	44.20	68.16	66.65	10.87	16.77	16.40		
$5d\,^2D_{3/2}$	133.46	189.66	185.07	32.83	46.66	45.53	46.23 [66]	44.5417(16) [63]
$6d\,^2D_{3/2}$	28.82	51.62	51.00	7.09	12.70	12.55		
$7d\,^2D_{3/2}$	12.76	22.65	22.44	3.14	5.57	5.52		
$5d\,^2D_{5/2}$	171.26	253.06	247.14	42.13	62.25	60.80	62.17 [66]	59.528(43) [63]
$6d\,^2D_{5/2}$	37.38	69.77	68.90	9.20	17.16	16.95		
$7d\,^2D_{5/2}$	16.60	30.64	30.35	4.08	7.54	7.47		

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

$$2T^{\mathrm{DF}} = 1.4482 \times 10^{-3}, \quad C^{\mathrm{DF}} = 2.2603 \times 10^{-5},$$
$$R^{\mathrm{DF}} = 2.6238 \times 10^{-3}. \tag{5}$$

Since the value of C^{DF} is smaller than the T^{DF} and R^{DF} by two orders of magnitude, I did not recalculate the C term in the SD approximation.

The expression for R is similar to that for α^{E1} (compare Eqs. (1) and (7) [69]). The difference is an additional factor of the diagonal hyperfine matrix element:

$$\langle 6s_{1/2} \| \mathcal{T} \| 6s_{1/2} \rangle^{(\mathrm{SD})} = 1.1971 \times 10^{-6} \text{ a.u.}$$

I evaluate matrix elements $\langle v \| rC_1 \| n \rangle$ in the SD approximation for $n \leqslant 26$. I use recommended NIST energies [75] for n up to $n = 12$ and SD energies for $13 \leqslant n \leqslant 26$. The sum of terms for $n \leqslant 26$ is $R_{n \leqslant 26} = 2.11051 \times 10^{-3}$. The remainder of the sum, evaluated in the DHF approximation, $R_{n>26} = 5.1 \times 10^{-7}$ is less than 0.03%. The expression for T includes sums over two indices m and n. To calculate the dominant part of T, I limit the sum over m to six states ($m = 6p_{1/2}$, $6p_{3/2}$, $7p_{1/2}$, $7p_{3/2}$, $8p_{1/2}$, and $8p_{3/2}$) and sum over ns to $n = 36$. It should be noted that I use E_{ns} energies and $\langle ns \| \mathcal{T}^{(1)} \| 6s \rangle$ and $\langle mp_j \| rC_1 \| ns \rangle$ matrix elements evaluated in SD approximation for $ns = 14s$-$26s$ and in the RPA approximation for $ns = 27s$-$36s$:

$$\begin{aligned}
T_{\substack{m\leqslant 3\\ n\leqslant 36}} = &-\frac{1}{2} \sum_{ns=6s}^{36s} \frac{\langle ns \| \mathcal{T}^{(1)} \| 6s \rangle}{(E_{ns} - E_{6s})} \\
&\times \left[\frac{\langle 6s \| rC_1 \| 6p_{1/2} \rangle \langle 6p_{1/2} \| rC_1 \| ns \rangle}{(E_{6p_{1/2}} - E_{6s})} - \frac{\langle 6s \| rC_1 \| 6p_{3/2} \rangle \langle 6p_{3/2} \| rC_1 \| ns \rangle}{(E_{6p_{3/2}} - E_{6s})} \right. \\
&+ \frac{\langle 6s \| rC_1 \| 7p_{1/2} \rangle \langle 7p_{1/2} \| rC_1 \| ns \rangle}{(E_{7p_{1/2}} - E_{6s})} - \frac{\langle 6s \| rC_1 \| 7p_{3/2} \rangle \langle 7p_{3/2} \| rC_1 \| ns \rangle}{(E_{7p_{3/2}} - E_{6s})} \\
&+ \left. \frac{\langle 6s \| rC_1 \| 8p_{1/2} \rangle \langle 8p_{1/2} \| rC_1 \| ns \rangle}{(E_{8p_{1/2}} - E_{6s})} - \frac{\langle 6s \| rC_1 \| 8p_{3/2} \rangle \langle 8p_{3/2} \| rC_1 \| ns \rangle}{(E_{8p_{3/2}} - E_{6s})} \right].
\end{aligned} \tag{6}$$

The sum of the six contributions from Eq. (6) is $1.325\,85 \times 10^{-3}$. The ratio of contributions to the sum from the $7p$ and $8p$ to $6p$ states are surprisingly very small (about 10^{-2}). The relatively small remainder $T - T_{\substack{m>7\\ n>36}} = 0.003\,5 \times 10^{-3}$ is evaluated in the DHF approximation, leading to a final value $2T^{(\mathrm{SD})} = 1.329\,4 \times 10^{-3}$. Combining these contributions, we obtain

$$2T^{\mathrm{SD}} + C^{\mathrm{DF}} + R^{\mathrm{SD}} = 3.4631 \times 10^{-3} \text{ a.u.} \tag{7}$$

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

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

is equal to $-0.425\,191$ for $F = 1$ and $0.255\,114$ for $F = 2$.

Using these values and the result from Eq. (7), we obtain

$$\alpha^{(3)}_{F=2}(0) - \alpha^{(3)}_{F=1}(0) = 2.355\,9 \times 10^{-3} \text{ a.u.}$$

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

$$\begin{aligned} k^{(\mathrm{SD})} &= -1.1780 \times 10^{-3} \text{ a.u.} \\ &= -0.293\,1 \times 10^{-10}\ \mathrm{Hz/(V/m)^2}. \end{aligned}$$

In the DHF approximation [Eq. (5)], we find $k^{(\mathrm{DF})} = -0.346\,6 \times 10^{-10}\ \mathrm{Hz/(V/m)^2}$.

The relative blackbody radiative shift β is defined as

$$\beta = -\frac{2}{15} \frac{1}{\nu_{\mathrm{hf}}} (\alpha\pi)^3 T^4 \alpha_{\mathrm{hf}}(6s_{1/2}), \tag{8}$$

where ν_{hf} is the ^{137}Ba II hyperfine ($F = 2$ and $F = 1$) splitting equal to 8 037.741 668 MHz and T is a temperature equal to 300 K. Using those factors, we can rewrite Eq. (8):

$$\beta = -1.071\,35 \times 10^{-12} \alpha_{\mathrm{hf}}(6s_{1/2}). \tag{9}$$

Using the SD value for $\alpha_{\mathrm{hf}}(6s_{1/2}) = 2.355\,9 \times 10^{-3}$ a.u., we obtain finally

$$\beta^{(\mathrm{SD})} = -0.252\,4 \times 10^{-14}. \tag{10}$$

This result is in a good agreement with results [−0.245(2)] given in Ref. [68].

IX. CONCLUSION

In summary, a systematic RMBPT study of the energies of the $ns_{1/2}$, np_j, and nd_j ($n \leqslant 12$) states in singly ionized barium is presented. The energy values are in excellent agreement with existing experimental data. Electric-dipole ($6s_{1/2}$-np_j, $n = 6$–26), electric- quadrupole ($6s_{1/2}$-nd_j, $n = 5$–26), and electric-octupole ($6s_{1/2}$-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 Ba II are evaluated, including matrix elements with high n up to $n = 26$. All of the aforementioned matrix elements are determined using the all-order method. Hyperfine A and B values are presented for the first low-lying levels up to $n = 8$. The quadratic Stark shift of the ground-state hyperfine interval in ^{137}Ba II is also evaluated. These calculations provide a theoretical benchmark for comparison with experiment and theory.

Throughout the article, I compare my all-order results with the RCC calculations of Refs. [44,66]. These works focused on the properties of the low-lying levels so relatively few comparisons could be made. In general, results of my work are in good agreement with RCC values. The comparison with experiment is not sufficiently conclusive to demonstrate better agreement of one method over the other. Both methods utilize the coupled-cluster approach but differ significantly in its implementation. Differences in the results are due to the inclusion or omission of different types of terms (nonlinear terms and triple excitations), the use of different basis sets (B-splines vs Gaussian-type orbitals) and different parameters of the nuclear distribution, and the completeness of the basis sets, including the use of the different numbers of the partial waves. For some properties, the discrepancies may be exacerbated owing to significant cancellations between certain terms. To provide more information regarding the importance of the triple excitations, I include both SD and SDpT values. These calculations omit nonlinear terms. However, it was shown in Ref. [89] that nonlinear terms tend to cancel nonperturbative triple excitations that are omitted in Refs. [44,66], and their inclusion may not lead to more accurate values. I use completely saturated B-spline basis sets and include more partial waves than RCC calculations that are important for certain properties. Since there are relatively few RCC data and precision experimental results available for comparison it does not appear possible to make general statements regarding the comparative accuracy of these two approaches. In the case of the $6p$ lifetimes, my SD data are expected to be in better agreement with experiment than SDpT data based on studies of the alkali-metal atoms. About 1% accuracy is expected for these values. Indeed, my SD values are in agreement with experiment and RCC data within the uncertainties. While central values of the RCC data are in closer agreement with experiment, the experimental precision is also on the order of 1.3–1.6%. The comparison of the all-order, RCC, and a number of experiment results for the $5d_j$ lifetimes is discussed in great detail in Ref. [1]. The values for A and B hyperfine constants are more sensitive to the differences in the methods discussed previously than the transition matrix elements. As a result, one can see somewhat larger differences between all-order and RCC data. The agreement with experiment is again not conclusive since all-order values are in closer agreement with experiment for the ground-state A constant and most B constants, while RCC data are in closer agreement for other cases. In conclusion, more precision experimental results would be useful for benchmark comparisons.

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