

# Lifetimes of the metastable ${}^2D_{3/2,5/2}$ states in $\text{Ca}^+$ , $\text{Sr}^+$ , and $\text{Ba}^+$

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Atomic properties involving the low-lying excited  ${}^2D_{3/2,5/2}$  states in alkaline-earth-metal ions are of current interest in many different applications ranging from tests of physics beyond the standard model to astrophysics. We have used the relativistic coupled-cluster theory to perform accurate calculations of the lifetimes of the lowest excited  ${}^2D_{3/2}$  and  ${}^2D_{5/2}$  states in singly ionized calcium, strontium, and barium. The importance of electron correlation in these calculations is emphasized. Our results are compared with the available experimental and theoretical data.

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## I. INTRODUCTION

Singly ionized calcium ( $\text{Ca}^+$ ), strontium ( $\text{Sr}^+$ ), and barium ( $\text{Ba}^+$ ) have been proposed as candidates for optical frequency standards [1–4] due to the long lifetime of their  ${}^2D_{3/2,5/2}$  states. These systems are important for quantum information processing [5]. A knowledge of the atomic properties of the  $5d\ {}^2D_{3/2}$  and  $5d\ {}^2D_{5/2}$  states in  $\text{Ba}^+$  is essential for the studies of atomic parity nonconservation (PNC) [6,7]. Forbidden transitions from the  $d$ -metastable states to their ground states in these systems are important in many astrophysical contexts [8]. Numerous experiments have been performed during the last decade to measure the lifetimes of these states using different approaches [9–14]. Additionally, several theoretical studies have been carried out using a variety of many-body approaches [15–18], but further progress is needed to obtain reliable values for the lifetimes of these excited  ${}^2D_{3/2,5/2}$  states. It is therefore desirable to use the relativistic coupled-cluster (RCC) theory [19,20] which is equivalent to all order relativistic many-body perturbation theory to perform these challenging calculations.

In the present work, we have employed the RCC theory to calculate the lifetimes of the  $nd\ {}^2D_{3/2}$  and  $nd\ {}^2D_{5/2}$  states in  $\text{Ca}^+$  ( $n=3$ ),  $\text{Sr}^+$  ( $n=4$ ), and  $\text{Ba}^+$  ( $n=5$ ). Less than one percent calculations of subtle effects that arise from parity [21] and time reversal violating interactions [22] have been reported recently using this theory.

## II. THEORY

According to the selection rules, the  ${}^2D_{3/2}$  states decay to the  ${}^2S_{1/2}$  states by both the  $E2$  and  $M1$  channels whereas the  ${}^2D_{5/2}$  states decay to  ${}^2S_{1/2}$  states only through the  $E2$  transition. The emission transition probabilities (in  $\text{sec}^{-1}$ ) for the  $E2$  and  $M1$  channels from state  $f$  to state  $i$  are given by

$$A_{f \rightarrow i}^{E2} = \frac{1.11995 \times 10^{18}}{[J_f] \lambda^5} S_{f \rightarrow i}^{E2}, \quad (2.1)$$

$$A_{f \rightarrow i}^{M1} = \frac{2.69735 \times 10^{13}}{[J_f] \lambda^3} S_{f \rightarrow i}^{M1}, \quad (2.2)$$

where  $[J_f]=2J_f+1$  is the degeneracy of  $f$  state,  $S = |\langle f | O | i \rangle|^2$ , for the transition operator  $O$  [in atomic unit (a.u.)], and  $\lambda$  (in Å) are the corresponding transition line strength and wavelength, respectively.

In addition, the  ${}^2D_{5/2}$  states can decay to the  ${}^2D_{3/2}$  states via  $E2$  and  $M1$  channels, hence the total transition probability of decay from the  ${}^2D_{3/2,5/2}$  states can be expressed as

$$A_{nd3/2} = A_{nd3/2 \rightarrow ms1/2}^{E2} + A_{nd3/2 \rightarrow ms1/2}^{M1},$$

$$A_{nd5/2} = A_{nd5/2 \rightarrow ms1/2}^{E2} + A_{nd5/2 \rightarrow nd3/2}^{E2} + A_{nd5/2 \rightarrow nd3/2}^{M1}, \quad (2.3)$$

where  $m$  and  $n$  represent the principal quantum numbers for the ground and metastable states of the corresponding systems. A schematic diagram of these transitions is shown in Fig. 1.

The lifetime of these states, which is the reciprocal of the transition probability, can be expressed as (in sec)

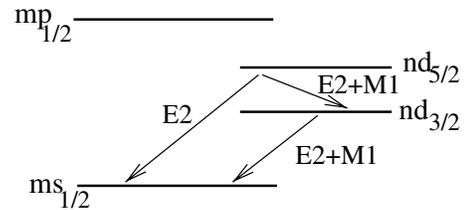


FIG. 1. Schematic diagram for the energy levels of the  $ms$ ,  $mp$ , and  $nd$  states transition lines in  $\text{Ca}^+$ ,  $\text{Sr}^+$ , and  $\text{Ba}^+$ . The  $m$  and  $n$  represent the principal quantum numbers of the ground and metastable states.

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$$\tau_{nd3/2} = \frac{1}{A_{nd3/2}},$$

$$\tau_{nd5/2} = \frac{1}{A_{nd5/2}}. \quad (2.4)$$

The single particle reduced matrix elements due to  $E2$  and  $M1$  operators, which are needed in calculating the line strengths, are given below.

For  $E2$ , in length gauge

$$\begin{aligned} \langle \kappa_f || e2^l || \kappa_i \rangle &= \frac{15}{k^2} \langle \kappa_f || C^{(2)} || \kappa_i \rangle \\ &\times \int_0^\infty dr \left\{ j_2(kr) [P_f(r)P_i(r) + Q_f(r)Q_i(r)] \right. \\ &+ j_3(kr) \left( \frac{\kappa_f - \kappa_i}{3} [P_f(r)Q_i(r) + Q_f(r)P_i(r)] \right. \\ &\left. \left. + [P_f(r)Q_i(r) - Q_f(r)P_i(r)] \right) \right\}, \quad (2.5) \end{aligned}$$

and in velocity gauge

$$\begin{aligned} \langle \kappa_f || e2^v || \kappa_i \rangle &= \frac{15}{k^2} \langle \kappa_f || C^{(2)} || \kappa_i \rangle \int_0^\infty dr \left[ 2 \frac{j_2(kr)}{kr} \right. \\ &\times [P_f(r)Q_i(r) - Q_f(r)P_i(r)] - \frac{(\kappa_f - \kappa_i)}{3} \\ &\times \left( -j_3(kr) + \frac{3}{kr} j_2(kr) \right) [P_f(r)Q_i(r) \\ &\left. + Q_f(r)P_i(r)] \right], \quad (2.6) \end{aligned}$$

and for  $M1$

$$\begin{aligned} \langle \kappa_f || m1 || \kappa_i \rangle &= \frac{6}{\alpha k} \langle \kappa_f || C^{(1)} || \kappa_i \rangle \int_0^\infty dr \frac{\kappa_f + \kappa_i}{2} j_1(kr) [P_f(r)Q_i(r) \\ &+ Q_f(r)P_i(r)]. \quad (2.7) \end{aligned}$$

Here,  $j$ 's and  $\kappa$ 's are the total and relativistic angular momentum quantum numbers, respectively. The radial functions  $P_i(r)$  and  $Q_i(r)$  are the large and small components of the  $i$ th single particle Dirac orbital. The Racah operators are given by

$$\langle \kappa m | C_q^{(k)} | \kappa' m' \rangle = (-1)^{j-m} \begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix} \langle \kappa || C^{(k)} || \kappa' \rangle, \quad (2.8)$$

with

$$\begin{aligned} \langle \kappa || C^{(k)} || \kappa' \rangle &= (-1)^{j+1/2} \sqrt{(2j+1)(2j'+1)} \\ &\times \begin{pmatrix} j & k & j' \\ 1/2 & 0 & -1/2 \end{pmatrix} \pi(l, k, l'), \quad (2.9) \end{aligned}$$

$$\pi(l_1, l_2, l_3) = \begin{cases} 1 & \text{for } l_1 + l_2 + l_3 = \text{even}, \\ 0 & \text{else.} \end{cases} \quad (2.10)$$

In the above expression, we define  $k = w\alpha$ , where  $w = \epsilon_i - \epsilon_f$  is the excitation energy at single particle levels,  $\alpha$  is the fine structure constant and  $j_l(kr)$  is a spherical Bessel function of order  $l$ . When  $kr$  is sufficiently small, one can apply the following approximation to calculate the above matrix elements

$$z^{-n} j_n(z) \approx \frac{1}{1 \times 3 \times 5 \times \cdots \times (2n+1)}. \quad (2.11)$$

### III. METHOD OF CALCULATION

The radial functions  $[P_i(r)$  and  $Q_i(r)]$  of the Dirac orbitals for a given angular momentum symmetry (for  $s, p, \dots$  orbitals) are expanded as a set of Gaussian type orbitals (GTOs) of the form [23]

$$F^\kappa(r_i) = \sum_j C_j^\kappa t_i^\kappa e^{-\alpha_j r_i^2}, \quad (3.1)$$

where  $C_j^\kappa$ ,  $i$  and  $j$  represent the expansion coefficients, radial grid points, and the number of GTOs for a given  $\kappa$  symmetry orbital, respectively. These grid points are defined in such a way that they construct sharp functions at the origin and diffuse functions at the asymptotic region of the nucleus. For the exponents, we use the even tempering condition

$$\alpha_j = \alpha_0 \beta^{j-1}. \quad (3.2)$$

The exact wave function, for a system with a single valence electron  $v$  in the framework of coupled-cluster theory can be written as [20,24]

$$|\Psi_v\rangle = e^T \{1 + S_v\} |\Phi_v\rangle, \quad (3.3)$$

with the reference state  $|\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle$ , where  $|\Phi_0\rangle$  is the Dirac-Fock (DF) state of the closed-shell system. We define  $T$  and  $S_v$  as the closed-shell and open-shell excitation operators, respectively. Assuming only singles and doubles excitations [coupled-cluster theory at singles and doubles (CCSD method)], we express  $T = T_1 + T_2$  and  $S_v = S_{1v} + S_{2v}$ . The corresponding cluster amplitudes are evaluated using the following coupled equations

$$\langle \Phi_L | \{He^T\} | \Phi_0 \rangle = E_0 \delta_{L,0}, \quad (3.4)$$

$$\begin{aligned} \langle \Phi_v^K | \{He^T\} S_v | \Phi_v \rangle &= -\langle \Phi_v^K | \{He^T\} | \Phi_v \rangle + \langle \Phi_v^K | S_v | \Phi_v \rangle E_v \\ &= -\langle \Phi_v^K | \{He^T\} | \Phi_v \rangle + \langle \Phi_v^K | S_v | \Phi_v \rangle \langle \Phi_v | \{He^T\} \{1 + S_v\} | \Phi_v \rangle, \quad (3.5) \end{aligned}$$

where the superscript  $L(=0, 1, 2)$  represents reference, singly, and doubly excited states from DF wave function for the closed-shell system, respectively, and  $K(=0, 1, 2)$  denotes reference, singly, and doubly excited states for the open-shell

system, respectively. We have considered all the nonlinear terms in solving the above equations. Contributions from the most important triple excitations to the  $S_v$  amplitude have been considered self-consistently through Eq. (3.5); this is known as the CCSD(T) method and it has been explicitly discussed elsewhere (for example, see Refs. [25,26]).

The transition matrix elements for an operator  $O$  can be expressed as

$$\begin{aligned} \langle O \rangle_{fi} &= \frac{\langle \Psi_f | O | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle} \sqrt{\langle \Psi_i | \Psi_i \rangle}} = \frac{\langle \Phi_f | \{1 + S_f^\dagger\} e^{T^\dagger} O e^T \{1 + S_i\} | \Phi_i \rangle}{\sqrt{1 + N_f} \sqrt{1 + N_i}} \\ &= \frac{\langle \Phi_f | \{1 + S_f^\dagger\} \bar{O} \{1 + S_i\} | \Phi_i \rangle}{\sqrt{1 + N_f} \sqrt{1 + N_i}}, \end{aligned} \quad (3.6)$$

where we define the effective operator  $\bar{O} = e^{T^\dagger} O e^T$  and for the valence electron  $v$ ,  $N_v = \langle \Phi_v | S_v^\dagger e^{T^\dagger} e^T S_v | \Phi_v \rangle$ . The above expressions are calculated using the method described earlier [25,26]. Contributions from the normalization factor can be expressed as

$$(\text{normalization factor}) = \langle \Psi_f | O | \Psi_i \rangle \left( \frac{1}{\sqrt{1 + N_f} \sqrt{1 + N_i}} - 1 \right). \quad (3.7)$$

#### IV. RESULTS AND DISCUSSIONS

In Table I, we present our lifetime results along with the other calculated and experimental results. It is clear from this table that most of the experimental results disagree with each other for all the transitions that we have considered. Similarly, there are discrepancies between the calculated results based on different many-body theories. Reliable calculations of the lifetimes are therefore necessary. Bearing this in mind, we have used the RCC theory to perform our calculations. The primary merit of this method is its ability to compute physical effects to all orders in the residual Coulomb interaction at any level of hole-particle excitation.

As given in Eq. (2.3), the  ${}^2D_{3/2}$  states decay to the ground states in the systems that we have considered by the  $E2$  and  $M1$  channels. However, the  $M1$  contributions are very small compared to those from  $E2$ . From Eqs. (2.1) and (2.2), one would expect that the contribution from the  $E2$  transition probabilities which depend on the reciprocal of the fifth power of the wavelength to be much smaller than the  $M1$  transition probabilities which depend on the reciprocal of the cubic power of the wavelengths, cf. Eq. (2.2). Also the line strengths of the  $M1$  transitions are so small that their contributions have very little effect on the lifetime and they had been neglected in the earlier calculations. We have considered both these transitions in our calculations for the sake of completeness.

The  ${}^2D_{5/2}$  states can decay either directly or via  ${}^2D_{3/2}$  states to the ground state,  ${}^2S_{1/2}$ , due to  $E2$  and  $M1$  transitions as shown in Fig. 1. In almost all calculations the latter contributions are neglected due to very small energy differences

TABLE I. Lifetimes of the  ${}^2D_{3/2,5/2}$  states in  $\text{Ca}^+$ ,  $\text{Sr}^+$ , and  $\text{Ba}^+$  in seconds.

Transitions	Experiments	Others	This work
<b>Ca<sup>+</sup></b>			
$3d\ {}^2D_{3/2} \rightarrow 4s\ {}^2S_{1/2}$	1.176(11) [9]	1.196(11) [9]	1.185(7)
	1.20(1) [10]	1.080 [15]	
	1.17(5) [28]	1.160 [32]	
	1.111(46) [29]	1.271 [16]	
	1.113(45) [30]	1.2 [17]	
	1.24(39) [31]	1.09 [33]	
		1.08 [34]	
		0.98 [35]	
		0.797 [36]	
		0.769 [37]	
	1.200 [38]		
$3d\ {}^2D_{5/2} \rightarrow 4s\ {}^2S_{1/2}$	1.168(9) [9]	1.165(11) [9]	1.110(9)
	1.168(7) [10]	1.045 [15]	
	1.152(20) [39]	1.07 [33]	
	1.177(10) [40]	1.163 [17]	
	1.100(18) [11]	1.140 [32]	
	1.09(5) [28]	1.236 [16]	
	0.969(21) [41]	0.774 [36]	
	1.064(17) [42]	0.769 [37]	
	0.994(38) [29]	1.14 [32]	
	1.054(61) [30]	1.06 [34]	
1.08(22) [43]	0.95 [35]		
1.24(39) [31]	1.170 [38]		
1.149(18) [44]			
<b>Sr<sup>+</sup></b>			
$4d^2\ {}^2D_{3/2} \rightarrow 5s^2\ {}^2S_{1/2}$	0.435(4) [12]	0.454 [16]	0.426(8)
	0.435(4) [13]	0.422 [13]	
	0.455(29) [13]	0.441 [38]	
	0.395(38) [45]	0.257 [36]	
$4d\ {}^2D_{5/2} \rightarrow 5s^2\ {}^2S_{1/2}$	0.3908(16) [46]	0.384 [13]	0.357(12)
	0.408(22) [13]	0.396 [38]	
	0.372(25) [47]	0.405 [16]	
	0.347(11) [48]	0.209 [36]	
	0.345(33) [45]		
<b>Ba<sup>+</sup></b>			
$5d\ {}^2D_{3/2} \rightarrow 6s\ {}^2S_{1/2}$	79.8(4.6) [14]	81.4 [50]	80.086(714)
	17.5(4) [49]	81.5 [18]	
		83.7 [16]	
		72.1 [51]	
		45.4 [36]	
$5d\ {}^2D_{5/2} \rightarrow 6s\ {}^2S_{1/2}$	34.5(3.5) [52]	85.5 [38]	
	32(5) [53]	36.5 [50]	29.856(296)
	47(16) [54]	30.3 [18]	
		37.2 [16]	
		33.2 [51]	
	19.0 [36]		
	38.7 [38]		

TABLE II. Reduced matrix elements of the  $E2$  transition operator using length gauge for the corresponding  ${}^2D_{3/2}$  states to the ground state in atomic unit.

RCC terms	Ca <sup>+</sup>	Sr <sup>+</sup>	Ba <sup>+</sup>
$\overline{E2}$	9.772	12.975	14.740
$\overline{E2S_{1i}}$	-1.408	-1.105	-1.395
$S_{1i}^\dagger \overline{E2}$	-0.298	-0.429	-0.459
$\overline{E2S_{2i}}$	-0.079	-0.056	-0.118
$S_{2i}^\dagger \overline{E2}$	-0.017	-0.038	-0.085
$S_{1i}^\dagger \overline{E2S_{1i}}$	0.087	0.092	0.148
$S_{1i}^\dagger \overline{E2S_{2i}}$	-0.008	-0.002	-0.005
$S_{2i}^\dagger \overline{E2S_{1i}}$	0.004	0.002	0.004
$S_{2i}^\dagger \overline{E2S_{2i}}$	0.049	0.079	0.156
Contributions from effective two-body terms			
$T_1^\dagger \overline{E2S_{2i}}$	-0.0008	-0.0012	-0.0054
$S_{2i}^\dagger \overline{E2T_1}$	-0.0010	-0.0011	-0.0059
$T_2^\dagger \overline{E2S_{2i}}$	0.000	-0.00001	-0.00001
$S_{2i}^\dagger \overline{E2T_2}$	0.0038	0.0053	0.0086
Normalization factor	-0.136	-0.178	-0.245
Total	7.973	11.332	12.734

between the  ${}^2D_{5/2}$  and  ${}^2D_{3/2}$  states giving large transition wavelengths, which is true in the case of Ca<sup>+</sup> and Sr<sup>+</sup>. On the contrary, one has to consider them in Ba<sup>+</sup> where the corresponding wavelength is small compared to the aforementioned two systems and they contribute significantly to improve the lifetime calculation of the  $5d\ {}^2D_{5/2}$  state.

The net errors associated with the lifetime calculations for the  ${}^2D_{3/2,5/2}$  states accumulate from the individual errors of the calculated wavelengths and the line strengths. Since the transition probabilities depend on the inverse of the third and fifth powers of the wavelengths, even small errors in the calculated wavelengths will give rise to relatively large errors in the lifetime calculations. The wavelengths of these transitions are known up to very high precision and we have taken them from the excitation energies available from the National Institute of Standards and Technology (NIST) [27] database for our lifetime calculations. The line strengths can be calculated to fairly high precision and they have been used in our determination of the lifetimes.

We have performed calculations for the  $E2$  amplitudes in the length and velocity gauges. The agreement between the results of these two gauges varies between 2–3 % for different ions and it can be improved further by using a larger basis. We have used the results of the length gauge in our calculations since they are more stable than the results of the velocity gauge.

In Tables II and III, we present the reduced transition matrix elements, whose squares give the line strengths of the corresponding transitions, using the relativistic CCSD(T) method. The trends of these results which are identical for all the systems, reflect the influence of pair correlation effects present in  $\overline{E2S_{1i}}$  and  $S_{1i}^\dagger \overline{E2}$ , which is important in the precise determination of the final results. The DF contribution resides in the  $\overline{E2}$  term. The core-polarization contributions are

TABLE III. Reduced matrix elements of the  $E2$  transition operator using length gauge for the corresponding  ${}^2D_{5/2}$  states to the ground state in atomic unit.

RCC terms	Ca <sup>+</sup>	Sr <sup>+</sup>	Ba <sup>+</sup>
$\overline{E2}$	11.976	15.992	18.349
$\overline{E2S_{1i}}$	-1.617	-1.268	-1.633
$S_{1i}^\dagger \overline{E2}$	-0.333	-0.529	-0.582
$\overline{E2S_{2i}}$	-0.057	-0.092	-0.143
$S_{2i}^\dagger \overline{E2}$	-0.009	-0.041	-0.081
$S_{1i}^\dagger \overline{E2S_{1i}}$	0.109	0.122	0.176
$S_{1i}^\dagger \overline{E2S_{2i}}$	-0.002	-0.003	-0.006
$S_{2i}^\dagger \overline{E2S_{1i}}$	0.005	0.003	0.005
$S_{2i}^\dagger \overline{E2S_{2i}}$	0.064	0.120	0.190
Contributions from effective two-body terms			
$T_1^\dagger \overline{E2S_{2i}}$	-0.0011	-0.0015	-0.0067
$S_{2i}^\dagger \overline{E2T_1}$	-0.0012	-0.0014	-0.0072
$T_2^\dagger \overline{E2S_{2i}}$	0.000	-0.00001	-0.00001
$S_{2i}^\dagger \overline{E2T_2}$	0.0051	0.0065	0.0104
Normalization factor	-0.165	-0.214	-0.298
Total	9.979	14.094	15.960

significant and they are present in  $\overline{E2S_{2i}}$  and  $S_{2i}^\dagger \overline{E2}$ . Contributions from the effective two-body terms from  $\overline{E2}$  are also not negligible. The total correlation effects for the  ${}^2D_{3/2}$  states are around 17%, 13%, and 28% with respect to the DF values in Ca<sup>+</sup>, Sr<sup>+</sup>, and Ba<sup>+</sup>, respectively, whereas, they are 17%, 12%, and 13% for the  ${}^2D_{5/2}$  states in Ca<sup>+</sup>, Sr<sup>+</sup>, and Ba<sup>+</sup>, respectively.

The following considerations have gone into the evaluation of errors in our calculations. The leading order contributions that have been neglected in our calculations come from the triple excitations in the CCSD(T) method. As has been shown, the unitary coupled-cluster theory at the singles, doubles and partial triples [UCCSD(T)] has some extra triple and quadrupole excitations compared to the CCSD(T) method [55]. We have taken the lower-order extra triple excitations that can only appear through the UCCSD(T) theory using the CCSD(T) amplitudes and the Coulomb interaction term. We have also compared these with the differences of the CCSD and CCSD(T) results and have obtained similar trends and hence, it seems appealing on physical grounds to consider this approach to estimate the errors for the calculated line strengths. Further, we have checked the convergence of the results with higher angular momentum orbitals. We increased the size of our single particle orbitals till the calculated values of our line strength remained unchanged. We have considered the small fluctuations in our results using different basis as a second source of errors.

Several calculations have been carried out on Ca<sup>+</sup> and among them Kreuter *et al.*'s results [9] are the most recent. These calculations are based on the RCC theory, but it does not take into account the nonlinear terms which are important for high precision calculations. In these calculations, it has been shown that the contributions from the Breit inter-

action are insignificant [9]. Other calculations by Guet and Johnson [16] are based on the second-order many-body perturbation theory which is a low-order approximation of the RCC theory, Liaw [15] has performed his calculation in the Bruckner approximation (BA), which is present in the RCC theory. Other calculations are based on different variants of the multiconfiguration Hartree-Fock (MCHF) method or just the Hartree-Fock (HF) approximation.

We have found that the main contribution to the lifetime of the  $3d^2D_{3/2}$  state comes from the  $E2$  transition amplitude. The reduced matrix element of the  $M1$  transition amplitude is around 0.0007 a.u. The lifetime of  $3d^2D_{5/2}$  state changes only in the third place of decimal due to the  $M1$  transition. The contribution to the  $E2$  reduced matrix element comes from the  $3d^2D_{5/2} \rightarrow 3d^2D_{3/2}$  transition is around 3.92 a.u., and the  $M1$  matrix element is about 1.54 a.u.

There are comparatively less studies on the lifetime of the  $4d$ - states in  $\text{Sr}^+$ . Two identical experimental results [12,13] for the lifetime of the  $4d^2D_{3/2}$  state have been reported, which are close to our calculated result. Other theoretical results have been performed using lower order many-body theories in contrast to our RCC theory. The  $M1$  reduced matrix element is 0.0005 a.u., which is smaller than that for  $\text{Ca}^+$ . The experimental results for the  $4d^2D_{5/2}$  state in this system are also given with different error bars. Other theoretical results computed with the lower order many-body theories are somewhat larger than the present work. Our results agree well with some of these experiments. The  $M1$  and  $E2$  reduced matrix elements are 1.55 a.u. and 6.196 a.u., respectively.

High precision measured values of the lifetimes of the  $5d^2D_{3/2,5/2}$  states in  $\text{Ba}^+$  are not available. In fact, the earlier and the recent experiments give dissimilar results for the  $5d^2D_{3/2}$  state [14,49]. The  $M1$  reduced matrix element for this state is 0.0008 a.u., which results in a negligible contribution to the lifetime of this state. As given in Table I, our lifetime result for the  $5d^2D_{3/2}$  state is more accurate than the earlier calculations. There are noticeable disagreements between the calculated lifetime of the  $5d^2D_{5/2}$  state in  $\text{Ba}^+$ .

Guet and Johnson [16] have calculated this result using the second-order many-body perturbation theory and Dzuba *et al.* [18] have calculated using a variant of the Green's function method. Geetha *et al.* [50] have calculated using the same RCC theory that is used in this work, but they did not consider the effective two-body terms in the reduced matrix element calculation for  $E2$  which are given explicitly in Tables II and III. The  $M1$  and  $E2$  reduced matrix elements are 1.54 a.u. and 6.83 a.u., respectively. This trend is similar to what we had obtained for  $\text{Sr}^+$ . We would like to emphasize that these contributions are significant for the lifetime of the  $5d^2D_{5/2}$  state. We have found that the lifetime of this state due to  $E2$  from the  $5d^2D_{5/2} \rightarrow 6s^2S_{1/2}$  transition is 35.539 sec, but due to the  $5d^2D_{5/2} \rightarrow 5d^2D_{3/2}$  transition it reduces to 29.856 sec.

## V. CONCLUSION

The work in this paper focuses on the calculation of the accurate line strengths for the low-lying metastable  $^2D_{3/2,5/2}$  states in  $\text{Ca}^+$ ,  $\text{Sr}^+$ , and  $\text{Ba}^+$  employing the RCC theory at the level of single, double, and also a leading class of triple excitations. Combining these line strengths with the available experimental wavelengths corresponding to different transitions, we have determined the lifetimes of the above states precisely. These results can serve as benchmarks for testing relativistic many-body theories in the future. Additionally, we have discussed the trends exhibited by the different many-body effects that play a crucial role in the present calculations.

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