Decay of the $1s^2 2s3p\ ^3P_0$ level in Be-like ions

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(Received 15 October 2012; published 29 November 2012)

The lifetime of the $1s^2 2s3p\ ^3P_0$ level of selected Be-like ions, from $Z = 5$ to $Z = 92$, is calculated using the multiconfiguration Dirac-Fock method including QED corrections. Full correlation up to the $4f$ subshell in both initial and final levels for all possible decay modes was included. The results are in reasonable agreement with the scarce existing experimental and theoretical data.

DOI: 10.1103/PhysRevA.86.052521 PACS number(s): 32.70.Cs, 32.70.Fw

I. INTRODUCTION

The knowledge of accurate values of atomic radiative and radiationless transition probabilities, level energies, and lifetimes is crucial in many fields of science, such as fundamental physics and precise measurements. From the theoretical point of view, the accurate calculation of transition probabilities and lifetimes for highly charged ions must include, among other effects, electron correlation, relativity, QED corrections, and nuclear structure. As the importance of these effects increases strongly with Z, simplifications based on perturbative treatments of relativistic and QED corrections may not be adequate in highly charged ions [1].

Be-like ions have been the object of intense theoretical research for several decades because their small number of electrons makes them manageable by different approaches, thus constituting a benchmark for testing atomic models and wave functions in many-body systems. Among these studies, the analysis of forbidden transitions provides better information on the quality of wave functions than energy calculations because the latter are insensitive to small changes in the wave function due to the variational technique usually applied; electronic correlation can dramatically change the lifetime of long-lived levels. The decay of atomic levels with total angular momentum $J = 0$, for instance, is particularly interesting because it can be heavily suppressed, due to angular momentum conservation, if no appropriate decay channel to $J \neq 0$ levels exists.

In a study concerning forbidden transitions in Be-like systems, Knystautas and Drouin [2] measured the lifetimes of ten terms in Be-like oxygen using the beam-foil technique. However, they were not able to discriminate between the initial levels of those terms because their energies are very close. Engström *et al.* [3] reported lifetime measurements for the $1s^2 2s3p\ ^3P_{0,1,2}$ levels in Be-like nitrogen, oxygen, and fluorine, also using the beam-foil method. The lifetime values reported are 5.26 ± 0.07 ns and 3.04 ± 0.04 ns for the $^3P_0$ level in Be-like oxygen and fluorine, respectively. In 1979, Glass [4] published calculated oscillator strength values for transitions in Be-like carbon, nitrogen, oxygen, and neon.

From the theoretical point of view, Träbert *et al.* [5] quoted the value of 1.2 ns for the Be-like silicon $^3P_{0,2}$ level lifetimes calculated by Fawcett. Tully *et al.* [6] calculated the transition probabilities for selected term transitions in Li-like nitrogen, oxygen, and neon. Chung and Zhu [7] calculated the energies and wave functions of the $1s^2 2snl$ states of the beryllium atom with a full core plus correlation method. The same authors [8,9] reported the calculation of energies and wave functions of the Be-like $1s^2 2snl$ ($n = 2,3$) terms for $5 \leqslant Z \leqslant 14$. They included intermediate coupling relativistic corrections, mass polarization, and QED effects. Energy values and transition probabilities for several $1s^2 2snp$ ($n = 2,3$) terms in Be-like nitrogen were computed by Ramsbottom *et al.* [10]. These authors used the R-matrix method to compute electron-impact excitation collision strengths, and Hibbert's code [11] to calculate oscillator strengths and transition probabilities.

Results from systematic multiconfiguration Hartree-Fock studies of the $1s^2 2s^2\ ^1S_0 \rightarrow 1s^2 2s3p\ ^1P_1$ transition in the Be-like sequence, in the range $Z = 4$–10, were reported for several electronic correlation models by Fischer *et al.* [12]. Safronova *et al.* [13] performed relativistic many-body calculations of transition probabilities for the $2l_1 l_2[LSJ]$–$2l_3 3l_4[L_0 S_0 J_0]$ lines in Be-like ions for Z between 6 and 100. The many-body perturbation theory (MBPT), including the Breit interaction, was used to evaluate retarded dipole matrix elements in length and velocity forms. The authors used first-order theory to obtain intermediate coupling coefficients and second-order theory to determine matrix elements. The transition energies used to evaluate transition probabilities were also obtained from second-order MBPT. Breit-Pauli results for energy levels, lifetimes, and some transition data were reported by Tachiev and Fischer [14,15] for all levels of the $2s^2$, $2s2p$, $2p^2$, $2s3s$, $2s3p$, and $2s3d$ configurations of the Be-like spectrum for $4 \leqslant Z \leqslant 12$. In the framework of the IRON project, Chidichimo *et al.* [16] calculated collision strengths for electron-induced transitions in the Be-like ion

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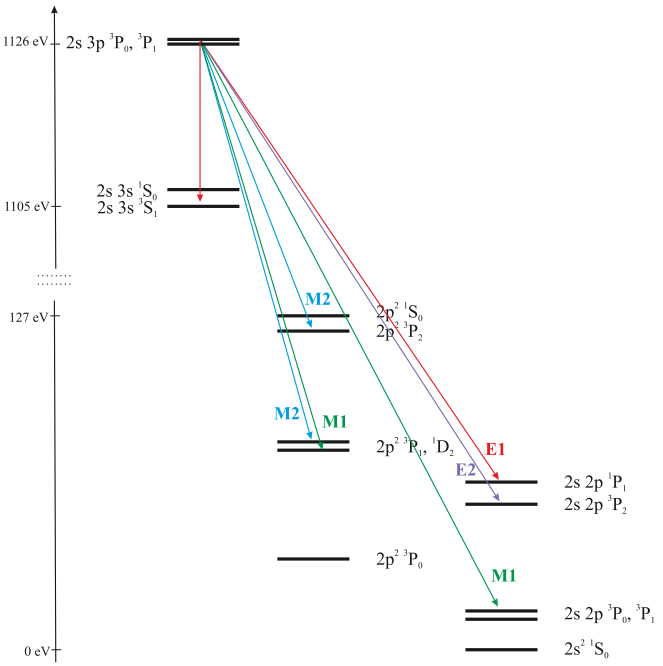

FIG. 1. (Color online) Energy levels for $Z = 26$ and decay channels from the Be-like $1s^2 2s3p\ ^3P_0$ level.

Fe^{22+} using the intermediate coupling frame transformation (ICFT) version of the *R*-matrix programs. Most recently, Li *et al.* [17] used the flexible atomic code (FAC) to calculate the collision strengths for some Be-like neon lines, based on the distorted-wave method with large configuration interactions included.

In this work, we used the multiconfiguration Dirac-Fock approach (MCDF), including correlation up to the $4f$ subshell, to calculate the transition-energy and -probability values for all possible decay channels of the $1s^2 2s3p\ ^3P_0$ level in Be-like ions in order to obtain the lifetime of this level for selected values of Z from 5 to 92. The importance of the different

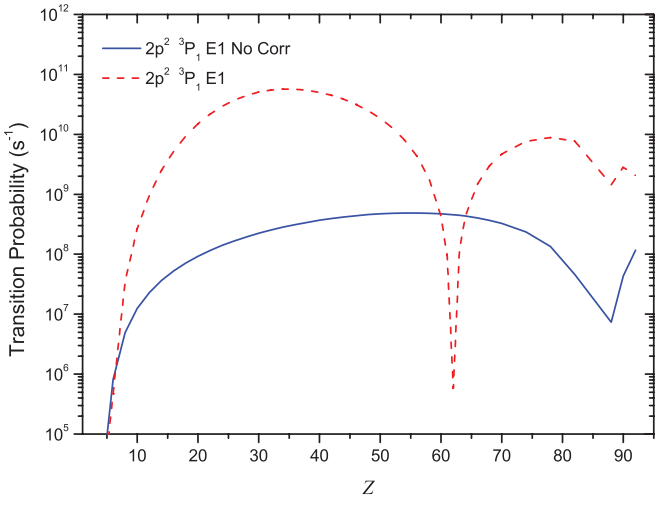

FIG. 2. (Color online) Transition-probability values for two-electron one-photon decay channel of the $1s^2 2s3p\ ^3P_0$ level to the $1s^2 2p^2\ ^3P_1$ level in Be-like ions as a function of Z, calculated with and without correlation.

decay channels is discussed and the results are compared to the scarce existing experimental values and available theoretical values. Indelicato [1] had used a similar approach to calculate the radiative deexcitation of the $1s^2 2s3p\ ^3P_0$ level in Be-like ions, for $Z = 26$,54, and 92, using a much smaller set of configurations than in the present work.

II. THE MCDF METHOD

The detailed calculations of the atomic energy levels and radiative transition probabilities were carried out within the multiconfiguration Dirac-Fock (MCDF) approach using the general relativistic code (MDFGME) developed by Desclaux and Indelicato [18–20]. The description of the code as well as the method is given in Refs. [21,22]. Complete correlation was included up to the $4f$ subshell.

In order to obtain the best possible transition energies and accurate values for two-electron one-photon (TEOP) transition probabilities, one must relax independently the initial- and final-state wave functions. Yet this leads to nonorthogonal spin

TABLE I. Transition-probability and -energy values for the $1s^2 2s3p\ ^3P_0 \rightarrow 1s^2 2s3s\ ^3S_1$ decay for several values of Z.

	Trans. Prob. (s^{-1})		Energy (eV)		
Z	This Work	NIST	This Work	NIST	Engström [3]
5	4.29×10^7	3.97×10^7	1.78	1.76	
6	8.23×10^7	7.24×10^7	2.74	2.67	
7	1.23×10^8	1.06×10^8	3.69	3.56	3.56
8	1.63×10^8	1.38×10^8	4.62	4.44	4.44
9	2.04×10^8		5.55		5.34
10	2.44×10^8	2.30×10^8	6.48	6.21	
11	2.84×10^8		7.40		
12	3.24×10^8		8.32		
14	4.04×10^8		10.15		
16	4.85×10^8		11.99		
18	5.67×10^8		13.85		
20	6.52×10^8		15.71		
22	7.39×10^8		17.59		
24	8.27×10^8		19.48		
26	9.18×10^8		21.38		
28	1.01×10^9		23.30		
30	1.11×10^9		25.23		
32	1.21×10^9		27.18		
34	1.31×10^9		29.16		
42	1.76×10^9		37.43		
46	2.01×10^9		41.74		
48	2.15×10^9		44.01		
50	2.30×10^9		46.35		
52	2.45×10^9		48.75		
54	2.62×10^9		51.22		
56	2.79×10^9		53.77		
62	3.39×10^9		61.94		
70	4.38×10^9		74.21		
74	4.98×10^9		81.01		
78	5.67×10^9		88.35		
82	6.48×10^9		96.37		
86	7.38×10^9		104.91		
90	8.18×10^9		113.16		
92	8.39×10^9		116.43		

orbitals of identical symmetry between the initial and final states. This nonorthogonality effect, described in Refs. [1,23], is taken into account using the formalism proposed by Löwdin [24].

It should be noted that the initial and final levels for each transition are defined in jj coupling since the MCDF method used is a fully relativistic method. However, for comparison with other published work where levels are characterized by their LSJ labels, we give in the tables, for each level, the most important LSJ set of values that results from the expansion of the jjJ wave function in terms of the LSJ ones.

All calculations were done for a finite nucleus using a uniformly charged sphere. The atomic masses and the nuclear radii were taken from the tables by Audi *et al.* [25] and Angeli [26], respectively. The length gauge was used for all radiative transition probabilities.

Radiative corrections are also introduced, from a full QED treatment. The one-electron self-energy is evaluated using the one-electron values of Mohr and co-workers [27–30] and corrected for finite nuclear size [31]. The self-energy screening and vacuum polarization are treated with methods developed by Indelicato and co-workers [19,20,32–34].

III. RESULTS AND DISCUSSION

Unlike the $1s^2 2s2p\ ^{1,3}P_J$ levels for which an experimental lifetime can immediately be converted to an oscillator strength or transition rate, the lifetimes of the $1s^2 2s3p\ ^{1,3}P_J$ levels in Be-like ions require the knowledge of the transition-probability values for all decay channels. In this work, we focused on the $1s^2 2s3p\ ^3P_0$ level lifetime.

An example of the structure of the lower levels of an highly charged Be-like ion is shown in Fig. 1. The $1s^2 2s3p\ ^3P_0$ level can decay by an $E1$ transition to the $1s^2 2s3s\ ^3S_1$ level, by an $E2$ transition to the $1s^2 2s2p\ ^3P_2$ level, and by two $M1$ transitions to the $1s^2 2s2p\ ^{1,3}P_1$ levels. It can also decay by a TEOP $E1$ transition to the $1s^2 2p^2\ ^3P_1$ level, and by two $M2$ transitions to the $1s^2 2s2p\ ^1D_2$ and $1s^2 2s2p\ ^3P_2$ levels, respectively.

TABLE II. Transition-probability and -energy values for the $1s^2 2s3p\ ^3P_0 \rightarrow 1s^2 2p^2\ ^3P_1$ decay for several values of Z.

	Trans. Prob. (s^{-1})				Energy (eV)			
Z	This work	NIST	Safronova [13]	Techiev [14]	This work	NIST	Tachiev [14]	Safronova [13]
5	4.86×10^4	5.40×10^4			5.45	5.59		
6	4.75×10^5	1.93×10^6			15.13	15.16		
7	8.28×10^6	1.51×10^7	1.48×10^7		28.54	28.56		28.64
8	3.48×10^7	5.57×10^7	6.12×10^7	5.79×10^7	45.76	45.77	45.75	45.84
9	1.14×10^8				66.77			
10	2.68×10^8	3.50×10^8			91.56	91.56		
11	5.42×10^8				120.12			
12	9.79×10^8	1.18×10^9			152.45	152.53		
14	2.53×10^9				228.39			
16	5.26×10^9				319.34			
18	9.41×10^9				425.27			
20	1.50×10^{10}				546.13			
22	2.19×10^{10}				681.88			
24	2.95×10^{10}				832.48			
26	3.73×10^{10}				997.87			
28	4.45×10^{10}				1178.00			
30	5.04×10^{10}				1372.81			
32	5.46×10^{10}				1582.23			
34	5.66×10^{10}				1806.18			
42	4.47×10^{10}				2845.63			
46	3.15×10^{10}				3450.16			
48	2.47×10^{10}				3773.20			
50	1.84×10^{10}				4109.90			
52	1.27×10^{10}				4460.13			
54	8.00×10^9				4823.71			
56	4.36×10^9				5200.46			
62	5.74×10^5				6407.75			
70	4.68×10^9				8188.05			
74	7.63×10^9				9145.81			
78	8.83×10^9				10144.63			
82	7.75×10^9				11180.78			
86	1.17×10^{11}				12250.49			
90	2.85×10^9				13347.07			
92	2.07×10^9				13904.95			

TABLE III. Transition-probability and -energy values for the $1s^2 2s 3p\ ^3P_0 \rightarrow 1s^2 2s 2p\ ^3P_2$ decay for several values of Z.

Z	Trans. Prob. (s^{-1})	Energy (eV)
5	6.14×10^3	13.25
6	5.10×10^4	25.80
7	2.35×10^5	42.14
8	7.82×10^5	62.26
9	2.11×10^6	86.16
10	4.94×10^6	113.83
11	1.04×10^7	145.28
12	2.00×10^7	180.49
14	6.23×10^7	262.21
16	1.61×10^8	358.98
18	3.66×10^8	470.77
20	7.51×10^8	597.55
22	1.42×10^9	739.29
24	2.54×10^9	895.94
26	4.31×10^9	1067.47
28	7.01×10^9	1253.81
30	1.10×10^{10}	1454.93
32	1.67×10^{10}	1670.76
34	2.47×10^{10}	1901.24
42	9.52×10^{10}	2968.17
46	1.69×10^{11}	3587.38
48	2.21×10^{11}	3918.05
50	2.86×10^{11}	4262.59
52	3.66×10^{11}	4620.87
54	4.64×10^{11}	4992.74
56	5.82×10^{11}	5378.02
62	1.10×10^{12}	6612.49
70	2.31×10^{12}	8433.25
74	3.24×10^{12}	9413.33
78	4.45×10^{12}	10435.91
82	5.98×10^{12}	11497.24
86	7.91×10^{12}	12592.74
90	1.03×10^{13}	13716.75
92	1.16×10^{13}	14287.36

We calculated the transition-energy and -probability values for all decay possibilities of the $^3P_0$ level for selected Be-like ions from $Z = 5$ to 92, using the method outlined in the previous section, in order to obtain the lifetime values of this level and the relative importance of the different decay modes.

In a preliminary calculation, all transition energies and probabilities were computed in a monoconfiguration approach. Afterwards, we used a virtual space spanned by single- and double-excited configurations, up to the $4f$ subshell, resulting from the excitation of $n = 1,2$, and 3 electrons in the upper and lower levels, to take into account electronic correlation. Concerning the transition-probability values, contrary to the transition-energy values, it was found that the correlation is important only for the TEOP $E1$ transition to the $1s^2 2p^2\ ^3P_1$ level, illustrated in Fig. 2.

One indicator of the accuracy of the present calculations is provided by the study of the transition-energy and -probability values as the virtual space is enlarged. From this study, we estimate a maximal relative uncertainty of 0.5% and 1.5% for the transition-energy and -probability values, respectively, obtained in this work.

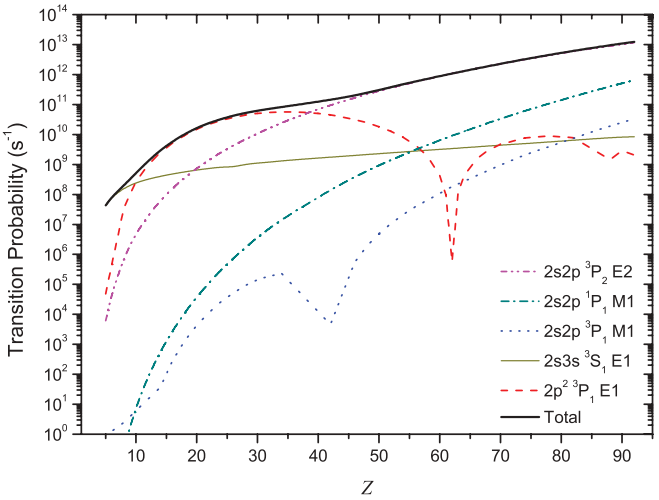

FIG. 3. (Color online) Transition probability for all possible decay channels of the $1s^2 2s 3p\ ^3P_0$ level in Be-like ions as a function of Z.

Figure 3 shows the transition-probability values that we obtained for all decay channels from the $1s^2 2s 3p\ ^3P_0$ level in Be-like ions as a function of Z. We notice that for $Z < 12$, the main decay mode is the $E1$ transition to the $1s^2 2s 3s\ ^3S_1$ level; for $12 \leqslant Z \leqslant 41$, the TEOP $E1$ transition to the $1s^2 2s 2p\ ^3P_1$ level becomes the most probable decay mode; and for $Z > 42$, the $E2$ transition to the $1s^2 2s 2p\ ^3P_2$ level is dominant.

Table I shows our values for the transition energy and probability to the $1s^2 2s 3s\ ^3S_1$ level, as well as the available values from the NIST tables and from Engström *et al.* [3]. We note that inclusion of the correlation raises the transition-probability values by about 10% for values of Z up to 60; this effect becomes negligible at around $Z \simeq 90$. In what concerns the transition energy, the influence of correlation is about 7% up to $Z \simeq 30$ and becomes negligible for high values of Z. To our knowledge, the only results available in the literature for this transition are in the range of atomic number Z between 5 and 10. Engström *et al.* [3] measured the wavelengths of these transitions for $Z = 7,8$, and 9 using the beam-foil technique. The relative difference between our calculated values for the energy and Engström's measured values are of the order of 4%. Our values are thus in good agreement with experiment.

Table II reports the probability and energy values for the $1s^2 2s 3p\ ^3P_0 \rightarrow 1s^2 2p^2\ ^3P_1$ TEOP $E1$ transition obtained in this work, together with the values obtained by other authors; this transition, as mentioned above, is the most probable decay mode in the region from $Z = 12$ to $Z = 41$. In a standard calculation performed with orthogonal spin orbitals in the initial and final states, and with no correlation configurations included, a TEOP $E1$ transition probability would be exactly zero because the transition operator is a two-electron operator. This is not the case in our work since we used separately optimized wave functions for the initial and final states and included correlation configurations, so that many matrix elements contribute to the final value. Up to $Z = 42$, correlation effects lead to an increase of the TEOP $E1$ transition probability by two orders of magnitude. For higher values of Z, the contribution of the correlation

TABLE IV. Energy of selected levels (in eV) of Be-like ions, relative to the ground level $1s^2 2s^2\ ^1S_0$, calculated in this work and by other authors.

	$Z = 8$		$Z = 10$			
Energy levels	This work	Fischer [15]	This work	Fischer [15]	Kramida [35]	Di [17]
$1s^2 2s3p\ ^3P_0$	72.02	72.28	127.42	127.55	127.50	127.48
$1s^2 2s3s\ ^3S_1$	67.60	67.84	121.23	121.35	121.29	121.08
$1s^2 2p^2\ ^3P_1$	26.26	26.53	35.86	36.03	35.94	36.46
$1s^2 2s2p\ ^3P_2$	9.96	10.22	13.87	14.00	13.97	14.15

to the transition probability decreases and, for $Z = 62$, the transition-probability values calculated with fully correlated wave functions are lower than the monoconfiguration ones. For $Z \geqslant 64$, the correlated results become again higher than the uncorrelated ones.

On the other hand, correlation does not appear to have an influence on the transition probabilities for the decay mode to the $1s^2 2s2p\ ^3P_2$ level, which is dominant in the $Z \geqslant 42$ region. The probability and energy values for this transition are listed in Table III. We highlight that for $Z = 92$, this transition probability is two orders of magnitude larger than the one corresponding to the next large decay mode, namely, the $M1$ transition to the $1s^2 2s2p\ ^1P_1$ level.

The transition-probability values for the $M1$ decay modes corresponding to transitions to the $1s^2 2s2p\ ^1P_1$ and $^3P_1$ levels, respectively, were found to be very small for small values of Z, but they become the second and third largest contribution, respectively, for high values of Z, as can be seen in Fig. 3.

A comparison of the energy values of the $1s^2 2s3p\ ^3P_0$, $1s^2 2s3s\ ^3S_1$, $1s^2 2p^2\ ^3P_1$, and $1s^2 2s2p\ ^3P_2$ levels, relative to the ground level, calculated in this work with all singly and doubly excited configurations up to the $n = 4$ shell, is made

TABLE V. Lifetime values (in s) of the $1s^2 2s3p\ ^3P_0$ level in Be-like ions for several values of Z.

Z	This work	Tachiev [14]	Engström [3]	Engström [3]	Lewis [36]
5	2.33×10^{-8}	8.32×10^{-8}			
6	1.21×10^{-8}	2.50×10^{-8}			
7	7.61×10^{-9}	1.35×10^{-8}	8.20×10^{-9}		$(10.08 \pm 0.57) \times 10^{-9}$
8	5.02×10^{-9}	8.34×10^{-9}	5.20×10^{-9}	$(5.26 \pm 0.07) \times 10^{-9}$	
9	3.13×10^{-9}	5.11×10^{-9}	3.40×10^{-9}	$(3.04 \pm 0.04) \times 10^{-9}$	
10	1.93×10^{-9}	3.04×10^{-9}			
12	7.56×10^{-10}	1.10×10^{-9}			
14	3.34×10^{-10}	6.94×10^{-10}			
16	1.69×10^{-10}				
18	1.13×10^{-9}				
20	6.09×10^{-11}				
22	4.16×10^{-11}				
24	3.04×10^{-11}				
26	2.35×10^{-11}				
28	2.35×10^{-11}				
30	1.60×10^{-11}				
32	1.38×10^{-11}				
34	1.21×10^{-11}				
42	7.05×10^{-12}				
46	4.92×10^{-12}				
48	4.02×10^{-12}				
50	3.25×10^{-12}				
52	2.61×10^{-12}				
54	2.10×10^{-12}				
56	1.69×10^{-12}				
62	2.61×10^{-12}				
70	4.25×10^{-13}				
74	3.02×10^{-13}				
78	2.19×10^{-13}				
82	1.62×10^{-13}				
86	1.20×10^{-13}				
90	9.25×10^{-14}				
92	8.12×10^{-14}				

in Table IV with the theoretical values of Tachiev and Fischer [14] for $Z = 8$, and the experimental values of Kramida and Buchet-Poulizac [35] for $Z = 10$. Our energy values agree with the former ones within 1.00% and with the latter ones within 0.04%.

From the calculated values of the transition probabilities for the $1s^2 2s3p\ ^3P_0$ level decay modes, the lifetime values of this level in Be-like ions were calculated for selected values of atomic number Z, and listed in Table V together with available values from other authors. The only values found in the literature are the theoretical ones from Tachiev and Fischer [14] for $4 \leqslant Z \leqslant 12$, and from Engström *et al.* [3] for $7 \leqslant Z \leqslant 9$, and the experimental results of the latter authors for $Z = 8$ and 9, and of Lewis *et al.* [36] for $Z = 7$. The results obtained in this work are in reasonable agreement with the results of Ref. [14] and the experimental results of Ref. [3]. The experimental result of Ref. [36] is $\simeq$25% higher than the other existing results.

IV. CONCLUSIONS

We used the MCDF method, with full correlation included up to the $4f$ subshell in both the initial and final states, to calculate the contributions of all possible modes for the decay of the $1s^2 2s3p\ ^3P_0$ level in Be-like ions for selected values of Z in the $5 \leqslant Z \leqslant 92$ range.

For $Z < 12$, we found out that the main decay mode is the $E1$ transition to the $1s^2 2s3s\ ^3S_1$ level, but, for $12 \leqslant Z \leqslant 41$, the two-electron one-photon $E1$ transition to the $1s^2 2p^2\ ^3P_1$ level becomes dominant. However, at $Z = 42$, a third decay mode, namely, the $E2$ transition to the $1s^2 2s2p\ ^3P_2$ level, becomes the most probable one for the remaining values of Z. At the same time, the transition probabilities for the $M1$ transitions to the $1s^2 2s2p\ ^1P_1$ and $^3P_1$ levels become important and, for high $Z \geqslant 82$, these transitions are more probable than the $E1$ transition to the $1s^2 2s3s\ ^3S_1$ level.

Concerning the influence of correlation on the transition probabilities, we conclude that it is relevant only in the two-electron one-photon $E1$ transition to the $1s^2 2p^2\ ^3P_1$ level and thus it will influence the total decay probability only for $Z < 42$.

The results obtained in this work are in reasonable agreement with the scarce existing data in the literature.

ACKNOWLEDGMENTS

This research was supported in part by FCT–Fundação para a Ciência e a Tecnologia (Portugal) through Projects No. PEstOE/FIS/UI0303/2011 and No. PTDC/FIS/117606/2010, financed by the European Community Fund FEDER through the COMPETE Competitiveness Factors Operational Programme. Laboratoire Kastler Brossel (LKB) is "Unité Mixte de Recherche du CNRS, de l'ENS et de l'UPMC No. 8552." We also thank the Allianz Program of the Helmholtz Association, Contract No. EMMI HA-216 "Extremes of Density and Temperature: Cosmic Matter in the Laboratory."

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