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Intercombination transitions in Be-like ions

Yu.V. Ralchenko[*]
Department of Particle Physics, Weizmann Institute of Science, Rehovot 76 100, Israel

L.A. Vainshtein[†]
P.N. Lebedev Physical Institute, Moscow 117 924, Russia

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Probabilities of intercombination transitions $2s^2\,{}^1S_0$ – $2s2p\,{}^3P_1$, $2s3p\,{}^3P_1$ for Be-like ions are calculated along the isoelectronic sequence for a large range of Z with the $1/Z$ expansion method. Results agree well with experimental data, including the recent ones. A comparison is also made with other theoretical calculations.

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Intercombination, or spin-forbidden, transitions are due to deviations from the pure LS coupling. Since their very existence, at least for small nuclear charges Z, is a consequence of the subtle relativistic spin-orbit interaction, the agreement between theoretical and experimental results is an important measure of our understanding of atomic structure and interactions. In addition, intercombination lines are very important for plasma diagnostics, for example, in astrophysics and tokamak studies [1].

Since spin-forbidden transitions for not too large Z are much weaker than spin-allowed ones, the reliable determination of their transition probabilities requires serious experimental efforts. Recently two important experiments on measurement of the intercombination transition probabilities in Be-like ions were carried out. Kwong *et al.* [2] have improved their ion trap experiment on the transition $2s^2\ {}^1S_0$ – $2s2p\ {}^3P_1$ 1909 Å in C III and obtained the value of $121 \pm 7\ \mathrm{s}^{-1}$, which differs considerably from the preliminary result of the same group $75\ \mathrm{s}^{-1}$ [3]. In another experiment Granzow *et al.* [4] have measured the probability of the $2s^2\ {}^1S_0$ – $2s3p\ {}^3P_1$ transition in Na VIII–Si XI ions. Similar measurements for smaller nuclear charges Z from N IV to Ne VII [5,6] were done more than ten years ago, so it is possible now to compare theoretical predictions along a larger interval of Z. These two latest experimental works initiated a wave of theoretical calculations [7–11] where most sophisticated and elaborate up to date methods were used, e.g., multiconfiguration Hartee-Fock (MCHF), multiconfiguration Dirac-Fock (MCDF), configuration interaction (CI) methods, and multiconfiguration relativistic random-phase approximation (MCRRPA). In this paper we report the results of calculations of $2s^2\ {}^1S_0$ – $2s2p\ {}^3P_1$ and $2s^2\ {}^1S_0$ – $2s3p\ {}^3P_1$ transition probabilities along [Be] isoelectronic sequence by the Z expansion method. This approach is known to be very accurate in determination of energy levels of few-electron multicharged ions but, as we will see in what follows, gives also good results for intercombination probabilities.

In these calculations we use the MZ computer code [12,13] based on the perturbation theory on a $1/Z$ parameter. The main principles of this approach and the code structure are described in Ref. [12] so we refer the reader to that book for details.

Both intercombination transitions studied in this paper arise from mixing of triplet terms with the singlet ones. This mixing not only makes the spin-forbidden transition to be possible but also influences the level energies. Therefore the correspondence between the experimental and theoretical energies is an additional important check for accuracy of the calculations. Earlier the MZ method was successfully applied for calculation of the level energies for configurations $1s^2 2l'nl''$ ($n = 2, 3, 4$) of Na VIII–S XIII ions [14,15]. These references contain detailed examination of energy calculations by MZ so here we immediately pass to the discussion of obtained results. In Table I we show the calculated energies for $2s2p\ {}^3P_1$ levels with respect to the ground state for $Z = 6 - 26$. Also presented are experimental energies [16] and the lat-

TABLE I. Energy of $2s2p\,{}^3P_1$ level (cm^{-1}). All experimental energies have been taken from Ref. [16].

Z	Experiment	MZ	Other calculations
6	52 391	52 399	52 397,[a] 52 372,[b] 53 327,[c] 52 369,[d] 52 343[e]
7	67 272	67 269	67 270,[a] 67 202,[b] 68 591[c]
8	82 075	82 096	82 075,[a] 82 015,[b] 83 733[c]
9	96 867	96 920	96 866,[a] 98 826[c]
10	111 710	111 783	111 696,[a] 113 922[c]
12	141 631	141 775	141 630,[a] 144 307[c]
14	172 144	172 346	172 150,[a] 172 453,[b] 175 207[c]
16	203 479	203 737	206 925[c]
18	235 843	236 181	
20	269 515	269 863	
22	304 566	304 933	
24	341 120	341 467	
26	379 160	379 484	382 591[b]

[a]Reference [17].
[b]Reference [10].
[c]Reference [9].
[d]Reference [7].
[e]Reference [8].

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[*] Electronic address: fnralch@plasma-gate.weizmann.ac.il
[†] Electronic address: vainsh@sci.lpi.ac.ru

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TABLE II. Energy difference $E(2s2p\ ^1P_1) - E(2s2p\ ^3P_1)$ (cm^{-1}). All experimental energies have been taken from Ref. [16].

Z	Experiment	MZ	Other calculations
6	49 961	50 171	49 974,[a] 50 353,[b] 52 542,[c] 50 325,[d] 50 230[e]
7	63 422	63 419	63 440,[a] 64 071,[b] 66 492[c]
8	76 720	76 616	76 743,[a] 77 412,[b] 80 185[c]
9	89 963	89 818	90 014,[a] 93 760[c]
10	103 234	103 070	103 291,[a] 107 308[c]
12	130 057	129 875	130 120,[a] 134 571[c]
14	157 532	157 365	157 622,[a] 158 261,[b] 162 434[c]
16	186 114	185 966	191 353[c]
18	216 337	216 235	
20	249 001	248 939	
22	285 092	285 088	
24	326 110	326 004	
26	373 600	373 336	374 234[b]

[a] Reference [17].
[b] Reference [10].
[c] Reference [9].
[d] Reference [7].
[e] Reference [8].

est other theoretical results [7–10,17]. One can see from this table that in most cases the difference between calculations in this work and experimental energies is of order of a few units of 10^{-4} or less. Note that experimental energies for levels $2s2p\ ^3P_1$ ($Z = 18 - 26$) have a stable shift of $\sim 350\ \mathrm{cm}^{-1}$ independent of Z, comparing to our results. Since all these energies were determined from the same experiment [18], it is quite possible that there was a systematic error in those measurements. Table II compares our results with other theoretical as well as experimental data for another important parameter, namely, the energy difference between $2s2p\ ^3P_1$ and $2s2p\ ^1P_1$ levels. This quantity enters the coefficient of mixing between two $J = 1$ levels and therefore strongly affects the intercombination transition probability. Finally, in Table III energies are shown for $2s3p\ ^3P_1$ levels

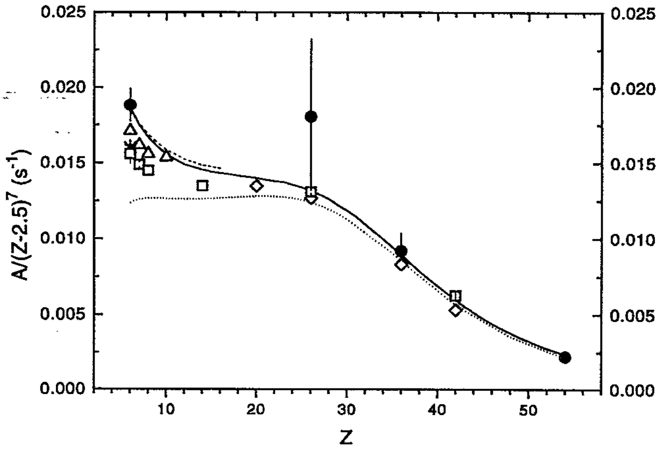

FIG. 1. Scaled transition probabilities for $2s^2\ ^1S_0 - 2s2p\ ^3P_1$ line in Be-like ions. Experiment •, Z=6 [2], Z=26 [22], Z=36 [23], Z=54 [24]; Theory: — this paper, △ [27], ◇ [28], ··· [26], + [7], × [8], – – – [9], □ [10].

TABLE III. Energy of $2s3p\ ^3P_1$ level (cm^{-1}). All experimental energies have been taken from Ref. [16].

Z	Experiment	MZ	Other calculations
6	259 711.22	259 613	259 713,[a] 259 736,[b] 258 032[c]
7	405 987.5	405 960	405 992,[a] 406 024,[b] 404 481,[c] 406 040[d]
8	582 839.8	582 871	582 839,[a] 582 908,[b] 581 446,[c] 582 770,[d] 582 400[e]
9		790 395	790 331,[a] 790 470,[c] 789 032[d]
10	1 028 519	1 028 591	1 028 505,[a] 1 027 307,[c] 1 028 680,[d] 1 028 100[e]
12		1 597 286	1 597 193,[a] 1 597 167,[b] 1 597 110,[d] 1 596 800[e]
14		2 289 640	2 289 539,[a] 2 289 507,[b] 2 289 390[d]
16		3 106 556	3 106 436,[b] 3 105 800,[d] 3 106 400[e]
18		4 049 225	4 049 147,[b] 4 048 890[d]
20		5 119 011	5 118 807,[b] 5 118 500,[d] 5 119 500[e]
22	6 316 700	6 317 338	6 317 314[b]
24	7 644 700	7 623 941	7 645 796[b]
26	9 076 100	9 074 279	9 106 017,[b] 9 074 190,[d] 9 076 400[e]

[a] Reference [17].
[b] Reference [19].
[c] Reference [20].
[d] Reference [11].
[e] Reference [21].

TABLE IV. Transition probabilities A (s^{-1}) of the intercombination line $2s^2\ {}^1S_0 - 2s2p\ {}^3P_1$ in [Be] ions from C III to Xe LI. Below a(b) means $a \times 10^b$. Experiment, footnotes a – d; theory, footnotes e – k.

Z	Experiment	MZ	Other calculations
6	121±7[a]	120	104±4,[e] 103 ± 3,[f] 110 ± 16.5,[g] 80,[h] 100.3 ± 4,[i] 118[j]
7		653	604.2,[g] 471,[h] 556.3±6,[i] 657[j]
8		2.54(3)	2.37(3),[g] 1.93(3),[h] 2.207±0.04(3),[i] 2.57(3)[j]
9		7.87(3)	6.20(3),[h] 8.00(3)[j]
10		2.08(4)	2.05(4),[g] 1.69(4),[h] 2.12(4)[j]
12		1.04(5)	8.80(4),[h] 1.06(5)[j]
14		3.87(5)	3.36(5),[h] 3.586±0.08(5),[i] 3.95(5)[j]
16		1.17(6)	1.04(6),[h] 1.19(6)[j]
18		3.04(6)	2.74(6)[h]
20		7.04(6)	6.43(6),[h] 6.77(6)[k]
22		1.48(7)	1.37(7)[h]
24		2.88(7)	2.69(7)[h]
26	7.14 ± 2.04(7)[b]	5.21(7)	4.91(7),[h] 5.186±0.04(7),[i] 5.01(7)[k]
36	4.35 ± 0.57(8)[c]	4.23(8)	4.04(8),[h] 3.93(8)[j]
54	2.13 ± 0.23(9)[d]	2.29(9)	2.10(9)[h]

[a] Reference [2].
[b] Reference [22].
[c] Reference [23].
[d] Reference [24].
[e] Reference [7].
[f] Reference [8].
[g] Reference [27].
[h] Reference [26].
[i] Reference [10].
[j] Reference [9].
[k] Reference [28].

along [Be] isoelectronic sequence up to Fe XXIII. These tables show very good agreement between MZ results and experimental data.

Until now only four experiments on the measurement of the $2s^2\ {}^1S_0 - 2s2p\ {}^3P_1$ transition probability were carried out, that is, for C III [2], Fe XXIII [22], Kr XXXIII [23], and Xe LI [24]. The best known in this list is the intercombination line 1909 Å in C III, which has been discussed in many theoretical papers (see references in Ref. [25]). As we have noted above, the recently reported experimental results on C III [2] do not overlap with the previous measurements of the same group for this transi-

TABLE V. Transition probabilities A (s^{-1}) of the intercombination line $2s^2\ {}^1S_0 - 2s3p\ {}^3P_1$ in [Be] ions from N IV to Fe XXIII. Below a(b) means $a \times 10^b$. Experiment, footnotes a – c; theory, footnotes d – g.

Z	Experiment	MZ	Other calculations
7	3.3±2.7(6)[a]	4.97(6)	1.33(6),[d] 3.07(6)[e]
8	2.2±0.6(7)[a]	2.22(7)	1.61(7),[d] 1.83(7)[e]
9	8.8±0.9(7)[a]	9.59(7)	8.39(7),[d] 8.86(7)[e]
10	4.3±0.6(8)[b]	3.70(8)	3.87(8),[d] 2.75(8),[e] 3.87(8),[f]
11	3.45±0.73(9)[c]	1.27(9)	1.52(9),[d] 1.34(9),[f] 1.50(9)[g]
12	5.55±0.96(9)[c]	3.97(9)	4.67(9),[d] 4.43(9),[f] 3.97(9)[g]
13	1.21±0.24(10)[c]	1.13(10)	1.37(10),[d] 1.36(10),[f] 1.24(10)[g]
14	2.50±0.54(10)[c]	2.97(10)	3.66(10),[d] 3.69(10),[f] 3.38(10)[g]
15		7.21(10)	9.21(10),[d] 8.32(10)[g]
16		1.60(11)	1.99(11),[d] 1.92(11),[f] 1.85(11)[g]
18		5.93(11)	6.63(11),[d] 6.56(11)[g]
20		1.52(12)	1.59(12),[d] 1.69(12),[f] 1.63(12)[g]
22		3.00(12)	
24		4.06(12)	
26		5.30(12)	4.84(12),[d] 4.95(12)[g]

[a] Reference [5].
[b] Reference [6].
[c] Reference [4].
[d] Reference [11].
[e] Reference [20].
[f] Reference [21].
[g] Reference [29].

tion probability [3]. The value $A_{\mathrm{C\,III}} = 121 \pm 7\ \mathrm{s}^{-1}$ agrees well with our result 120 s^{-1} and the MCRRPA value of 118 s^{-1} [9] but contradicts the latest CI [7], MCHF [8], and MCDF [10] calculations which give 104 ± 4, 103 ± 3, and $100.3 \pm 4\ \mathrm{s}^{-1}$, respectively. As one can see from Table IV and Fig. 1, the agreement between MZ probabilities and available data for Fe, Kr, and Xe is also good. In addition to the above mentioned CI, MCDF, MCHF, and MCRRPA calculations, we included in this table the extensive MCDF calculations for Be-like ions up to Xe LI [26], model potential results [27], and MC calculations with SUPERSTRUCTURE code [28] as well. Although different theoretical results give practically the same Z dependence and absolute values of probabilities for large $Z \geq 26$, the situation for small nuclear charges is not very clear yet and new accurate measurements for $Z < 10$ would be of great importance.

In Table V and in Fig. 2 the theoretical and experimental results for the transition probability $A(2s^2\ {}^1S_0 - 2s3p\ {}^3P_1)$ for $Z = 7-26$ are shown. At present there are old experimental data for $Z = 7-9$ [5], $Z = 10$ [6], and the latest data for $Z = 11-14$ [4]. The theoretical results in Table V include MCDF [11], MCHF [21], CI [20], and HF-with-relativistic-corrections [29] calculations. As was shown by Fritzsche and Grant [11], for small Z the MCDF method is rather slow convergent with an increase of the number of configurations included. This is probably a reason for the large discrepancy between that paper and the results of Kim *et al.* [19]. It is seen from Fig. 2 that different theoretical approaches show again similar Z dependence, except for smallest Z, where more accurate measurements would be desirable. The experimental results by Granzow *et al.* [4] seem to give a Z dependence rather different from the theoretical one, although in a sufficiently narrow region. At least for Na VIII the value of A is considerably larger than most recent theoretical results. This feature needs further investigation, especially since the authors claim that this value appears to be an overestimate.

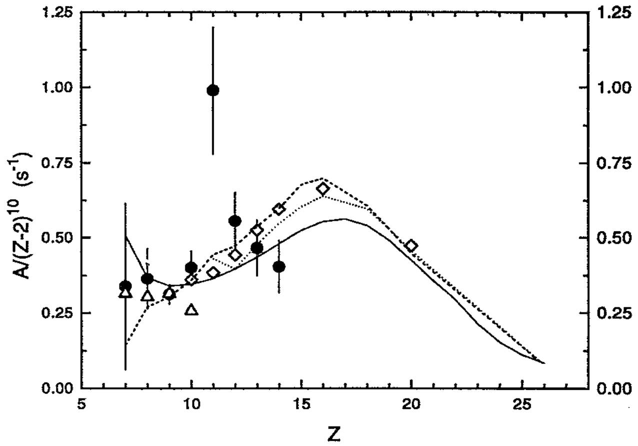

FIG. 2. Scaled transition probabilities for $2s^2\ {}^1S_0 - 2s3p\ {}^3P_1$ line in [Be] ions. Experiment: ●, Z=7–9 [5], Z=10 [6], Z=11–14 [4]; Theory: — this paper, △ [20], ◇ [21], – – – [11], · · · [29].

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