The Double-Configurational Approximation in the Case of Carbon-like Atoms

A. B. BOLOTIN, I. B. LEVINSON AND L. I. LEVIN
Vilna State University

(Submitted to JETP editor May 29, 1954)
J. Exper. Theoret. Phys. USSR 29, 449-453 (October, 1955)

Parametric values of analytical one-electron wave functions are presented for C, N^+, O^{++}, $F^{3+}$and Ne^{4+} in the configurations $1s^2 2s^2 2p^2$, $1s^2 2s 2p^3$ and $1s^2 2p^4$. Corrections to the energy in the double-configurational approximation for the fundamental configurations of the above atoms were determined in the double-configurational approximation $1s^2 2s^2 2p^2 - 1s^2 2p^4$. The theoretical values obtained for the energy are compared with experimental data. The total dipole strengths and the probabilities of the transitions $1s^2 2s 2p^3 - 1s^2 2s^2 2p^2$ were determined in both the single- and double-configurational approximations.

INTRODUCTION

A poly-configurational approximation for beryllium and boron-like atoms and its effect on quantities in the theory of transitions were investigated in the work of reference 1 by means of analytical one-electron wave functions. The present work is devoted to the study of carbon-like atoms by means of the above wave functions.

A poly-configurational approach for the case of the carbon atom was studied in detail in reference 2, using wave functions of a self-consistent field without quantum exchange. From this work it follows that in the case of the fundamental configuration of carbon-like atoms, the poly-configurational approximation reduces in practice to the double-configurational $1s^2 2s^2 2p^2 - 1s^2 2p^4$. Furthermore, the manner of consideration proposed in part 2 of reference 3 leads to the conclusion that as long as we use one-electron wave functions determined in the single-configurational approximation, then in the case of the configuration $1s^2 2s 2p^3$ the poly-configurational approach reduces to the single-configurational approximation. Therefore, in the investigation of quantities in transition theory for the configuration $1s^2 2s^2 2p^2$ we use a double-configurational approach and for $1s^2 2s 2p^3$ a single-configurational approach.

2. PARAMETERS OF THE ONE-ELECTRON WAVE FUNCTIONS

The expressions for the wave functions and all the notations used in reference 1 are retained in the present work. The parameters η, a, b and c were found by a graphical method from the condition of minimum total energy in the single-configurational approximation. The numerical values of these parameters and the total energy for the configurations $1s^2 2s^2 2p^2$, $1s^2 2s 2p^3$and $1s^2 2p^4$ are presented in Table I for the atoms C, N^+, O^{++}, F^{3+} and Ne^{4+}. Experimental data for the total energy, compiled with the aid of reference 4, are also included in the Table.

By means of the data in Table I, values were determined for the correction to the energy of the fundamental configuration in the double-configurational approximation $1s^2 2s^2 2p^2 - 1s^2 2p^4$, and for the constant a_{12}; the absolute value of the latter is the weight of the configuration $1s^2 2p^4$ relative to $1s^2 2s^2 2p^2$. The results are entered in Table II.

3. THE TOTAL DIPOLE STRENGTH AND THE TRANSITION PROBABILITY IN THE DOUBLE-CONFIGURATIONAL APPROXIMATION

For the total dipole strength in the double-configurational approach we obtain the following expression:

$$S(SL', SL) = \frac{\alpha}{1+a_{12}^2}[N(r2s, 2p)_{13} + a_{12}\beta N(r2s, 2p)_{32}]^2, \quad (1)$$

[1] A. B. Bolotin and A. P. Iutsis, J. Exper. Theoret. Phys. USSR 24, 537 (1953).

[2] A. P. Iutsis, J. Exper. Theoret. Phys. USSR 19, 565 (1949).

[3] A. P. Iutsis and V. I. Kavetskis, J. Exper. Theoret. Phys. USSR 21, 1139 (1951).

[4] C. E. Moore, Atomic Energy Levels, Nat. Bur. Stand. Cir. 467, Washington (1949).

TABLE I *

Values of the parameters in the wave functions for the configurations $1s^2 2s^2 2p^2$, $1s^2 2s 2p^3$, $1s^2 2p^4$ of the carbon-like atoms C, N^+, O^{++}, F^{3+}, Ne^{4+} (energies in atomic units).

Configuration	a	ηa	b	ηb	$2\eta c$	2η	$E_{theor.}$	$E_{exper.}$
$1s^2 2s^2 2p^2$								
^3P	3.61	5.70	3.25	5.14	3.10	3.16	−37.600	−37.855
	3.34	6.71	2.90	5.83	4.14	4.02	−53.765	−54.072
	3.15	7.72	2.73	6.62	5.29	4.90	−72.940	−73.317
	3.00	8.72	2.60	7.55	6.28	5.81	−95.120	—
	2.90	9.72	2.50	8.38	7.30	6.70	−120.285	—
^1D	3.60	5.69	3.20	5.06	3.10	3.16	−37.530	−37.809
	3.37	6.71	2.97	5.97	4.14	3.98	−53.685	−54.005
	3.16	7.71	2.75	6.71	5.22	4.88	−72.835	−73.225
	3.01	8.72	2.62	7.59	6.20	5.79	−94.985	—
	2.95	9.72	2.50	8.35	7.21	6.68	−120.140	—
^1S	3.60	5.69	3.18	5.02	3.10	3.16	−37.435	−37.757
	3.39	6.71	2.99	5.92	4.12	3.96	−53.555	−53.926
	3.18	7.71	2.80	6.79	5.20	4.85	−72.675	−73.120
	3.03	8.72	2.65	7.63	6.16	5.76	−94.790	—
	2.92	9.72	2.55	8.49	7.13	6.66	−119.900	—
$1s^2 2s 2p^3$								
^1P	3.52	5.68	3.20	5.15	3.03	3.22	−36.995	−37.309
	3.25	6.65	2.93	5.99	4.17	4.09	−52.980	−53.315
	3.07	7.64	2.72	6.77	5.13	4.98	−71.985	−72.358
	2.93	8.64	2.55	7.52	6.14	5.90	−93.985	—
	2.80	9.63	2.45	8.43	7.22	6.88	−119.010	—
^1D	3.53	5.68	3.23	5.20	3.06	3.22	−37.065	−37.409
	3.30	6.66	2.87	5.80	4.08	4.04	−53.065	−53.418
	3.07	7.64	2.75	6.84	5.18	4.98	−71.950	−72.465
	2.93	8.62	2.60	7.65	6.29	5.88	−94.115	—
	2.81	9.60	2.55	8.71	7.31	6.83	−119.155	—
^3P	3.42	5.67	2.90	4.81	3.12	3.32	−37.245	−37.512
	3.12	6.65	2.75	5.86	4.09	4.26	−53.295	−53.577
	2.97	7.64	2.65	6.81	5.19	5.14	−72.370	−72.668
	2.87	8.64	2.55	7.68	6.20	6.02	−94.425	—
	2.77	9.64	2.50	8.70	7.17	6.96	−119.505	—
^3D	3.45	5.67	3.15	5.18	3.13	3.29	−37.305	−37.563
	3.22	6.62	3.00	6.22	4.14	4.14	−53.380	−53.655
	3.05	7.65	2.70	6.78	5.17	5.02	−72.470	−72.770
	2.89	8.64	2.55	7.62	6.22	5.98	−94.555	—
	2.77	9.64	2.40	8.35	7.24	6.96	−119.660	—
^3S	3.55	5.69	3.22	5.16	3.01	3.20	−37.045	−37.373
	3.35	6.69	3.00	5.99	4.07	3.99	−53.050	−53.368
	3.18	7.68	2.78	6.71	5.17	4.83	−72.070	−72.419
	3.03	8.68	2.60	7.45	6.19	5.73	−94.105	—
	2.88	9.66	2.50	8.39	7.24	6.71	−119.135	—
^5S	3.48	5.66	3.14	5.10	3.12	3.25	−37.030	−37.702
	3.25	6.64	2.95	6.03	4.17	4.09	−53.050	−53.860
	3.05	7.63	2.82	7.05	5.25	5.00	−72.085	−73.042
	2.97	8.62	2.72	7.90	6.27	5.80	−94.105	—
	2.90	9.61	2.67	8.85	7.29	6.63	−119.140	—
$1s^2 2p^4$								
^3P	3.59	5.67	—	—	3.00	—	−36.820	—
	3.30	6.67	—	—	4.04	—	−52.735	—
	3.05	7.67	—	—	5.08	—	−71.660	−72.024
	2.89	8.66	—	—	6.10	—	−93.595	—
	2.80	9.66	—	—	7.10	—	−118.535	—

TABLE I (*continued*)

Configuration	a	ηa	b	ηb	$2\eta c$	2η	$E_{theor.}$	$E_{exper.}$
^1D	3.59	5.67	—	—	3.00	—	— 36.760	—
	3.30	6.67	—	—	4.04	—	— 52.650	—
	3.05	7.66	—	—	5.08	—	— 71.555	—71.958
	2.89	8.65	—	—	6.10	—	— 93.470	—
	2.78	9.64	—	—	7.14	—	—118.390	—
^1S	3.59	5.67	—	—	3.00	—	— 36.660	—
	3.20	6.67	—	—	4.04	—	— 52.520	—
	3.05	7.66	—	—	5.08	—	— 71.400	—71.753
	2.89	8.64	—	—	6.10	—	— 93.275	—
	2.78	9.63	—	—	7.14	—	—118.165	—

* Precision of the parameter values ± 0.02, and of the energy ± 0.005.

TABLE II

Corrections to the energy in the double-configurational approximation for the investigated configurations, values of the constant a_{12} and of the non-diagonal element of the energy.

Entity	C	N^+	O^{++}	F^{3+}	Ne^{4+}
		^3P			
ΔE^1	—0.018	—0.023	—0.027	—0.031	—0.035
E_{12}	0.118	0.153	0.186	0.218	0.249
a_{12}	—0.15	—0.15	—0.14	—0.14	—0.14
		^1D			
ΔE^1	—0.018	—0.022	—0.026	—0.030	—0.034
E_{12}	0.120	0.153	0.185	0.217	0.248
a_{12}	—0.15	—0.14	—0.14	—0.14	—0.13
		^1S			
ΔE^1	—0.068	—0.084	—0.100	—0.116	—0.131
E_{12}	0.240	0.305	0.372	0.434	0.495
a_{12}	—0.28	—0.28	—0.27	—0.27	—0.26

wherein

	$^1P-{}^1S$	$^1P-{}^1D$	$^1D-{}^1D$
α	4	5	15
β	+1	—1	+1

	$^3P-{}^3P$	$^3D-{}^3P$	$^3S-{}^3P$
α	9	15	12
β	—1	+1	+1

The integrals $N(nl, nl)_{13}$ and $N(nl, nl)_{32}$ are equal to unity within the limits of error and are omitted in Eq. (1). To obtain Eq. (1) it is convenient to use the methods applied in references 5 and 6. Formula (4.3) of reference 1 was used for the determination of transition probabilities. The values of the total dipole strength and probability of transitions determined with the use of the

[5] G. Racah, Phys. Rev. 62, 438 (1942).
[6] G. Racah, Phys. Rev. 63, 367 (1943).

Table III

Values of the total dipole strength and transition probability for carbon-like atoms. (The transition probability is in units of 10^8 per second, all other quantities are in atomic units).

Entity	C	N^+	O^{++}	F^{3+}	Ne^{4+}	
$N(r2s, 2p)_{13}$	1.64	1.25	1.00	0.842	0.712	^3S—^3P
$N(r2s, 2p)_{32}$	1.63	1.26	1.02	0.855	0.732	
$S(^3S, ^3P)$ a	10.8	6.25	4.00	2.84	2.07	
b	7.62	4.40	2.88	2.04	1.49	
$W(^3S, ^3P)$ a	130	160	190	210	220	
b	100	125	145	165	175	
$N(r2s, 2p)_{13}$	1.61	1.25	1.00	0.841	0.725	^3P—^3P
$N(r2s, 2p)_{32}$	1.59	1.22	0.995	0.838	0.722	
$S(^3P, ^3P)$ a	7.78	4.69	3.00	2.12	1.58	
b	10.2	6.02	3.82	2.70	2.01	
$W(^3P, ^3P)$ a	8.20	11.5	14.0	16.5	17.5	
b	12.5	17.0	21.0	24.0	25.5	
$N(r2s, 2p)_{13}$	1.60	1.24	1.00	0.839	0.719	^3D—^3P
$N(r2s, 2p)_{32}$	1.60	1.24	1.00	0.840	0.723	
$S(^3D, ^3P)$ a	12.9	7.69	5.02	3.52	2.58	
b	9.11	5.43	3.63	2.55	1.87	
$W(^3D, ^3P)$ a	4.70	6.20	7.35	8.90	9.00	
b	3.95	5.20	6.30	7.30	7.70	
$N(r2s, 2p)_{13}$	1.64	1.24	1.02	0.848	0.725	^1P—^1S
$N(r2s, 2p)_{32}$	1.62	1.25	1.01	0.845	0.723	
$S(^1P, ^1S)$ a	3.59	2.05	1.29	0.959	0.701	
b	1.74	0.979	0.694	0.478	0.360	
$W(^1P, ^1S)$ a	21.5	27.5	32.5	34.5	35.0	
b	16.0	20.5	24.5	26.5	27.0	
$N(r2s, 2p)_{13}$	1.64	1.24	1.01	0.847	0.725	^1P—^1D
$N(r2s, 2p)_{32}$	1.62	1.25	1.01	0.845	0.723	
$S(^1P, ^1D)$ a	4.48	2.56	1.70	1.20	0.876	
b	5.78	3.27	2.17	1.52	1.11	
$W(^1P, ^1D)$ a	48.5	63.0	74.0	85.0	89.5	
b	69.5	88.5	103	115	120	
$N(r2s, 2p)_{13}$	1.63	1.26	1.00	0.833	0.719	^1D—^1D
$N(r2s, 2p)_{32}$	1.62	1.26	1.00	0.845	0.723	
$S(^1D, ^1D)$ a	13.3	7.88	5.00	3.47	2.53	
b	9.40	5.70	3.62	2.50	1.90	
$W(^1D, ^1D)$ a	58.0	73.0	86.5	97.5	105	
b	46.0	58.0	69.0	78.0	83.5	

Note: a – denotes the single-configurational approximation; b – the double-configurational.

parameters in Table I and of the quantities in Table II are represented in Table III.

4. CONCLUSIONS

From Table II it is seen that the correction to the energy in the double-configurational approach in the case of carbon-like atoms increases in absolute value with increase in nuclear charge, while decreasing percentagewise. In the cases of C and O^{++}, the correction to the energy in the double-configurational approximation and the constant a_{12} agree with the results of references 7 and 8.

The results in Table III show that the total dipole strength in the double-configurational approximation is increased 1.3-2.0 times or decreased in the same amount, depending on the sign of β in (1). The transition probabilities ^3S - ^3P, ^3D - ^3P, ^1P - ^1S, ^1D - ^1D are reduced by 1.2-1.3 times, while the transition probabilities ^3P - ^3P, ^1D - ^1D are increased by 1.4 -1.5 times.

In the case of carbon-like atoms the total dipole strengths of the transitions ^3S - ^3P, ^3P - ^3P, ^3D - ^3P have the ratios 12:9:15 in the single-configurational approximation and 8.5:11:10 in the double-configurational, while for the transitions ^1P - ^1S, ^1P - ^1D, ^1D - ^1D the ratios are 4:5:15 and 2:6:11 in the single- and double-configurational approximations, respectively.

The authors consider it their pleasant duty to express deep thanks to Prof. A. P. Iutsis for his suggestion of the topic and his constant attention to the work.

[7] A. Iutsis, Proc. Roy. Soc. (London) **A173**, 59 (1939)

[8] D. R. Hartree, W. Hartree and B. Swirles, Phil. Trans. Roy. Soc. **A238**, 229 (1939)

Translated by R. L. Eisner
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