

Efficient Method to Account for Correlation Effects when Generating Atomic Parameters for Complex Atoms

P. Bogdanovich, G. Gaigalas and Z. Rudzikas
*State Institute of Theoretical Physics and Astronomy,
A. Gostauto 12, 2600 Vilnius, Lithuania*

1 Introduction

The potential of a simplified method of superposition of configurations for studying the energy spectra of atoms and ions has been discussed in some earlier papers[1-4]. In this method a part of admixed configurations, obtained mainly by one-electron excitations, is taken into account directly when calculating the multi-configurational energy matrix, whereas the correlation corrections, connected with the majority of configurations, obtained by virtual two-electron excitations, are accounted for in second-order perturbation theory as corrections to Slater integrals and similar quantities [4]. Such an approach allows us to take into consideration a fairly large number of admixed configurations, preserving a comparatively small order of the matrix to be diagonalized. This is of extreme importance for calculations of energy spectra of complex configurations.

The possibility to approximately account for a large number of admixed configurations (in the second order of perturbation theory) has allowed us to avoid the use of solutions of multi-configurational equations and to employ the so-called transformed radial orbitals, obtained from Hartree-Fock functions of the configuration considered, with the help of simple algebraic multipliers of the type of various positive degrees of a radial variable. The main advantage of this approach is the exceptional simplicity of the generation of the basis combined with its fairly high efficiency. Recently a similar approach has been also applied to the relativistic Dirac-Hartree-Fock approximation [5,6].

This paper is aimed at exploring the possibility to apply such a method for calculations of electronic transitions in atoms and ions. We expect a fairly high efficiency because of the following facts:

- 1) The transformed radial orbitals are fairly useful for calculations of matrix elements of the operators of electronic transitions [7].
- 2) It follows from the above-mentioned publications that the approach under consideration allows the determination of fairly accurate wavelengths. This is rather important when calculating the majority of characteristics of electronic transitions.
- 3) The high accuracy of the energy levels of a configuration leads to sufficiently accurate weights of the wave functions of a pure coupling scheme, obtained after diagonalization of the energy matrix. This also contributes to an increase in the accuracy of the matrix elements of the electronic transitions.
- 4) The approach used allows us to include in the multi-configurational wave function practically all necessary configurations - both giving the principal contributions to the expansion as well as the most important ones for the electronic transition considered.

2 Results of the Calculation of the Transition $2s^2 2p^2 - 2s 2p^3$ in O III

Let us consider the electronic transitions $2s^2 2p^2 - 2s 2p^3$ in O III. These transitions were studied by many authors, therefore we can compare our results with fairly accurate theoretical and experimental data. Moreover, the role of correlation effects is very important for these configurations. Therefore, it will be possible to estimate how accurately we are taking them into account.

The transformed radial orbitals were defined as follows:

$$P_{TR}(n' l' / r) = N \cdot r^k \cdot P_{HF}(nl / r),$$

(N is the normalizing factor). They are orthogonalized to all Hartree-Fock and transformed functions already included in the basis used. The values of $n'l'$, k and nl are presented in Table 1.

Table 1: Parameters of the transformed radial orbitals used.

$n'l$	k	nl	$n'l$	k	nl	$n'l$	k	nl	$n'l$	k	nl	$n'l$	k	nl
<u>5s</u>	1	2s	<u>5p</u>	1	2s	<u>5d</u>	2	2s	5f	3	2s	5g	4	2s
<u>6s</u>	1	2p	6p	1	2p	<u>6d</u>	1	2p	6f	2	2p	6g	3	2p
6h	3	2p	7s	2	2s	7p	2	2s	7d	3	2s	7f	4	2s
7g	5	2s	8s	2	2p	8p	2	2p	8d	2	2p	8f	3	2p
8g	4	2p	8h	5	2p	9s	1	1s	9p	1	1s	9d	2	1s

The quantum numbers of the radial orbitals which according to [7] play the main role while refining the matrix elements of the transition operator are underlined. In this approach the principal quantum numbers n have no physical meanings and they have nothing to do with the numbers of nodes of the radial orbital considered. Their values starting with $n = 5$ were used.

While calculating the energy matrix and, correspondingly, multi-configurational wave function (as in [4] for calculations of the energy spectra), the fairly important quasidegenerate configuration $2p^4$ was admixed to $2s^2 2p^2$, as well as all configurations obtained from these two by one-electron excitations. Moreover, all configurations necessary to improve the matrix element of the transition operator and obtained from the configuration $2s 2p^3$ by one electron excitations in states of opposite parity [7] were automatically included in the matrix. The contributions of the remaining possible admixed configurations were taken into consideration in second order perturbation theory in terms of the corrections to the radial integrals of electrostatic interactions and similar quantities. The configuration $2s 2p^3$ has no configurations of the same parity which are quasidegenerate to it. When improving it, all possible one-electron admixed configurations were taken into account to form the energy matrix as well as the configurations obtained from $2s^2 2p^2$ and, due to strong mixing, from $2p^4$ by one-electron excitations in the states of the opposite parity [7]: $2s^2 2pn,s$; $2s^2 2pn,d$. It is necessary to underline that according to the above-mentioned list, configurations of the kind $2p^3 n,s$ and $2p^3 n,d$ must be included. However, they already appeared earlier as the result of one-electron excitation of the configuration considered.

The results obtained for some transitions are presented in Table 2. It contains the experimental wavelengths and the oscillator strengths (gf) of electric dipole transitions, calculated in the single-configuration Hartree-Fock (HF) approximation and with the method of simplified superposition of configurations (SSC) as well as calculated with the usual superposition of configurations approach with the same radial orbitals accounting for a complete set of possible

admixed configurations (SC). In the latter case the order of the matrix to be calculated and diagonalized increases many times. The table also contains recommended data on oscillator strengths [8] as well as the results of multi-configuration calculations [9]. Our results are presented for both the “length” (L) and “velocity” (V) forms of the transition operator. Moreover, the upper lines contain *ab initio* values whereas the lower ones contain data obtained using experimental energy values.

As seen from Table 2, the results obtained in the SSC and SC approaches differ insignificantly, especially for the case of the “length” form of transition operator. They are very close to the data found using more elaborate methods [8,9] and are not significantly improved when using experimental energy values. As was expected, the largest discrepancies occur when calculating intercombination transitions. The SSC data, obtained for the “velocity” form of the transition operator, are slightly less accurate. This may be an indication that the basis of radial orbitals used is not sufficiently complete while using this operator.

3 Conclusion

The numerical data presented indicate that the method of simplified superposition of configurations (SSC), in which only part of the admixed configurations is directly taken into account when calculating the energy matrix, whereas the majority of admixed configurations, obtained by two-electron virtual excitations, are accounted for in second-order perturbation theory, is fairly efficient not only for calculations of the energy spectra, but also for studies of electronic transitions. This method may be easily applied to study complex electronic configurations, having several open shells, and, thus, may efficiently contribute to the generation of accurate atomic data for relevant databases..

References

- [1] P. Bogdanovich, G. Zukauskas, *Sov. Phys. Collection* **23**, No. 3, 13-26 (1983)
- [2] P. Bogdanovich, G. Zukauskas, S. Sadziuviene, *Sov. Phys. Collection* **24**, No. 3, 27-37 (1984)
- [3] P. O. Bogdanovich et al, *Izvestija vuzov SSSR. Fizika* **33**, 6-17 (1990)
- [4] P. Bogdanovich, G. Gaigalas, A. Momkauskaite, Z. Rudzikas, *Physica Scripta* **56**, 230-239 (1997)
- [5] V. A. Dziuba, V. V. Flambaum, M. G. Kozlov, *28th EGAS, Abstracts*, 62, 1996
- [6] V. A. Dziuba, V. V. Flambaum, M. G. Kozlov, *Phys. Rev. A* **54**, 3948-3959 (1996)
- [7] P. Bogdanovich, *Lithuanian Physics Journal* **31**, 79-83 (1991)
- [8] W. L. Wiese, J. R. Fuhr, T. M. Deters, *J. Phys. Chem. Ref. Data, Monograph* 7, (1996)
- [9] H. Nussbaumer, P. J. Storey, *Astron. Astrophys.* **99**, 177-181 (1981)

Table 2: Oscillator strengths (gf) for some electric dipole transitions in OIII.

LSJ-L'S'J'	λ_{exp} (Å)		HF	SSC	SC	[8]	[9]
$^3P_2-^3D_3$	835.289	L	0.841 0.856	0.431 0.433	0.456 0.451	0.438	0.44
		V		0.492 0.489	0.464 0.469		
$^3P_0-^3D_1$	832.929	L	0.203 0.207	0.104 0.105	0.110 0.109	0.106	0.107
		V		0.118 0.118	0.112 0.114		
$^3P_2-^3P_2$	703.854	L	0.541 0.550	0.499 0.499	0.524 0.516	0.510	0.505
		V		0.515 0.516	0.522 0.530		
$^3P_2-^3S_1$	508.178	L	1.392 1.343	0.906 0.918	0.945 0.932	0.935	0.925
		V		1.014 1.002	0.976 0.990		
$^3P_0-^3S_1$	507.388	L	0.277 0.268	0.180 0.183	0.188 0.186	0.186	0.185
		V		0.202 0.199	0.194 0.197		
$^1D_2-^1D_2$	599.590	L	2.682 2.557	1.414 1.438	1.485 1.469	1.455	1.460
		V		1.674 1.647	1.557 1.574		
$^1D_2-^1P_1$	525.794	L	1.008 0.972	1.158 1.163	1.209 1.188	1.195	1.160
		V		1.199 1.194	1.225 1.246		
$^1S_0-^1P_1$	597.814	L	0.668 0.684	0.241 0.242	0.246 0.244	0.240	0.250
		V		0.312 0.311	0.269 0.272		
$^3P_2-^1D_2$	535.481	L	1.01-4 .959-4	.440-4 .444-4	.525-4 517-4	.555-4	.585-4
		V		.428-4 .424-4	.553-4 .561-4		
$^1D_2-^3D_3$	1002.49	L	.347-4 .364-4	.179-4 .181-4	.190-4 .190-4	.190-4	.200-4
		V		.343-4 .338-4	.319-4 .319-4		