

## THEORETICAL ATOMIC DATA FOR ASTROPHYSICS

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**Abstract.** Modern methods of theoretical description of the structure and spectral characteristics of many-electron atoms and ions are analyzed. In order to achieve fairly accurate results, one has to account for correlation and relativistic effects. The latter may be considered either as corrections in a Breit-Pauli approximation (if they are small) or one starts with relativistic wave functions. Correlation effects may be taken into consideration in the framework of superposition-of-configurations method, multiconfigurational approach and stationary many-body perturbation theory, making use of the simplified methods of their accounting for. Existing universal computer programs are surveyed and examples of the calculations are presented.

**Key words:** atomic data: wavelengths, transition probabilities, radiative lifetimes

### 1. Introduction

The application of atomic data to astrophysics is one of the most important domains of the usage of theoretical atomic spectroscopy. In such a case the role of theory becomes extremely important, because fairly often astronomers observe objects or phenomena, which can be hardly reproduced in laboratories. In many cases, the astrophysical models require enormous amount of spectroscopic information, which has to be stored in computerized data banks, including both the experimental and theoretical data. Moreover, only extensive theoretical calculations employing various methods and approaches give a reliable estimation of the quality of experimental and theoretical results.

An important peculiarity of astrophysical applications of atomic theory are the high requirements of accuracy in the calculations. However, in the case of many-electron atoms, which are of particular importance for astrophysics, theoretical data on wavelengths are, as a rule, much less accurate compared to the experimental ones and, therefore, quite often do not satisfy the requirements of astrophysicists. Fortunately, this is not the case for the other characteristics of electronic transitions (oscillator strengths, transition probabilities, lifetimes, etc.). The accuracy of these experimental quantities is usually rather low. Moreover, the discrepancies between the data of various authors often differ considerably more than the error bars indicated. It seems to us that nowadays the calculations of just such characteristics are the most promising applications of the atomic theory to astrophysics.

## **2. Methodology**

Contemporary theory of many-electron atoms or ions is based on a wide utilization of the group-theoretical methods and of the angular momentum technique (Jucys and Bandzaitis 1977, Jucys and Savukynas 1973). Two approaches are the most frequently used nowadays: variational (Froese-Fischer 1977, Cowan 1981) and perturbation theory (Lindgren and Morrison 1982, Safronova and Senashenko 1984). The latter has a number of advantages (strictness of the method used, possibility to obtain the results for the whole isoelectronic sequence at the same time, etc.). Unfortunately, so far it was successfully applied only to relatively simple systems, not exceeding, as a rule, ten electrons.

A variational approach, having practically no restrictions on the complexity of the system under consideration, requires for obtaining highly accurate results some experience in calculations, because it is less limited by the framework of the mathematical method. Now there is a tendency of rapprochement of both these methods. This must lead to a further successful development of atomic theory and to the possibilities to achieve the more accurate results in the near future.

Practically, all versions of the variational approach are based on the usage of the solutions of the nonrelativistic Hartree-Fock (HF) equations as an initial approximation (Hartree 1957). While considering multiply charged ions, when the ionization degree reaches a few dozens, the relativistic Dirac-Hartree-Fock (DHF) equations

giving relativistic wave functions must be applied (Stanley 1960, Grant 1970). However, such objects are not very interesting for astronomers, because the outer layers of stars, from which the radiation is usually observed, are too cool to create so highly stripped atoms. For astrophysical applications it seems sufficient to use the so-called Hartree-Fock-Pauli (HFP) approximation, when radial orbitals (r. o.) are obtained solving the HF equations neglecting relativistic corrections, whereas the relativistic effects are taken into consideration while forming the energy matrix and accounting for all terms of the order  $\alpha^2$  ( $\alpha$  stands for the fine structure constant) in the Breit energy operator. The diagonalization of such matrices, written for a single atomic configuration, gives us an initial approximation for both the energy levels and eigenfunctions. The latter are expressed in terms of a linear combination of the wave functions of the initial pure coupling scheme chosen. The energies and eigenfunctions are further used to calculate the characteristics of electronic transitions. These methods are well known and are described in many monographs. Their astrophysical applications may be found in the monographs of Nikitin and Rudzikas (1983) and Rudzikas et al. (1990).

### 3. Energy levels and wavelengths

Table 1, containing the wavelengths of the transitions  $1s^22s^22p^53d - 1s^22s^22p^6$  for Fe XVII and Mo XXXIII, illustrates the accuracy of various methods for this quantity. It indicates that even for such a highly ionized atom as Mo XXXIII the HFP approximation gives the results very close to those of the DHF. However, with a further increase of the ionization degree, the HFP fails to describe accurately the electronic properties.

**Table 1.** Wavelengths (Å) of the transitions  $1s^22s^22p^53d - 1s^22s^22p^6$  for Fe XVII and Mo XXXIII

Atom	$2p^53d - 2p^6$	PT	HFP	DHF	Exper.
Fe	$^3P_1 - ^1S_0$	15.484	15.457	15.460	15.453
	$^3D_1 -$	15.274	15.263	15.268	15.261
	$^1P_1 -$	15.023	14.996	15.004	15.012
Mo	$^3P_1 - ^1S_0$	4.869	4.860	4.854	4.847
	$^3D_1 -$	4.812	4.802	4.803	4.804
	$^1P_1 -$	4.643	4.637	4.630	4.630

Further improvement of the initial approximation described above (often called as accounting for correlation effects) is complicated by the fact that quantum numbers describing many-electron atomic configuration are not always accurate enough, because the matrix of the energy operator of electrostatic interaction between electrons is not diagonal with respect to those quantum numbers. Hence, one has to carry out the diagonalization of the energy matrices calculated in the basis of several (many) configurations. The simplest way to achieve this is to use the so-called superposition-of-configurations (SC) method. Generally speaking, the larger number of configurations is taken into consideration, the more accurate are the results obtained.

In this approach, the question arises of what sort of r. o. must be utilized to describe these admixed configurations. It is well known that the usage of standard HF functions for such purposes leads to slow convergence of the method and requires to account for a very large number of such configurations, including even electrons of continuous spectrum. The best convergence may be achieved, if one uses the solutions of the multi-configurational Hartree-Fock-Jucys (HFJ) equations. The methods of their numerical solution are described by Froese-Fischer (1977).

Unfortunately, the solution of the HFJ equations for complex many-electron atoms is extremely cumbersome and requires very powerful computing facilities. To overcome these difficulties, we have worked out a method for obtaining the so-called transformed r. o., when the radial wave function of an admixed configuration is found from that of the main configuration by multiplying it by a simple function of its distance from the nucleus. The calculations show that such transformed r. o. are very close in their form to the solutions of the HFJ equations, approximate them fairly accurately and allow to take into account an essential part of the correlation effects. Various ways of obtaining them, as well as their properties are discussed by Bogdanovich (1986). They are particularly efficient, taking into account the correlation corrections of separate configurations in a simplified way (SCC) in the second order of perturbation theory. This approach was preliminary described in Rajnak and Wybourne (1963) and Wybourne (1965) and later on developed for practical applications by Bogdanovich and Žukauskas (1983) and Bogdanovich et al. (1984).

Table 2 lists the energy levels and eigenfunctions multiplied by 1000 for the configurations  $3d^2$  Fe VII, obtained in a single-

configuration HFP approximation, by using the transformed functions to account for correlation effects (SCC), in a semiempirical approach (SE) and the experimental data. It shows that SCC improves essentially both the energy values (its bottom line contains the root-mean-square deviations  $\sigma$  of the calculated results from the experimental data) and the weights of the functions of an intermediate coupling scheme. Let us notice that the usage of the SCC method is very simple, because the energy matrix still remains single-configurational after accounting in this way for correlation effects.

**Table 2.** Energy levels ( $\text{cm}^{-1}$ ) and eigenfunctions of the configuration  $3d^2 \text{Fe VII}$

$J$	HFP		SCC		SE		Exper.
	$E$	1000 $\Psi$	$E$	1000 $\Psi$	$E$	1000 $\Psi$	
2	0	$999.^3F+48.^1D$	0	$999.^3F+53.^1D$	0	$999.^3F+57.^1D$	0
3	1050	$1000.^3F$	1061	$1000.^3F$	1026	$1000.^3F$	1047
4	2369	$999.^3F-22.^1G$	2377	$999.^3F-24.^1G$	2302	$999.^3F-24.^1G$	2327
2	21259	$974.^1D-220.^3P-$ $-47.^3F$	17695	$919.^1D-50.^3F-$ $-391.^3P$	17457	$966.^1D-252.^3P-$ $-57.^3F$	17475
0	24492	$999.^3P+30.^1S$	20117	$999.^3P+34.^1S$	20017	$999.^3P+35.^1S$	20037
1	24875	$1000.^3P$	20506	$1000.^3P$	20394	$1000.^3P$	20428
2	25759	$976.^3P-9.^3F+$ $+220.^1D$	21443	$920.^3P-19.^3F+$ $+290.^1D$	21284	$968.^3P-12.^3F+$ $+292.^1D$	21275
4	32455	$999.^1G+22.^3F$	30376	$999.^1G+24.^3F$	28899	$999.^1G+24.^3F$	28915
0	78705	$999.^1S-30.^3P$	68266	$999.^1S-34.^3P$	65691	$999.^1S-35.^3P$	65707
$\sigma$	3442		762		20		

The computer programs allowing us to simultaneously account for correlation corrections to several strongly mixing configurations are in preparation now. Such an approach looks very promising while calculating the spectra of complex configurations containing open  $nd^N$  shells.

Utilization of the transformed r.o. allows one to generate easily the basis of the wave functions in which the energy matrices may be calculated. However, the number of admixed configurations, which may be taken into consideration in this basis by the superposition-of-configurations method, becomes very large, and the choice of the most important configurations is a rather complicated problem. In order to simplify this procedure, a special computer program has been written. It calculates, by the formulas taken from Karazija (1991), the squared interconfigurational matrix elements of

the energy operator, averaged over all terms (for a given principal configuration and for all admixed configurations allowed in a given basis of the wave functions). After that, using these quantities as well as the differences of mean energies between configurations, the program estimates in the second order of perturbation theory the role of each allowed admixed configuration. The same program evaluates the efficiency of any basis of the r. o. employed.

#### 4. Transition probabilities and radiative lifetimes

Multi-configurational eigenfunctions of an intermediate coupling scheme are further used to calculate the matrix elements of electronic transitions. Line and oscillator strengths as well as transition probabilities are expressed in terms of these matrix elements squared. As it follows from Bogdanovich (1991), the utilization of the transformation  $P^*(n'l'|r) = NrP(nl|r)$  allows one to describe fairly accurately the correlation effects while studying the electric dipole transitions (SCTF). There exists the generalized form of the operator of electric multipole transitions, containing arbitrary value of gauge condition of electromagnetic field potential (Nikitin and Rudzikas 1983). However, so far usually two special forms ("length"  $L$  and "velocity"  $V$ ) of this operator are utilized. In a single-configuration HF approximation, the transition quantities obtained while using these two forms of the operator may differ substantially. Only superposition of configurations implemented in a fairly extensive and properly chosen basis leads to highly accurate results, practically coinciding for both forms of the transition operator.

The efficiency of the usage of the transformed functions to account for correlation effects (SCTF approximation) while calculating probabilities of transitions between configurations  $1s^22p^2 - 1s^22s2p$  in C III is demonstrated by the data of Table 3. As it is seen, the SCTF approach not only diminishes essentially the discrepancies between  $A_L$  and  $A_V$ , but also completely changes some transitions compared to a single-configuration approximation. It is also worthwhile to emphasize that in this case a comparatively small basis of admixed configurations was employed. Data on transition probabilities for C III presented in Table 3, as well as similar data for N IV and O V have been already successfully used to study the spectra of planetary nebulae.

**Table 3.** Transition probabilities ( $10^8 \text{ s}^{-1}$ ) between the levels of configurations  $1s^2 2p^2 L_1 S_1 J_1 - 1s^2 2s 2p L_0 S_0 J_0$  for C III

Transition $L_1 S_1 J_1 - L_0 S_0 J_0$	HF		SCTF		PT	SC+SE	SC
	$L$	$V$	$L$	$V$			
$^1S_0 - ^1P_0$	7.35	8.47	22.3	25.5	16.6	21.1	18.6
$^3P_0 - ^3P_1$	15.3	10.8	13.8	14.9	12.7	13.3	13.6
$^3P_1 - ^3P_0$	5.11	3.60	4.60	4.96	4.25	4.4	4.55
$^3P_1 - ^3P_1$	3.83	2.70	3.44	3.72	3.18	3.3	3.41
$^3P_1 - ^3P_2$	6.36	4.50	5.73	6.19	5.30	5.5	5.67
$^3P_2 - ^3P_1$	3.83	2.70	3.45	3.72	3.19	3.3	3.42
$^3P_2 - ^3P_2$	11.5	8.11	10.3	11.2	9.55	10.0	10.2
$^1D_2 - ^1P_1$	1.78	5.28	1.30	1.30	1.50	1.4	1.46

The results of calculations of transition probabilities, when  $\Delta n \neq 0$ , are presented in Table 4. The following superposition of configurations, influencing most of the transition probabilities, has been chosen:

$$\begin{aligned}
 & 3s^2 3p^2 4s + 3s 3p^4 + 3s^2 3p^2 3d + 3s^2 3p^2 4d + 3s 3p^3 4p \rightarrow \\
 & \rightarrow 3s^2 3p^3 + 3s^2 3p 4s^2 + 3s^2 3p^2 4p + 3s 3p^3 4s + 3s 3p^2 4s 4p + \\
 & \quad + 3s^2 3p 3d 4s + 3s^2 3p^4 4s 4d.
 \end{aligned}$$

The calculations have been carried out using only the HF r. o. (SC) or adopting the transformed r. o. to describe  $4p$  and  $4f$  electrons (SCFT). The last line of Table 4 contains the root-mean-square deviation values  $\sigma^{LV}$  of the transition probabilities obtained using two forms ( $L$  and  $V$ ) of the transition operator. It follows from Table 4 that inclusion into the basis of the transformed r. o. allows one to achieve not only a high agreement between the transition probabilities found using two forms of the transition operator, but also a fairly good agreement of these results with the data obtained in a semiempirical approach combined with an extensive superposition of configurations (SC+SE).

**Table 4.** Transition probabilities ( $10^8 \text{ s}^{-1}$ ) between the configurations  $3p^2 4s - 3p^3$  for Fe XII

Transition	HPF		SC		SCTF		SC+SE
	<i>L</i>	<i>V</i>	<i>L</i>	<i>V</i>	<i>L</i>	<i>V</i>	
$^2P_{1/2} - ^2P_{1/2}$	514	498	394	410	464	484	444
$^2S_{1/2} - ^2P_{1/2}$	631	532	605	629	566	542	272
$^4P_{1/2} - ^4S_{1/2}$	742	646	687	729	654	651	417
$^2S_{1/2} - ^2P_{3/2}$	864	735	858	919	772	753	439
$^2P_{1/2} - ^2D_{3/2}$	1990	1820	1780	1880	1830	1830	1990
$^2P_{3/2} - ^2P_{1/2}$	297	284	234	245	269	280	275
$^2D_{3/2} - ^3P_{1/2}$	131	119	97	101	109	113	108
$^4P_{3/2} - ^4S_{3/2}$	735	633	682	715	649	438	350
$^2P_{3/2} - ^2P_{3/2}$	537	517	412	429	478	495	425
$^2D_{3/2} - ^2P_{3/2}$	656	606	545	575	592	607	647
$^2P_{3/2} - ^2D_{3/2}$	33	30	26	27	31	31	45
$^2D_{3/2} - ^2D_{3/2}$	741	638	697	731	661	645	609
$^2P_{3/2} - ^2D_{5/2}$	1610	1450	1450	1530	1470	1460	1500
$^4P_{5/2} - ^4S_{3/2}$	737	625	689	713	653	632	310
$^2D_{5/2} - ^2P_{3/2}$	227	210	172	178	198	204	175
$^2D_{5/2} - ^2D_{3/2}$	192	166	165	167	171	165	247
$^4P_{5/2} - ^2D_{5/2}$	45	42	37	42	36	38	18
$^2D_{5/2} - ^2D_{5/2}$	969	841	891	933	867	851	796
$\sigma^{LV}$	90		40		13		

The radiative lifetimes of the excited levels are usually defined as an inverse quantity of the sum of probabilities of the transitions from a given level into all lower-lying levels. It is interesting to notice that sometimes only the usage of a single-configuration approximation leads to the results fairly accurately coinciding with the experimental ones. This may be explained by the fact that the errors of particular transition probabilities may partially compensate each other, while summing them up. In papers by Bogdanovich et al. (1985, 1988) it was suggested not to calculate individual transition probabilities but to use instead the formulas obtained for a very simple and fast theoretical estimation of lifetimes. In Table 5 there are presented the radiative lifetimes (ns) of the levels of the configuration  $3p^4 3d$  Ar II, obtained by a successive summation of all transitions and by the usage of two kinds (a and b) of simplified

formulas. It is seen that the utilization of the second kind of formulas (b) allows one to describe fairly accurately the lifetimes considered, having in this way the differences from the successive method of calculation essentially smaller than those obtained using two forms of the transition operator or the error bars of the measurements.

**Table 5.** Radiative lifetimes (ns) of the levels of the configuration  $3p^43d$  Ar II

$(L_0S_0) LSJ$	Successive		Simplified				Exper.
	$L$	$V$	a		b		
			$L$	$V$	$L$	$V$	
$(^3P) ^4D_{3/2}$	4.17	4.33	3.7	4.0	4.15	4.27	$4.7 \pm 0.6$
$(^1D) ^2D_{3/2}$	0.65	0.70	0.57	0.62	0.63	0.69	$3.2 \pm 0.4$
$(^3D) ^4P_{5/2}$	3.72	4.15	3.7	4.1	3.87	4.10	$3.9 \pm 0.4$
$(^3P) ^4D_{5/2}$	4.18	4.34	3.7	4.1	4.16	4.28	$4.6 \pm 0.6$
$(^1D) ^2D_{5/2}$	0.51	0.63	0.62	0.66	0.59	0.65	$3.5 \pm 0.3$
$(^3P) ^4D_{7/2}$	4.21	4.35	3.7	4.1	4.17	4.28	$4.1 \pm 0.4$
$(^3P) ^2F_{7/2}$	3.75	4.18	3.7	4.1	3.75	4.14	$4.4 \pm 0.4$
$(^3P) ^4F_{7/2}$	3.99	4.27	3.8	4.1	3.96	4.22	$4.9 \pm 0.4$
$(^3P) ^4F_{9/2}$	4.02	4.28	3.8	4.1	3.96	4.22	$5.0 \pm 0.4$
$(^1D) ^2G_{9/2}$	3.98	4.26	3.7	4.1	3.93	4.20	$4.5 \pm 0.4$

When it is not possible to achieve high accuracy of the lifetimes in a single-configuration approach, one faces the necessity to employ the superposition-of-configurations method. The efficiency of the application of the transformed functions in this case is demonstrated in Table 6. It contains the radiative lifetimes of the levels of the configuration  $5d^96p$  Hg III, calculated in two approaches. The transitions into two configurations ( $5d^96s$  and  $5d^{10}$  for the levels with  $J = 1$ ) were considered. As one can see, the usage of the SCC approach allows us to obtain very close lifetime values, when using transition probabilities calculated with two forms of the transition operator. Achievement of such correspondence is a fairly reliable guarantee of the high accuracy of the results obtained.

**Table 6.** Radiative lifetimes (ns) of the levels of the configuration  $5d^9 6p$  Hg III

<i>LSJ</i>	HFP		SCTF	
	<i>L</i>	<i>V</i>	<i>L</i>	<i>V</i>
$^3P_2$	1.12	1.60	1.79	1.34
$^3F_3$	1.09	1.59	1.71	1.32
$^3F_4$	0.70	1.37	1.13	1.20
$^3P_1$	0.51	0.68	0.69	0.63
$^1D_2$	0.72	1.38	1.20	1.18
$^3D_3$	0.59	1.30	1.05	1.12
$^3F_2$	1.02	1.55	1.65	1.32
$^1P_1$	0.24	0.27	0.27	0.26
$^3P_0$	0.82	1.44	1.35	1.31
$^3F_3$	0.72	1.38	1.20	1.24
$^3D_1$	0.49	0.87	0.76	0.80
$^3D_2$	0.61	1.31	1.08	1.13

## 5. Conclusion

Using the modern methods of theoretical atomic spectroscopy and the computer programs available, one is in a position to perform fairly accurate, purely theoretical (*ab initio*) or semiempirical calculations of the energy spectra, transition probabilities and other spectroscopic characteristics, as well as their isoelectronic sequences, in principle, for any atom or ion of the periodical table revealing in this way their structure and properties. This makes it possible to model the processes in low and hot temperature plasma and to help to interpret the interesting phenomena found from experimental studies and astrophysical observations.

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