

Calculations of radiative transition probabilities for forbidden lines

ABSTRACT

A review is presented of some typical results illustrating the level of accuracy reached in recent theoretical calculations of radiative transition probabilities for forbidden lines. The emphasis of the present paper is put on results obtained with the computer program SUPERSTRUCTURE, but comparisons with other studies allow for an assessment of the data and comments are made on the present state of the art. Most of the transitions considered here are between levels in the ground configurations $2p^{2,3,4}$ and $3p^{2,3,4}$, but some other cases are mentioned briefly.

INTRODUCTION

It has been known for some time that well-chosen forbidden lines arising through electric quadrupole (E2) and magnetic dipole (M1) transitions can be used as a basis for electron temperature and/or density diagnostics both in astrophysics and fusion research (see, for example, Seaton, 1968, Osterbrock, 1974 & 1989, or Hinnov & Suckewer, 1980). For these diagnostics to be meaningful, there are two obvious requirements: good observations and accurate atomic data, such as collision strengths and radiative transition probabilities. I shall be looking at the latter in the present paper. To treat the subject exhaustively would take a much longer talk. Many reviews and compilations exist, which have been widely consulted by users of atomic data and by atomic physicists who want to decide which case to tackle next (see, for example, Wiese et al, 1966 & 1969, Garstang, 1968, Eidelsberg et al, 1981, Mendoza, 1983, Kaufman & Sugar, 1986). Biémont & Zeippen (1989) have started an extended review of recent developments. Here, although some other cases will be mentioned very briefly, we shall mainly

content ourselves with the important transitions in the ground configurations $2p^{2,3,4}$ and $3p^{2,3,4}$ for comparatively light elements. Indeed, the importance of relativistic effects increases and that of correlation effects decreases as Z becomes larger. All calculations then tend to converge in the middle- Z range until the Breit-Pauli approximation ceases to hold and only fully-relativistic structure programs give reasonable data. Here, the emphasis will be on values obtained with the code SUPERSTRUCTURE, but comparisons will of course be made with other theoretical findings. It should be noted that very few experimental results exist in this field, which makes all the more crucial the need for assessing various sets of theoretical data yielded by methods and codes as different as possible.

THE METHODS

The code SUPERSTRUCTURE (Eissner et al, 1974) has been used extensively to produce accurate transition probabilities. It is a configuration-interaction (CI) computer program which accounts for fine-structure and other relativistic effects in the low- Z Breit-Pauli approximation. The one-electron radial orbitals P_{nl} are computed using a Thomas-Fermi statistical model (SM) potential (Eissner & Nussbaumer, 1969), or are obtained from the Coulomb potential. In the version of the code modified by Nussbaumer & Storey (1978), there is one scaling parameter per (n,l) , allowing for much flexibility in building the orbitals. Those scaling parameters are determined through term energy minimization procedures. The Breit-Pauli Hamiltonian is treated as a perturbation and the expansion of the relativistic wavefunctions may be improved by means of the term energy correction (TEC) procedure described by Zeippen et al (1977).

The probability for a transition between levels i and j , forbidden for electric dipole (E1) radiation but not for E2 and M1 radiation is taken to be

$$A_{ij} = A_{ij}(E2) + A_{ij}(M1) \quad (1)$$

$$\text{with} \quad (2)$$

$$A_{ij}(E2) = 2.6733 \cdot 10^3 (E_i - E_j)^5 / g_i S_{ij}(E2) \text{ s}^{-1}$$

$$\text{and} \quad (3)$$

$$A_{ij}(M1) = 3.5644 \cdot 10^4 (E_i - E_j)^3 / g_i S_{ij}(M1) \text{ s}^{-1}$$

S_{ij} is the line strength and energies are expressed in Rydbergs and lengths in Bohr radii.

Relativistic corrections to the M1 operator are included, i.e.

$$S_{ij}(M1) = |\langle i | Q | j \rangle|^2 \quad (4)$$

where

$$Q = Q^0 + RC = \sum_{m=1}^N \{ \mathbf{L}(m) + \sigma(m) \} + RC \quad (5)$$

Q^0 is the usual lowest-order M1 operator, corresponding to the magnetic moment and the sum runs over all N electron coordinates. Expression (5) is implemented in DIPOLE, a program complementary to SUPERSTRUCTURE and written by Eissner & Zeippen (1981). The expressions for the operators labelled RC can be found in Drake (1971) or Sucher (1978).

Another CI code which has been used extensively to compute transition probabilities is CIV3 (Hibbert, 1975). It calculates Slater-type orbitals using Hartree-Fock functions like those of Clementi & Roetti (1974), together with correlation orbitals, to provide initial estimates. The parameters defining the orbitals are obtained through minimization procedures similar to the ones in SUPERSTRUCTURE. There is a relativistic version of the code (Glass & Hibbert, 1978) incorporating the Breit-Pauli Hamiltonian.

Combining the Hartree-Fock, Breit-Pauli and CI formalisms is the computer program MCHF-BP (Froese Fischer, 1978 & 1983). Firstly, a non-relativistic MCHF calculation produces a set of radial functions for a given LS term, providing the basis for an interaction matrix to be determined in the BP approximation for a wavefunction expansion over a large set of configurations which may interact electrostatically or through relativistic corrections, for one or more J-values of interest.

The semi-empirical framework of HXR and HFR self-consistent-field methods have been implemented in the Cowan-Zealot suite of programs (Bromage, 1978) which are used in connection with Cowan's (1981) atomic structure codes. The self-consistent-field method with relativistic corrections is used to set up the radial wavefunctions. Energies and spectra are then computed with the help of conventional Slater-Condon theory with configuration mixing.

The relativistic equivalent to the MCHF code described above is the multiconfiguration Dirac-Fock program written by Desclaux (1975). The MCDF computer program is based on a more rigorous theory than the codes incorporating the Breit-Pauli formalism. It does not introduce adjustable parameters in building the wavefunctions and it treats the leading correlation and relativistic effects on an equal level. Note that the variational

principle gives a stationary solution in this case and not a minimum, as the Dirac equations have two solutions.

Finally, among many other methods, I shall also mention the non-closed-shell-many-electron theory (NCMET) of atomic structure developed by Sinanoglu et al (see, for example, Sinanoglu, 1969) or the FOTOS formalism (see, for example, Nicolaidis & Beck, 1978).

THE ASTROPHYSICAL IMPORTANCE OF THE DIAGNOSTICS BASED ON FORBIDDEN LINES

Rosa (1989) explains in detail the importance of atomic data in the study of gaseous nebulae. Suffice to say here that some forbidden line intensity ratios are sensitive to electron temperature and/or density and that some of those are powerful tools to analyze the spectra from nebulae, on condition that the quality of observations is matched by that of atomic data and vice versa.

For instance, the ratio $I(3729 \text{ \AA})/I(3726 \text{ \AA})$ in O II is of great importance (see, for example, Seaton & Osterbrock, 1957, Canto et al, 1980, O'Dell & Castaneda, 1984, Zeippen, 1980 & 1987). A good illustration of the interplay between observations and atomic data is the high-density limit $r(N_e \rightarrow \infty)$ of the ratio $I(3729 \text{ \AA})/I(3726 \text{ \AA})$ which is equal to $3/2 A(2D_{5/2} - 4S_{3/2})/A(2D_{3/2} - 4S_{3/2})$, thus allowing for a "direct" check of consistency between observed intensities and atomic data: the theoretical value for $r(\infty)$ must never be superior to the one observed in nebulae with high electron density. This is but one example where one may consider, with great caution (after all, there are still many uncertainties in our knowledge of nebulae...), the universe as a large laboratory.

Another ratio of interest is $I(4741.5 \text{ \AA})/I(4712.7 \text{ \AA})$ in Ar IV (see the recent study by Zeippen et al, 1987), which is a good companion to the equivalent ratio in O II, as their ranges of sensitivity complement one another.

Finally, it is worth mentioning the work recently completed by Stanghellini & Kaler (1989) who analyzed 146 planetary nebulae and showed, in particular, how new atomic data change the conclusions drawn.

FORBIDDEN LINES IN THE $2p^2$ CONFIGURATION

The most complete SUPERSTRUCTURE calculation to date is by Nussbaumer & Rusca (1979) who considered all the members of the isoelectronic sequence up to Ni XXIII. There is good

agreement with the work of Nicolaides & Sinanoglu (1971 & 1973). In the case of O III, the values obtained by Baluja & Doyle (1981), using CIV3, and by Nussbaumer & Storey (1981), using SUPERSTRUCTURE, agree rather well with each other and with the earlier work of Nussbaumer & Rusca (1979). Based on a smaller configuration basis set, the values computed with SUPERSTRUCTURE by Kastner et al (1977) differ markedly from the latter. Recent MCHF+BP calculations were performed by Froese Fischer & Saha (1985) who also present a detailed comparative discussion of the main sets of probabilities available in the literature for this case. Using a large number of configurations, Froese Fischer & Saha (1985) obtained good agreement with the relativistic MCDF results of Cheng et al (1979) and the data computed by Fawcett (1978) using the Cowan-Zealot package. However, the discrepancies with the SUPERSTRUCTURE or CIV3 results can be important for some E2 transitions. For the M1 transitions, there is reasonable agreement between all main studies. In view of this situation, a new and more ambitious effort using SUPERSTRUCTURE might be timely.

FORBIDDEN LINES IN THE $2p^3$ CONFIGURATION

The ground configuration $2p^3$ of N-like ions is a tricky case because it has a half-filled outer shell. In this case, the first-order spin-orbit interaction vanishes and second-order effects become important (see the discussion in Eissner & Zeippen, 1981). Trying to solve the inconsistencies between observed and calculated values for $r(\infty)$ pointed out by Seaton & Osterbrock (1957) in their study of O II forbidden lines, Zeippen (1980) showed that the usual lowest-order M1 transition operator was not adequate to treat the most "sensitive" transitions and that the inclusion of relativistic corrections (RC in formula (5) above) was required. Eissner & Zeippen (1981) confirmed this viewpoint and proposed new forbidden transition probabilities which yielded, in particular, a value for $r(\infty)$ close to the one observed in nebula NGC 7027 for the high-density limit of the ratio $I(3729 \text{ \AA})/I(3726 \text{ \AA})$. Zeippen (1982) extended the calculation to the first twenty members of the isoelectronic sequence. A detailed comparison with previous work (including Garstang, 1972, Fawcett, 1978, Cheng et al, 1979, Bhatia & Mason, 1980a & 1980b) was also carried out by this author. Using a larger configuration basis set in the MCHF+BP code, Godefroid & Froese Fischer (1984) were able to show that some important correlation effects had been neglected so far and publi-

shed improved probabilities, with the qualification that the RC operators were not included in their expression for the M1 transition operator. Taking full advantage of the progress in computing facilities and of the findings of all the previous studies, Butler & Zeippen (1984), Zeippen (1987) and Becker et al (1989) have now produced what should be the most accurate transition probabilities to date for this sequence up to Fe XX, with an estimated uncertainty within 10%. Note that the agreement between the new SUPERSTRUCTURE results and the MCHF+BP values for the same quantities has now reached a good level. Finally, it should be said that the theoretical value for $r(\infty)$ is now smaller than the one observed in nebulae with high electron density, which is not inconsistent.

FORBIDDEN LINES IN THE $2p^4$ CONFIGURATION

For this isoelectronic sequence, no extended SUPERSTRUCTURE calculation has been reported, apart from the preliminary results of Mendoza & Zeippen quoted by Mendoza (1983). There are calculations by Kastner et al (1977) and Bhatia et al (1979) but those are based on a limited number of configurations. A study of the sequence has been performed by Baluja & Zeippen (1988) who used CIV3, including the intrashell correlations within the $n=2$ complex and the intershell correlations between the $n=2$ and the $n=3$ complexes. They calculated E2 and M1 transition probabilities for 17 species, obtaining good agreement with two experimental results for O I (McConkey et al, 1966, Corney & Williams, 1972). In this paper, a detailed comparison is made with the MCHF+BP results of Froese Fischer & Saha (1983) who include the $n=2$, $n=3$ and $n=4$ complexes in their calculations, and with the relativistic data of Cheng et al (1979). The agreement between the three sets of results is generally good, although some discrepancies can be seen. The differences between the MCHF+BP and the CIV3 data are smaller than the ones with the MCDF values. Other studies include the work of Garstang (1951), Nicolaides & Sinanoglu (1971) and Fawcett (1978). It could be worthwhile to perform a large-scale SUPERSTRUCTURE calculation for this sequence, as the preliminary results of Mendoza & Zeippen (see Mendoza, 1983) tend to agree rather well with the most reliable data available.

FORBIDDEN LINES IN THE $3p^2$ CONFIGURATION

The three main recent calculations performed for this case will be considered here. The SUPERSTRUCTURE study of the isoelectronic sequence up to Ni XV is by Mendoza & Zeippen (1982b) who used a 7-configuration basis set and improved over earlier work by Czyzak & Krueger (1963) or McKim-Malville & Berger (1965). Biémont & Bromage (1983) produced results for alternate ions from S III to Sn XXXVII with the help of the HXR self-consistent-field method and Slater-Condon theory. The agreement between the SUPERSTRUCTURE and HXR results is good, which is significant as the two methods and physical models differ markedly. A relativistic MCDF computation has been done by Huang (1985) who takes all the configurations in the $n=3$ complex into account. Unfortunately, this author included no comparison with previous work in his paper. A quick assessment shows the usual trend of some discrepancies at the neutral end of the isoelectronic sequence and converging results as Z increases. Only a more detailed comparative study will tell if there is a need for further work on this case.

FORBIDDEN LINES IN THE $3p^3$ CONFIGURATION

Again, as in the case of $2p^3$, second-order effects play an important rôle, but to a smaller extent as Z is higher for $n=3$ than for $n=2$ and the higher-order corrections decrease as Z increases (see the discussion in Eissner & Zeippen, 1981). The first "modern" computation was performed by Mendoza & Zeippen (1982a) using a 7-configuration basis set in SUPERSTRUCTURE and its companion DIPOLE. They obtained some sizeable changes as compared to previous work (Czyzak & Krueger, 1963 & 1965, Garstang, 1968 & 1972). Biémont & Hansen (1985) provided a check on those new results with the help of the HXR and HFR self-consistent-field methods. They found reasonable agreement but noted that the discrepancies were more substantial for this isoelectronic sequence than in the case of $3p^2$, which is not surprising in view of the more complex problem in hand. Froese Fischer & Godefroid (1986) published some MCHF+BP results, in particular for S II and Ni XIV. Their detailed comparison with the work of Mendoza & Zeippen (1982a) and with the MCDF results of Huang (1984) shows a reasonable agreement between the three studies. The general conclusion here must be that there seems to be room for improvement of at least some of the forbidden transition probabilities available in the literature for the $3p^3$

isoelectronic sequence.

FORBIDDEN LINES IN THE $3p^4$ CONFIGURATION

Mendoza & Zeippen (1983) based their SUPERSTRUCTURE calculation on an 8-configuration basis set, obtaining reasonable agreement with previous work by Czyzak & Krueger (1963) and McKim-Malville & Berger (1965). The HXR/HFR results were obtained by Biémont & Hansen (1986b) and their values were found to be in satisfactory agreement with the SUPERSTRUCTURE data, although there are some sizeable discrepancies. Very recently, a relativistic MCDF computation was performed by Saloman & Kim (1989). These authors compare their results with the two previous sets of data and they conclude that the differences can be explained by the approximations and adjustments used in the HXR/HFR and SUPERSTRUCTURE studies and by the limitation of their own calculations at low Z (small number of configurations in the physical model). It should be noted that the values of Biémont & Hansen (1986b) and those of Mendoza & Zeippen (1983) tend to agree better with one another than with the MCDF results.

SOME OTHER CASES

Due to the narrow scope of this talk, it will be impossible to describe in detail many other studies of interest, such as the recent application of the HXR/HFR method to configurations $4p^2$, $4p^3$ and $4p^4$ by Biémont & Hansen (1986a & 1986b), or the attempt of Nussbaumer & Storey (1980), using SUPERSTRUCTURE for treating the forbidden lines of Fe II. All this will have to be assessed in further surveys.

I will conclude by mentioning the forbidden lines between the $3p^6 4s \ ^2S_{1/2}$ and the $3p^6 3d \ ^2D_{3/2, 5/2}$ levels in K-like elements. These lines are of astrophysical interest in Ca II (see, for example, Hobbs et al, 1988). There have been two recent calculations by Ali & Kim (1988), using a single-configuration approximation in the MCDF code, and Zeippen (1989), using some amount of CI in SUPERSTRUCTURE. The agreement between the two sets of results is good, even though more sophistication seems necessary to reach a definitive conclusion. The experimental result for K by Hertel & Ross (1969) looks too large, but reasonable agreement is obtained with the theoretical result of Langhoff et al (1985) for the same atom. The earlier transition probabilities of Osterbrock (1951) for Ca II are most probably overestimated.

CONCLUSION

In this necessarily limited review, while providing a sample of references which could be of practical use to the reader, I hope I have shown how much effort by many teams goes into supplying accurate data to astrophysicists and fusion specialists. In this presentation, I have tried to illustrate the idea that detailed comparisons between different sets of results is essential in assessing the accuracy of the data proposed to the user, but also in understanding (and perhaps attenuating) the weaknesses of the various theoretical methods. Saloman & Kim (1989) state that these approximations which include adjustable parameters require experience and judgment on the part of physicists in order to yield reliable results. I would happily extend their view to most methods, as none of them, however rigorous and foolproof in principle, can be treated in practice as a "black box". We all suspect that human beings are still needed in the age of computers: it is certainly true of forbidden line transition probability calculations!

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