Update of UCL computer codes for the calculation of fine-structure electron–atom collision cross-section

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**ABSTRACT**

To calculate fine-structure electron–atom collision cross-section, a set including 3 codes was developed at University College London, presented in Computer Physics Communications: SUPERSTRUCTURE (1974), UCL Distorted wave (1998), JAJOM (1972, 1978). Due to improvements in computers, more ambitious calculations of atomic data were performed. Unfortunately, unexpected problems have appeared which required an update version of these codes, presented here.

1. Introduction

The original version of University College London (UCL) codes was developed around 1970 to interpret XUV spectra of astrophysical and laboratory plasmas. In this paper, we only consider the set of 3 codes computing fine-structure electron–atom collision data: SUPERSTRUCTURE (SS, [1]), UCL Distorted wave (DW, [2]) and JAJOM [3]. It has produced many accurate data and is still in use [4]. DW and JAJOM are available in the CPC Program Library but SS does not belong to it. Nevertheless, it is easy to get a copy of this later code from the authors. Since 1970, this set has been improved and corrected a few times.

JAJOM computes electron collision strengths for transition between fine-structure levels of an (ionised or neutral) atomic target. It requires, from DW, non-relativistic reactance matrices and, from SS, “Term Coupling Coefficients” (TCC). Both SS and DW are expected to provide, for the target, the same non-relativistic LS eigenfunctions. The same energy ordering of the corresponding LS eigenterms is also expected. Unfortunately, experience has shown that some unwanted and not foreseen problems could appear. The purpose of the present paper is to propose suitable updates in DW to enforce a coherence with SS data. JAJOM does not need any modification.

2. Identification of problems

Different behaviours have been identified in SS and DW. First of them is in the energy ordering of target terms. Already for H and H-like ions, there is a well-known problem of energy degenerescence of $n\ell$ orbitals and terms, for example the energy ordering of 2s and 2p terms. Problems can also occur for Ne and Ne-like ions, for example the energy ordering of 1s$^2$2s$^2$2p$^3$3p$^1$P and $^3$P terms (see Table 1, terms 7 and 8). Moreover similar energy ordering problems also appear in heavier closed shell neutral or ionised atoms, for example some 3d$^9n\ell$ terms. This energy degenerescence can be proved theoretically but numerically, computers may apply a random ordering, different in SS and DW. Due to recent computer performance improvements, another case of different energy ordering has been identified in the energy ordering of 1s$^2$2s$^2$2p$^3$3p$^1$P and $^3$P terms (see Table 1, terms 7 and 8). Moreover similar energy ordering problems also appear in heavier closed shell neutral or ionised atoms, for example some 3d$^9n\ell$ terms. This energy degenerescence can be proved theoretically but numerically, computers may apply a random ordering, different in SS and DW. Due to recent computer performance improvements, another case of different energy
ordering in SS and DW has appeared for large multiconfiguration expansions. Such large expansions produce many terms, some of them being very close to each other. A small difference in the calculation of radial functions \((nl \text{ orbital})\) has a direct effect on the energy matrix giving the \(LS\) energy eigenvalues, and therefore inversions may appeared.

More exceptional behaviour has also been identified in SS and DW. Both codes include in the diagonalisation procedure the Jacobi method but SS allows also the use of QR decomposition method. For large dimension matrices obtained usually in SS relativistic part, QR can be very efficient. But for JAJOM use, to get the same Slater state term expansions one must use the same diagonalisation method in both codes.

### 3. Description of SS and DW codes

SS and DW have similar structure made of \(2\) algebraic parts followed by \(2\) analytic parts (see Fig. 1). In fact, the target term calculations are handled in the following parts: \((1)\) and \((3)\) of SS and \((5)\) and \((7)\) in DW. The target algebraic part is considered in \((1)\) and \((5)\) and the target analytic part in \((3)\) and \((7)\). In shorter words, the algebraic parts consider the orbital angular and spin integrals whereas the analytic parts consider the radial integrals. The algebraic parts are independent of the nuclear charge and of the energy of the projectile electron.

In SS, in parts \((1)\) and \((3)\) are computed non-relativistic \(LS\) eigenstates which are transformed to \(J\) semi-relativistic eigenstates in parts \((2)\) and \((4)\), by inclusion of Breit–Pauli relativistic corrections. The transformation matrix between \(J\) semi-relativistic eigenvalues and \(LS\) non-relativistic eigenterms (coupled to give \(J\) levels) is called Term Coupling Coefficients (TCC). In DW, similarly to SS, in parts \((5)\) and \((7)\) are computed \(LS\) eigenstates which, for different projectile electron energies, are used to compute reactance matrix \(R(\text{LS})\) elements (parts \((6)\) and \((8)\)).

### 4. Code modifications

In a normal run, SS is used only one time, whereas DW might be used many times, for many projectile energies and/or for many partial waves. The most efficient way is therefore to extract from SS the target data which will be read by DW to replace similar data calculated by DW. DW update version is made such as users can choose either the original or modified version. More precisely, the first line of DW inputs includes now a flag IX09: original version, IX09 = 0; modified version, IX09 = 1. In the later case, an output file from SS is expected, the name of it being read on the next DW input line. All target informations being included in this file, no more information is provided to DW. In particular for IX09 = 1, it avoids to type different target configurations in SS and DW. The following lines of DW input include only informations concerning the projectile, for example its energy.

SS input data have not been modified in the update version: configurations, nuclear charge \(Z\), radial potential scaling parameters, etc. To construct the output target file, only a few WRITE statements have been included in SS. In part \((1)\), subroutine ALGEB1, are extracted \(LS\) eigenvalues and \(LSM_1M_S\) eigenvectors for \(M_z = 0\) and \(M_S = 0\) or \(1/2\), projected on the Slater states basis (called the Vector-Coupling Coefficients). In part \((3)\) of SS, subroutine DIAGON, are extracted \(LS\) energy eigenvalues, called target terms, and \(LS\) energy eigenstates projected on the configuration-\(LS\) terms, the so-called configuration mixing coefficients. Moreover in subroutine RADIAL, all the parameters required to calculate the radial functions (orbitals) are written in the SS output file.

DW structure has not been changed but only modified slightly. The SS output data replace the similar data computed by DW. In part \((5)\), subroutine ONE, are inserted the configuration list and, subroutine ONEONE, the algebraic matrix elements from part \((1)\). In part \((7)\), subroutine TWOONE, SS data from part \((3)\) are also inserted. Radial parameters have been input in subroutine TWOBON and to avoid radial function iterations, a command line was inserted in subroutine RADWAV.

### 5. Conclusion

In this paper, a potential problem in using UCL fine-structure collision codes is pointed out. The problem is due to instable iterations which can occur, for instance, in diagonalisation methods. To remedy such problems, updates are presented and applied. A few tests have been performed, as example for Ne-like ions. Interested readers can get this updated version from the authors.

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### References