2028-1

Joint ICTP/IAEA Workshop on Atomic and Molecular Data for Fusion

20 - 30 April 2009

Calculation of Atomic Data for Fusion

Robert E.H. CLARK
IAEA, Div. of Physical & Chemical Science
Dept. of Nuclear Sciences & App. A-1400
Vienna
Austria

Calculation of atomic data for fusion

Presented at the Workshop on Atomic and Molecular Data for Fusion Energy Research

20 – 30 April, 2009
International Centre for Theoretical Physics

Lectures Notes

R.E.H. Clark
International Atomic Energy Agency

1. Introduction

The devices used in fusion energy research require generating and containing a plasma consisting of isotopes of hydrogen as well as a number of more complex atoms and their ions. These complex atoms and ions enter the plasma in a variety of ways and have a variety of effects on the plasma. In order to accurately understand the behavior of the plasma, details of a variety of processes involving these atoms and ions must be understood, with data for a large number of processes collected and used in large computer codes for modelling the plasma.

Impurities may enter the plasma of a fusion device from different processes. In all machines there will inevitably be some interaction with plasmas and the wall materials. This will lead to introduction of wall material into the plasma. Some diagnostic procedures inject specific materials into the plasma to see the resulting spectral signatures for use in determining plasma parameters. It has been proposed to implant impurities of differing atomic number at different depths in tiles facing the plasma so that as the tiles erode it will be possible to determine the rate of erosion. In the divertor region of machines there are various schemes of introducing inert gases to moderate the plasma. All of these processes require modelling the plasma with these impurities, which requires a large amount of data for a number of processes.

The modelling of the plasma includes solution of the collisional radiative problem. To understand the extent of this problem, consider extreme cases of plasmas, high density and low density.

In a high density plasma each process is balanced by the inverse process. For example, collisional excitation is balanced by collisional de-excitation. With such balancing it is readily shown that the populations of all levels and all ionization stages are determined solely by the energy levels and statistical weights of the levels. This is called local thermodynamic equilibrium (LTE). For a plasma in LTE it is not necessary to know the data for any collisional processes, as each is balanced by its inverse. The only data needed are the energy levels and statistical weights, along with radiative process for calculation of spectral features and for calculations of total radiated power from such a plasma.

For a very low density plasma when an excitation takes place the excited state will decay to the ground state before interaction with other plasma constituents. This is the situation in many astrophysical plasmas and is known as coronal equilibrium. This simplifies the modelling of the plasma because no collisional processes from an excited state need be considered, only processes from the ground state.

The plasmas found in fusion energy research fall between these two extremes. In this case, the plasma is not in LTE, nor is it in the coronal regime. This means that some excited states may be significantly populated, and that the processes and their inverses do not balance each other. Therefore, it is necessary to have data for all processes connecting all such levels to each other and to adjacent ionization stages. This is the idea behind a collisional-radiative (CR) model. Such a model requires a large database for a number of processes.

This series of lectures will focus on the types of data needed, how such data are obtained, where some databases can be accessed, and examples of using these data to do some simple plasma modelling. The types of data include atomic structure, radiative processes, cross sections for electron impact excitation and ionization, photo-ionization and autoionization as well as their inverse processes. There are other types of processes talking place in fusion plasmas, such as molecular processes, collisions between ions and atoms with charge transfer and a variety of plasma interactions with surfaces. These topics will be covered in other lectures in this workshop.

In this series of lectures I will focus on the structure of atoms and ions of atoms and their collisions with electrons, and the use of those processes in modelling calculations. Hereafter I will use the term ion to mean an atom or atomic ion.

2. Atomic Structure

All data for processes in ions rely on atomic structure for defining the states of the ion. For example, either a measurement or a calculation of the cross section for electron impact excitation must specify the initial and final states of the target ion and the difference of energy in order to by useful in a modelling calculation. A typical method of calculating atomic structure is the Hartree-Fock method. An extensive description of calculation of atomic structure is given by Cowan [1]. I will summarize some aspects of atomic structure here.

Cowan uses the well-known Hartree-Fock method for obtaining the radial wave functions of a complex ion. In this method one first makes an initial approximation to each electronic orbital. With the potential determined from these orbitals, each electron has a new orbital calculated by solving the Schroedinger equation from the potential calculated from the first approximation to the other electronic orbitals. This process is iterated until the orbitals converge.

Atomic structure can be calculated fully relativistically or non-relativistically. It is possible to include some of the important relativistic effects in a non-relativistic code, such as the mass and Darwin effects in the radial wave functions and the effect of spin-orbit interaction in obtaining the fine structure energy levels. For most cases in fusion, except for very heavy elements, such a semi-relativistic approach is sufficient.

As most of you know there are different methods for specifying the levels of an ion, with the most common being LS and jj labelling. Since for most fusion energy applications the semi-relativistic data will be sufficient, I will use LS labelling throughout. As a refresher, let us consider an ion of carbon, C^{+4} in the electron configuration 1s2p. The orbital angular momenta of the two electrons are l=0 for the 1s and l=1 for the 2p electrons, respectively. The only total angular momentum possible from coupling these two electrons is L=1, or P. However, there are two possible couplings of the spins, resulting in S=0 or S=1. In LS notation it is customary to label a term by the notation ^{2S+1}L so that we can have two terms from the above electron configuration

1s2p ^1P

1s2p ^3P

The final step is to couple the total spin and total orbital angular momentum to form a total angular momentum, J. With the ^1P there is only one J possible, J=1, because the J is determined by $|L-S|\leq J\leq L+S$ and for L=1 and S=0, J must be 1. For the ^3P, we have L=1 and S=1. We can then have J=0, J=1, and J=2. Therefore the final result is that the 1s2p configuration has four fine structure levels,

1s2p $^1P_1$

1s2p $^3P_0$

1s2p $^3P_1$

1s2p $^3P_2$

It should be noted that under the jj coupling scheme the same number of fine structure levels will be arrived at, but through a different method of coupling. Also note that there are other coupling schemes in use.

It turns out that no coupling scheme is perfect in describing an ion. For light elements the LS scheme is reasonably good, while for heavy elements the jj scheme is better. In both cases it is possible to improve the calculation of energies by using perturbation theory and using the pure states as basis states. A complete solution of the structure problem then brings in a mixture of the initial basis states with mixing coefficients. In the semi-relativistic case the effects of spin can be brought in through spin-orbit interaction, which leads to mixing of the LS basis states. Coulomb interactions lead to mixing of the electron configurations. The result is that a final state will be a mixture of different configurations and LS terms. For further information on the details of such calculations, I refer you to Cowan's book, or the work of C. Froese-Fischer [2]. For a fully relativistic treatment, there are many references, the work of I.P. Grant [3] being widely used.

Once the basic atomic structure has been calculated, including the mixture of basis states, it is possible to calculate radiative transitions between the states. As you know, radiative transitions must follow selection rules due to the dipole nature of radiative transitions. Therefore, the initial and final states must differ in parity. For pure LS states, the value of L must change by one, and the spin must not change. However, when mixing of basis states occurs, those rules may apparently be violated, leading to so-called forbidden transitions. As an example, the transition

$1s^2\,{}^1S_0 \rightarrow 1s2p\,{}^3P_1$

would be forbidden in pure LS coupling because the spin is not permitted to change in an optical transition. However, the 1s2p $^3P_1$ state is actually a mixture:

$$1s2p\ ^3P_1 = A\ (1s2p\ ^3P_1) + B\ (1s2p\ ^1P_1)$$

where A and B are the mixing coefficients. One readily sees that the transition contains a component of an allowed transition to a singlet state. For light elements the mixing between singlet and triplet states will be small, the B coefficient will not be large. The result is that the oscillator strength will be small for such transitions. However, for highly charged heavier ions the mixing can be quite large with the result that there is nearly no difference in the so-called spin allowed and spin forbidden transitions. As a specific example, in he-like carbon the values of the mixing coefficients in the above expression are approximately:

$$A = 0.99995,\ B = 0.00041$$

Note that the normalization of the mixing coefficients is $A^2 + B^2 = 1$, NOT $A+B=1$. Going to heavier elements, for he-like argon,

$$A = 0.99286,\ B = 0.11933$$

And for he-like iron

$$A = 0.95922,\ B = 0.28266$$

One clearly sees that the mixing of the spin states increases with nuclear charge. This has an effect on calculations of many quantities in a plasma, such as spectral features, radiated power, and even charge state distribution. This also causes different levels of treatment to be required for different types of elements.

As an example, it is normally desirable to run a CR calculation with the fewest number of levels consistent with a good solution. Often simply using electronic configurations is sufficient. However, in the case of carbon one can see a potential problem. In that case the solution would predict that any collision from the $1s^2 \rightarrow 1s2p$ would radiatively decay, because this is a dipole allowed transition. However, if one were to use fine structure levels one would see that collisions leading to the $1s2p\,^3P_1$ would radiatively decay very slowly and they would have time to either collisionally de-excite, or collisionally ionise. In either case, the total radiated power predicted from the electronic configuration model would be too large. In addition, the ionization balance would likely not be correct, because the cross section for ionization from the $1s2p\,^3P_1$ is much larger than from the $1s^2$ configuration and if the excited level is populated appreciably, it would lead to enhanced ionization to the hydrogen-like ion stage. However, as the nuclear charge increases, you can readily see that the metastable levels will quickly reach a point where they can be considered radiatively allowed and the model based on just electronic configurations will be much better.

2.1 Obtaining information on atomic structure

The Internet has become a powerful tool for gathering data for atomic processes. There are a number of sources now available for obtaining detailed information on atomic structure. As an example, the IAEA A+M Unit has collaborated with colleagues at the Los Alamos National Laboratory to make the atomic structure code of Cowan available through a web interface. Through this interface it is possible to calculate atomic structure parameters for any ion stage of any elements of interest to fusion. It is possible to use this interface to obtain energy levels in the Hartree-Fock approximation for an arbitrary atomic ion and to use those approximate energy levels to search more sophisticated databases for specific measured properties of ions.

3. Transition Processes

There are a number of possible transitions that can take place in an ion that are needed in the CR model. Such processes include electron impact excitation and ionization, autoionization and photoionization. Other processes, such as heavy particle collisions leading to excitation, ionization, and charge transfer are also important, but are covered in other sets of lectures.

Of course, it is also necessary to obtain the cross sections for the inverse of each of the above process. However, this is accomplished from the principle of detailed balance. Recall that in LTE the energy levels are determined by energy and statistical weight alone. The requirement that at LTE each process is balanced by its inverse means that:

$$n_i R_{ij} = n_j R_{ji}$$

where R represents a rate coefficient and n represents a level population, and from which it follows that

$$R_{ji} = \frac{n_i}{n_j} R_{ij}$$

The LTE distribution is just the Maxwell-Boltzmann distribution from which it follows that:

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} e^{\frac{-E}{kt}}$$

where g represents a statistical weight, so that we arrive at the relationship:

$$R_{ji} = \frac{g_i}{g_j} e^{\frac{-E}{kt}} R_{ij}$$

where R_{ij} and R_{ji} are the cross sections for the direct and inverse processes respectively. This type of relationship allows one to find the cross sections for all inverse processes, and from those cross sections, an integration over a velocity distribution for electrons will yield the rate coefficients.

There are experimental measurements for these processes for an increasing number of transitions in many ions. However, in general, as the stage of ionization is increased, the cross sections become quite small and beam dispersion becomes large so that the experiments become difficult. For that reason, the bulk of the data actually used in CR calculations have been generated from theoretical calculations. I should be noted that the experimental results are extremely valuable in determining the level of accuracy of theoretical methods. There are a variety of methods used to measure cross sections which will not be detailed in this set of lectures; instead a brief description of the leading theoretical methods will be given for each process.

3.1 Electron Impact Excitation

There are many methods for the theoretical calculation of electron impact excitation cross sections of ions. These different theories span a range in complexity and in computational time required. A complete understanding of any of the methods would require much more time that we can spend, so only a brief survey will be given here.

The general problem of calculating a cross section for excitation involves a coupled set of equations involving the states of the target and the free electron. In the simpler methods, the problem is largely decoupled, leading to a two state problem, with an initial target state and free electron, and a final target state and free electron at a lower energy. The main feature of the two state solutions is in the method of describing the free electron wave functions. In the coupled methods, a full range of target functions is included in the problem and the full set of coupled equations is solved to obtain cross sections. Each method has advantages and drawbacks.

It should be noted that often, for ions, a quantity called a collision strength is used instead of a cross section. The reason for the use of the collision strength is that the dominant energy dependence of the cross section has been removed, and the collision strength is symmetric with respect to direction of transition. The relation between the cross section and collision strength is:

$$Q_{i \to j} = \frac{\pi a_0^2}{g_i E_i (Ryd)} \Omega(i, j)$$

where Q is the cross section, i is the initial state of the target ion, j is the final state of the target ion, g_i is the statistical weight of the initial state of the target, a_0 is the Bohr radius and Ω is the collision strength.

3.1.1 Plane wave Born

The simplest two state method is the plane wave Born (PWB) approximation. In this approximation the free electrons are described as plane waves and the details of the potential of the target is completely ignored. In this case it is possible to obtain the total cross sections from the atomic structure without any detailed calculation of wave functions for the free electron at all. Cowan [1] gives a description of this method, using a generalized oscillator strength.

The main advantage to the PWB calculation is that it is extremely fast computationally. The disadvantage is that it has poor accuracy at energies that are low compared to the transition energy. The accuracy is usually acceptable for energies above five to ten times the transition energy, and often at even lower energies. However, below a few times the transition energy the results can be quite unreliable, in error by over a factor of two. Efforts are sometimes made to mitigate these low energy errors, with some success. Some comparisons have been made by Clark and Collins [4].

In spite of the potential for large errors, the PWB results are often quite useful, especially for transitions between two excited states. As you will recall, such transitions are needed in the CR model, as the excited states may have significant population. An attractive feature of the PWB cross section is the accuracy generally is good for impact energies above several times the transition energy. For many ions, the first excited state is at an energy considerably above the ground state, often over half way to the next ion stage. This means that the transition energy from one excited state to another will generally be small compared to the ionization energy. This in turn means that the impact electron energies that are often several times the threshold energies for these transitions and the PWB cross sections may be adequate for most of these types of transitions. This is a strategy employed by some models of plasmas for fusion. The normal procedure is to calculate PWB cross sections for all transitions possible. More complex theory can then be used on transitions originating from the ground states of the ions, for which the transition energy is large. In this way the more time consuming calculations are limited to those transitions for which they are truly needed and the rest are done adequately with the PWB theory.

3.1.2 Coulomb Born

The next step from the PWB is to assume the free electron is in a Coulomb potential. In that case the free electron wave function depends only on the residual nuclear charge and the energy. This method had been coupled with hydrogenic wave functions for target states by Samson and co-workers [5,6]. This method is quite well suited for highly charged ions. In the method employed by Sampson the matrix elements used in calculating the cross sections scale with nuclear charge, so the results could be easily applied to an isoelectronic sequence. Large numbers of cross sections of reasonable accuracy were calculated using this method at a time when computational facilities were relatively primitive.

3.1.3 Distorted wave

The next logical approximation is to use the actual potential from the target state to solve for the free electron wave function. This is the distorted wave approximation (DWA), so-called because it introduces a distortion from the Coulomb function due to the target electron distribution. Distorted wave methods represent the best of the simple two state approaches.

There are several varieties of the DWA, depending on the details of the potential. For instance, in the standard distorted wave method as described in Mott and Massey [7], and as used by Mann [8], the potential for the incoming free electron uses the electron distribution of the initial state of the target, while the outgoing free electron is calculated using the potential derived from the final state of the target. An argument can be made that the collision takes place over some time and that it is actually better to use the same potential for both incoming and outgoing free electron. This is incorporated in the first order many body theory (FOMBT), as described by Csanak and Cartwright [9].

In addition to the direct part of the potential, there are a variety of methods to deal with part of the potential due to exchange. A number of possible approximations have been detailed by Riley and Truhlar [10].

A further approximation to the DWA has been made by Peek and Mann [11]. The main goal of this approximation, called the average approximation (AA) is to handle a rapidly fluctuating function resulting from the product of free and bound state wave functions. The AA gives a good approximation to the standard DWA for energies above about twice threshold and is not terribly inaccurate for energies approaching the threshold energy. A version of the AA, along with an atomic structure calculation is available on-line at the A+M Unit web page.

3.1.4 Close coupling

As mentioned at the start of this section, the actual solution of the excitation problem requires solving a complete set of coupled equations describing the bound and free electrons. Doubly excited states of the next lower ionization stage can be included in such a solution, which can give rise to reonances to the cross sections. These double excited states generally lie above the continuum and can autoionize to a singly excited state. As an example, consider the direct transition in C^{+4}:

$e + 1s^2 \rightarrow 1s2p + e'$

in configuration average notation, where e is an incoming free electron and e' is the outgoing electron, at lower energy. At certain discrete energies it is possible for the incoming electron to cause an excitation and simultaneously be captures in a high rydberg state. As an example, the following transition is possible:

$e + 1s^2 \rightarrow 1s3dnl$

where nl is a high-lying shell of the ion. The resulting doubly excited ion has the possibility to autoionize in the following manner:

$1s3dnl \rightarrow 1s2p + e'$

which means that the final state of the ion is the same as the direct excitation result. However, this enhancement is possible only for the energy which allows the capture of the free electron into the nl state while one 1s electron is excited to the 3d. Thus this gives a resonant enhancement to the direct cross section. You can easily see that there is the potential for a number of such resonances for differing values of nl. Furthermore, another set of resonances will arise from the 1s3snl configurations. In fact it is easy to see that the general configuration type $1snln'l'$ will give resonances to the direct transition.

Proper use of the close coupling techniques brings in the appropriate resonances automatically. The close coupling technique also correctly handles the effects of quantum interferences between all included states. Several different methods have been developed over the years to solve the close coupling equations, for example the R-matrix [12] and the convergent close coupling (CCC) theory [13]. In general, it takes considerable computing power to solve the equations, but the results are the best theoretical calculations of cross sections available.

3.2 Electron impact ionization

If the impact electron has sufficient energy, it can cause a bound electron to be knocked completely off the ion. This is the process of electron impact ionization. This process is more challenging to calculate due to the presence of two outgoing free electrons, which will share the total energy available, requiring a quadrature over the splitting of the outgoing energy distribution. As in the excitation processes, there are several levels of approximation, with the CCC method being the best, and the CCC method has been applied to electron impact ionization by Bray et. al. with very good results [13,14].

3.2.1 Lotz formula

A popular approximation formula for ionization cross sections is due to Lotz [15]. This formula is based on observation of a number of measurements of cross sections. A formula with the correct asymptotic high energy behavior was used to fit these data. A number of fit parameters have been published for application of the Lotz formula to a number of ions. In general the formula reproduces known cross sections well, but is not very reliable for extrapolation to new ion stages. However, in cases where no other data were available, the Lotz formula provided at least an estimate of the cross sections for ionization cross sections that were useful in CR models.

3.2.2 Scaled hydrogenic-Coulomb Born

The Coulomb Born theory using hydrogenic target functions used by Sampson and colleagues for excitation has also been applied to ionization with adequate success. Detailed calculations have been made for ionization of nl shells of hydrogenic ions for nl ranging from 1s to 6h [16,17,18,19,20]. Using some approximations, it is also possible to use these hydrogenic results for complex ions, and with inclusion of angular factors and mixing coefficients for the target states, to give approximate cross sections for fine structure levels in complex ions. In most cases the results are of reasonable accuracy. The major errors occur for targets that are most different from hydrogenic target states, mainly for nearly filled shells, such as a neon like ion with the shell structure of $1s^2 2s^2 2p^6$. The method also encounters difficulties for energies near threshold.

This cross section method is based on the reduced hydrogenic cross sections developed by Sampson and colleagues. The relationship between the hydrogenic cross section and the reduced hydrogenic cross section is:

$$Q_{nl}^{HR}(u) = \left(\frac{Z}{n}\right)^4 \frac{Q_{nl}^{H}(u)}{\pi a_0^2}$$

where HR is the reduced hydrogenic, u is the impact electron energy in threshold units, Z is the nuclear charge and a_0 is the Bohr radius. Sampson and colleagues calculated a number of the reduced cross sections and applied the results to complex ions. They did this by noting that for an outer electron in a complex ion, the nuclear charge is screened by the inner electrons. Thus, the outer electron "sees" an effective nuclear charge, Z_{eff}. Using this, along with the number of electrons in a shell, r_{nl}, the result for a complex ion is:

$$Q(u) = \pi a_0^2 \left(\frac{n}{Z_{eff}} \right)^4 r_{nl} Q_{nl}^{HR}(u)$$

One further modification has been made to the above formula. It is noted that for a hydrogenic ion the ionization energy on rydbergs is:

$$E^I = \left(\frac{Z}{n} \right)^2$$

It is then assumed that a good approximation to the effective nuclear charge is the one that satisfies this equation for the calculated or observed ionization energy of a complex ion. This results in the prescription for the cross section in terms of the reduced hydrogenic cross section as:

$$Q(u) = \frac{\pi a_0^2}{\left(E^I\right)^2} r_{nl} Q_{nl}^{HR}(u)$$

where E^I is in rydberg units.

By examining the large number of reduced hydrogenic cross sections it was possible to formulate a general fit to those cross sections as a function of impact energy and shell [21]. The result is:

$$Q_{nl}^{HR}(u)=\frac{1}{u}\left[\left(C_1+\frac{C_2+C_3 l}{n}\right)\ln(u)+\left(C_4+\frac{C_5+C_6 l}{n}\right)\left(1-\frac{1}{u}\right)+\left(C_7+\frac{C_8+C_9 l}{n}\right)\left(1-\frac{1}{u}\right)^2\right]$$

A least squares fit over reduced hydrogenic cross sections from the 1s to 6h shells and for impact electron energies from 1.125 to 6 times threshold reproduced the cross sections with an average error of 2.5% and a maximum error of 10%. These fit parameters are shown in the table. This formula can thus be used to give an estimate for the electron impact ionization cross section for any complex ion with the only required data being the ionization energy.

Coefficients for calculating Reduced Hydrogenic Cross Sections

Coefficient	Value
C_1	1.5369
C_2	0.99656
C_3	-0.61916
C_4	2.4463
C_5	-2.4773
C_6	3.2151
C_7	-1.4512
C_8	1.7230
C_9	-0.47075

3.2.3 Distorted wave

The same basic distorted wave method from excitation can be applied in a straightforward way to ionization. As noted above the presence of two outgoing electrons means that calculations must be done on several different splits of the energy between the two and a quadrature performed. However, this generally is not extremely difficult and the resulting cross sections are reasonably accurate, except for neutral atoms and near threshold energy.

3.2.4 Close coupling

The CCC method has been applied to ionization with quite good success by Fursa and Bray [13, 14]. The results of this method represent the best theoretical calculations of electron impact ionization to date. Note that as in excitation it is also possible to have resonances to the ionization processes and that the close coupling methods will include these automatically.

3.3 Photoionization

The process of photoionization is the absorption of a photon by an ion with the energy going to removal of an electron from the ion. In plasmas typical of current fusion devices, the plasma is optically thin and direct photoionization is not a factor in the CR model. However, the photoionization cross sections are still needed for the important inverse process of radiative recombination. As mentioned earlier, for an LTE plasma each process will be exactly balanced by the inverse process and the cross sections for radiative recombination can be obtained form the photoionization cross section. This is important because the radiative recombination is often the dominant recombination mechanism. This due to the low electron density in fusion devices. The inverse process of electron impact ionization, three body recombination, depends strongly on the electron density and at the densities typical of fusion devices, this mechanism can be ignored. Thus, the main recombination process is often radiative recombination. Therefore, in order to carry out a successful CR calculation for a fusion plasma photoionization cross sections are needed. These are readily obtained using a radial dipole calculation with the initial target function and the ion with a free electron determined from the potential. Photoionization cross sections can be calculated from Cowan's atomic structure code [1, 22].

3.4 Autoionization

As noted in the discussion of close coupling, it is possible for an ion to be in a doubly excited state with sufficient energy to ionise; this is the process called autoionization. The inverse process of the capture of an electron into a doubly excited state is called di-electronic recombination (DR). Often there is a close balance between the two processes with a net result that the overall effect on the ionization balance is small. However, in many ionization stages it is possible for the DR to be large and to even be the main method of recombining. Therefore it is necessary to include these processes in a CR calculation.

As with photoionization, autoionization cross sections can also be obtained from Cowan's [1] code. However, a newer multipurpose code has also been developed at Los Alamos to handle electron impact ionization, photoionization and autoionization for all transitions between two adjacent ions. This code uses input from a modified version of Cowan's structure code. A general purpose code for calculation of DWA excitation cross sections has also been written. The Atomic and Optical physics group in the Los Alamos National Lab has collaborated with the A+M Unit to make these codes available through a web interface. A link to the interface can be found on the A+M home page.

4. Collisional radiative modelling

We are now in a position to look into solving the CR model. In general, the solution to the CR model will give the populations of each level of each stage of ionization of the element in question. In addition it is possible from the populations and the data for radiative processes to calculate the total radiated power from the plasma. If desired, it is also possible to construct a detailed synthetic spectrum for emission from the plasma, i.e. radiation versus wavelength. This is what is generally meant by solving the CR model.

4.1 The equations

We now need to specify the equations that must be solved in the CR model. There are two cases, time dependent and steady state. The time evolution of the population is [23]:

$$\frac{dN_{i\,j}}{dt} = \sum_k R^I_{i-1_{k-j}} N_{i-1_k} - \sum_k R^I_{i_{j-k}} N_{i_j} + \sum_k R^R_{i+1_{k-j}} N_{i+1_k} - \sum_k R^R_{i_{j-k}} N_{i_j}$$

where the R’s represent rate coefficients, the superscript I represents ionization, the superscript R represents recombination, and the subscript represents ion stage and level. In effect this says that the change in an ion stage is due to ionisations and recombinations into and out of the stage in question. The R values are determined by integrating the cross sections over an electron velocity distribution to form a rate coefficient:

$$R = \int F(E,T)v(E)\sigma(E)dE$$

where F(E,T) is the electron distribution, normally a Maxwellian, v(E) is the velocity of the electron and σ is the cross section.

Normally, the plasma in a fusion device has time to reach a steady state, meaning that the populations of the ion stages are constant with time. This is the condition that:

$$\frac{dN_i}{dt} = 0$$

which can easily be seen to lead to the relation:

$$\frac{N_i}{N_{i-1}} = \frac{R_i^R}{R_i^I}$$

This relates each ion stage population to the adjacent ion stage. The condition that the sum of the ion stages must equal the total number of ions is then sufficient to determine the populations of all the ion stages, provided that all of the rate coefficients are known. Thus it is seen why the databases are essential to solution of the CR calculation.

It should be emphasized that in carrying out a CR model calculation there are several requirements of a database.

First, the database should be consistent. This means that the entries to the database should share a common set of energy level labels, and cross sections for all processes should be related to those energy levels. This is often a problem in attempting to use cross sections from several different sources in building a model. Different sources will have used different methods of arriving at energy levels, even employing different labelling schemes. Furthermore, some calculations will include resonance effects, while others may not. In addition, it is possible for a CR model to follow doubly excited states explicitly. This can cause a problem if some cross sections include resonances, as this is bringing in the effect of those states independently.

Second, the database for a CR model needs to be as complete as possible. It is often preferable to have a complete set of processes calculated with a relatively simple approximation rather than a small set of processes calculated with the best theory available.

Finally, the database should be as accurate as possible. This is of highest importance for plasmas that are not in LTE, such as fusion plasmas. As noted previously, for LTE plasmas the actual rate coefficients do not matter, because of the balance between each process and its inverse. However, for non-LTE plasmas the accuracy is important because that balance does not exist. Thus, one process may populate an excited level and a completely different process may depopulate that level. If either rate coefficient is in error, the resulting calculation of populations will be in error.

4.2 Special cases

4.2.1 Coronal limit

As mentioned previously, for low density plasmas, the excited states will decay before interacting with the plasma, so that all of the ion stages will be in the ground state. In that case, the populations of the excited states do not need to be calculated at all. It is assumed that every excited state results in radiation and there are no excited to excited state transitions. As noted above, this is not the case in most fusion research machines, so will not be pursued here, except to point out that this can serve as a check on a full CR calculation. Since the coronal model is easily solved, it can be compared to the results from a full CR calculation at progressively lower densities. At some density the two methods should approach very closely in all respects. If they do not, this usually indicates an error in the full CR model.

4.2.2 Local Thermodynamic Equilibrium (LTE)

As mentioned earlier, as the density increases, the populations of all levels will be determined solely by the energy levels and statistical weights. This occurs at much higher densities than found in fusion research devices, but again this limit is a good test of a full CR code. The LTE populations are easily determined and can be directly compared to the full CR model run at progressively higher densities. If the full CR model does not approach the LTE result, this indicates a problem with the CR model. Thus, there are very tight checks on both low and high density limits for the CR model.

4.2.3 Time dependent calculations

In the general case, it may be necessary to carry out the integration over time of the general CR equations. In that case the full set of equations for the description of the change of each level population must be integrated over time. This can be a very lengthy problem computationally. In many applications this is not necessary, as the plasma is mostly in a steady state, so that the change in population with respect to time is zero.

4.2.4 Effective rate coefficients

It is possible to carry out the solution of a CR model on a grid of temperature and density and to save certain aspects of the solution. It is then possible to reconstruct the solution with appropriate interpolation within the temperature and density grids. The main parameters to be stored are effective rate coefficients, ion stage populations, and radiation per ion stage. If spectral data are desired, it is also possible to store an output spectrum from each ion stage.

In the steady state case it is readily shown that the populations of the ion stages can be found by simply interpolating on the stored populations. Thus, it is not necessary to solve any rate equation at all in the steady state case, if the populations have been saved on reasonable density and temperature grids. Furthermore, it can also be shown that the total radiated power can also be interpolated from the stored quantities. It is also possible to obtain the spectra from the stored spectrum per ion multiplied by the ion stage population. It is not necessary to save any populations for specific energy levels, nor is it necessary to solve any rate equations at all. Thus, once a number of steady state solutions have been generated for a particular element over a range of temperature and density, the solution for any point within the grids can be found with only trivial computational effort.

In the case of a time dependent situation, it is also possible to make use of data from the steady state solution. The important data are effective rates for ionization and recombination from each ion stage. The main difficulty in solving the time dependent case is the solution of the rate equations for a very large number of levels. In many cases there may be thousands of important energy levels in each ion stage. This makes solving the time dependent equations quite computationally intensive. However, it is possible to sum all of the rates for ionization for one ion stage and to derive an effective ionization rate coefficient for that ion stage. In a similar way an effective recombination rate coefficient can be obtained. In order to solve a time dependent case, it is then only necessary to use two effective rate coefficients for each ion stage. The resulting CR model is very easily solved. There are, however, some inaccuracies. The effective rate coefficients are determined from the steady state solution, not from the actual time dependent solution, so the initial conditions of the true problem are not matched. This will cause the very short time behaviour of the solution to be inaccurate. However, in a short time, the approximate solution will closely approximate the correct behaviour of the plasma. For example, the case of a neutral atom injected into a hot plasma will show initial ion stages that are not correct. However, the calculation of the time required for the injected material to reach equilibrium with the plasma will be quite good and for most of the time the details of the behaviour will be acceptable. Therefore, it has been found useful to use the stored effective rate coefficients to give estimates of the behaviour of a time dependent plasma.

During the course of a Co-ordinated Research Project (CRP) at the IAEA, some large scale models for several elements of interest to fusion were developed at the Los Alamos National Laboratory. Atomic structure calculations were carried out for approximately 1000 configurations for each ion stage. PWB cross sections were calculated for all possible transitions. FOMBT cross sections were calculated for all transitions from the ground and lowest excited states. Electron impact ionization calculations using the scaled hydrogenic method were carried out from each configuration of each ion stage. Autoionization cross sections were calculated. The resulting data sets were used to solve the CR equations for a temperature range of 1 to 100000 eV for densities of 10^{13} to 10^{16} per cc. The populations of all levels of all ion stages were determined as well as the total radiated power from the plasma. Results were reported in the APID series of the IAEA [24,25,26]. These results along with the rate coefficients have been stored on the IAEA web server. This provides the capability to determine the populations of ion stages, as well as the radiated power for any of five elements at arbitrary temperature and density within those ranges. In addition it is possible to use the effective rate coefficients to carry out a time dependent calculation on fusion relevant plasmas.

5. Data on the Internet

There are a number of databases on the Internet. There are a variety of types of data. The main categories are numerical and bibliographic.

Often it is useful to locate a reference to a particular type of data so that all details of the data generation can be found. There are bibliographic databases in several locations, such as the IAEA, NIFS in Japan, GAPHYOR in France, and Oak Ridge and NIST in the USA.

There are also a number of numerical databases on-line. There are several with data for radiative processes, such as NIST, the Opacity Project, and others. For electron impact collisions the main sources are the IAEA and NIFS. In addition to these on-line numerical databases, there are collections of data on the Internet, which may be useful, but are not easily searchable.

To facilitate the search for data on the Internet two search engines are under development, GENIE for numerical data and DANSE for bibliographic data. These search engines have been developed by Y. Ralchenko and D. Humbert.

In addition to the search engines there is now the possibility to run a calculation of atomic structure and electron impact cross sections using the average approximation. This is available through the IAEA A+M Unit home page. A similar capability has been developed at the Los Alamos National Laboratory which gives access to the fine structure atomic structure calculations, ionization cross sections, and distorted wave excitation cross sections. A similar interface has also been developed for calculations of ion-ion cross section calculations.

References:

1. R.D. Cowan, *Theory of Atomic Spectra*, (University of California Press, Berkely), 1991.
2. C.F. Froese-Fischer, *Computational Atomic Structure: An MCHF Approach*, (Lund University, Sweden), 1997.
3. I.P. Grant, *Relativistic Atomic Structure Theory* in *Methods in Computational Molecular Physics*, (Plenum, New York), 1992.
4. R.E.H. Clark and L.A. Collins, Los Alamos Report LA-10192-MS, *Plane-Wave Born Collision Strengths for Electron-Ion Excitation: Comparison with Other Theoretical Methods*, 1984.
5. D.H. Sampson, Ap. J. Suppl., **28**, 309, (1974).
6. R.E.H. Clark, D.H. Sampson and S.J. Goett, Ap. J. Suppl., **49**,545 (1982).
7. H.F. Mott and H.S. Massey, *Theory of Atomic Collisions*, (3rd edition, Oxford University Press, London), 1965.
8. J.B. Mann, At. Nuc. Data Tables, **29**, 497 (1983).
9. D.C. Cartwright and G. Csanak, Phys. Rev. A, **51**, 454 (1995).
10. M.E. Riley and D.G. Truhlar, J. Chem. Phys., **63**, 2182 (1975).
11. J.M. Peek and J.B. Mann, Phys. Rev. A, **16**, 2315 (1977)
12. K.A. Berrington and C.P. Balance, J. Phys. B, **35**, 2275 (2002).
13. D.V. Fursa and I. Bray, Phys. Rev. A, **52**, 1279 (1995).
14. I. Bray, D.V. Fursa, A.S. Kheifets, and A.T. Stelbovics, J. Phys. B, **35**, R117 (2002).
15. W. Lotz, Z. Phys., **232**, 101 (1970).

16. L.B. Golden and D.H. Sampson, J. Phys. B, **10**, 2229 (1977).

17. L.B. Golden, D.H. Sampson and K. Omidvar, J. Phys. B, **11**, 3235 (1978).

18. D.L. Moores, L.B. Golden and D.H. Sampson, J. Phys. B, **13**, 385 (1980)

19. L.B. Golden and D.H. Sampson, J. Phys. B,**13**, 2656 (1980)

20. R.E.H. Clark and D.H. Sampson, J. Phys. B, **17**, 3311 (1984).

21. R.E.H. Clark, J. Abdallah and J.B. Mann, Ap. J., **381**, 597 (1991).

22. R.E.H. Clark, R.D. Cowan, and F.W. Bobrowicz, At. Data Nuc. Data Tables, **34**, 415 (1986).

23. J. Abdallah and R.E.H. Clark, Los Alamos Manual No. LA-11926 (1990).

24. R.E.H. Clark and J. Abdallah, APID, **11**, 1 (2003).

25. J. Abdallah and R.E.H. Clark, APID, **11**, 21 (2003).

26. R.E.H. Clark, J. Abdallah and C.J. Fontes, APID, **11**, 49 (2003).

Atomic structure exercises

1. Go to the A+M Unit home page at the URL:
http://www-amdis.iaea.org/
Click on the label:
LANL Codes
Use the codes to find the configuration energies for the configurations $2s^2$ and 2s2p in C^{+4}. Find the first few energy levels for He-like xenon. Compare the radial distances at which the 1s orbitals reach their maxima in these two cases.

2. What is the approximate energy of the 1s3p configuration of C^{+4} (using the LANL codes) relative to the ground level? How about the 1s4p? The 1s10p? What appears to be the series limit? What does this limit represent? Does it appear reasonable (use hydrogenic theory with screening)? To confirm this use the ionization feature of the LANL codes.

3. Run the code in configuration mode for ionization of C^{+4} and observe the ionization energy for the $1s^2$ shell. How does this compare to the Koopman theory result (use the interface to find the shell energies)? Do the same for Fe $^{+24}$. Does it appear that the Koopman theory is a good approximation? Now try the same test for neutral argon and look at ionization from the $3p^6$ shell. How does the koopman theory work now? Why is this?

4. Run the configuration mode for ionization of the C^{+4} case and observe the ionization energy. Now use the idea of hydrogenic ionization energy and assume that each 1s electron completely screens the other. What is the result of the hydrogenic theory? Now assume that two electrons in the same shell are only ½ effective in screening. Does this improve the calculated ionization energy? Repeat for several different ions.

5. Run the codes in fine structure mode for C^{+2} with the $2s^2$ and 2s2p configurations (you have done this in configuration mode for exercise 1). How do the energies of the fine structure levels compare to the configuration average energy? Now do a similar comparison for Fe^{+22} and compare. How do the results for Be-like iron differ from the carbon?

6. For Si^{+4} find the approximate energy for ionization in configuration mode. Now find the energy of the 1s1 2s2 2p6 3p1 configuration relative to the ground level. What do you conclude about this configuration? Now find the energy of the 1s2 2s1 2p6 3p1 configuration. What do you conclude about this configuration? Now look at the fine structure levels. Now do the same comparisons for Ar^{+8}. What differences do you see?

7. Run a fine structure calculation for C^{+2} with only the $2s^2$ and 2s2p configurations. Look at the mixing of the 2s2p $^3P_1$ fine structure level. Now go back and include the 2s3p configuration and check the 2s2p $^3P_1$ fine structure level mixing again. What do you see? Now repeat the same but for the Fe^{+22} ion. How does the mixing differ? Now include the 2p3s configuration and see how this affects the mixing. Try adding other configurations to see if there is any other significant change to this level.

Excitation cross section exercises

1. Go to the Unit home page and click on the AAEXCITE for the Average Approximation. Calculate cross sections for C^{+4} from the $1s^2$ ground configuration to all nl with $2s \leq nl \leq 4f$. Note which transition is the largest overall and which is the smallest. For the largest and smallest, run the LANL codes in configuration mode and compare the results to the AA results.

2. Find cross sections for the $1s^2 \rightarrow 1s2p\ ^1P$ transition in C^{+4} from the NIFS database. How many entries are there? Find entries for the same transition in the ALADDIN database. How do the results from different authors compare?

3. Run the LANL codes on the $1s^2 \rightarrow 1s2p\ ^1P$ transition (note than only J=1 is possible for this case) in C^{+4} and compare to the results found in exercise 2. How do the LANL results compare to the others. You may convert from cross section or collision strength to rate coefficient in the interface.

4. Run the AA calculation for the configuration mode for the $1s^2 \rightarrow 1s2p$ transition in C^{+4}. To compare to the LANL results, you will need to also run the $1s^2 \rightarrow 1s2p\ ^3P_J$ transitions where $1 \leq J \leq 3$.

5. Compare the relative cross sections for $1s^2 \rightarrow 1s2p\ ^1P_1$ to those for $1s^2 \rightarrow 1s2p\ ^3P_1$ in C^{+4}. What happens to the spin forbidden cross section at high energy? Make the comparison for the same transition in Fe^{+24}. It is instructive to view the rate coefficient.

Ionization exercises

1. From earlier exercises you know the ionization potential for C^{+4}. Use this in the formula for scaled hydrogenic cross sections to find the electron impact ionization cross section at several energy points. Go to the NIFS database and find other tabulated cross sections and compare to the result from the scaled hydrogenic method.

2. The LANL codes include the scaled hydrogenic method as well as distorted wave and binary encounter. Make a comparison of all three methods for the case given in exercise 1. How do the more approximate methods compare to the distorted wave?

3. Now make a comparison for electron impact ionization using the same three methods for the neutral argon case. How do the methods compare for this case?

4. Set up an ionization case in configuration mode for C^{+2}. For the initial ion include the configurations $2s^2$ and $3s^2$. For the C^{+3} ion include the $2s^1$ and $2p^1$ configurations. Observe the energies of the C^{+2} ion. Continue through the calculation to the results page. After the electron impact ionization and photoionization cross sections you should find autoionizations. Observe that it is possible to autoionize from the $3s^2$ configuration of C^{+2} to the $2p^1$ configuration of the C^{+3} ion with outgoing electron energy of 10.018 eV, and to the $2s^1$ configuration with an energy of 18.03 eV. Consider the inverse process of the latter, describe the process and the final state. From the calculation you have run, what is a possible end result of this state? This is

the basic idea of a resonance to an excitation. Consider other possible configurations that could give rise to reonances.

Collisional-radiative exercises

1. Go to the Rates page from the A+M Hime page. Suppose it is desired to use an inert gas in the divertor region of a fusion machine to radiate power. The temperature is 10 eV and the electron density is 10^{14} per cc. Does neon or argon make the more efficient radiator under these conditions? How about for a temperature of 40 eV? Suppose that the gas diffuses into the core of the plasma at a temperature of 5000 eV? Which element will be more of a problem?

2. Neutral argon is injected into a plasma with a temperature of 200 eV and electron density of 10^{14} per cc. Find the approximate time for the argon to reach equilibrium with the plasma. Find the time if the electron density is 10^{13}.

3. A full stripped ion of iron migrates to a plasma region with electron temperature of 20 eV and electron density of 10^{15}. How long does it take for the ion to equilibrate and what is its final average charge state? How about for an electron density of ^{13}?

4. At what temperature does Ti have its maximum radiated power for an electron density of 10^{13}?

5. How does the radiated power from iron at electron temperature of 5000 eV and electron density of 10^{13} compare to an electron density of 10^{16}? Do the same comparison for neon.

6. Go to the interface for data sensitivity for CR models:

http://www-amdis.iaea.org/DATASENS/

and start with Be. For this element, confine electron temperatures to the range of 1 to 100 eV. Run a base calculation. View the output generated. Now try varying the input data by factors up to a factor of 10, in both random and non-random fashion. Repeat for Ar, but remember to reset the temperature range to 500 to 5000 eV.