CHIANTI

An Astrophysical Database for Emission Line Spectroscopy

CHIANTI TECHNICAL REPORT for version 11

Advanced Models for Higher Density Plasma

Ver. 1.0, 15-Mar-2024, Roger Dufresne

1 Outline of the concepts

One principal assumption within CHIANTI from the beginning has been that the plasma is in ionization equilibrium, and the ion abundances have been pre-calculated assuming the so-called 'coronal approximation' (e.g. Eq. 24 of Del Zanna & Mason, 2018). This assumes that, for ionization and recombination purposes, atoms and ions are entirely populated in their ground state. Many of the other key assumptions in the coronal approximation are suitable only for high temperature, low density plasma; however, even at typical electron densities of the quiet-Sun corona some of the assumptions break down. The problem is magnified further in the higher density transition region (TR).

Various effects have been invoked in the atomic modelling over the years to improve the agreement between observations and theory for the TR. Atomic energy levels which have no rapid, dipole-allowed decays to lower energy levels can become significantly populated in certain conditions. For instance, in high electron densities they become populated through the balance of collisional excitation and de-excitation. Such energy levels are denoted as metastable levels. Rate coefficients for collisional ionization (CI) from metastable levels are generally larger than those from the ground level in the same ion because metastable levels are closer to the continuum. The overall ionization rate coefficient out of the ion is the sum of the total ionization rate coefficient from each initial level weighted by the relative population of the level. When metastable levels become populated in higher density plasma the overall ionization rate coefficient is higher than in a low density plasma. This causes the ions to form at lower temperature (Nussbaumer & Storey, 1975). The coronal approximation only includes ionization from the ground level, and cannot take account of this effect. Similarly, since metastable levels are further away in energy from levels in the next lower charge state than the ground level, rate coefficients for radiative recombination (RR) and dielectronic recombination (DR) are generally smaller for metastable levels than the ground. This produces an additional shift to lower temperatures when metastable levels become populated compared to the coronal approximation.

DR mostly goes through highly excited, Rydberg levels close to the continuum. In higher density plasma these levels are rapidly ionized by free electrons before decays to lower levels take place. The effects are not easy to calculate, as they require complex collisional-radiative models and a large number of rates which are not easy to calculate accurately. Simple hydrogenic models with very approximate atomic rates were developed by Burgess & Summers (1969, 1976). Following this, the tables of the resulting effective recombination rates obtained by Summers (1974) have been used by various authors (Jordan, 1969; Vernazza & Raymond, 1979; Judge et al., 1995) to approximate DR suppression. In a recent version of CHIANTI (v10, Del Zanna et al., 2021) the Nikolić et al. (2018) approximation to reproduce the suppression seen in the Summers (1974) rates was introduced. We use the Nikolić et al. (2018) approximation in the present advanced models to reduce the DR rates for both the ground and metastable levels. Although the same ionization and recombination rates are being used for the present models as Dufresne et al. (2021a,b), there are some differences in the ion balances because the earlier works use DR suppression factors taken from the Summers (1974) tables.

Another physical effect that changes significantly the ion balance for some ions in the chromosphere and TR is charge transfer (CT) during collisions with the most abundant species: hydrogen and helium. Charge transfer is the exchange of an electron that takes place between two colliders during atom-ion or ion-ion collisions. The process is variously known as charge transfer, charge exchange and electron capture. Baliunas & Butler (1980) demonstrated that silicon is strongly affected in

the solar atmosphere, but it was only relatively recently that more accurate, quantum-mechanical calculations became available, many of which included rates for metastable levels. Earlier calculations used the rather approximate Landau-Zener method, but its assumptions are more suitable for higher collision energies (Bates & McCarroll, 1962). The CT rate also depends on the number density in the plasma of the relevant perturber, atomic or ionized hydrogen or helium in this case, and its ion fractions. Self-consistent calculations of these values are not feasible and they are usually taken from model atmosphere calculations.

2 Methods used in the advanced models

2.1 Collisional ionization

Collisional ionization rates for ground and metastable states of carbon and oxygen were calculated in Dufresne & Del Zanna (2019) and Dufresne et al. (2020), respectively. Flexible Atomic Code (FAC, Gu, 2008) was used for direct collisional ionization and Autostructure (Badnell, 2011) for excitation–auto-ionization (EA, or indirect collisional ionization). The cross sections were benchmarked against many of the same experiments as Dere (2007), whose ground-level CI rates have been used in CHIANTI for the default ion balances until now.

To provide a consistent set of rates for the advanced models, the rate coefficients from Dufresne & Del Zanna (2019) and Dufresne et al. (2020) are used for ground and metastable levels of carbon and oxygen, with one exception. Comparison of the ion balances from Dufresne & Del Zanna (2019) and the default in CHIANTI for C II shows a significant difference at low density. This arises from the ground level ionization cross section, which is 25% higher than experiment in Dufresne & Del Zanna (2019). For this level, CHIANTI uses the Dere (2007) cross section, which for this level was matched with the experiment of Yamada et al. (1989). Consequently, we retain the Dere (2007) cross sections for the ground level and incorporate the Dufresne & Del Zanna (2019) cross sections for the metastable levels, which were in good agreement with the R-Matrix calculation of Ludlow et al. (2008).

For other ions included in the advanced models the same method is used as Dufresne et al. (2021b). The rate coefficients of Dere (2007) are used for the ground levels. To estimate rates for metastable levels, the Burgess & Chidichimo (1983) CI approximation for low charge ions is used to calculate the ratio of the metastable to ground rate coefficients. The Dere (2007) rate coefficients are multiplied by this ratio to estimate those for the metastable levels. This is an equivalent way of estimating the constant C in the Burgess and Chidichimo formula.

The ionization potentials required by the Burgess & Chidichimo (1983) approximation are taken from experimental values stored in CHIANTI for each ion. Dufresne et al. (2021b) compared the oxygen ion balance obtained using this approximation with that using *ab initio* CI rate coefficients; differences in the ion balance were negligible. The effective number of electrons in each isoelectronic sequence, required by the Burgess & Chidichimo (1983) formulation, have been fixed in an array within the present programs. The present implementation could be improved because currently it uses the number of equivalent electrons for the ground level, but some metastable levels have a different number of equivalent electrons. A more accurate method is found in the thesis by Dickson (1993[1]), which additionally calculates rates resolved by final level using coefficients of fractional

[1] https://www.adas.ac.uk/theses/dickson_thesis.pdf

parentage.

2.2 Recombination involving free electrons

We use the RR rate coefficients calculated by Badnell (2006). The DR rate coefficients for ground and metastable levels have so far been calculated for all ions of hydrogen to zinc in the H-like to P-like isoelectronic sequences by the DR Project (see Badnell et al., 2003, for the first paper in the series). Rate coefficients were calculated for all ground and metastable levels up to the first dipole allowed transition in the ion. Previous versions of CHIANTI only included the RR and DR rate coefficients for ground levels, using the fitting coefficients made available by N.R. Badnell[2]. We now include in CHIANTI the RR and DR rates for metastable levels using the same set of data. Rate coefficients were calculated to final resolved states at zero density in those works; here, we use total rate coefficients resolved by initial level to the next lower charge state.

In a recent version of CHIANTI (v10, Del Zanna et al., 2021) the Nikolić et al. (2018) approximation to reproduce the suppression seen in the Summers (1974) rates was introduced. We use the Nikolić et al. (2018) approximation in the present advanced models to reduce the DR rates for both the ground and metastable levels. Although the same ionization and recombination rates are being used for the present models as Dufresne et al. (2021a,b), there are some differences in the ion balances because the earlier works use DR suppression factors taken from the Summers (1974) tables. The Nikolić et al. approximation is used because it is significantly slower to interpolate the Summers data in both temperature and density to obtain suppression factors for the models. Comparisons of different ionisation equilibria showed that it is more important to have an estimate of DR suppression than ignore it altogether. Differences between the two methods has only been assessed for elements in the advanced models and it is not switched on for other cases. The user can include it for all elements using the '`dr_suppression`' keyword, if desired.

2.3 Charge transfer and associated model atmospheres

Dufresne et al. (2021a,b) made a comparison of all CT cross sections available for the low charge ions of the elements being modelled. The preference was given for results from more accurate methods and those which included metastable levels. Rate coefficients were calculated from the cross sections if not published in the original articles. All except one calculation was in LS-coupling and rate coefficients were split according to statistical weights of the initial levels in each term; ground and metastable levels are populated in these ratios for all the ions under consideration in the solar TR. Double electron capture is also possible and was included in the earlier models, but the ion balances were not affected by this and it has been neglected in CHIANTI.

The CT rate also depends on the number density in the plasma of the relevant perturber, atomic or ionized hydrogen or helium in this case, and its ion fractions. Self-consistent calculations of these values are not feasible and they are usually taken from model atmosphere calculations. The relevant number densities from the model atmospheres are interpolated in temperature over the temperature grid required for the ion balance. Model atmospheric data can be tabulated and read in for the calculation. A number of files have been prepared for the present version, including those of Avrett & Loeser (2008) and Fontenla et al. (2014); data from the latter includes the quiet Sun,

[2]http://apap-network.org/

an active region, plage and facula. The files are located in the '`ancillary_data/advanced_models`' directory of the CHIANTI database.

2.4 Solving the ion balances

One of the main differences here compared to the earlier TR models is the solution of the ion balances. The earlier models included in one large matrix all the level-resolved rates (except RR and DR) between neighbouring charge states, plus all the rates required within each ion. The matrix was then inverted to find the populations of all the levels of all the charge states at once. We adopt here a simplified, faster method.

In Dufresne et al. (2021a) the level populations were solved using models in which CI and CT were fully level-resolved. In densities typical of the solar TR, they found that the level populations were all within 2% of the level populations from the CHIANTI independent atom model, except one level in O II which had a difference of 7%. This is because, for the main lines under consideration in the advanced models, collision rates between levels in an ion are much faster than processes connecting ions. It means in these conditions total CI and CT rates can be used, that is, rates which are resolved only by initial level and not final level. (Dufresne et al. 2021a and the other related models used total RR and DR rates. Level populations can be affected by level-resolved RR and DR, but such models are too large and complex to be included in the CHIANTI models. The issues associated with such models can be found in Del Zanna et al. 2020, for example.)

These conditions allow the independent atom model already implemented in CHIANTI to be exploited. The level populations within each ion are calculated first to find the ground and metastable populations. From these, overall ionization and recombination rates out of the ion can be calculated. For example, if S_i is the ionization rate from level i, which has a fractional population n_i, then the overall ionization rate out of the ion is

$$S \; = \; \sum_i \; n_i S_i \; , \tag{1}$$

where the sum is over all metastable levels. This replaces S_g, the total ionization rate from the ground level, used to solve the coronal-approximation ion balance.

For neutrals, the CHIANTI routine '`metastable_levels`' is used to define the levels for which ionization data is included. In the routine, metastable levels are defined as those levels for which there is no decay rate above $10^5\,\mathrm{s}^{-1}$. For ions, however, the only metastable levels included in the overall rates are those for which recombination data has been calculated, (see the section on recombination data above for the criteria). The ions included in the advanced models are given in a new master list. For all other ions it is assumed, as previously, that the population is in the ground state for ionization and recombination purposes, and there is no suppression of DR rates with density.

Once the overall rates are calculated, the same method previously used in CHIANTI to calculate the ion populations is used. Essentially, the ratio of the populations of two successive charge states is proportional to the ratio of the ionization/recombination rates. We have verified that the large matrix approach and the independent atom model produce the same ion abundances, within a fraction of a percent. The ion charge states can be both calculated on-the-fly and stored in CHIANTI-format files for later use. The IDL software has been modified to calculate the advanced

ion models by default, and a program has been provided to compare different ionization equilibria. More details are provided below and in the software notes.

3 Description of the routines

3.1 The main routine

The main new code is called '`ch_calc_ioneq`' and is used to calculate the ion charge states for any choice of temperatures and either a fixed density or pressure. Alternatively, a grid of temperatures and related densities can be imported from a file. The advanced models are switched on by default using the keyword '`advanced_model`', but can be switched off. Charge transfer is switched off by default and can be switched on by using the keyword '`ct`'. It is strongly advised that CT is switched on when modelling any TR ions of Si. Examples of calling the routine are

```
IDL> data=ch_calc_ioneq(dens=1.e10,/adv,ele='C')
IDL> iontemp=10.^(findgen(61)*0.05+3.5)
IDL> data=ch_calc_ioneq(iontemp, pressure=3e14,/adv, ele=['C','N','O'])
IDL> data=ch_calc_ioneq(iontemp, dens=1.e10,/adv,/ct,$
IDL>   out='all_ions_ne=1e10.ioneq')
IDL> data=ch_calc_ioneq(outname='all_ions_zero_density.ioneq')
```

3.2 Retrieving global parameters

A subroutine called '`ch_adv_model_setup`' is called to import the various parameters used throughout the calculation. Primarily it reads the recombination fitting coefficients, the list of ions included in the advanced models, and the number of levels included in the level population solution. (The latter two are contained in a new file called '`advmodel_list.ions`'.)

It optionally obtains the model atmosphere parameters required for the charge transfer (CT) calculation. ATM_PARAMS provides as an input the model atmosphere file, which contains the temperature, density, pressure, total hydrogen density, H and optionally He ion fractions. If He fractions are not provided, it obtains these from the default CHIANTI ion fraction file. Data for a few model atmospheres have been made available for the convenience of the user. If He abundance is not provided relative to H, it obtains this from the default abundance file. The routine then interpolates the parameters over the temperature grid used as an input, which is the grid used for the ion balance calculation. Because the interpolation of the rates for the ion balance calculation is over temperature, the model atmosphere parameters will be truncated below and above any temperature minimum and maximum in the file.

```
IDL> temp=10.^(findgen(61)*0.05+3.5)
IDL> params=ch_adv_model_setup(temp)
IDL> params=ch_adv_model_setup(temp,/ct,atm=!xuvtop+ $
IDL>   '/ancillary_data/advanced_models/model_atmospheres/avrett_atmosphere.dat')
```

3.3 Retrieving the atomic rates

From this point, the ionization and recombination rates are loaded for each ion using the routine '`ch_adv_model_rates`'. If available, level-resolved, direct and indirect ionization rate coefficients are stored in files ending '`.dilvl`' and '`.ealvl`', respectively, while CT ionization and recombination rate coefficients are stored in files with suffixes '`.ctilvl`' and '`.ctrlvl`', respectively. The rates for the individual atomic processes are retrieved using the routine '`ch_ioniz_rate_lr`', which reads the files and interpolates the rates over the temperature grid of the ion balance calculation. Fitting coefficients for the recombination rates are passed to the routine '`calc_recrates_fits`', which calculates the rates. DR suppression is calculated in the routine '`ch_nikolic_dr_suppression`'. This is a minor modification of '`ch_dr_suppress` to output only the suppression factor.

Overall rates are calculated by finding the level populations of an ion at each point in the temperature and density grid using the routine '`get_populations`' and then multiplying the initial-level resolved rates by the fractional population of each ground and metastable level. The overall rates are passed back as the output.

For those who wish to retrieve overall rates, the subroutine and can be called to return overall rates in the following way:

```
IDL> temp=10.^(findgen(61)*0.05+3.5)
IDL> dens=fltarr(61)+1.e11
IDL> metastable_levels,gname,metas,quiet=quiet
IDL> meta=where(metas eq 1)+1
IDL> recs=fltarr(24,n_elements(meta))

IDL> rates=ch_adv_model_rates('c_1',meta,temp,dens,recs)
```

A few measures have been introduced to speed up the routines. The primary one is in the calculation of the overall ionization and recombination rates, which requires the relative populations of the ground and metastable levels. For the advanced models only, the number of levels included for calculating the level populations has been reduced for some ions. The number of levels for each ion is found next to the ion name in the '`advmodel_list.ions`' list. In doing this, it is ensured that the populations of the metastable states are not affected by more than 1% when reducing the number of levels. The large models are mostly those that include autoionizing states, and so the optional keyword '`no_auto`' has been implemented. This removes the autoionizing states from the level population calculation, since they are only relevant when modelling satellite lines in the X-rays.

3.4 Solving the ion fractions and comparing ionisation equilibria

The resulting ion balances can be saved into a standard CHIANTI format file and/or used on-the-fly by other programs which calculate line contribution functions or intensities. Another time-saving device has been to calculate ion balances only for individual elements being modelled by the on-the-fly routines. Many existing programs have been modified to incorporate the advanced models. More details can be found in the headers of the programs.

A new program, '`ch_compare_ioneq`', has been provided to compare different ionization equilibria. Using the examples provided above, two equilibria can be compared in the following way:

```
IDL> ch_compare_ioneq,'C',files=['all_ions_ne=1e10.ioneq',$
IDL>   'all_ions_zero_density.ioneq'],lab=['Ne=1e10','Ne=0'],$
IDL>   /top,/right,psym=[6,5],lines=[0,2],ion=[1,4]
```

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