VOTADA - VO TOOLS AND ATOMIC DATA FOR ASTROPHYSICS

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ABSTRACT

An overview of the VOTADA project is presented, with highlights of progress made and various issues related to the provision of atomic data to the astrophysical community.

Key words: Atomic data; Virtual Observatory.

1. INTRODUCTION

The VOTADA project aims at providing accurate basic atomic data (and derived products), together with tools for astrophysical applications, within the Astrogrid[1] (PPARC/STFC funded) and the Virtual Observatory. The VOTADA is principally aimed at the interpretation of optically-thin emission from plasmas collisionally excited and in equilibrium, however it also provides basic ion atomic data that are useful for other modelling purposes.

In optically-thin plasmas, spectral line intensities are directly proportional to $N_j\ A_{ji}$, where A_{ji} is the spontaneous transition probability, $N_j(X^{+r})$ is the number density of the upper level j of the emitting ion (X^{+r}). In low density plasmas the collisional excitation processes are generally faster than ionization and recombination timescales, therefore the collisional excitation is dominant over ionization and recombination in populating the excited states. The intensity is then proportional to

$$A_{ji}\frac{N_j(X^{+r})}{N(X^{+r})}\ \frac{N(X^{+r})}{N(X)}\ \frac{N(X)}{N(H)}\frac{N(H)}{N_e}\ N_e \qquad (1)$$

where $\frac{N_j(X^{+r})}{N(X^{+r})}$ is the fractional population of ions $\mathrm{X^{+r}}$ lying in the state j; $N(X^{+r})/N(X)$ is the ionization ratio of the ion X^{+r} relative to the total number density of element X; $Ab(X) = N(X)/N(H)$ is the elemental abundance relative to Hydrogen; $N(H)/N_e$ is the Hydrogen density relative to the free electron density (often assumed equal to 0.83 whenever H, He are fully ionised).

The fraction $\frac{N_j(X^{+r})}{N(X^{+r})}$ can be calculated once all the important collisional and radiative excitation and de-excitation rates between all important levels are known. Similarly, the ionization ratio can be calculated once all the ionization and recombination rates are known.

The product $\epsilon_{ji} = A_{ji}\ \frac{N_j(X^{+r})}{N(X^{+r})}$ is the *line emissivity* and expresses the number of photons emitted per unit time by the transition $j \rightarrow i$. The line emissivity depends on both the temperature and the density of the emitting plasma. The ionization ratio is strongly dependent on the temperature with some density dependence.

Once theoretical emissivities are know, it is relatively straightforward to use them to infer plasma parameters such as electron densities, temperatures from a set of observed spectral lines. Once ionization fractions are known, relative abundances of different elements can also be found. All this is routinely done with data from XUV spectra (e.g. XMM-Newton/RGS, Chandra/HETG and LETG, SOHO/CDS and SUMER, Hinode/EIS, just to mention a few.)

Conversely, theoretical emissivities are needed for the forward modelling process, i.e. to predict spectral line intensities and profiles (or synthetic broad-band images) based on specific models. This is relatively straightforward once instrument properties are known.

For the design and interpretation of broad-band data, theoretical emissivities are commonly used to calculate instrument response functions as a function e.g. of the plasma temperature and density. Conversely, broad-band data can be used to measure properties such as plasma densities and temperatures, once the instrument response functions are know (although severe limitations often exist, due to non-isothermal responses in the filters).

Finally, theoretical emissivities are necessary to calculate the radiative losses via bound-bound emission, needed for any study of the energy balance within a plasma.

[1] http://www2.astrogrid.org/

The ever larger amount of atomic data and observations to be interpreted is challenging. In solar physics, the amount of XUV data per day is already very large, but soon (2008) one single mission (SDO) will add 1Tb/day. It is obviously necessary to develop tools for quick-look data analysis and for handling large amounts of data. VOTADA is a first attempt in this direction.

2. ATOMIC DATA CALCULATIONS FOR IONS

Accurate atomic physics calculations are of paramount importance for the interpretation of astrophysical spectra. Over the years, a large amount of accurate atomic data have been produced, for a number of ions, by the Iron Project [2] and UK Rmax[3] collaborations. The UK RmaX network was formed to calculate electron and photon collisional properties with atoms and ions for transitions at X-ray wavelengths. The focus was on K-, L- and M-shell electron- and photon-impact excitation and ionization. The follow-up of UK RmaX is a recently PPARC/STFC funded network named APAP (Atomic Processes in Astrophysical Plasmas). The APAP network will take advantage of automated codes for the calculation of a very large number of new atomic data for all astrophysically-important ions.

Many other groups world-wide are also providing ever larger atomic datasets, thanks to the increased computing power. One of the problem from an user-community point of view is the lack of standards in the output results, and often the lack of complete datasets so the published atomic data cannot directly be used to compute e.g. spectral line intensities.

3. ATOMIC ION DATABASES

Unfortunately, there are no standards among the various atomic ion databases that are available. In many cases, atomic databases are only specific to a set of ions or to research groups. For example, TIPTOPbase[4] is a public, interactive database service implemented to access the atomic data computed by the Opacity Project (OP) and the IRON Project (IP).

Many published atomic ion data are the result of ab-initio calculations, and wavelengths of spectral lines are normally inaccurate, so the data cannot directly be compared to observations. One of the reasons why the CHIANTI[5] package (Dere et al., 1997; Landi et al., 2006) has become so succesfull (more than 800 citations) is the inclusion of observed wavelengths. Another one is the inclusion of all the necessary rates to calculate line emissivities, in an homogenous standard way (from all available literature). But most of all, the inclusion of programs to perform all necessary calculations and user-friendly graphic user interfaces. One drawback is the limited number of rates included for each ion, and the fact that the software is written in IDL, which does not make it directly available to users that do not have IDL licences.

One important issue for any atomic database or package concerns the various limitations for their use, which the users must always be aware. In the case of CHIANTI, many restrictions are described in the user guides and within each data file, but there are no automatic ways to warn the users of improper use. Another important issue is the need to propagate references to any original atomic physics calculation or measurement. Quite often atomic databases are used as 'black boxes', and references are lost. Also, atomic data can become ingested into other databases. For example, CHIANTI atomic data are included in many other spectral codes such as: XSTAR, APED/ATOMDB, XSPEC, ISIS, PINTofALE. It is obviously not simple to struck a good balance between making atomic data as widely available as possible, and retain important information for the end users.

Another important issue is the need to assess/benchmark atomic calculations against observations, so the best calculations can be chosen.

4. BENCHMARK OF ATOMIC DATA

For many ions, a large number of atomic levels are not known. Indeed, a large number of spectral lines, from the X-rays to the UV, have not been identified yet. Also, some line identifications that are found in the literature turn out to be incorrect, and a lot of work is still needed to revise/complete atomic data for the XUV. The most complete database of observed wavelengths and energy levels for ions is the NIST[6] compilation. This compilation in turn relies on original work mostly done in the 70's (but even earlier, following pionerring work by researchers such as B. Edlen, B.C.Fawcett), based on laboratory measurements and simple atomic structure calculations (due to the limited computing power at the time).

In the last few years, I have embarked in a long-term project of benchmarking atomic data (cf. Del Zanna et al. (2004) and following papers). One important step forward has been the use of large structure calculations to confirm the reliability of collisional rates, and provide accurate radiative rates. The structure calculations are done with semi-empirical adjustements. All previous identifications are reviewed and assessed by comparing not only predicted wavelengths and gf-values (as mostly done in previous literature), but also by comparing line intensities with observations. In this way, a large number of new lines and energy levels have been identified and given uncertainties. Transition probabilities are also benchmarked with lifetimes measured with beam-foil spectroscopy. The estimates of line intensities for

[2] http://www.usm.uni-muenchen.de/people/ip/iron-project.html
[3] http://amdpp.phys.strath.ac.uk/UK_RmaX
[4] http://vizier.u-strasbg.fr/topbase/
[5] www.chianti.rl.ac.uk
[6] http://physics.nist.gov/PhysRefData/ASD/index.html

each laboratory or astrophysical source also allows to point out when lines are blended (a common feature even for the highest-resolution spectrometers).

5. ATOMIC DATA ACCESSIBLE VIA ASTROGRID AND THE VO

Making existing atomic databases and programs accessible through the VO can be done in many different ways. As a first step, it seemed best to make the CHIANTI package available, starting with some basic atomic data. Currently, for each ion CHIANTI has a set of three minimum ascii files that contain: 1) Energy levels (theoretical, observed), level descriptions 2) Transition probabilities, gf values, theoretical and observed wavelengths 3) spline fits to Maxwellian-averaged electron collision strengths, from which rates for excitation, de-excitation can be reconstructed. Additional files/data are included for many ions. They include spline fits to proton collision rates, and ionization/recombination rates.

A subset of CHIANTI data have been imported into a MySQL database. A Table named **SpectralLines** containing all information for each spectral line in the database has been created. This includes ion, observed and theoretical wavelengths, transition probability, weighted oscillator strength, full spectroscopic notation together with observed and theoretical energies of initial and final levels, and finally full reference to original publications, with comments. The table **SpectralLines** can easily be accessed and queried via the AstroGrid Workbench[7]. The output results of the query can be saved as a Votable and browsed with e.g. TOPCAT[8].

As a second step, the idea was to make derived products such as line emissivities available. Instead of writing wrapper scripts which would then call the existing software, it seemed best to make line emissivities directly available. This has been done by creating a Table named **LineEmissivities** which contains the values of the spectral line emissivities calculated for a grid of electron temperatures and densities. The table can be queried via the AstroGrid Workbench, and its values can be used to e.g. obtain theoretical ratios of lines as a function of temperature or density. The emissivities in the table are calculated adopting standard options and do not include photo-excitation (an option available within the CHIANTI package).

A further step, to be completed, involves the calculation of actual line intensities, which requires the inclusion of the element and ion abundances. CHIANTI line intensities are currently calculated for plasmas in ionization equilibrium, and element and ion abundances are stored in tables. These tables are going to be included within the CHIANTI-VOTADA. Work still to be done includes writing workflows/scripts, perhaps in Python, to manipulate the data stored in the various tables.

In the future, continuum emission will be included. Another interesting application would be the inclusion of a treatement of non-equilibrium, non-Maxwellian plasmas. The CHIANTI team is building a database of radiative and dielectronic recombination rates, as well as collisional and photo-ionization rates / cross-sections tocalculate time-dependent ionization.

[7] See details in http://www2.astrogrid.org/science/misctutorials/chianti-on-astrogrid/

[8] http://www.star.bris.ac.uk/ mbt/topcat/

6. CONCLUSION

The ever growing amount of atomic data and spectral observations is challenging, so making data and tools VO-enabled can be a significant aid for data analysis. The effort of defining, within the IVOA, standards for atomic data and their access is very welcomed. In particular, the Atomic and Molecular Lines Data Model and the SLAP (Simple Line Access Protocol) appear as a first step in the right direction. For example, when SLAP will become publicly available, the CHIANTI-VOTADA atomic data could be made easily accessible to VOSpec via a SLAP interface, using the ESAC DAL Toolkit to install a SLAP server. It is however of paramount importance that all atomic/molecular data providers around the world are involved with these developements, so standards useful to a variety of communities can be defined.

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