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The ionization balance of a non-equilibrium plasma

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Most of the quantitative information we have about the cosmos comes from spectroscopy. Whether it is the cosmic expansion, deviations within the CMB, the chemical evolution of galaxies, or the events that occur during a supernova explosion, our knowledge can be traced back to the analysis of a spectrum of some sort.

The gas in a stellar atmosphere is often dense enough for equilibrium thermodynamic to apply. In this case a local temperature is meaningful and the excitation and ionization of the gas will follow from thermodynamic principles. The text Mihalas (1978) gives much of the underlying physics for this "local thermodynamic equilibrium" (LTE) case.

The LTE limit is seldom achieved in emission-line objects. Emission lines are commonly observed when energy is deposited into a gas by some external process, perhaps mechanical or by exposure to ionizing radiation, so that the gas becomes hot. If the column density is small enough for the gas to be optically thin to continuous absorption, an emission-line spectrum will result.

Complications are introduced because of the low density of most emission-line gas. Collisions between various constituents are too slow for different species to share their energy and for kinetic equilibrium to dominate. This means that a variety of processes, some with a vast range of energies, determine the properties of the gas. An atom may be irradiated by the CMB, a true blackbody with a low temperature; starlight, with typical energies of 10^4 K to 10^5 K but highly diluted; and by emission from neighboring atoms. Cosmic rays, with relativistic energies, are often present. Collisions between various constituents of the gas are not fast enough to bring them into statistical equilibrium. Even if a temperature is defined by a Boltzmann equation, that temperature would be different for each ion and level.

The result is that the level populations and the observed spectrum are quite sensitive to microphysical details. This is why the spectrum reveals so much about the intrinsic properties of the gas, such as its composition, heating, temperature, and pressure. But this is a two-edged sword. We need to understand the microphysical processes that govern the ionization, excitation, and chemistry of the gas to harvest the information present in a spectrum.

The Arnaud & Rothenflug (1985, hereafter AR85) paper, and the supplement for Fe by Arnaud & Raymond (1992, hereafter AR92), did much of the difficult work needed to assemble the data base that is essential for understanding the properties of a low-density gas. These two papers have over 1300 citations at the time of this writing, placing them in the highest "renowned" citation category recognized by SPIRES. A good part of these citations are because of the quality and comprehensiveness of the work. But another reason is that basic atomic rates have universal value. The data derived by AR85 can be applied to regions ranging from the solar corona to the intergalactic medium. Such atomic data are among the foundations for how we understand the universe giving them timeless value.

The final product of AR85/AR92 was the calculation of the ionization distribution of a gas where ionization was produced by collisions between an ion and a free electron. It is generally a safe assumption that, because of the very fast electron-electron elastic collisions, electrons have a thermal distribution (Spitzer 1962). The problem is to find a rate coefficient, the integral of a cross section over this electron velocity distribution function.

A dense gas will recombine following a three-body collision, $A^{+n} + 2\mathrm{e} \rightarrow A^{+n-1} + \mathrm{e}^*$. Energy is exchanged between the two free electrons to produce an electron in a bound state and an energetic free electron. The balance equation, assuming that every collisional ionization is followed by a three-body recombination, is $n_\mathrm{e} n(A^{+n-1}) q_\mathrm{ion} = n_\mathrm{e}^2\, n(A^{+n}) \alpha_3$ where α_3 is the three-body recombination-rate coefficient and q_ion the collisional-ionization rate coefficient. Three-body recombination can be thought of as the time reversal of collisional ionization, so q_ion and α_3 are related by detailed balance. The balance equation can be posed into the continuum form of the Boltzmann equation. The atomic cross sections will cancel out leaving us with the familiar Saha equation for ionization balance, in which the ionization ratio $n(A^{+n-1})/n(A^{+n})$ only depends on the density and temperature. This is the LTE limit.

There are few emission-line regions in which this LTE limit will apply. At low densities collisional ionization will be followed by radiative and dielectronic recombination. The balance equation will have the form $n_\mathrm{e} n(A^{+n-1}) q_\mathrm{ion} = n_\mathrm{e} n(A^{+n}) \alpha$ where α is the total recombination rate coefficient. Radiative recombination can be thought of as the time reversal of photoionization, while dielectronic recombination is the reversal of autoionization. The ionization and recombination terms have the same density dependence, so the ionization balance is independent of density. Neither recombination process is directly related to collisional ionization, so the ionization balance depends on the gas kinetic temperature and the cross sections for electron impact

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ionization, photoionization, and the properties of autoionizing levels. This is the key complication.

The challenge is to compute the ionization and recombination rate coefficients and then solve a simple set of balance equations to determine the ionization balance. The first step, and the majority of the work, is to assemble the atomic data, often published in a wide range of physics and chemistry journals, and integrate these to produce rate coefficients.

In a collisionally-ionized gas, the typical kinetic energy of the free electrons, kT, is similar to the ionization potential of the most common ions. The dominant ionization process will be electron-impact ionization from the ground state. AR85 improved upon previous work, which largely had been based on the semi-empirical work of Lotz (1967), with a variety of experimental and theoretical studies. The temperature dependencies of the resulting rate coefficients were fitted by relatively simple formulae and the fitting coefficients given in appendices. Their derived rates are generally not too different from the best values today.

Radiative recombination rates are computed from the photoionization cross sections using the "Milne equation" (Osterbrock & Ferland 2006). Photoionization cross sections must be known for all bound levels of the recombined species to find a total recombination rate coefficient. Fortunately, this is relatively easy since excited states will be fairly hydrogenic and ground states had been explicitly computed by other groups (Reilman & Manson 1979) interested in the photoionization equilibrium problem. In this way AR85 built upon the previous best calculations, those of Aldrovandi & Péquignot (1972, 1974).

The gas recombines, in most cases, by dielectronic rather than radiative recombination. In this process the free electron loses energy following an internal excitation of the ion. The electron is captured and forms a recombined ion in a doubly-excited autoionizing state. In most cases this state does auto-ionize, but in some small fraction of the time one of the excited electrons decays to a lower level, producing an emission line, and then forms a stable recombined atom. For a collisionally-ionized gas the kinetic energies are high enough to reach highly-excited Rydberg levels near the continuum of the recombined species. The large number of Rydberg levels makes a simple statistical calculation of the dielectronic recombination (DR) rate possible (Burgess 1965).

DR is the main area where today's best results differ the most from AR85/AR92. Two additional channels are present and cause large increases in the DR rate coefficient. The original work considered changes in the bound electron electronic *configuration* before recombination. The energies required are large so the rate coefficient is fast only at high temperatures. When changes in electron *term* were considered (Nussbaumer & Storey 1983, 1984, 1986, 1987, only the first of these was published in time to be considered by AR85), the rate coefficient sometimes increased as much as 1 dex at lower temperatures. The most recent work, a series of A&A papers with Altun et al. (2007) among the more recent, considers changes in both electron term and *level*. This produces another increase in the DR rate. A summary of the A&A publications, and fitting coefficients, are on Nigel Badnell's web site `http://amdpp.phys.strath.ac.uk/tamoc/DR/`. The total DR recombination rate is now substantially higher at temperatures below the ionization peak with the result that the gas tends to be more neutral (Bryans et al. 2006, 2009).

Besides these ionization and recombination processes, AR85 also summarized charge-transfer rates, a process in which an atom and ion form a quasi molecule and exchange electrons. Charge-transfer rates were later revised by Péquignot & Aldrovandi (1986) and Kingdon & Ferland (1996). This process is generally far less important in collisional plasmas but should still be included.

All of the AR85 results were presented as fitting coefficients in relatively simple interpolation formulae. This ease of access was a major contributor to the wide adoption of their results in many different applications and codes. Although the AR85 basic data were intended for application to a collisionally-ionized plasma, a very large number of studies of photoionized plasmas were done by combining their data with Reilman & Manson (1979). The lesson is again the universal applicability of basic atomic data.

Spectroscopic instrumentation improves with each new mission or telescope. If the density of the object under study is too low for LTE to apply, true for most objects, the ionization of the elements will be determined by the processes described by AR85. Of the processes they consider, the DR rates remain the largest source of uncertainty. DR occurs through autoionizing levels that have energies only slightly above the ionization energy. The positions of many of these levels have not been measured experimentally and energies must be obtained from theoretical calculations. The uncertainties intrinsic to such a calculation are often similar to the separation between a level and the continuum edge. The result is "threshold straddling" – it is not known whether a level is above or below the continuum. More precise DR rates will require more precise experimental energies.

Finally, this series of commentaries is a reflection back upon the first forty years of A&A. AR85, along with some of the others paper discussed, are very highly cited presentations of fundamental atomic and molecular data. Such studies, which have become a hallmark of A&A, are the foundation of how we understand the universe. The recent DR calculations (Altun et al. 2007, and earlier), which substantially increase the rates presented in AR85, have appeared as a series of A&A papers. The Iron Project papers (see, for example, Butler & Badnell 2008) are also found in A&A. These represent the hard and diligent work of a large body of gifted researchers. That these papers have all found a home in A&A is a testimonial to the very high standards set by both this journal and the European Astronomical community.

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