Atomic Processes and Overview

UV and X–ray Spectroscopy in Astrophysics

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ABSTRACT

Spectroscopy is an extremely powerful tool for measuring the physical conditions in astronomical plasmas, including the density, temperature, ionization, radiation intensity, and magnetic field. Application of spectroscopic analysis is more straightforward for diffuse plasmas, such as those in stellar coronae and the interstellar medium, since the effects of radiative transfer are less important there; this brief review focuses on such plasmas. The composition of stars and the interstellar medium is inferred from spectroscopy. Line profiles reveal the dynamics of astrophysical plasmas, and spectra calculated from global dynamical models can be compared with observation to obtain a more complete understanding of the dynamics. Both spectropolarimetry and the technique of "reverberation mapping" permit one to deduce the structure of astronomical sources on scales too small to be resolved directly. However, the potential of astrophysical spectroscopy can be realized only if accurate atomic data are available; dielectronic recombination is cited as an example.

1 THE POWER OF ASTROPHYSICAL SPECTROSCOPY

Astronomy is an unusual science in that it is based on observation instead of experiment. The astronomer must rely on analyzing the radiation that happens to reach the Earth from whatever source is being studied. There is a good deal of information in the distribution of this radiation on the sky and, for variable sources, its time evolution. However, the information content is multiplied manyfold when the radiation is broken down into different frequencies, its spectrum.

Here I shall present a brief and idiosyncratic look at some of the properties of astrophysical plasmas that can be inferred from spectroscopy, particularly spectroscopy of sufficiently high resolution that individual lines can be observed. A paper this brief is not a review and cannot be complete. In keeping with the topic of this conference, I shall focus on UV and X-ray spectroscopy, but I shall comment on techniques from other parts of the electromagnetic spectrum where appropriate. Furthermore, I shall concentrate on the spectroscopy of diffuse gases, such as stellar coronae and the interstellar medium (ISM), since then deductions from spectroscopic observations are less dependent on the effects of radiative transfer. First I discuss how spectroscopy can be used to infer the physical conditions in an astrophysical plasma, such as the density, temperature, and magnetic field. In some cases more subtle measurements

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are possible, so that, for example, the velocity distribution function of the emitting plasma is accessible to observation. The composition of astrophysical plasmas is determined by spectroscopic observations. Astrophysical plasmas are often violent, with flares, winds, and shock waves generating high velocities and temperatures, which are revealed by spectroscopy. Finally, it is possible to use spectroscopy to study the geometry of sources on very small scales by using spectropolarimetry or by using the technique of "reverberation mapping".

1.1 Physical Conditions

1.1.1 Density

The density of a plasma can be inferred from the intensity ratio of two lines of the same ion, at least one of which is not a permitted transition. For example, the relative populations of the $2\ ^3S$ and $2\ ^3P$ states in He–like ions are sensitive to the density, making the ratio of the forbidden and intercombination lines resulting from the decay of these states to the ground state a density diagnostic useful for stellar coronae (Gabriel and Jordan 1969). The excitation of Fe L–shell lines in X–ray photoionized nebulae has been studied by Liedahl *et al.* (1992a), and they have shown that the collisional excitation of metastable levels in an Fe ion of charge $Z+1$ affects the recombination spectrum of the Fe ion Z in a manner that permits the estimation of densities in the range $10^{12} - 10^{15}$ cm^{-3}. The density can also be estimated from absorption line observations, if one of the lines arises from an excited state.

If both emission and absorption line observations are available, it is even possible to estimate the density from observation of a single line: The intensity of the emission line can be written as $I_l = n_e N(X) C(T) h\nu/4\pi$, where $N(X)$ is the column density of the lower state of the emission line and $C(T)$ is the collisional excitation rate coefficient. Provided $C(T)$ is a weak function of temperature, as it generally is for photon energies $h\nu \lesssim kT$, one can infer the electron density n_e from observations of the emission line intensity $I_l \propto n_e N(X)$ and the absorption column density $N(X)$. Martin and Bowyer (1990) have applied this technique to estimate the density of the C IV emission region in the Galactic halo, finding $n_e \sim 0.01$ cm^{-3}.

1.1.2 Temperature

The temperature can be inferred from intensity ratios of permitted lines of the same ion. For example, transitions from the $2s2p^2$ excited states to the $2s^22p$ ground state in the B isoelectronic sequence provide a useful temperature diagnostic for the solar chromosphere (Zirin 1966). The dielectronic satellites of H–like and He–like ions are sensitive to the temperature (Gabriel 1972). Liedahl *et al.* (1992b) have shown that the widths of the recombination continua in X–ray photoionized nebulae

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are relatively narrow and provide a good temperature diagnostic. Observations of line profiles in either emission or absorption give an upper limit on the temperature of the plasma, since bulk flows can also contribute to the line width.

1.1.3 Pressure

If both the density and temperature of the plasma can be determined, then the pressure is known. The pressure can thus be determined by using pairs of line ratios that depend on density and temperature, as described above. A good example of the determination of the pressure of an astronomical plasma is provided by the study of the resonant absorption lines from the excited fine structure states of neutral carbon in the cold phase of the ISM (Jenkins and Shaya 1979). Observation of absorption in the C I multiplets λ 1261, λ 1280, and λ 1329 showed that most of the cold gas in the ISM is at a pressure $P/k \lesssim 10^4$ K cm^{-3}, but that some is at pressures exceeding 10^5 K cm^{-3}.

1.1.4 Ionization

Comparison of the intensities of lines from different stages of ionization allows one to infer the degree of ionization in the plasma; when combined with an estimate of the temperature, one can infer whether the ionization is collisional [$kT \sim (0.1 - 0.3)E_i$, where E_i is the ionization potential of the dominant ion] or due to photoionization ($kT \ll E_i$). Collisionally ionized plasmas in stellar flares or in supernova remnants (SNR) are often not in ionization equilibrium. Deviations from ionization equilibrium in such plasmas can be measured from observations of the ratio of the forbidden [$1s^2 - 1s2s(^3S_1)$] to resonance [$1s^2 - 1s2p(^1P_1)$] lines in He–like ions (Vedder *et al.* 1986): the recombination contribution to the lines favors the forbidden line more than does the collisional excitation, so the forbidden/resonance ratio is reduced for ionizing plasmas. Vedder *et al.* used this diagnostic to demonstrate that the X–ray emitting plasma in the Cygnus Loop is not in ionization equilibrium.

The level of ionization can also be inferred from absorption observations. For example, Green *et al.* (1990) have used the first observation of the absorption edge of neutral helium in the ISM to infer the He I/ H I ratio in the local ISM from the EUV spectrum of the white dwarf G191-B2B; they found that this ratio is about 0.06 to within a factor of 1.5.

1.1.5 Local intensity of radiation

Atomic levels can be excited by radiation as well as by collisions, and this can often be used to infer the intensity of the local radiation field. Perhaps the most famous example of this procedure is the measurement of the temperature of the cosmic microwave background from absorption line observations of the ratio of the $R(0)$ and

$R(1)$ lines of the CN molecule at λ3874 Å (e.g., Field and Hitchcock 1966). The excitation of the lower state of the $R(1)$ line is due almost entirely to the absorption of radiation by the $R(0)$ ground state at a wavelength $\lambda = 2.64$ mm. Meyer and Jura (1985) inferred a radiation temperature of 2.70 ± 0.04 K at this wavelength, in quite good agreement with the subsequent measurement by the Cosmic Background Explorer, 2.735 ± 0.06 K (Mather *et al.* 1990). The Bowen fluorescence mechanism provides another example: He II Lα at λ 304 excites a characteristic set of lines in O III in the near UV, so that measurement of the O III line intensities can be used to determine the intensity of He Lα. Schachter *et al.* (1990) have used observations of the Bowen lines in a sample of Seyfert galaxies to infer the properties of the emitting regions in these objects.

The level of ionization in photoionized plasmas depends on the ionization parameter $\Gamma = n_\gamma/n$ or, equivalently, $\Xi = u_\gamma/P$, where n_γ and u_γ are the number and energy density of ionizing radiation, respectively (e.g., Krolik *et al.* 1981). Observation of the level of ionization together with a determination of the density then allow one to infer the intensity of the ionizing radiation and thus the size of the source, a procedure commonly used to estimate the size of the broad emission line regions of active galactic nuclei. An ingenious variant of this approach has been developed by Bajtlik *et al.* (1988) to infer the intensity of the intergalactic ionizing radiation field at high redshift: They noted that the number of Lα absorption systems seen in quasar spectra was smaller at redshifts near that of the background quasar (the "proximity effect"). By attributing this decrease to the rise in the level of ionization as one approached the quasar, they were able to infer the distance out to which the quasar radiation dominated that of the background and thus the intensity of the background radiation itself. With this technique, it is possible in principle to measure the evolution of the intensity of the ionizing background with cosmic time.

1.1.6 Velocity distribution in shock fronts

Shocks generate non–Maxwellian velocity distributions, and for shocks in partially ionized gases this distribution is accessible to spectroscopic observation (Chevalier and Raymond 1978). The ionized component of the plasma is promptly heated and accelerated by collisionless processes (e.g., McKee and Draine 1991). The neutral component of the plasma can interact with the hot plasma only through collisions. Some of these collisions will excite the atoms, producing emission lines with the narrow profile characteristic of the ambient plasma; some of the collisions will ionize the atoms; and some will result in charge exchange, producing fast neutral atoms that emit lines with the profile appropriate to the shocked plasma. In a gas of cosmic abundances, the line emission from such shocks is predominantly in the Balmer lines of hydrogen, and as a result these shocks are often referred to as Balmer–dominated shocks.

Observation of the narrow and broad components of the emission lines from

Balmer–dominated shocks provides a number of important diagnostics of the shock (Raymond 1991): First, the profile of the broad lines gives a direct measure of the proton temperature. Next, the ratio of the narrow to the broad lines depends on the electron/ion temperature ratio behind the collisionless shock, which is not known theoretically. Some of the shock energy goes into accelerating cosmic rays, and in principle this fraction can be determined from observations of face–on shocks by comparing the velocity shift of the shocked gas (which is 3/4 the shock velocity) with the observed ion temperature. If the fraction of the shock energy going into the protons can be determined, then the shock velocity can be inferred from the temperature; observation of the proper motion of edge–on shocks can then be used to measure the distance to the shock. Measurement of these effects in the spectrum of helium would be extremely challenging, but useful.

1.1.7 Magnetic fields

Magnetic fields lead to a Zeeman splitting of $h\Delta\nu = 0.058(B/10^7 \text{ G})$ eV for an unpaired electron, where the normalization has been chosen to represent the typical fields found in magnetic white dwarfs (Angel 1977). These fields are generally measured in the optical region of the spectrum, but are accessible to UV spectroscopy as well. Much larger fields are found in neutron stars, and these can be measured only in the X–ray region of the spectrum since the cyclotron absorption resonance occurs at $11.6(B/10^{12} \text{ G})$ keV. For example, two gamma ray bursts have been observed with features at about 20 and 40 keV, and these observations have been interpreted as the first and second harmonics of the cyclotron resonance in a field of 1.7×10^{12} G (Murakami *et al.* 1988). These observations are consistent with the conventional view that gamma ray bursts arise from old neutron stars.

1.2 Abundances

Our knowledge of the composition of stars and the interstellar medium comes entirely from spectroscopy. In some cases, the composition can be measured by summing up the abundances in each ionization state, but this becomes more complicated if some of the atoms are in molecules or in grains. UV absorption line studies of the ISM provide the main source of information on the abundances in the ISM (Jenkins 1987). The difference between the observed abundances and the solar values is attributed to depletion onto grains. With this interpretation, there is no evidence for significant variations in abundances in the solar neighborhood. A direct confirmation of the result that interstellar abundances are in fact close to solar can be made by observing the K–shell absorption of an element, since the absorption cross section is almost unaffected by whether the atom is in a grain. *Einstein* observations of the Crab Nebula with the Focal Plane Crystal Spectrometer show that the oxygen abundance in the intervening ISM is indeed consistent with the solar value.

with the measurement giving an oxygen abundance 1.1 ± 0.3 times the solar value (Schattenburg and Canizares 1986).

Another technique for inferring the abundances in astrophysical plasmas is by direct comparison of the spectrum with a similar solar spectrum, thereby circumventing uncertainties in the atomic data. Applying this technique to the SNR Puppis A, Canizares and Winkler (1981) find that the strengths of the H and He–like lines of oxygen and neon compared to the expected lines of Fe XVII indicate that oxygen and neon are enhanced relative to iron by a factor $\sim 3-5$. They argue that this is not due to depletion onto grains, both because silicon does not appear to be depleted and because the high temperatures in the remnant are expected to destroy the grains; on the other hand, the results are consistent with the injection of about 3 $M_\odot$ of oxygen and neon by a supernova in a star of mass $\gtrsim 25M_\odot$.

1.3 Dynamics

Line profiles are a direct manifestation of the dynamics of the emitting gas. P Cygni profiles in the spectra of early type stars indicate substantial mass loss in winds with velocities of order 3000 km s^{-1}. Such winds have a dramatic effect on the evolution of the star and on the ambient interstellar medium; in addition, they substantially complicate the interpretation of the underlying stellar spectrum (Kudritzki and Hummer 1990). Far more dramatic outflows are evident in the spectra of some quasars, the broad absorption line quasars, where line widths well in excess of 10^4 km s^{-1} are commonly observed (e.g., Turnshek *et al.* 1988). In many cases, the equivalent width of the emission is much less than that of the absorption, in contrast to the stellar case; this indicates that the high velocity outflow covers only part of the sky as seen from the quasar, and thus that a substantial fraction of quasars must have such outflows.

For the flows just described, the width of the line accurately portrays the velocity of the gas. This need not be the case, however, if the opacity in the line is large enough so that the line width is due to the damping wings. An interesting example of this is provided by the acceleration of Lα photons by shocks (Neufeld and McKee 1988). Shocks in atomic gas emit copious amounts of Lα radiation, which is effectively trapped by the large neutral hydrogen opacity on either side of the shock. Each time a Lα photon crosses the shock, it is blue–shifted by a process directly analogous to first order Fermi acceleration of cosmic rays in shocks. The Lα line profile of the radio galaxy 3C326.1 has a strong blue wing which Neufeld and McKee interpreted as being due to such acceleration. The peak of the profile of the accelerated photons occurs at a velocity of $270(N_{20}v_{s7})^{1/3}$ km s^{-1}, where N_{20} is the H I column density in units of 10^{20} cm^{-2} and v_{s7} is the shock velocity in units of 10^7 cm s^{-1}; widths substantially in excess of the shock velocity are possible. Low dust to gas ratios are required in order to ensure that the Lα photons survive.

It is also possible to use spectroscopy to study the dynamics of a system by developing a dynamical model of the system, calculating the resulting spectrum, and comparing with the observed spectrum. A good example of this procedure is provided by the modeling of the X–ray spectrum of Tycho's supernova remnant by Hamilton *et al.* (1986). They used the observed age, angular diameter, and X–ray flux as inputs to their model, and assumed that the supernova ejected a mass of 1.4 $M_\odot$. They used an analytic representation for the dynamics of the expanding SNR, including the blast wave in the ISM and a reverse shock expanding back into the ejecta of the supernova. By adjusting the composition of the ejecta, they were able to get good agreement with the *Einstein* spectra, and they inferred the distance to the remnant, the energy of the original explosion, the density of the ambient medium, and a number of parameters describing the SNR. This approach will become increasingly powerful as spectra of higher resolution become available.

1.4 Mapping the Source Geometry on Small Scales

1.4.1 Spectropolarimetry of NGC 1068

One of the remarkable applications of spectroscopy is in the measurement of the geometrical properties of the source on scales far too small to be spatially resolved. Some information on the structure of the source can be gleaned from measuring the polarization of the spectrum. A good example of the effectiveness of this procedure is the discovery that NGC 1068, a classical Seyfert 2 galaxy, is in fact a Seyfert 1 with an obscured broad emission line region (Antonucci and Miller 1985). Seyfert galaxies are characterized by bright nuclei with strong emission lines; those with line widths well in excess of 10^3 km s^{-1} are termed Seyfert 1, and those with narrower lines are termed Seyfert 2. The spectrum of NGC 1068 has the intense, narrow lines of a Seyfert 2 galaxy, but Antonucci and Miller showed that the *polarized* spectrum has the broad lines of a Seyfert 1. They interpreted this as indicating that the the broad emission line region is obscured by dust; the polarized flux was attributed to electron scattering by a plasma that has a clear line of sight both to us and to the central source, and that is confined to a region too small to be resolved optically.

A means of confirming this picture was proposed by Krolik and Kallman (1987): the same gas that we observe by its scattering in the optical region of the spectrum should also convert continuum X–rays to Fe Kα lines with a relatively large equivalent width. This prediction was soon confirmed by the *Ginga* satellite (Koyama *et al.* 1989). The efficiency of this process is enhanced by about a factor 2 due to resonant scattering of the continuum by the large number of Kα lines in the various stages of ionization of Fe (Band *et al.* 1990). In addition, Band *et al.* pointed out that strong Fe L–shell emission should be present. Such emission has recently been observed with BBXRT (Marshall *et al.* 1992); the emission is centered at 870 eV, with a width of 120 eV and an equivalent width of 340 eV. The quantitative interpretation of the X–ray spectrum of NGC 1068 should shed new light on the nature of Seyfert galaxies.

1.4.2 Reverberation mapping

A detailed picture of both the geometrical structure and the dynamics of a relatively compact, photoionized source can be obtained through the technique of reverberation mapping (Blandford and McKee 1982). Consider the broad emission line region of an active galactic nucleus (AGN) or the accretion disk of an X–ray binary, for example. Now imagine that the central source produces a brief flash of ionizing radiation, $L_c(t) = \delta(t)$. When this burst of radiation reaches an element of gas in the system, it will cause a brief change in the intensity of the emission line spectrum of the gas. The observer will see this emission shifted in both frequency and in time, with the frequency shift corresponding to the radial velocity of the emitting gas, v, and the time delay τ corresponding to the additional light travel time associated with the longer pathlength. Each emission line in a given source is thus characterized by a *transfer function* $\Psi(v, \tau)$ which gives the response of the line to a flash of ionizing radiation as a function of the delay time and of the frequency (measured in velocity units). The transfer function is the projection of the six dimensional phase space of the source (emissivity as a function of position and velocity) onto two dimensions: the spatial information is integrated over a paraboloid corresponding to the surface of constant delay time τ, and the velocity information is reduced to the radial velocity v. As such, it is impossible to completely reconstruct the source from the transfer function, but, particularly if the source has an underlying symmetry (spherical or axial, for example) it is possible to learn a great deal. Graphic depictions of the transfer function for different models have been presented by Welsh and Horne (1991).

Real sources generally do not oblige us with flashes of ionizing continuum radiation, and the line luminosity observed at a time t is an integral over the past history of the continuum emission of the source:

$$L_l(v, t) = \int_0^\infty \Psi(v, \tau) L_c(t - \tau) d\tau. \tag{1}$$

With an extensive set of observations of the continuum and line fluxes, this equation can be formally inverted using Fourier transforms to find the transfer function $\Psi(v, \tau)$ (Blandford and McKee 1982). A more robust method of evaluating the transfer function is to use the maximum entropy method, and this has been done by Krolik *et al.* (1991) using the extensive IUE data on the NGC 5548 (Clavel *et al.* 1991). The accuracy of the data gathered in this extensive campaign was in fact only adequate to determine the velocity–integrated transfer function, $\Psi(\tau) = \int \Psi(v, \tau) dv$. The high–ionization lines show a peak near zero time delay, and fall off to a lower value in 15–20 days. The low ionization line C III] λ1909 shows a quite distinct behavior, with a peak in the transfer function at a lag of 25 days and a gradual roll off thereafter. Eventually, it should be possible to obtain the full transfer function $\Psi(v, \tau)$, and in that case Blandford and McKee have shown how the transfer function can be formally inverted to determine the emissivity and the moments of the velocity distribution of the emitting gas.

The technique of reverberation mapping should be particularly effective for X–ray sources, since the variability occurs on timescales of seconds to minutes for compact galactic X–ray sources and hours for AGN. For an accretion disk, it is possible to infer both the mass of the central object and the inclination of the disk (Blandford and McKee 1982; Stella 1990). AGN produce a greater observed flux of X–rays in a Schwarzschild crossing time than do galactic X–ray sources, and so they should be particularly amenable to this treatment (Stella 1990).

2 ATOMIC DATA

As the foregoing discussion has demonstrated, astrophysical spectroscopy is an extremely powerful tool for elucidating the physical processes occurring in astronomical sources of radiation as well as their geometrical and dynamical structure. However, this potential can be realized only if the atomic and molecular data used to interpret the observations are of sufficient quality. Here I shall illustrate this with a single example, that of dielectronic recombination rates.

The realization that dielectronic recombination is the dominant recombination process for incompletely ionized plasmas over a wide range of temperature was a major advance in our understanding of astrophysical plasmas (Burgess 1964). In this process, an incident electron is captured by an ion, forming a doubly excited state; usually, the ion autoionizes without recombining, but sometimes it radiates into a bound state. Since the original work of Burgess, a good deal of effort has gone into calculating more accurate dielectronic rates. In particular, Jacobs *et al.* (1980 and references therein) pointed out that it was essential to include autoionization to excited states of the recombining ion, a change which substantially reduced the dielectronic rate for a number of ions. Some of the transitions included by Jacobs *et al.* are energetically inaccessible, however (e.g., Smith *et al.* 1985). Using a quantum defect method similar to that of Jacobs *et al.,* Romanik (1988, 1992) has calculated dielectronic rates of astrophysical interest by considering only energetically allowed transitions and by including captures to forbidden doubly excited states. Rates for the He, Li, Be, and Ne isoelectronic sequences were presented in the first paper; the rates for the remaining sequences between H and Ca are presented in the second. He has obtained good agreement with recent *ab initio* distorted wave calculations (e.g., Roszman 1987a,b). Fig. 1a shows a comparison between Romanik's (1992) results and Roszman's results for Fe XVIII; the discrepancy between the two may be due to the fact that Roszman used configuration–averaged energies in his calculation. In general, Romanik's results are intermediate in value between those of Jacobs *et al.* and those obtained with the original Burgess formula.

The values of the dielectronic recombination rates can have a substantial effect on the ionization equilibria of collisionally ionized plasmas. Romanik's (1992) results are compared with those of Shull and van Steenberg (1982a,b), who used the rates of Jacobs *et al.,* in Fig. 1b. The temperature at which a given ion reaches its peak