Emission Lines: Past and Future

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In the first half of this century many emission lines were or had been identified. Noteworthy moments were the identification of the Nebulium lines (λ 4959/5007) as forbidden lines of O^{++} (Bowen 1927) and of the strong solar green coronal line λ 5303 as due to Fe^{13+} (Edlen 1942). In addition, a first quantitative understanding of some aspects of nebular spectra was obtained: the Balmer decrement was calculated by Menzel and associates (1937), the temperatures of the central stars of planetary nebulae were inferred by Zanstra (1927), and the first information on elemental abundances in nebulae was gained.

In the second half of this century a much more detailed understanding of emission spectra was acquired. Emission lines assumed a fundamental role for the diagnostics of conditions in nebulae. As a result electron densities N_e and temperatures T_e as well as elemental abundances became known in many objects. Excitation and ionization conditions in nebulae were found to be frequently radiative (photoionization), but shocks and perhaps fast particles were also found to play a role. Non-equilibrium conditions were seen to be important especially in the hot, tenuous plasmas revealed by X-ray observations: the ionization state was often different from that expected from the temperature, and even T_e and the temperature of the proton gas could be different.

Chemistry was found to play a role in many emission nebulae. Numerous new molecules were observed, especially by radio observations in cool, dense media. Dust was found to strongly affect the appearance of spectra, not only by absorption and scattering but also by its effects on abundances. And finally observations of emission lines gave much information on velocity fields in nebulae and also on magnetic and electric fields.

These developments resulted from improvements in atomic and molecular parameters, in observations and in modelling. The calculation and sometimes measurement of transition probabilities, photoionization cross-sections, collisional cross-sections and recombination coefficients were an obvious prerequisite for the quantitative analysis of emission line spectra. Observations improved in precision, and perhaps almost more important in dynamic range, by the introduction of new detectors, in particular CCD's. And the initially limited wavelength range over which optical emission lines had been observed was extended to include lines in the MHz region of the radio spectrum to the gamma-ray lines associated with nuclear rather than atomic processes.

The interpretation of these data was much strengthened by the introduction of sophisticated modelling techniques: Self-consistent photoionization models play an increasing role, radiative transfer calculations have been substantially improved, hydrodynamics has become a new ingredient, reaction networks of chemical or nuclear nature have been included as having non-equilibrium processes. As a result, a deeper insight has been obtained in the origin and evolution of emission nebulae.

It is particularly appropriate that this symposium be held in honor of Mike Seaton and Don Osterbrock, who have contributed decisively to give the subject its present more quantitative shape.

Seaton's first paper was, I believe, written in 1949 (with Bates) on the continuous absorption of O, N, and C. In 1953 and 1954 followed two papers which were fundamental for the understanding of the spectra of planetary nebulae, HII regions and supernova remnants. The first paper contained the calculation of the electron collision cross-sections of the ground states of N^+, O°, O^+, O^{++}, Ne^{++}, S^+, and in the second paper the blue [OII] and the [SII] doublet ratios as a function of N_e were explicitly given. With the data of these two papers it became possible to quantitatively understand the stronger forbidden lines in the nebular spectra.

Osterbrock started out in 1951 with a paper on transition probabilities of [Ca II], [Fe XV], etc. Four years later he measured the [OII] doublet ratios in the Orion Nebula and confirmed Seaton's calculations. In a subsequent joint paper (Seaton & Osterbrock 1957) they studied the red [OII] doublet, which again gives valuable information on N_e. The same year Osterbrock determined N_e in the filaments of the Crab Nebula from the λ 3727 doublet ratio.

I came into the subject myself in 1957 with the analysis of Mayall's spectra of the Crab Nebula and was lucky enough to find that all the atomic data needed to determine the conditions in the Nebula had just been calculated. This led to the conclusion that abundances in the Crab Nebula were rather normal (except for helium) and that the ionization could be understood as being due to the ultraviolet extension of the synchrotron radiation spectrum of the Nebula.

This point was taken up again by Williams (1967) who constructed a photoionization model for the "Ionization and thermal equilibrium of a gas excited by uv synchrotron radiation" from which line intensities were predicted. This was the first of the power-law type photoionization models which has blossomed into a whole industry for Active Galactic Nuclei. In the meantime similar approaches had been followed by Hjellming (1966) for HII regions excited by hot stars and for Planetary Nebulae by Goodson (1967). The main additions to these models made since then are the charge exchange reactions and the di-electronic recombination.

While as a result of these developments no major problems remained in understanding the intensities of the lines of the more common elements, a curious anomaly was noted by Dennefeld and Péquignot (1983) who measured the [Ni II] lines λ 7378/7411 in the Crab Nebula and found an overabundance of Ni with respect to iron of a factor of around 60. It then was noticed that similar but less strong anomalies existed in other supernova remnants and even in the Orion Nebula (see also Osterbrock *et al.* 1992 for the latter object). The matter was discussed by Henry (1984) who attempted to see if there could be problems with the ionization equilibrium of Ni, with the atomic parameters or with differential condensation into grains of Fe and Ni. None of these approaches was found to be very promising. Also in Seyfert galaxies (Halpern and Oke 1986) and in Herbig-Haro objects the anomaly was found. Stahl and Wolf (1986) found the same in the Luminous Blue Variables in the Large Magellanic Cloud. The most extreme result was obtained by Johnson *et al.* (1992) who found in the P Cygni Nebula an overabundance of Ni by a factor of 2000!

As noted by Lucy (1994), the latter result makes it impossible to believe that real overabundances are the cause of the observed line strengths. Instead he considers the radiative excitation (of 284 levels) by continuum radiation in the 900–2200 Å range and calculates their effect on the level populations. A good fit is obtained for the P Cygni Nebula with a predicted intensity ratio λ 7378/λ 7411 of 3.5, close to the observed value (Barlow *et al.* 1994), but far from the factor of 10–11 for pure collisional excitation. However, Lucy also finds that radiative excitation is inadequate in the case of the highly diffuse radiation field in the Crab Nebula. This would then indicate a real overabundance which could be produced during the supernova outburst by nuclear reactions in an unusually neutron-rich environment. It is, of course, the case that in all supernova explosions nickel is produced in the form of ^{56}Ni, but this rapidly decays into Co and then

Fe. However, before this conclusion can be entirely convincing, it would be necessary to understand the curious geometry of the [Ni II] emission; according to results reported at this meeting by Mac Alpine the [Ni II] emission is strong on the side of the filaments which faces the pulsar. Also the results of Hudgins *et al.* (1990) from the [Ni II] line at 1.19 μm indicate a smaller apparent overabundance (factor of 6) of Ni. While on the subject of the Crab Nebula, I also note that Murdin (1994) appears to have detected the long sought for halo. Though extremely faint, it could contain several solar masses of hydrogen and represent a relic of the stellar wind in an earlier evolutionary phase (Chevalier 1977). The spectroscopic detection of the narrow Hβ emission and the absence of the braod [O III] lines make it rather clear that scattered light from the Nebula is not a problem.

Returning to the photoionization models, these have been particularly elaborated in the context of quasars and Seyfert galaxies. Various complications have been added to the models, including optical depth effects, clouds of high N_e, scattering of electrons and/or dust, and an intercloud medium. Perry and Dyson (1985) have added shocks in the Seyfert winds, while Osterbrock and Parker (1965) tried to add ionization by fast protons.

Perhaps the most enduring problem for the pure photoionization models has been to explain the very strong Fe II emission seen in Seyferts and quasars. Already in 1979 Collin-Souffrin *et al.* concluded that "the Fe II region should be thermally heated, excited and ionized," essentially because with photoionization most Fe would be Fe^{++}. While in the meantime the models have been stretched to explain some of the spectra, cases like PHL 1092 with its almost pure Fe II spectrum (Bergeron & Kunth 1980) remain far beyond the possibilities. Very strong Fe II emission has also been observed in some luminous IRAS galaxies and interpreted as due to shocks in a starburst environment (Lipari *et al.* 1993). The foregoing discussion shows the difficulties of dealing with elements like Fe and Ni with their complex atomic structures which result in thousands of lines.

As suggested by Antonucci & Miller (1985), scattering may help to explain the Seyfert 2 galaxies as heavily obscured Sy 1's. Lower ionization than in the Seyferts is found in the LINERS identified as a group by Heckman (1980). At first, these were believed to be shock excited objects, but Ferland & Netzer (1983) showed that photoionization with a softer radiation field could also explain the spectra.

Shocks produce a hot gas which tends to have a rather narrow range of states of ionization, unless very different shock velocities occur in the medium. Photoionization by power-law type radiation fields tends to give a broader range of stages of ionization, the energy of the highest ionization stages corresponding to the hardest photons in the ionizing spectrum. As a result, coronal lines may appear. Fe 6^+ was detected in the spectrum of NGC 1068 by Seyfert (1943), following its earlier identification in the planetary NGC 7027 by Bowen and Wyse (1939). In some Seyferts also Fe^{9+} and Fe^{10+} are seen in the optical. Many such lines are also found in the IR. Osterbrock *et al.* (1990) found [S VIII] at 0.99 μm, and Oliva *et al.* (1994) observed lines of Si^{5+}, Si^{6+}, Si^{8+}, S^{8+} and Ca^{7+} in the 1–4 μm region. Observations of such lines are particularly useful to ascertain the shape of the ionizing radiation field.

Variability in the recombination lines of a Seyfert galaxy was first found in NGC 3516 (Andrillat & Souffrin 1968), where the Hβ line had much weakened relative to [O III] since the first observations by Seyfert (1943). Many variable Seyferts have been found since. From IUE observations the variations of the ionizing radiation have been inferred. The variations in the emission lines show a time lag and this allows a determination of the characteristic size of the Broad Line Region which is found to be of the order of a pc for luminous Seyferts or weak quasars. Precise observations over long enough periods allow mapping of the BLR to be done. If moreover accurate line profiles are measured, also information about the kinematics in different parts of the BLR may be obtained. These variations provide a unique tool for resolving the BLR. Unfortunately they take much telescope time and are difficult to schedule at the larger telescope facilities. Recent results include the multi-author studies on NGC 3516 (Wanders *et al.* 1993), NGC 3783 (Reichert *et al.* 1994) and NGC 5548 (Peterson *et al.* 1994), as well as the line profile studies of Rosenblatt *et al.* (1994).

Absorption by dust makes the interpretation of the optical spectra more difficult and may render invisible part of the nuclear region of an AGN. In this respect observations in the IR have a major advantage. For example in Cygnus A an absorption of $A_V = 20$–80 magnitudes has been inferred (Djorgovski *et al.* 1991) for the nucleus which begins to be visible only for $\lambda > 2.4\ \mu$m. IR observations are also important for abundance observations. Some stages of ionization of common elements have no accessible lines in the optical part of the spectrum (Ne^+, etc.). Also the broader wavelength range obtained by including the IR sometimes gives very sensitive diagnostics. For example the intensity ratio of the [Ne III] lines at 15.5 μm and at 3869 Å changes by a factor of 100 if T_e varies from 5000 to 15000 K, essentially independently of N_e (Pottasch *et al.* 1984), while the ratio of the [Ne V] lines at 14.3 μm and at 3425 Å changes by a factor of 25 if N_e changes from 3×10^3 to 5×10^5 cm^{-3}, with only a relatively weak dependence on T_e (Pottasch *et al.* 1986).

Photoionized plasmas tend to have temperatures around 10^4 K. Much hotter conditions are found in supernova remnants, shock heated to 10^6–10^8 K or more, and in the chromospheres and coronae of stars (10^4–10^7 K). In both cases collisional ionization and excitation predominate, and accurate collisional cross-sections are essential.

Still much atomic physics is needed to understand the uv and X-ray spectra. For example, Arnaud & Raymond (1992) recently recalculated the ionization equilibrium of iron at 4×10^6 K. The abundance of Fe^{18+} turns out to be six times larger and that of Fe^{15+} six times smaller than in previous calculations, mainly because of improved dielectronic recombination coefficients. Such results are of importance in the calculation of abundances which in the solar corona sometimes show unexpected behavior. For instance it is found that the ratio of the Ne and Mg abundances in the solar wind is ten times smaller than in the photosphere (Widing & Feldman 1992).

Other effects that may be of importance include non equilibrium ionization and unequal temperatures for different plasma constituents. Delayed ionization in shocks was first noted by Itoh (1977) and turns out to be of essential importance in the interpretation of the X-ray spectra of supernova remnants. Inferred abundances of elements like Ca or Si could be in error by a factor of 100 or more if these effects are not properly taken into account. Similar effects may occur in the solar corona due to microflares (see the review by Mason and Monsignori Fossi 1994).

In young, rapidly expanding supernova remnants even the temperatures of the neutral H and of the proton gas may be very different. Chevalier and Raymond (1978) showed that charge exchange between the hot protons behind the shock separating the remnant and the interstellar medium and neutral H swept up by the shock may produce broad wings in the Balmer lines. These have actually been observed in Tycho's SNR and in SNR 1006 as well as in some remnants in the Large Magellanic Cloud. The narrow components in the Balmer lines would be due to collisional excitation of the neutral H before its ionization. However, the width of these narrow components (40 km s^{-1}) is much larger than would be expected for interstellar H atoms and some kind of a precursor would be needed to stir up the gas; the nature of this precursor is not understood (Smith *et al.* 1994).

Emission lines from cool gas (T < 100 K) are also of much importance in the interstellar medium and in particular in dense molecular clouds. Lines of H_2, CO and a plethora of molecules have been discovered at mm and submm wavelengths. Again, laboratory measurements are needed for line identifications, collisional cross-sections and transition probabilities. The large number of chemical reactions between complex molecules and the importance of the surface effects on dust grains make this a complex subject outside the range of this review. Of particular interest are the possibilities for measuring isotope ratios, but also here chemistry plays a confusing role.

At the other end of the spectrum are the gamma-ray lines resulting from nuclear decays. Observations are difficult because of the low photon fluxes and high instrumental backgrounds. The main observational results to-date include the lines from the $^{56}\mathrm{Ni} \rightarrow {}^{56}\mathrm{Co} \rightarrow {}^{56}\mathrm{Fe}$ decay in SN 1987A which lead to quantitative results concerning the iron production in supernovae (Teegarden 1994), the line of ^{26}Al in the interstellar medium resulting from (super)novae, W.R. stars, etc. (Diehl *et al.* 1994), the e^+e^- annihilation lines occurring in some ill understood objects (Churazov *et al.* 1994), and the decay lines of ^{44}Ti. The latter decay $^{44}\mathrm{Ti} \rightarrow {}^{44}\mathrm{Sc} \rightarrow {}^{44}\mathrm{Ca}$ has been observed in Cas A (Iyudin *et al.* 1994). Two different measured values for the lifetime of ^{44}Ti of 78 and 96 years lead to values of 3.2 respectively 1.4×10^{-4} $M_\odot$ for the production of Ti in the supernova. Again, the essential importance of accurate values for the nuclear constants is much in evidence.

The future

Order of magnitude improvements in the observation of emission lines may be expected in the near future, largely as a result of a number of forthcoming space missions. In the submm and IR part of the spectrum the Infrared Space Observatory—a 60 cm cryogenically cooled telescope—is scheduled to be launched late in 1995 by the European Space Agency. Among the instruments are spectrographs covering the wavelength range of 2.5–197 μm with spectral resolutions mainly between 100 and 20000. ISO should take observations for about 18 months. While much of the program will be concerned with cooler gas, observations of the emission line spectra of supernova remnants and of (dusty) AGN should also take place. ISO possibly will be followed by SOFIA (airplane) and SIRTF, two infrared facilities under consideration at NASA. FIRST—a 3-m telescope for submm observations (85–900 μm)—should be launched by ESA in 2006.

HST, IUE and the Extreme Ultraviolet Explorer should continue to produce spectral results, HST with high spatial resolution and IUE with easier availability for long time series. The spectroscopic capabilities of HST should become very substantially increased when STIS (the imaging spectrograph) is installed by NASA in 1997. STIS should give spectral resolutions from around 10^3 to 10^4 in the optical and 10^5 in the uv in combination with spatial resolutions of $0\overset{''}{.}12$–$0\overset{''}{.}06$. IUE has now been functioning for nearly two decades and there is some fear it may not live forever; its loss would be a severe blow to the mapping of the BLR in Seyferts.

The X-ray domain will be well served: Astro E (Japan), XMM (ESA) and AXAF (NASA) are all three scheduled for launch around 1999. The spectral resolution in these missions would be much better than available today (in the range of 100–1000), and as a result individual lines should be resolved in AGN, SNR (also with improved spatial resolution) and stars. More gamma-ray line observations should come from continued use of the GRO (NASA) and from INTEGRAL to be launched in 2002 by ESA.

Finally detailed spectra of the solar chromosphere and corona in the wavelength range 160–1600 Å should be obtained by SOHO, an ESA/NASA cooperative project to be launched in 1995. Spectral resolutions range up to 40,000 with angular resolution in the range of 2–3 arcsec.

As noted earlier, the IR is a particularly propitious wavelength region for the observation of emission lines in Seyferts, quasars and other objects, in part because it is still very much underexplored and in part because of the much reduced interstellar absorption. Space missions by necessity have relatively small telescopes and therefore poor angular resolution in the IR. It is in this area that the new large ground-based telescopes can make a major contribution. Also their high photon collecting power will allow the full dynamic range of the new optical detectors to be exploited and thereby fainter lines to be observed. As reported at this meeting by Péquignot, the first lines of elements beyond the iron group have now been observed in planetary nebulae and this may become a subject of importance for nucleogenesis.

Seeing the continuing stream of high quality data and new results on AGN obtained by Osterbrock and his many students, we can still look forward to much in the future. But all the observations of emission lines will be of no avail without reliable atomic data. We can only wish that Seaton and his many followers will continue the good work they have been doing during the past half century for the benefit of all of us.

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Atomic Data for the Analysis of Emission Lines

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Within the last decade or so new atomic data has become available for most atomic systems of interest in astrophysics. Recent progress in atomic processes relevant to spectral formation is reviewed and the data sources are listed. Recommended transition probabilities and effective collision strengths are presented for a number of nebular emission lines.

1. Introduction

In a pioneering study on the electron impact excitation of atomic oxygen, Seaton (1953) formulated the now well known close-coupling approximation of atomic collision theory, which he termed the "continuum state Hartree-Fock method", reflecting the physical picture that the new method was an extension of the bound state method to the continuum region that encompassed electron-ion scattering and photoionization phenomena. For nearly three decades, the close coupling approximation has been widely employed to calculate the most accurate low-energy cross sections for excitation and photoionization, and radiative transition probabilities. Large computational packages were developed, mainly at University College London and the Queen's University of Belfast, to carry out the enormous task of fulfilling the needs of astrophysicists and plasma physicists. In particular, the R-matrix method developed by Burke and associates (Burke *et al.* 1971) has proved to be computationally very efficient for large-scale calculations.

A huge amount of radiative atomic data was produced, during last 10 years or so, under the auspices of an international collaboration of atomic physicists and astrophysicists, called the Opacity Project, led by Seaton (Seaton *et al.* 1994). Photoionization cross sections and oscillator strengths were calculated using the R-matrix method (Seaton 1987; Berrington *et al.* 1987) for almost all astrophysically abundant elements in various ionization stages. The calculations were carried out for LS multiplets; fine structure was not considered as it is relatively less important for the calculation of stellar opacities, which was the express aim of the Project. Recently, employing the basic tecniques of the Opacity Project and new developments incorporating relativistic effects into the R-matrix method, a new project called the Iron Project has been initiated (Hummer *et al.* 1993) that aims to compute accurate cross sections for electron impact excitation of most astrophysical ions including fine structure. The main aim of the Iron Project is the calculation of precise atomic data for the Iron group elements that are astrophysically very important but for which little reliable data is presently available. Thus the Opacity Project and the Iron Project are now providing much of the atomic data needed by astronomers.

This report consists of a review of data sources for:

- Electron impact excitaton
- Photoionization
- Radiative transition probabilities
- Electron-ion recombination

For completeness, data sources are also given for line broadening, recombination lines, electron impact ionization, charge exchange, proton impact excitation, isotopic and hyperfine structure, and energy levels and wavelengths. With the exception of energy levels,

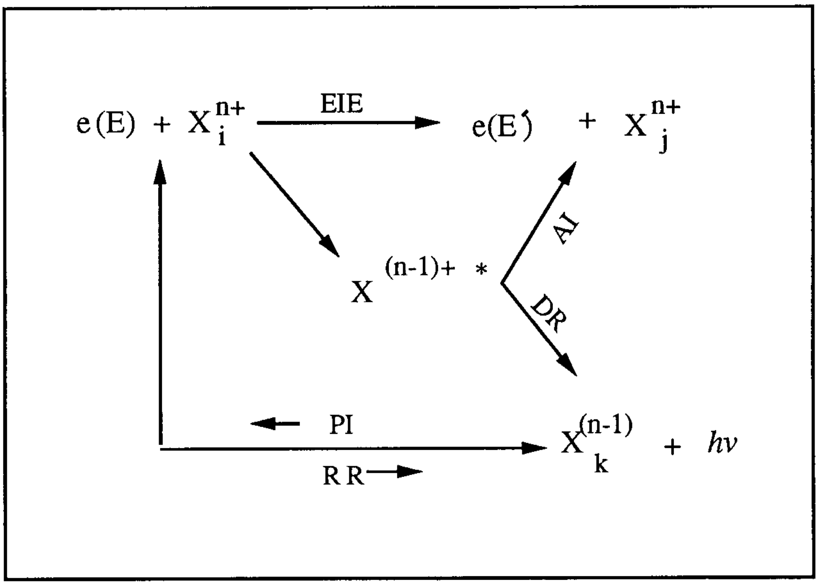

FIGURE 1. Inter-related radiative and collisional atomic processes: EIE - electron impact excitation, AI - autoionization, DR - dielectronic recombination, PI - photoionization, RR - radiative recombination

very little of the data is experimental; we confine ourselves mainly to a discussion of the theoretical data. A general bibliography for most of these atomic processes has been presented by Butler (1993).

The prominent spectral lines in nebular astrophysics are mostly due to forbidden transition among low-lying levels of atomic ions. In an attempt to update and extend the extremely useful compilation by Mendoza (1983) more than a decade ago, recommended data for electron impact excitation and transition probabilities for emission lines in AGN's, nebulae and other sources are tabulated.

2. Theoretical considerations

Electron-ion interactions may be depicted by the following diagram:

Quantum mechanically *all* of the atomic processes shown may be treated by a wavefunction expansion that represents the total e+ion system in terms of the coupled eigenfunctions of the "target" or the "core" states of the ion, i.e.

$$\Psi(E) = A\sum_i \chi_i\theta_i + \sum_j c_j\Phi_j, \tag{2.1}$$

where χ_i is the target ion wave function in a specific state $S_i\ L_i$ and θ_i is the wave function for the free electron in a channel labeled as $S_iL_ik_i^2\ell_i(SL\pi)$; k_i^2 being its incident kinetic energy. While the close coupling approximation (e.g. the R-matrix method) includes coupling between the target states of the ion, simpler approximations such as the distorted wave or the central field approximations neglect the coupling effects which may be important at low energies.

One particularly important coupling effect manifests itself as autoionizing resonances, from doubly-excited states of the e+ion system (the center of the Fig. 1), that can substantially enhance the cross sections and rates for excitation, photoionization and recombination. The near threshold region of the cross sections, that dominates the rate of electron excitation and line formation for forbidden and intercombination transitions, may be particularly affected by broad and extensive resonance structures. Dipole allowed transitions are less affected. In general therefore it is necessary to employ the accurate close coupling approximation for the forbidden and the intercombination lines, but for the dipole allowed transitions the distorted wave approximation often suffices to obtain rates to 10–30% uncertainty.

A brief discussion of a few points related to the atomic processes is given below.

2.1. *Electron impact excitation*

The quantity usually computed for electron impact excitation is denoted as $\Omega(i,j)$, which was introduced by Hebb & Menzel (1940) and later termed the "collision strength" by Seaton, in analogy with the line strength for radiative transitions. The Ω is dimensionless and symmetric with respect to initial and final states. It is related to the cross section as

$$Q(i,j;k_i^2) = \frac{\Omega(i,j)}{k_i^2 g_i}(\pi a_o^2), \tag{2.2}$$

in units of the area of the H atom.

The usually tabulated quantity is the maxwellian averaged collision strength, also called the effective collision strength,

$$\Upsilon(i,j) = \int_0^\infty \Omega(i,j) exp\left(\frac{-\epsilon}{kT}\right) d\left(\frac{\epsilon}{kT}\right). \tag{2.3}$$

The excitation rate coefficient, in cm^{3}sec^{-1}, is defined as

$$q(i,j) = \frac{8.63\times10^{-6}}{g_i T^{1/2}}\Upsilon(i,j) exp\left(\frac{-\Delta E_{ij}}{kT}\right), \tag{2.4}$$

related to the de-excitation rate coefficient ($E_i < E_j$) as

$$q(j,i) = \frac{g_j}{g_i} q(i,j). \tag{2.5}$$

The influence of autoionizing resonances may be seen in Fig. 2.

A detailed discussion on the analysis of collision strengths and rate coefficients is given by Burgess & Tully (1992), who describe analytic fitting procedures to $\Omega(E)$ and $\Upsilon(T)$ for interpolation and extrapolation in a compact form for the different types of transitions.

2.2. *Photoionization cross sections*

The availability of a very large number of photoionization cross sections from the Opacity Project is likely to influence considerably the modeling of radiative and collisional plasmas. There are two main features of these data: (i) inclusion of autoionizing resonances in the near-threshold region, (ii) cross sections for many excited states, typically several hundred bound states for each atom or ion. Prior to the Opacity Project, such data was available mainly for the ground states of relatively few ions, and the excited states were treated in either the hydrogenic approximation or with some Coulomb screening (such as in the quantum defect method).

Fig. 3 shows the photoionization cross section of a complex system, Fe II, illustrating the effect of resonances and the covergence of the close coupling wavefunction expansion. A total of 83 states of the core ion Fe III were included in the R-matrix (Nahar & Pradhan 1994a). In comparison, the central field calculations of Reilman & Manson (1979) underestimate the cross sections by several factors in the near threshold region, although at higher energy the discrepancy is relatively small. Comparison is also made