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A. Dalgarno
Chairman of Working Group

WORKING GROUP 4: LINE BROADENING

There has been quite a renewal of interest in the field of line broadening during the last three years and the proceedings of the Eight International Conference on Spectral Line Shapes (1) showed the general state of progress of this topic. It is not the purpose of this report to be exhaustive, so we will simply give a number of useful results for astrophysical purposes and indicate some new fascinating directions in this research theme.

1. Line Broadening and Shifts in Low to Moderately Dense Plasmas

1.1 HYDROGEN OR HYDROGENIC LINES

The ionic broadening of hydrogen or hydrogenic lines in plasmas has been considered as quasistatic during the last decades. In fact, this quasistatic ion assumption is only valid at quite high densities. At low or moderate densities, ion dynamics play an important role near the center as confirmed by new experimental results (2,3,4) for Lyman and Balmer lines. Computer simulations were employed successfully for investigations of these effects (5-8). In these computations, electron broadening is accounted for using an impact operator; the ionic contribution is obtained by numerical integration of the atomic Schrödinger equation for a set of ionic mocrofield formed by superposition of Debye-screened fields from uncorrelated particles. At typical astrophysical densities (smaller than 10^{14} cm^{-3} for Ly$_\alpha$) these results are in a relatively good agreement with analytic formulae giving the line halfwidth in the impact model (9). New calculations have been performed for the Ly$_\alpha$ profile for detunings ranging from the center to the near line wings (10) (< 10 Å). At these low densities, the fine structure splitting is not negligible and its subsequent effect on the profile has been investigated (11).

New theoretical data for the broadening of far infrared and submillimeter as well as radio (13) lines are now available.

The shift of hydrogen or hydrogenic ion lines (He II) in plasmas has become a subject of interest both from an experimental (14, 15) or a theoretical (17) point of view. This shift, important at high densities, becomes negligible in stellar atmospheres conditions.

In spite of these results, much work remains to be done in the future and particularly extensive results for Lyman, Balmer and Paschen series are required.

1.2 STARK BROADENING OF ISOLATED LINES IN MODERATELY DENSE PLASMAS

First it is necessary to present the Opacity Project in (1) page 583) which represents a major new effort to make extensive calculation of atomic data required for opacity determination. Professor M.J. Seaton assumes the responsibility of this project which is being pursued by research groups in Belfast, Boulder, Caracas, London, Munich, Paris and Urbana. The work includes accurate calculations of atomic energy levels, oscillator strengths, photoionization cross-sections and parameters for Stark broadening of spectral lines. For atoms (except H) or non hydrogenic ions, the dominant contribution to the broadening is likely to be due to electronic collisions. According to plasma line broadening theory, these electron impacts induce a Lorentzian line profile whose width given in terms of elements of the scattering matrices. The R-matrix method of computation chosen in the Opacity Project allows computation of elements of the scattering matrices. However it is not practical to use close coupling methods to calculate line broadening parameters between highly excited states. So it is proposed to make systematic studies of these parameters for transitions between states that are not too highly excited in order to obtain approximate formulae which can be used for the highly excited states. Such calculations are already under way for various isoelectronic sequences and will be published in Journal of Physics B. This work seems of particular interest for theories of stellar structure and stellar pulsations.

Another interesting and complementary direction for research concerns investigations of systematic trends of Stark broadening parameters as function of the principal quantum number and the ionization potential. Regularities of these parameters within a multiplet or a supermultiplet or within spectral series and homologous atoms have been investigated (18-23) in order to provide a simple method for critical evaluation of existing data and interpolation of new data. These regularities in Stark broadening parameters are directly related to regularities in the atomic structure, so one can expect that these studies become inadequate for complex atoms, when a large configuration mixing strongly perturbs the levels. Semi empirical methods have also been developed for ion lines (24-28) and neutral atom lines (29). Such approaches which give a good average accuracy while the accuracy for a particular line is rather poor, allow a rapid estimation of the width and may be very useful for evaluating a large amount of data.

2. Hot and Dense Plasmas

The study of spectral line profiles in hot and dense plasmas is one of the major subjects of research in the field of line broadening. In recent years, renewed interest has mostly been stimulated by inertial confinement research. Astrophysics should greatly benefit from this effort especially the physics of white dwarfs or neutron stars.

An interesting theoretical work on the so called "ion dynamics" effects on the broadening has been done by various approaches. The problem of incorporating time dependent many body ionic interactions is well taken into account by computer simulations. The field can be accurately approximated by Monte-Carlo or molecular dynamics simulations (46). It has been shown that the effects of ion dynamics may be of the order of or larger than the Doppler effects. However such computer simulation methods are computer time consuming and it appears quite important that other theoretical approaches namely the Model Microfield Method (47) or semi-analytical methods (48) should be developed at the same time. Fine structure effects (49-52) as well as coupling between Doppler and Stark broadening (46) have been investigated.

Another important problem arises in these plasma conditions as strong correlation effects appear between the internal structures of the radiating ions and the perturbing plasma. In this field ions are assumed to be static and the electric microfield produced by screened ions induces the Stark effect and causes the spectral series to merge. Correlations can be included in the microfield distribution function using a pair correlation function which yields the Debye Hückel theory at moderate densities for weakly coupled plasmas and the results obtained by Monte-Carlo method for strongly coupled plasmas (53). The ionic microfield leads to frequency shift and line broadening, and produces a potential barrier which leads to an advance of the recombination continuum and to an ionization of bound states by tunnel effect corresponding to attenuated line intensities. Actually, the physical limit between bound and free states becomes a function of the density and the temperature of the surrounding ions (54). Such studies lead to interesting improvements of the Inglis Teller formula.

Moreover there has been a controversy about the "plasma polarization shift" which must be described by an unified approach (55-57). This shift may be significant at large densities and for heavy stripped radiating ions. For densities close to the solid state densities the mean free path might be reduced to values smaller than the wavelength of the line leading to some reduction of the thermal Doppler broadening (58). But we have yet no experimental test of this assumption.

3. Line Broadening by Foreign Gases and Molecular Line Broadening

As the broadening of the sodium D lines by collisions with atomic hydrogen is very important in the studies of the chemical composition of the Sun and other stars, the determination of the width and the shift of these lines has been the subject of many experimental (59) and theoretical (60) efforts. All available theoretical and experimental results have been reviewed (61). According to the discussion given here, it appears that the latest experiment (59) agrees well with empirical determination obtained from the solar spectrum. No fully satisfactory theory exists, due essentially to inaccuracies in the intermediate range of the relevant interatomic potentials inducing the broadening effect. This particular case illustrates quite well the general situation of the atomic line broadening theory: methods for the description of detailed dynamics are efficient and accurate but depend drastically on molecular structure calculations. An important effort concerning interatomic potentials is continuing and there is now a very good agreement with experimental results for alkali-metal-atoms + rare gas systems (62) indicating large improvements on all previous results when accurate potential data are available. Therefore, one can observe that the physicists' present preoccupations are far from astrophysical applications owing to this particular difficulty. There is a great need for work in this topic.

Concerning pressure broadening of molecular lines, many important results have been obtained; for astrophysical purpose we will quote particularly the calculation of the line widths of H_2O (63), N_2 and H_2 (64) broadened CO rovibrational lines, an experimental determination of collision broadened half widths of lines of the ν_9 fundamental band of C_2H_6 (12μm) (65,66). This band seen in the spectra recorded on board Voyagers 1 and 2 is an important emission feature in the thermal infrared spectrum of Titan. Measurements of pressure broadened half width have been performed for some vibration rotation lines in bands of methane (67a,b) and ammonia (68a,b). These results are of particular importance for the modelling of planetary atmospheres. The measurement of line strengths and pressure broadening coefficients of the ν_3 band R_0 and R_1 transitions of GeH_4 (69) allows the interpretation of recent observations in the atmospheres of the outer planets. Studies on the collisional broadening of H_2O (70, 71) lead to precise knowledge of water absorption required in atmosphere physics applications and for space investigations.

Owing to recent observations recorded by Voyager space craft in the infrared region, many rototranslational collision induced spectra have been obtained both experimentally and theoretically for H_2-H_2 (72),N_2-N_2 (73),N_2-H_2 (74), H_2-He (75), CH_4-H_2 (76). There is an overall good agreement for the features of free-free, free-bound and bound-bound transitions. This work is of interest for the modelling of Titan's atmosphere in the far infrared and for the determination of the vertical temperature spectra. These results will convince easily the reader that recent molecular broadening studies lead to very fruitful collaboration between physicists and astrophysicists.

4. Collisional Redistribution of Radiation and Related Topics

Collisional redistribution has been reinvigorated these last years by much experimental and theoretical work, and has been reviewed recently (79). From a theoretical point of view, the processes of absorption or emisison of radiation when collisions occur lead to different problems such as the statistics of the collision events, the correlation between photons absorbed and emitted during the same collision, the modification of atomic collision dynamics in intense fields. In view of astrophysical interest, we will focus our attention on the problem of redistribution of weak radiation at low perturber densities. It has been shown (79,80) that absorption during a collision can be thought of as populating the molecular states of a transient molecule. The observed fluorescence comes either from the same collision leading to the possibility of correlated photons or from another collision corresponding to less correlated events.

The mechanism of collisional redistribution is now understood and the theoretical description is well established (81,82). Many experimental and theoretical results have been devoted to simple systems (Sr, (83,84) or Ba (85,86) or Na (87-89) perturbed by rare gas atoms) with a particularly good agreement for redistribution of polarized radiation studies when accurate interatomic potentials exist (Na): the dependence of the far wing excited state orientation or alignment versus the detuning can be interpreted in terms of reorientation of molecular orbitals o-curing during the collision. Contrarily to some appropriate model predictions, depolarization may not be total in the far wings and depends on the details of the collision. Obviously, such work is of interest for the problem of polarized line radiation transfer for which the first experimental result has been obtained (90). Redistribution by hydrogen in plasma requires a very complicated formulation and more work is needed in this topic. It is interesting to notice that collisional redistribution and photodissociation processes are closely related problems.

Beside this field of research, one may stress the progress of theoretical work along new interesting directions such as the theory of Stark broadening in the presence of magnetic fields (91) and more generally the study of spectral lines in plasmas in the presence of external fields or turbulence (92). A workshop on "Spectral Line Formation in Plasmas Under Extreme or Unusual Conditions" has been devoted to this subject, invited papers will be published in J.Q.S.R.T. Finally, there has been some new work concerning the computation of the Voigt function (93,94).

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N. Feautrier
Chairman of Working Group

WORKING GROUP 5: MOLECULAR STRUCTURE AND TRANSITION DATA

Research in molecular spectroscopy has continued to grow over the past three years. The spectral range has expanded from the far ultraviolet to millimeter wavelengths. The report has been limited to molecular spectroscopy of relevance to astronomy and has been compiled from edited contributions sent to me in the fall of 1987.

Sumner P. Davis and John G. Phillips have reported studies at the Berkeley laboratory on the molecules C_2, CN, FeH, InI, SH, Si_2, SiC_2, $TiC\ell$, TiO, ZrO, ZrS of either analysis of spectral structure or measurements of lifetimes and oscillator strengths. FeH is of special interest. A complete table of excitation energies for its complex infrared system has been prepared, and a set of tables for far infrared and radio wavelengths assembled to predict spectrum lines which may exist in stellar spectra or in the spectrum of matter in interstellar space. Underway are analysis of the blue-green system of the FeH molecule, measurements of radiative lifetimes for FeH, radiative lifetimes of CaH, transition strength for A-X and B-X systems of CaH, measurement of $CaC\ell$ transition strength (collaboration with J.E. Littleton), analysis and tabulation of infrared OH and OD bands (collaboration with R. Engleman) and analysis of ZrS in the infrared (collaboration with R. Winkel).

The bimonthly Berkeley Newsletter on Analyses of Molecular Spectra compiled by Davis, Phillips and Eakins continues to be the invaluable, timely bibliography of molecular spectra. There is about 150 recipients of the Newsletter.

Takeshi Oka has reported from the University of Chicago, laboratory spectra observed of the following molecular ions, H_3^+, H_2D^+, HeH^+, NeH^+, ArH_3^+, NH_4^+, NH_3^+, NH_2^+, H_3O^+, H_2O^+, OH^+, $HCNH^+$, CH_3^+, $HCCH^+$, $C_2H_3^+$, OH^-, C_2^-. A search for interstellar infrared absorption spectrum of H_3^+ was conducted; the result is inconclusive though promising.

Kurt Dressler has reported from ETH Zurich work on the electronic transition