

SUMMARY OF THE JOINT DISCUSSION

Atomic Data of Importance for Ultraviolet and X-Ray Astronomy

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Abstract. This Joint Discussion is in two parts. The first part is a description of recent observations which illustrate the need for atomic data and the second part is a description of what atomic data are available or could readily be produced by the latest theoretical and experimental methods. The purpose of this summary is to highlight the immediate requirements for atomic data of current observations which are not met by our present knowledge and thereby indicate where further work is necessary in providing atomic data.

Although this is a discussion of atomic data the problems of assuming local thermodynamic equilibrium have inevitably been raised. The importance of considering whether departures from LTE are significant or not in the interpretation of observations is clearly illustrated by the work of the Harvard group on the Lyman continuum emitted by the Sun which has shown a departure coefficient as large as 200 for the ground level of hydrogen.

1. Line identification

As new observations are made line identification will be a continuing problem. Although rapid progress has been made in line identification there are still some old outstanding problems, for example the diffuse interstellar absorption lines discovered 25 yr ago are still not identified though recently there have been suggestions of auto-ionizing levels.

Because of the low density of radiation and matter in interstellar space, the interstellar ions will be observed only in their resonance lines. Further work would be useful on specifying the resonance lines of the lowly ionized stages of the more common elements.

It is the Sun that has really provided most of the work recently in line identification. Only about half of the coronal lines measured at an eclipse several years ago by Jefferies have so far been identified. The recent joint experiment which gave the first flash spectrum in the ultra-violet has given many new lines. Even one of the brightest lines in the spectrum was not immediately identifiable. Most of the new coronal lines in the region 1000–2000 Å are probably forbidden transitions between levels of ground configurations. Further work is needed on intersystem lines, particularly in the Mg I, Al I, Si I and Cl I sequences.

There are many lines of photospheric absorption obtained at high resolution in the region 2000 Å to 3000 Å which require further work for their identification.

Perhaps the most exciting developments have been flare spectra obtained by satellite observations in the range 1 Å to 2 Å which have produced identifications of lines of ions like Fe XXV, Fe XXIV, Fe XXIII. Future work on flare spectra is sure to produce more problems of interpretation in this interesting region.

The problems of line identification in UV stellar spectra are only just beginning.

In the spectrum of a BO supergiant between 1000 Å and 2000 Å only about half the lines have been identified.

2. Transition Probabilities and Collisional Cross-Sections

Considerable progress has been made here in recent years. Transition probabilities have been determined theoretically and experimentally and furthermore the numerical values have been critically tabulated by the group at the National Bureau of Standards. There remains perhaps a gap in the transition probabilities available for some of the subordinate lines observed in stellar spectra.

The calculation of line blanketed stellar models requires a knowledge of many hundreds of gf -values for the absorption lines present in a given star. The need here is perhaps for some statistical representation of the lines important in a line blanketed model which will allow the temperature structure of a model atmosphere to be calculated accurately. The profiles of individual lines are then easily computed individually for comparison with the observations.

The interpretation of each of the many lines emitted by the solar transition region and corona requires the knowledge of a large number of cross-sections for collisional ionization, excitation and dielectronic recombination. Fortunately computer programs are now available which can calculate many excitation cross-sections. Recent observations of the Sun need particularly the excitation cross sections for the forbidden lines that might occur in the coronal spectrum.

There is an even greater need for the comparison of cross-section calculations with experiment or observation. The recent work at Culham and Harvard on the interpretation of Beryllium-like ions shows difficulties, which may be due to a lack of knowledge of the physical conditions of that part of the Sun emitting these lines, but which may also be due to inconsistencies in the cross-section calculations.

3. Photo-Ionization Cross-Sections

The most persistent demand in this Joint Discussion has been for further work on photo-ionization cross-sections.

Further study of interstellar ions requires the photo-ionization cross-sections of the ions present, and particularly of the ions of carbon and silicon, so that the ionization balance of interstellar matter under the influence of ionizing radiation from the stars can be calculated.

Recent UV observations of the Sun and stars have brought conflicts between the theory and the observations. The observed C I and Si I edges in Sirius require either a larger abundance or a different photo-ionization cross-section.

There is a discrepancy of 10% between the observed continuum between 1700 Å and 2100 Å and the theory which included the photo-ionization of silicon, carbon and sulphur in Gingerich's solar model atmosphere. In particular the calculated Si I edge is much too large. These discrepancies could be removed by including

line blanketing or by some extra source of opacity such as carbon monoxide.

There is a discrepancy of a factor of 3 between the calculated and observed continuum in the range 2500–3500. Is the MgI photo-ionization cross-section wrong? Is there some other source of opacity? Is the solar model wrong? Or is there an experimental error?

4. Pressure Broadening

While the theory of pressure broadening seems well established for a few of the important lines, there seems to be a lack of good pressure broadening calculations for the bulk of lines observed in UV stellar spectra. Observations of lines of ions like CIV, CIII, SiIV, FeII, etc., in the range of 1000 Å to 1800 Å from hot stars do not agree well with the calculations. The calculated line shapes do not agree with the observations nor do the temperatures of the stars for which the lines have a maximum intensity agree with the calculations, though this may well be explained by the importance of departures from LTE in the stellar atmosphere.

Recent experimental work of D. Burgess on the measurement of the absorption profile of $2P-4F$ forbidden line of HeI at 4470 Å does not agree with the latest theories, and this discrepancy is supported by the recent comparison of the calculated profile with the profile measured in some hot stars by Snijders and Underhill. There is clearly need for further work on the theory of pressure broadening of such forbidden lines.

Lastly in calculations for interstellar hydrogen there is the question whether the usual Lorenz profile is valid at 10^4 damping widths from the centre of the line.

5. Molecules

Very little is known about collisional processes and transition probabilities for molecules. These are becoming increasingly important. CO is a favourite molecule for increasing certain opacities in the Sun.

An increasing number of molecules have been observed as absorption lines from the interstellar matter, one of the most recent being H₂. There is much that still needs to be known about the wavelengths, transition probabilities and collisional excitation rates of the types of common molecules that might be expected in interstellar matter. A study of similar molecules is also needed for model atmospheres of cool stars.

Although maser action is perhaps now accepted as an explanation of the 18 cm emission of OH from HII regions, there is still no accepted theory for the formation of the OH ions and their excitation.

6. Other Processes

There are some other atomic processes which should be remembered in a joint discussion on atomic data. In the study of the ionization balance of interstellar matter,

ionization and excitation by cosmic rays having energies of many MeV appear to be important.

Auto-ionization can affect the ionization balance of some species, not only by increasing directly the rate of ionization, but also by the contribution of the inverse process to dielectronic recombination.

7. Dissemination of Atomic Data

In many respects the production of atomic data is coming to the manufacturing stage. There are computer programs available now which can compute a wide variety of atomic data, and some experiments also produce a large volume of data.

One might doubt whether the open literature should be burdened with such a large weight of data. Perhaps it would be better disseminated by other means. The setting up of data centres for atomic data is already being considered.

However there is certainly a need for good review articles which describe the physical basis of the present computational methods in a way that the general reader can understand.

There is another problem connected with the very flexible computer programs now developed, that is that the production work will last many years. This is obviously much less fun for the authors than the original development. There are those who advocate "every user his own computer program." This probably considerably underestimates the difficulties of running somebody else's computer program as a black box even on a slightly different machine. This would also lead to a very wasteful duplication of atomic data calculations. There is no doubt however that offers by groups to cooperate in a systematic fashion in the production work will be very gratefully received.