Physics of Formation of Fe II Lines Outside LTE

R. Viotti
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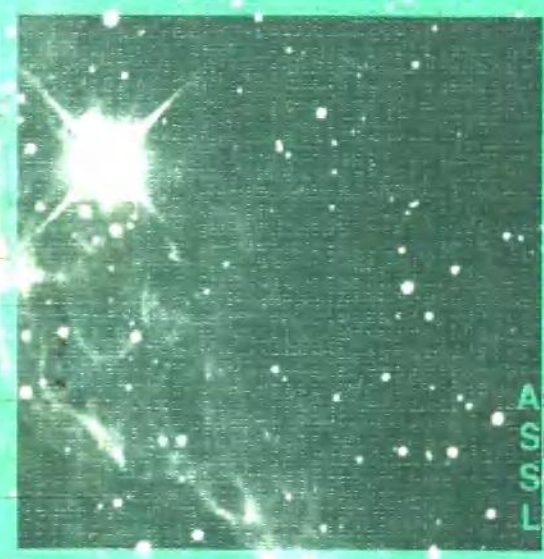
(editors)



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PREFACE

The same kind of physics is frequently common to very different fields of Astrophysics, so experts in each of these fields have often much to learn from each others. It was therefore logical that the International Astronomical Union should sponsor a colloquium about an ion which produces many spectral lines that can be used as a diagnostic for many sorts of objects, and which may sometimes have a major influence on physical processes occurring in astrophysical sources.

The lines of singly ionized iron (FeII) are present in absorption and emission in the spectra of objects such as the Sun, cool stars, circumstellar envelopes of hot stars, novae, diffuse nebulae including the supernova remnants, and active galactic nuclei. These lines are very often formed far from LTE, and their interpretation is not easy in view of the complex Grotrian diagram for FeII, and the gaps in the knowledge of various physical parameters. In addition, the density of very strong FeII lines becomes very large in the ultraviolet, and the lines can play a major role in the line blanketing. They need therefore to be taken into account in any energy balance argument.

This volume presents the proceedings of what we think to have been only the second meeting on this subject (*), and the first sponsored by the International Astronomical Union. Specialists in many different fields came to the Capri Colloquium on the 'Physics of Formation of FeII Lines Outside LTE' and gave their contribution to the discussion on many aspects of the problem. Different sessions of the colloquium were devoted to: (1) Basic atomic data. (2) Observation of FeII in different astrophysical objects from the solar photosphere to stellar chromospheres and winds, from novae to active galactic nuclei. (3) Theory of line formation and models, including data analysis techniques and spectral synthesis. (4) Prospects of future research, including new laboratory work, ground and space observations.

There were 29 invited and contributed papers and 13 posters. Each talk was followed by lively discussions which unfortunately could not be included in the proceedings owing to the constraints on the size of the book.

(*) A previous meeting on FeII was organized by M. V. Penston at the European Space Agency IUE Station of Villafranca (Madrid, Spain) on 3-5 October 1979, and was reported in Nature, Vol.282, p.557 (1979).

Both recent progress and outstanding problems were highlighted. Work is still very much humpered by the lack of good atomic data. Though oscillator strengths are beginning to be well known, much work is still required on collision strengths and particularly on ionization parameters. Nobody seems to be working on the latter, while the difficulties of interpreting the FeII spectra of active galactic nuclei could be only due to badly known physical quantities. In addition, theory and observations are often far apart; the theoretical calculations of line intensities and semi-empirical methods of analysis of observed line intensities, need to be brought closer together. Thus much work still remains to be done before the 'FeII Problem' can be considered to be solved.

This Colloquium was sponsored by IAU Commission 29 (Stellar Spectra), and co-sponsored by IAU Commissions 12 (Radiation and Structure of the Solar Atmosphere), 14 (Fondamental Spectroscopic Data), 36 (Theory of Stellar Atmospheres) and 48 (High Energy Astrophysics). We would like to thank the Presidents of these Commissions for their support.

We are very grateful to the many organizations which also sponsored the Colloquium, the Osservatorio Astronomico di Capodimonte, the Consiglio Nazionale delle Ricerche, the Istituto Astrofisica Spaziale, the Ministero della Pubblica Istruzione, and the Regione Campania.

The scientific organization was undertaken with the enthusiastic help of all the members of the Scientic Organizing Committee, and largely profited for the wide use of the Earnet/Bitnet computer network. From this point of view we believe that this was the first international meeting for which this network has placed such a large role.

We are indebted to the Local Organizing Committee for making perfect arrangements on the island of Capri. We have also greatly appreciated Lidia Barbanera, Teresa Ievolella and Dario Mancini for their helpful cooperation before and during the meeting.

The Editors.

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GENERAL INTRODUCTION TO THE "FE II PROBLEM" *

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ABSTRACT. A largely historical introduction is given to selected problems connected with observations and interpretations of iron lines in astronomical objects.

1. INTRODUCING THE LINE-RICH AND UBIQUITOUS SPECTRUM OF FE II

When asked to give a general introduction to the topic of this Colloquium, I was reluctant to accept because it seemed to me that everyone but me knew what the "Fe II problem" is. Assured, however, by Dr. Viotti that I would be essentially free to decide what to say and that a historical and even subjective introduction would be welcome, I'm going to try to present to you some old and new problems associated with iron in the universe. In this, I will not say much about to atomic physics aspects of Fe II as this is dealt with by the next speaker.

Why is it that Fe II attracts so much attention that an entire IAU Colloquium is devoted to this ion? First, iron is one of the abundant elements in the universe. With an abundance by number of $3\cdot 10^{-5}$ of that of hydrogen, it ranks only after H,He,C,N,O, and Ne in the solar composition, and is comparable in abundance to S,Mg, and Si. Then, Fe II has a very line-rich spectrum and the laboratory work on it is by no means completed. Numerous allowed and forbidden lines show up in the optical range and have long been observed in a variety of astronomical sources (cf. the Grotrian diagram by Merrill, 1956). In recent times, also the ultraviolet lines of Fe II became accessible to observation, mostly through satellites.

The richness in lines of Fe II originates in its about half-filled 3d-shell. Let us compare Fe II (ground configuration $1s^2 2s^2 2p^6 3s^2 3p^6 \cdot 3d^6 4s$) with Ca II in the ground state of which ($1s^2 2s^2 2p^6 3s^2 3p^6 \cdot 3d^0 4s$)

* This paper is dedicated to the memory of *Johannes Richter* (1925-1986) of the Institut für Experimentalphysik, University of Kiel, whose measurement of oscillator strengths for iron and other elements has helped to put astronomical spectroscopy on a firmer foundation.

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the 3d-shell is not occupied. While in Ca II between the three lowest terms $3d^0 4s\ ^2S$, $3d\ ^2D$, and $3d^0 4p\ ^2P$ two multiplets with together five (allowed) line transitions occur, namely the H and K lines and the infrared triplet around 8500 Å, the number of terms in Fe II is increased to 24 for the $3d^6 4s$ configuration, to 8 for $3d^6 \cdot 3d = 3d^7$, and to 68 for $3d^6 4p$ leading to far more than 10 000 lines if one further accounts for the increased multiplicity (maximum 6).

At last, the excitation and ionization conditions for populating Fe II levels are very favourable in a great number of astronomical objects. Due to the ionization potential of 7.9 eV for Fe I and 16.2 eV for Fe II, moderately hard ultraviolet photons ($\lambda \lesssim 1570$ Å) are sufficient to ionize neutral iron,and temperatures between about 5000 to 20 000 K are typical for producing strong Fe II lines. Consequently, we observe Fe II absorption lines in stellar photospheres of "intermediate" temperatures, and a few lines absorbed by the interstellar medium. Allowed as well as forbidden Fe II emission lines arise from thin "envelopes" around a variety of objects such as novae and supernovae, Be stars, T Tau stars, symbiotic stars, the solar and stellar chromospheres, H II regions, and the active nuclei of Seyfert 1 galaxies and quasars. Particularly complicated Fe II line profiles comprising emission and absorption components are observed in variable supergiants like S Dor and η Car.

This ubiquity and variety of Fe II lines in the universe makes their analysis such a fascinating topic. Furthermore, the interpretation of the complicated spectrum of Fe II demands "interdisciplinary" collaboration, in particular between atomic physicists and astrophysicists to provide the large amount of atomic data required for the kinetic rate and radiative transfer equations.

2. EARLY SPECTROSCOPY

After I. Newton's discovery of the spectral dispersion of the white sunlight in 1666, it still took about 150 years before spectral *lines* were observed. While in 1802 W. Wollaston could resolve 7 lines (or groups of lines) in the solar spectrum, by 1812/14 thanks to improved instrumentation J. Fraunhofer succeeded in seeing 10 strong lines (named A a B C D E b F G H) and almost 600 fainter absorption lines, among them the "d line" at 4383.6 Å which is - as we know today - the strongest Fe I line.

The first successful photographic recording of the Fraunhofer lines was accomplished by E. Becquerel in 1842. In the same year, Ch. Doppler formulated his law of the change of wavelength according to relative motions which could later be verified by astronomical observations of radial velocities.

The long-standing problem of the origin of the Fraunhofer lines required many steps (e.g. by L. Foucault 1849, A.J. Ångström 1855) before the "discovery of spectral analysis" by G. Kirchhoff and R. Bunsen (1859) in Heidelberg opened the door for quantitative spectroscopy. Kirchhoff and Bunsen themselves succeeded 1860/61 with the first spectroscopic discovery of new elements in terrestrial material, of caesium and rubidium, named after their blue-gray and red lines, respectively.

Already in 1861/63 G. Kirchhoff performed the first analysis of the solar spectrum by comparing the Fraunhofer lines with the laboratory spectra of 33 elements most of which had been recorded by himself. In particular, the coincidence of 60 lines in the spectrum of iron with solar lines established the existence of this element in the photosphere without any doubt. (Fortunately, this procedure was successful because the Sun is a relatively cool star with ionization and excitation conditions not greatly different from those in the laboratory sources).

From the 1860s onward, stellar and nebular spectroscopy made rapid progress due to the work of W. Huggins, W.A. Miller, L.M. Rutherfurd, A.Secchi, G. Airy and others. It was soon recognized that everywhere in the universe the same elements are found as on Earth. The observations of previously unknown spectral lines in astronomical sources were repeatedly attributed to "new" elements. In the case of helium, the "solar element", observed by the 5876 Å line in the chromospheric flash spectrum at the eclipse of 1868, a new element was actually discovered, in other cases, discoveries led to the recognition of unusual physical conditions such as the "nebulium" lines 4957/5007 Å and the "coronium" line 5302 Å which only decades later could be identified as forbidden lines of O III and Fe XIV, respectively.

Shortly before the discovery of the electron in 1897 by J.J. Thomson, N. Lockyer noted that the "white stars" exhibit the socalled enhanced or spark lines and put forward the hypothesis that the atoms are composite and break up at high temperatures to yield proto-elements, e.g. proto-iron or, as we would say today, Fe II. Perhaps we may define 1897 as the birth year of the Fe II problem?

The theory of ionization in stellar atmospheres was not formulated until 1920 by M.N. Saha.

3. EARLY QUANTITATIVE STELLAR ANALYSES

Quantitative spectroscopy became possible when from the 1920s onward quantum mechanics began to provide the necessary physical background, in particular absorption coefficients, oscillator strengths, data on pressure broadening etc.

The extensive pioneering analysis of the solar spectrum by Russell (1929) still had to be based upon eye estimates of the Fraunhofer line intensities which were calibrated by means of relative intensities within a multiplet, furthermore absolute f-values were not yet available. Nevertheless, Russell was able to derive solar abundances which are remarkably close to the modern values. In particular, he found that Fe, Mg and Si have about the same abundance.

Russell's deep insight into the line formation in a stellar analysis may be illustrated by a few quotations from his Halley Lecture (Russell, 1933): "Only a fraction, often a very small fraction indeed, of the atoms of a given element are at work in the production of a given line. They must be not only of the right degree of ionization but in a definite state of excitation, and, even so, some will produce one line and some another, in accordance with definite transition probabilities".., "The absence of many familiar elements from the solar spectrum, which was long unexplained, is now easy to understand. It arises, not in the sun at all, but in the earth's atmosphere. A small but mischievous amount of ozone in the higher regions, utterly beyond the reach of aircraft or even of sounding balloons, cuts off all entering radiations shorter than 2,900 Angstroms. This is the great tragedy of terrestrial astrophysics, for the region thus hopelessly barred to us contains more of interest and importance than any other part of the spectrum".

Russell determined an ionization potential of 8.5 eV of "an element whose atoms would be just half ionized" and recognized that e.g. iron is mostly singly ionized in the photosphere : "A great majority of the metals have ionization potentials lower than this, so that they are preponderantly ionized in the sun. Yet the solar spectrum is usually described as characterized by the arc lines of the metals. The earth's atmosphere is again to blame. For most of the richer metallic spectra... the strongest enhanced lines lie beyond λ 3,000, and are missed out. Could we enter the forbidden region, we would doubtless find the enhanced lines stronger. Only one group of the greater ones is accessible - the H and K lines of Ca^+. These dwarf all other observable lines; but the great magnesium pair at 2795, 2802 - just out of reach - probably much surpass them". A remarkable prediction of ultraviolet line strengths!

Problems with the determination of the abundance of the dominant element H in the sun could be resolved when Wildt (1939) relized the negative hydrogen ion as the main absorber.

The first detailed quantitative analysis of a stellar spectrum, that of the BO V star τ Sco, was performed by Unsöld (1941/44). The interesting question of the iron abundance in such a hot, young star could hot be answered at that time as the spectral resolution was not sufficient to recognize the faint Fe III lines.

4. REMARKS ON FE II EMISSION LINES

In view of the contributions by Dr. Gratton and Dr. Viotti at this Colloquium, I will restrict myself to only a few remarks on the early quantitative analyses of iron emission lines.

The observations of 1937/39 of the emission lines of H, He I, and Fe II in the Be star γ Cas were analysed by Wellmann (1951). Of the 21 Fe II lines between 4173 and 5317 Å neither b-factors nor absolute f-values were known. By assuming a common b-factor for the levels and applying relative f-values within multiplets and supermultiplets, however, Wellmann could draw the following conclusion: the dilution factor W is important for the line strengths; due to the spread in radial velocities there is hardly any self-absorption; the emission originates from a region separated from the star, and iron is dominantly in the form of Fe III. Characteristic parameters are $W \simeq 10^{-2}$, electron density $N_e \simeq 10^9$ cm^{-3}, and $T \simeq 15\ 000$ K.

Regarding the interpretation of forbidden Fe II lines in the sun and stars, e.g. in η Car, I mention the work of Pagel (1968) and Viotti (1969).

5. THE "IRON PROBLEM" OF THE 1960s

Based upon improved observational material Goldberg, Müller and Aller (1960) published a very detailed analysis of the solar photospheric spectrum. In order to derive element abundances they utilized a model atmosphere in combination with weighting functions and collected the measured and calculated oscillator strengths which had by then become available in increasing number. The abundance of iron was determined from Fe I only, using the relative f-values of King and King (1938) and Carter (1949) on the absolute scale of Bell et al. (1958). The result was lg N(Fe)/N(H) = 6.5 with the usual normalization lg N(H) = 12.0 (and the small correction by Zwaan, 1962). In contrast to Russell's (1929) earlier result and to the meteoritic data where Fe and Si are of comparable abundance, this new abundance of iron came out about a factor of 10 lower. The problem became more serious in 1963/67 when - after the pioneering work of Woolley and Allen (1948) - detailed studies of the abundances in the solar corona by Pottasch (1963/64) and Jordan (1966) yielded a high iron abundance of about 7.5. A similar value also resulted from the forbidden photospheric [Fe II] lines (Swings, 1965).

It is interesting to recall that Groth (1961) derived a "high" iron abundance of 7.5 from low-excitation Fe I lines in the supergiant α Cyg (A2Ia). He considered this as a probably real deviation from the solar abundance.

As we have seen, Fe II is the dominant ion in the solar photosphere so that it would be best to use its lines to derive the iron abundance. Oscillator strengths, however, became available only by Roder's (1962) experimental work (besides "astrophysical" f-values). Roder's absolute scale was linked to that of the Fe I socillator strengths. However, since photospheric Fe II lines yielded an iron abundance which differed from that based on Fe I lines, Baschek et al. (1963) suggested a correction to Roder's absolute f-values - unfortunately a wrong conclusion due to their belief in the correctness of King and King's Fe I oscillator strengths.

The solution of the solar iron problem emerged around 1967/69 by improved and new experimental methods to measure f-values, e.g. wall-stabilized arcs (Garz and Kock, 1969), shock-tube measurements (Huber and Tobey, 1968; Grasdalen et al., 1969), and beam-foil techniques (Whaling et al. 1969) and resulted in a revision of the Fe I oscillator strengths of King and King whose high-excitation lines turned out to be systematically too large (corresponding to an error in their furnace temperatures by a few 100 K). With the revised f-values, the photospheric iron abundance now because 7.5, too. New measurements of Fe II oscillator strengths (Baschek et. al.,1970) essentially confirmed Roder's values and resulted in a photospheric iron abundance of 7.6. For more details, see e.g. Garz et al. (1969) and Withbroe (1971).

A different "iron problem" of the 1960s arose from a series of papers by Pecker and collaborators in the Ann. d'Astrophysique (1959/61) where non-LTE effects in the sun of an order of magnitude were claimed for metals such as iron, a result not confirmed by subsequent studies (cf.e.g. Cayrel, 1965). The non-LTE analysis of Athay and Lites (1972) was based on 15 levels of Fe I; modern calculations include of the order of 100 levels of Fe I/II and show that non-LTE effects are modest for Fe I and only small for Fe II in A to G stars (e.g. Saxner, 1984; Steenbock, 1985; Gigas, 1986).

6. OUTLOOK: SOME PRESENT-DAY FE II PROBLEMS

Line spectroscopy of Fe II during the last years is characterized on the one hand by observations in the ultraviolet which, for fainter sources, have become feasible particularly through the IUE satellite (launch in 1978), on the other hand by the rapid increase of the sensitivity of optical detectors.

In this concluding section I will first briefly refer to my own recent work on Fe II, and then sketch some more or less arbitrarily selected recent Fe II problems in other fields.

High-resolution ultraviolet spectra of early-type stars obtained with IUE exhibit numerous absorption lines of which at most half can at present be identified (cf. e.g. Baschek, 1983). In particular for A stars, Fe II is very likely to contribute to a larger number of the unidentified lines. We began a collaboration between the atomicphysics group at Lund and the theoretical astrophysics group at Heidelberg on laboratory ultraviolet analysis of Fe II based upon new hollow-cathode spectra in the range 1300 to 3200 Å where many lines including strong ones are as yet not identified. As a first result we founde some 120 new doubly excited Fe II lines in the ($3d^5 4s4d + 3d^5 4p^2$) configuration system of which many could be identified in the IUE high-resolution spectrum of the sharp-lined B 9.5 V star 21 Peg. For further details, we refer to the poster contributions at this Colloquium by Baschek and Johansson, by Brage et al., and by Adam et al. and to Adam et al. (1986).

A very active field of research is the diagnosis based upon Fe II and [Fe II] lines of low-density plasmas around a variety of different objects with the aim to obtain a model for the stratification, the velocity fields, the excitation conditions etc. Of interest are - and will be discussed at this Colloquium - e.g. stellar chromospheres, Be stars, ζ Aur systems, S Dor variables, novae and supernovae. Out of recent discoveries I would like to mention here that [Fe II] lines have even been observed in the jet of the Herbig-Haro object HH 34 (Bührke and Mundt, 1986), and that the infrared [Fe II] line at λ 1.644 μm (a^4F-a^4D) has been detected in the supernova SN 1983 N (Graham et al., 1986) so that the "formation" of about 0.3 $M_\odot$ of Fe by the decay of $^{56}Ni \rightarrow {}^{56}Co \rightarrow {}^{56}Fe$ can be inferred directly.

Finally, strong Fe II emission in the optical as well as in the ultraviolet is observed in many quasars and Seyfert 1 galaxies following the first detection of optical Fe II lines in 3 C 273 by Wampler and Oke (1967). There seems to be a problem in these "Fe II galaxies" since the total emission in the Fe II lines exceeds that in Lyman α (cf. e.g. Wills et al., 1985). Possible excitation mechanisms are radiative excitation or fluorescence either by Lα, by the Mg II lines or by numerous lines within Fe II itself. The optical thickness of the clouds surrounding the active galactic nucleus essentially determines the ratio of optical to ultraviolet Fe emission.

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