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Tracing Iron Abundance with Fe II Spectra in Astrophysical Plasma

E. VERNER
IACS/Dept. of Physics, Catholic Univ. of America
and
NASA/Goddard Space Flight Center Greenbelt MD 20771

Abstract

This talk focuses on Fe II emission model developments and applications of Fe II emission models to the interpretation of observational data. The quantitative models have been used to simulate emission spectra of H II regions, partly-ionized regions and Broad Line Regions of Active Galactic Nuclei. Due to the richness of the Fe II spectra and the sensitivity to the excitation conditions the Fe II emission spectra analysis provides a powerful tool for diagnostics of physical conditions and Fe abundance in a variety of astronomical objects.

1.1 Introduction

A large number of the allowed and forbidden Fe II lines are present in a broad range of emission spectra in a variety of astronomical sources. The Fe II emission spectrum arises from thin "envelopes" around a variety of objects such as stars, H II regions, novae, supernova remnants, active galaxies and quasars. The high abundance of iron in the Universe and the very rich spectrum of Fe II explain why this is so. The iron abundance ranks only after H, He, C, N, O, and Ne in a solar composition, and is comparable in abundance to S, Mg, and Si.

Fe II has a very line-rich spectrum. The richness in lines of Fe II originates in its about half-filled 3d-shell. The pioneering work on the term analysis of singly ionized iron (Russell 1926) reported 61 energy levels. Now more than 1000 energy levels of Fe II are known (Johansson private communication 2002). The Fe II spectrum has a rich and complicated mixture of forbidden and permitted lines. The first permitted transition is possible only from 64^{th} level to the first one, and this transition produces a strong UV line. Netzer, Wills (1983) and Verner et al. (1999) discussed the critical density for this transition, and it is about 10^{10} cm^{-3}. In a case when only lower levels are populated, only forbidden lines take place. With the increasing density, higher levels are populated by collisions, and the permitted lines are observed. Many tens of terms, corresponding to hundreds of levels, contribute. Laboratory spectroscopy is not complete and only in the past few years have many of the radiative and collision rates been determined. First optical and then UV and IR spectral windows have become available to measure the full spectrum in astrophysical sources.

The excitation and ionization conditions for populating Fe II levels are very favorable in a great number of astronomical objects. Because the ionization potential of 7.9 eV for Fe I and 16.2 eV for Fe II the energy of hard ultraviolet photons ($\lambda <$ 1570 Å) is sufficient to ionize neutral iron. Electron temperatures between about 5000 to 20000 K are typical for producing strong Fe II lines. The atom is far from equilibrium in most emission objects, so the spectrum is sensitive to the detailed local conditions. A simulation of the physical processes affecting the Fe II spectrum would make it possible to deduce the density, temperature, and iron abundance of the emitting regions. One fourth of all energy emitted by Broad Emission Line clouds may come from Fe^+ emission. Fe^+ is the main coolant at high densities. Some stars also show extreme Fe^+ emission. For example, K-giant radiates most of its energy by Fe^+ (Carpenter & Wing, 1985).

The long-term hope is to determine the abundance of iron. Most of the evolutionary models of galaxies predict increase in Fe abundances after 1-2 Gyr by factors of 2 to 10 relative to solar (Hamann & Ferland, 1993). This overabundance might explain the strong Fe II emission observed in many QSOs and AGN. The expected 1 Gyr delay from the onset of star formation could therefore be used as a clock to constrain QSO ages if accurate Fe abundances are measured. If star formation has a significant contribution from very massive objects (Heger & Woosley 2002), then substantial Fe production can occur at times earlier than 1 Gyr. The answer to this question has important consequences not only for the evolution of the elements, but possibly for understanding the formation of AGNs as well.

1.2 Fe II Emission from H II Regions

A very active field of research is the diagnostics based upon [Fe II] lines of low-density plasmas around a variety of different objects with the aim to obtain consistence with velocity field, excitation conditions etc. H II regions are good laboratories to check how Fe II emission works. Recent studies of the [Fe II] lines observed in the Orion nebula have shown that some intensities ratios cannot be explained by only collisional excitation at the densities $n_e < 10^4$ cm^{-3}. Lucy (1995) has shown that the line ratios of [Ni II] can be explained by considering the fluorescent excitation of Ni^+ levels by UV nebular radiation. The same effect may be important for Fe II line formation process and Fe II emission can be explained by presence of continuum pumping (Baldwin et al. 1996, Verner 2000).

One of the simplest applications of the Fe II emission model is the interpretation of the forbidden infrared and optical [Fe II] lines from H II regions. The Orion Nebula is the defining blister H II region (Zuckerman 1973, Balick, Gammon, & Hjellming 1974). A star cluster ionizes the skin of the molecular cloud, causing an expansion away from the molecular cloud towards us. The H II region is in photoionization equilibrium with a density in concert with that of the background photodissociation region (Tielens & Hollenbach 1985), and both regions are dusty with high depletions of the refractory elements (Rubin, Dufour, & Walter 1993).

Our photoionization calculations made with the parameters taken from (Baldwin et al. 1991) with improved gas-phase elemental abundances based on results from (Osterbrock et al. 1992) and Rubin et al. (1991). Model has the incident continua from the Trapezium stars and total (gas and radiative) pressure is kept constant. Our photoionization models of the [Fe II] spectrum with parameters close to those found by (Baldwin et al. 1991) predict a spectrum in good overall agreement with observations. The infrared [Fe II]lines are produced by collisional excitation, and the optical [Fe II] lines by photon pumping by the ultraviolet continuum in a region of moderate density, $n_e \approx 10^4$ cm^{-3}. Fe/H must be depleted, 3×10^{-6} cm^{-3}.

1.3 Fe II Emission from the BD Blobs of Eta Carinae

In 1986, the object known as Eta Carinae was resolved by speckle interferometry into four components (Weigelt & Ebersberger, 1986). Today we name them the Weigelt components A, B, C, and D. The bright component A is due to the central star, while B through D are bright gaseous condensations. The size of the Weigelt Blobs B & D (thereafter BD) are about that of our Solar System (Davidson & Humphreys 1997). More detailed spectra of the central source, Eta Carinae and the BD Blobs have been obtained with the Space Telescope Imaging Spectrograph (STIS/HST) (Gull et al. 1999). The radial velocity measurements suggest they are slow moving gaseous ejecta with radial velocity about - 45 km s^{-1}. The angular distance from the BD Blobs to the central stellar source is $\approx 0.1''$. Thus, it is large enough to be spatially resolved in STIS/HST long-slit spectra. The spectrum of the BD Blobs differs from that of the central source. The stellar spectrum is rich in broad H I and Fe II permitted lines (Hillier et al. 2001). In contrast, narrow forbidden Fe II lines dominate in the BD spectrum.

In spite of considerable uncertainties in the atomic data and complexity of physical processes, we present the first quantitative model for the Fe II and [Fe II] emission in the BD knots (Verner et al. 2002). We focus on explaining the Fe II and [Fe II] emission spectrum in the wavelength range 4000–10000 Å. Specifically we address the following questions: Why do we see so many strong Fe II and [Fe II] lines? What is temperature and density of the emitting region? What excitation process dominates: collisional excitation, pumping by the incident stellar continuum, or fluorescence by Lyα? And, can we explain the Fe II emission by a single density model?

The BD Blobs spectrum of Eta Carinae is uniquely rich in Fe II and [Fe II] lines. The Fe II studies reveal details of physical conditions in the emitting region, and indicate shortcomings in the atomic data for Fe^{+} ion. We conclude that Fe II and [Fe II] lines in BD Blobs spectrum are due to the dominant excitation mechanisms: 1) Pumping by the blackbody-like stellar radiation field from the central source of Eta Carinae produces the strong and rich spectrum in 4000–6500 Å. Most of observable [Fe II] and Fe II lines have accurate A-values (Quenet et al. 1996). These lines are in a good agreement with model predictions. 2) Primary cascades after Lyα fluorescence is responsible for 24 strong Fe II lines in 8000–10000 Å and in particular Fe II 2507, 2509 Å in the BD Blobs. Secondary cascades have much weaker effects. However, they contribute to the strengths of many other Fe II emission lines. We have postulated a large Lyα flux along with a broad emission profile to explain the observed Fe II primary cascades. In our future work we will study Lyα pumping in greater details. The Fe II level mixing, the number Fe II channels involved in excitation, the Lyα intensity as well as profile width and shape are the most important unknown factors. 3) Collisional excitation dominates in the formation of strong [Fe II] lines in the 7000–9000 Å. For n_e = 10^{5} - 10^{7} cm^{-3}, the lowest levels of Fe^{+}. can be populated by collisions. The strength of the [Fe II] 7156 Å is systematically underpredicted for a constant density model. It is not clear if its intensity is due to lower density component (B or D), uncertainties in atomic data, or geometric effects. Small collisional strengths or an overlooked excitation route might also affect the predicted intensity.

We have used the Fe II spectrum to derive physical conditions in BD Blobs. The best fit to the observed spectrum is achieved in the 4000 - 6000 Å range at constant density $n_e = 10^{6}$ cm^{-3}, and $T_{bb} \approx$ 15,000K. The dominant Fe^{+} ionization fraction and rich Fe II spectrum suggest the electron temperature range T_e = 5,000 - 7,500K. Our model predicts that the

Fe^{+}/Fe^{2+} has very sharp transition due to collisional ionization at 10 ^{6} cm^{-3}, and the size of blob about 10^{15} cm. The Fe ionization structure, low electron temperature in plasma, the shape of blackbody radiation and intense Lyα radiation provide conditions favorable for a rich Fe II spectrum. Blackbody radiation and Lyα -pumping are the main excitation mechanisms for the *Fe II* ion in the BD Blobs. As our first step, we have focused on Fe II emission analysis of the spectrum of the BD Blobs from 1998 observations. Extensive STIS/HST Eta Carinae observations at different positions and during other epochs are available. The morphology of the Homunculus Nebula, surrounding Eta Carinae is very complex. Line profile analysis by Viotti et al. (1989) and Davidson et al. (1995) suggest a wider range of velocities than expected from spherical geometry. In addition, an inhomogeneous dust distribution may selectively obscure the radiation field. As a result any of considered above combinations (e.g. collisions, blackbody radiation) may be responsible for Fe II and [Fe II]emission spectrum at other than BD positions. For the first time we have used detailed non-LTE Fe II models to bracket physical parameters of Fe^{+}-rich plasma in the BD Blobs of Eta Carinae. Most of [Fe II]and Fe II lines that predicted by our model are in a good agreement with observations.

1.4 Fe II Emission from Active Galactic Nuclei

Fe II emission was first seen in extragalactic objects by Greenstein and Schmidt (1964) for quasars 3C48 and 3C273. Features near 4450-4650 and 5100-5500 Å were reobserved by Wampler and Oke (1967) who suggested their identification with blended Fe II multiplets. Later, Sargent (1968) made the same identification in the Seyfert 1 galaxy, IZw1. From the absence of [Fe II], Wampler and Oke concluded that the emission region has n_e > 10 ^{6} cm^{-3} or higher. More Seyfert galaxies were observed (e.g., Fairall 1968, DeVeny and Lynds 1969, Adams and Weedman 1972, Baldwin 1975, Boksenberg and Netzer 1976, Oke and Shields 1976) and other Fe II emission features were recognized. A forest of thousands of Fe II lines competes with Lyα as the strongest contributor to the broad emission line spectrum of QSOs, the nuclei of radio galaxies and Seyfert 1 galaxies. The most prominent feature, always presented in broad line spectra, is between 2000 and 3500 Å. The Fe II lines in the optical region, strongest near 4600 Å, vary widely in strength from one object to another.

The ionization structure in AGN is very different from that of H II regions. The clouds can be thick enough to be highly ionized (N^{4+},O^{5+}) at their illuminated face and almost completely neutral at the back. The large flux of X-ray photons maintains a low degree of ionization (10Such extended low ionization regions are thought to be the origin of the strong Fe II and Mg II lines. The low excitation lines of Fe II are produced in the partly neutral region of the BLR clouds. They are characterized by T_e = 10 ^{4} K. Because of the extremely complicated energy level configuration of the Fe II atom, line intensities are not simple to calculate. There are several hundreds transitions of Fe II to be considered, many with large optical depth. An additional complication is the large number of wavelength coincidences of different Fe II lines. Their number at high densities (>10 ^{10} cm^{-3}) can reach 1000. Line overlap and self-pumping is a very important population process for the levels that must be taken into account.

1.4.1 Improved Fe II Ion Model

Our earlier 371-level Fe^+ ion model (for energies < 11.6 eV), incorporated into the code CLOUDY, predicts the emission of 68,635 Fe II lines (Verner et al. 1999). Tests of the new, expanded 830-level model (344,035 transitions) have already demonstrated greatly improved results. We found and resolved many discrepancies between our earlier model and Eta Carinae observations. Where A-values were absent for many semi-forbidden transitions, and rate coefficients uncertain for Lyα pumping channels and primary cascades, we inserted reasonable estimates. Our model now uses new experimental energy levels (Johansson 2002) and the A-values from the Amsterdam database (ftp://ftp.wins.uva.nl/pub/orth/iron, see also Raasen 1998). The increased number of atomic levels is crucial to predicting a more appropriate Fe II pseudo-continuum in QSO spectra (Verner et al. 2003).

1.4.2 Fe II /Mg II Emission Ratios

The observed ratio of Fe II UV emission flux (2000–3000 Å; hereafter Fe II (UV)) to that of the Mg II resonance doublet at 2800 Å in broad-line regions (BLRs) of quasars has a strong potential for being a fundamental cosmological metallicity indicator. The answer to whether the Fe/α abundance ratio has a sharp break at 1 Gyr has important consequences not only for the evolution of the elements, but possibly for understanding the formation of active galactic nuclei (AGN) as well. Whether the Fe/α enrichment is due to SN Ia or SN II explosions is a key problem to be addressed in constructing our picture of galactic evolution in the Early Universe.

The delay time in Fe enrichment can be estimated from observations by plotting the observed Fe II (UV)/Mg II emission ratio (or the Fe/Mg abundance) as a function of redshift. Recent Fe II (UV)/Mg II emission ratio measurements (e.g. Iwamuro et al. 2002; Dietrich et al. 2002; Freudling et al. 2003) show a wide range of values. That obscures any dependence on redshift. It is still unclear: (1) whether a dependence on redshift exists; and (2) whether the derived observed Fe II /Mg II values are sensitive to other physical parameters besides Fe abundance.

How the observed Fe II (UV)/Mg II emission ratio varies with physical conditions must be resolved before one can develop a reliable model that accurately predicts the Fe II emission line spectra in the BLRs of luminous AGNs. The large velocity dispersion of Fe II emission in BLRs, the large number of overlapping lines, and the overall richness of the Fe II spectrum (Verner et al. 1999) forms broad emission blends, producing a "Fe II pseudo-continuum" and/or prominent features from the UV through visual (4000–6000 Å; hereafter *Fe II* (Optical)) to IR. This necessitates a complete simulation of the physical processes affecting the Fe^+ ion to deduce how the Fe II emission varies with properties of the radiation field, density, temperature, and Fe abundance in the emitting regions. To investigate what really makes *Fe II* emission strong in the rest-UV, we have used a new Fe^+ model ion (up to ≈ 14 *eV*). By applying the new 830-level model ion for Fe^+, which is incorporated into detailed photoionization calculations, we have probed the feasibility of using the strong *Fe II* emission seen in quasar spectra to derive accurate Fe/Mg abundance enrichments. This *Fe II* emission would be especially important in determining the enrichment as a function of redshift and the nature of star formation in the Early Universe. We conclude that abundance is not the only factor that makes Fe II emission strong over a wide range of wavelengths and is not even the strongest factor. Our modeling indicates that microturbulence also leads to preferential strengthening of the *Fe II* emission in UV.

On the basis of the calculations, we concluded:

1. In contrast to recent observational *Fe II/Mg II* measurements, we emphasize the need for low-z quasar observations to calibrate detailed modeling as used here. Our model clearly demonstrates that a simple Fe II template cannot be applied for all quasars, because the Fe II sensitivity to radiation and turbulence is much stronger than that of the Mg II doublet. Only detailed modeling that includes the all these effects can provide more accurate Fe II templates.

2. Due to strong Fe II line overlap, we must adopt a wavelength band approach to get constraints on density, radiation field, and turbulence in BLRs.

3. Model comparisons with high S/N observations of quasars, and of even higher resolution observations of objects like Eta Carinae, will produce better atomic parameters, and more detailed understanding of the effects of the radiation field in astronomical objects. Future work using improved atomic data to fully explore effects of the radiation field is in progress.

4. These results clearly illustrate that the continuum of AGNs is greatly affected by *Fe II*. The spectrum of Fe II simply cannot be ignored. Understanding Fe II is crucial for obtaining realistic modeling of restframe AGN spectra from the UV through the IR. Studies in the expanded spectral range, much wider than used in any previous efforts, are required.

5. We suggest that our model is to be applied to low-redshift quasars spanning both a wide luminosity range, and the 1,000 − 10,000 Å restframe wavelength range. As the first step in this direction, the STIS and NICMOS capabilities can be used immediately to study low-redshift quasars. The Near Infrared Spectrograph (NIRSpec) on board the James Webb Space Telescope (JWST) would make it possible to measure spectra from 0.6 to 5 micron with resolving power in the range needed to obtain Fe II (UV) and Fe II (Optical) bands from low-redshift to high-redshift quasars.

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References

Adams, T. F., & Weedman, D. W., 1972, ApJ, 173, L109
Baldwin, J. A., 1975, ApJ, 196, L91
Baldwin, J. A., et al., 1996, ApJ, 468, L115
Baldwin, J., Ferland, G., Martin, P., Corbin, M., Cota, S., Peterson, B., & Slettebak, A. 1991, ApJ, 374, 580
Balick, B., Gammon, R. H., & Hjellming, R. M., 1974, PASP, 86, 616
Boksenberg, A., and Netzer, H., 1977, ApJ, 212, 37
Carpenter, K. G., Wing, R. F., & Stencel, R. E., 1985, ApJS, 57, 405
Davidson, K., et al. 1997, AJ, 113, 335
Davidson, K., & Humphreys, R. M. 1997, ARA&A, 35, 1
Davidson, K., Ebbets, D., Weigelt, G., Humphreys, R.M., Hajian, A.R., Walborn, N.R., & Rosa, M. 1995, ApJ, 109, 1784
DeVeny, J. B., & Lynds, C. R. 1969, PASP, 81, 535
Dietrich, M., Appenzeller, I., Vestergaard, M., & Wagner, S. J. 2002, ApJ, 564, 581
Freudling, W., Corbin, M., & Korista, K. 2003, ApJ, 587, L67
Fairall, A. P., 1968, PASP, 80, 235
Hamann, F., & Ferland, G. 1993, ApJ, 418, 11
Heger, A., & Woosley, S. E. 2002, ApJ, 567, 532
Hillier, D., Davidson, K., Ishibashi, K., & Gull, T. 2001, ApJ, 553, 837

Greenstein, J. L., & Schmidt, M., 1964, ApJ, 140, 1
Gull, T ., Ishibashi, K., Davidson, K., 1999, in ASP Conf. Proc. 179, Eta Carinae At The Millennium, ed. J. A. Morse, R. M. Humphreys, and A. Damineli (San Francisco: ASP), 144
Gull, T., Ishibashi, K., Davidson, K., Collins N., 2001, in ASP Conf. Proc. 242, Eta Carinae and Other Mysterious Stars ed. T. Gull, S. Johansson, and K. Davidson (San Francisco: ASP), 391
Iwamuro, F., Motohara, K., Maihara, T., Kimura, M., Yoshiii, Y., & Doi, M. 2002, ApJ, 565, 63
Kawara, K., Murayama, T., Taniguchi, Y., & Arimoto, N. 1996, ApJ, 470, L85
Korista, K., Baldwin, J., Ferland, G., & Verner, D. 1997, ApJS, 108, 401
Lucy, L., 1995, A&A, 294, 555
Netzer, H., & Wills, B. 1983, ApJ, 275, 445
Netzer, H., 1988, in Physics of Formation of FeII Lines Outside LTE, eds. R. Viotti, A. Vittone, & M. Friedjung, p. 247
Oke, J. B., & Shields, G. A., 1976, ApJ, 207, 713
Osterbrock, D., Tran, H., & Veilleux, S., 1992, ApJ, 389, 305
Quinet, P., Le Dourneuf, M., & Zeippen, C. J. 1996, A&AS, 120, 361
Raassen, A. J. J., & Uylings, P. H. M. 1998, A&A, 340, 300
Rubin, R. H., Dufour, R. J., & Walter, D. K., 1993, ApJ, 413, 242
Rubin, R., Simpson, J, Haas, M., & Erickson, E. 1991, ApJ, 374, 564
Russell, H. N., 1929, ApJ, 70, 11
Sargent, W.L.W., 1968, ApJ, 152, L31
Tielens, A. G. G. M., & Hollenbach, D., 1985, ApJ, 291, 722
Verner E. M., Verner, D. A., Korista, K.T., Ferguson, J. W., Hamann, F., & Ferland, G. J. 1999, ApJS, 120, 101
Verner, E., Verner, D., Baldwin, J., Ferland, G., & Martin P. 2000, ApJ, 543, 831
Verner, E. M., Gull, T. R., Bruhweiler, F., Johansson, S., Ishibashi, K., & Davidson, K. 2002, ApJ, 581, 1
Verner, E., Bruhweiler, F., Verner, D., Johansson, S., & Gull, T., 2003, ApJ, 592, L59
Viotti, R., Rossi, L., Cassatella, A., Altamore, A., Baratta, G., 1989, ApJS, 71, 9832
Wampler, E. J., & Oke, J. B., 1967, ApJ, 148, 695
Weigelt, G., & Ebersberger, J. 1986, A&A, 163, L5
Wills, B. J., Netzer, H., & Wills, D. 1985, ApJ, 288, 94
Yoshii, Y., Tsujimoto, T., & Kawara, K. 1998, ApJ, 507, L113
Zuckerman, B., 1973, ApJ, 183, 863