Lyα FLUORESCENT EXCITATION OF Fe ii IN ACTIVE GALACTIC NUCLEI

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ABSTRACT

We have calculated Fe ii emission-line strengths for active galactic nuclei broad-line regions using precise radiative transfer and Iron Project atomic data. We improve the treatment of all previously considered excitation mechanisms for the Fe ii emission, continuum fluorescence, collisional excitation, fluorescence by self-overlap among the iron lines, and fluorescent excitation by Lyα. We demonstrate that Lyα fluorescence is of fundamental importance in determining the strength of the Fe ii emission. In addition to enhancing the ultraviolet and optical Fe ii flux, Lyα fluorescence also results in significant near-infrared Fe ii emission in the 8500–9500 Å wavelength range. New observations are suggested to probe this effect in strong Fe ii-emitting quasars.

Subject headings: line: formation — quasars: emission lines — radiative transfer

1. INTRODUCTION

One of the most puzzling instances of Fe ii line formation occurs in the spectra of active galactic nuclei (AGNs) with broad-line regions (BLRs) that exhibit strong ultraviolet Fe ii emission (UV ≈ 2000–3000 Å) and often strong optical Fe ii emission (OP ≈ 3000–6000 Å) as well. The widths of the iron lines indicate formation in the dense BLRs, yet standard photoionization calculations, successful in interpreting many other BLR features, fail to account for the strength of the Fe ii emission (Wills, Netzer, & Wills 1985; Joly 1993). Observed total Fe ii/Hβ ratios are ≈ 12, whereas standard models predict ratios less than 8, typically 3 – 5, with the largest values resulting from enhanced iron abundances. There is also a class of “superstrong” Fe ii emitters with Fe ii/Hβ ≈ 30 which seem unexplainable by traditional photoionization modeling (Joly 1993; Graham, Clowes, & Campusano 1996).

Excitation mechanisms advanced for the Fe ii emission include continuum fluorescence via the UV resonance lines, self-fluorescence via overlapping Fe ii transitions, and collisional excitation, with the latter thought to contribute the bulk of the Fe ii emission. However, Wills et al. (1985) demonstrated that model BLR calculations including these excitation mechanisms cannot account for the observed strengths of the Fe ii lines. Elitzur & Netzer (1985, hereafter EN) extended this calculation to include Lyα fluorescent excitation but found its contribution to be negligible. Nevertheless, Penston (1987) argued that strong indirect observational evidence for the importance of Lyα fluorescence is found in the presence of unexpected UV Fe ii multiplets in the spectrum of the symbiotic star RR Tel that seem attributable only to cascades from higher levels pumped by Lyα fluorescence. The emission nebulae of symbiotics offer densities and ionization parameters similar to the BLRs of AGNs. Recently, Graham et al. (1996) have identified emission from these UV Fe ii multiplets that is expected to be preferentially strengthened by Lyα in the spectrum of the ultrastrong Fe ii emitter 2226 – 3905.

In this Letter, we improve the modeling of all of the mentioned excitation mechanisms by using new, accurate atomic data and precise radiative transfer, and we demonstrate that fluorescent excitation by Lyα can be of prime importance. A key feature of Lyα fluorescent excitation of Fe ii is significant near-IR Fe ii emission in the wavelength range 8500–9500 Å. We suggest that a currently well-known, but unidentified, emission feature near 9200 Å in AGN spectra may be, at least in part, a spectral signature of this process.

2. CALCULATIONS

Fe i–iv were considered, with Fe i, Fe iii, and Fe iv each represented by a ground-state photoionization cross section and total, unified radiative plus dielectric recombination rate from the Iron Project calculations (see Bautista & Pradhan 1998). The Fe ii atomic model consists of 262 fine-structure levels with energies from Johansson (1978; 1992, private communication). The model atom is complete in quartet and sextet levels for energies below 0.849 ryd, allowing full inclusion of all Lyα fluorescently excited transitions from a′D. This atom is a subset of the much larger 827 level Fe ii atom used by Sigut & Pradhan (1996).

Transition probabilities for Fe ii were drawn from three sources, Fuhr, Martin, & Wiese (1988), Nahar (1995), and R. L. Kurucz (1991, private communication). Over 3400 Fe ii radiative transitions were included in the non-LTE solution. Photoionization cross sections for all Fe ii levels were taken from Nahar & Pradhan (1994). A level-specific radiative plus dielectric recombination coefficient was used for each Fe ii quartet and sextet level. For the collisional excitation of Fe ii, we adopted the R-matrix results of Zhang & Pradhan (1995) and Bautista & Pradhan (1998) and used the Gaunt factor formula for all remaining high-lying, dipole transitions. The charge transfer recombination rates to Fe ii and Fe iii were taken from Kingdon & Ferland (1996). Charge transfer ionization of Fe ii was also included, because Fe iii + e – recombination is to the Fe ii ground state (Neufeld & Dalgarno 1987).

The coupled equations of radiative transfer and statistical equilibrium were solved with the accelerated lambda-iteration method of Rybicki & Hummer (1992). Overlap between the Fe ii transitions is complex, the full preconditioning strategy was implemented. Complete frequency redistribution (CRD) over depth-dependent Doppler profiles was assumed for all iron transitions. The calculations were performed in plane-parallel.
one-dimensional, continuum-illuminated clouds, each computed for a given ionization parameter and total particle density, assuming constant total pressure. The run of $T_e$ and $N_{e}$ the photoionizing radiation field, and the continuous opacities and source functions were obtained with the CLOUDY code (Ferland 1991). This cloud structure was fixed during the iron non-LTE calculation. The solar iron abundance was used, $\log (N_{Fe}/N_{H}) + 12 = 7.477$.

The Ly$\alpha$ source function can be written without significant error as

$$S_{Ly\alpha}^{\ell} = \left( \frac{n_{2p} A_{2p,1s}}{n_{1s} B_{1s,2p} - n_{2p} B_{2p,1s}} \right) \frac{\psi_{\ell}}{\phi_{\ell}},$$  

where $\gamma_{\ell}$ of Ly$\alpha$ photons is coherently scattered in the atom’s rest frame, the ratio of emission to absorption profile is

$$\frac{\psi_{\ell}}{\phi_{\ell}} = 1 + \gamma_{\ell} \left( \frac{\int_{\nu} a_{\ell \sigma} \phi_{\ell} d\nu - \int_{\nu} a_{\ell \sigma} \phi_{\ell} d\nu'}{\phi_{\ell} \int_{\nu} d\nu'} \right),$$

separately with an iterative technique, and then the Ly$\alpha$ source function and opacity were incorporated into the appropriate monochromatic source functions during the solution of the radiative transfer equations for the Fe $\Pi$ transitions. We have verified our solution of equation (2) by matching the Ly$\alpha$ profiles tabulated for BLR clouds by Avrett & Loeser (1988) using their models and hydrogen populations.

3. RESULTS

Figure 1 compares the predicted Fe $\Pi$ flux with and without Ly$\alpha$ pumping in BLR models with two different ionization parameters ($U_{\text{ion}}$), 10$^{-2}$ and 10$^{-3}$. These values are chosen to be representative of typical Fe $\Pi$–emitting clouds but do not exhaust the range of possibilities. Both models assumed a total particle density of $4 \times 10^{28}$ cm$^{-3}$, a total column density of $10^{23}$ cm$^{-2}$, and zero microturbulence. The shape of the photoionizing continuum was that of Mathews & Ferland (1987). For $U_{\text{ion}} = 10^{-2}$, the influence of Ly$\alpha$ is large, more than doubling the total emitted flux, giving Fe $\Pi$/H$\beta$ = 2.4 for UV emission and 0.78 for optical emission, as compared with 1.1 and 0.29, respectively, without Ly$\alpha$ (the H$\beta$ flux was taken from the CLOUDY model). The strongest flux enhancements occur as noted by Penston (1987). The most important fluorescent excitation rates are from low-lying $a^D$ levels to the $4^D$, $4^F$, $4^P$, $4^S$, and $4^E$ symmetries of the $3d^n(D)5p$ configuration (Johansson & Jordan 1984). Cascades from these levels to $e^D$ and $g^D$ produce strong emission lines in the range 8500–9500 Å (see Fig. 2). In turn, cascades from $e^D$ and $g^D$ to odd parity levels near 5 eV enhance multiplets 399, 391, 380 ($\sim$2850 Å), 373 ($\sim$2770 Å), and 363 ($\sim$2530 Å); these lines are the unexpected UV multiplets in the RR Tel spectrum noted by Penston (1987) and the multiplets identified by Graham et al. (1996) in 2226–3905. Penston estimated that $\approx$20% of the UV Fe $\Pi$ flux comes out in these multiplets, which

Fig. 1.—The predicted Fe $\Pi$ spectrum. The spectra were convolved with a Gaussian of 1e width of 2000 km s$^{-1}$. Covering fractions of the illuminated and shielded cloud faces were assumed to be 5% each. The ratios of Fe $\Pi$ fluxes with H$\beta$ are computed with the OP and UV wavelength regions defined in § 1.
Fig. 2.—An enlargement of the near-IR Fe ii spectrum for the \(U_{\text{ion}} = 10^{-2}\) model of Fig. 1. The spectra were convolved with a Gaussian of 1/e width of 500 km s\(^{-1}\). “Ly\(\alpha\) (1/10)” indicates that the \(A_i\) values of the pumped Fe ii transitions within \(\pm 3\) \&\& are scaled by 0.1. Fe+(IR) refers to the flux between 0.7 and 1.0 \&\&.

comparss comparifies with the \(\approx 30\%\) found in the current model. Subsequent cascades then enhance the optical and UV fluxes from transitions among the lower levels. While transitions from \(a^D\) within \(\pm 3\) \&\& of Ly\(\alpha\) are the most important in the fluorescent process (see the listing of Johansson & Jordan 1984), our treatment of Ly\(\alpha\) includes the entire profile within \(\sim 50\) \&\&. Including pumping only within \(\pm 3\) \&\& reduces the flux ratios to 2.1 for UV emission and 0.70 for optical emission for the case of \(U_{\text{ion}} = 10^{-2}\).

For \(U_{\text{ion}} = 10^{-3}\), the effect of Ly\(\alpha\) pumping is not as large, particularly on the UV flux. The Fe ii/H\(\beta\) ratio generally increases with decreasing ionization parameter (even without Ly\(\alpha\) pumping) because of the larger sensitivity of the hydrogen level populations to temperature.

As noted by Penston (1987), and confirmed by the current calculation (Fig. 2), strong observational evidence for Ly\(\alpha\) pumping of Fe ii would come from the identification of the initial decays from the pumped 5\& levels to \(e^D\) and \(e^D\) that give rise to transitions in the 8500–9500 \&\& wavelength range. We note that there is a prominent unidentified feature near 9200 \&\& in quasar spectra, as discussed by Morris & Ward (1989) and Osterbrock, Shaw, & Veilleux (1990). An identification as solely H i Pa\(\lambda\) 9229 would render it anomalously strong compared with Pa8 and Pa10. Morris & Ward tentatively assign this feature to Mg ii \(4p^2P_{3/2,1/2} - 4s^2S_{1/2}\) (\(\lambda\)9218, 9244) as formed by cascades from \(5p^2P_{3/2,1/2}\) pumped by Ly\(\beta\). They discuss possible contributions from Fe ii but discount this possibility based on the apparent absence of a line at 8927 \&\&. Our calculations indicate that the Fe ii \(\lambda\)8927 line is significantly weaker than the main feature near 9200 \&\& (see Fig. 2). We have performed a preliminary non-LTE calculation for Mg ii, including Ly\(\beta\) fluorescence in a manner similar to that described for Ly\(\alpha\) (but with \(\gamma_e = 0.4\)), and find that while the Mg ii transitions in this region are strengthened by Ly\(\beta\) by nearly a factor of 5, they are still only minor contributors to the flux in the 9200 \&\& region (<5%). Hence, the \(\lambda\)9200 feature may be, in part, a spectral signature of Ly\(\alpha\) pumping of Fe ii. As noted by Osterbrock et al. (1990), observations in this wavelength region are hampered by telluric H\(\text{O}\) absorption bands, which require careful removal and, for available observations, falling CCD responses in the near-IR. New observations of this wavelength region are warranted.

The current efficiency of Ly\(\alpha\) pumping is in disagreement with the EN calculation. An important difference is in the adopted oscillator strengths of the pumped transitions from \(a^D\). The Kurucz (1981) values are roughly a factor of 10 smaller than those obtained by either Nahar (1995) or R. L. Kurucz (1991, private communication). Reducing the oscillator strengths for the pumped transitions within \(\pm 3\) \&\& of Ly\(\alpha\) by a factor of 10 results in a strong reduction in the effect of Ly\(\alpha\) fluorescence, giving, for the \(U_{\text{ion}} = 10^{-2}\) model of Figure 1, Fe ii/H\(\beta\) ratios of 1.28 for UV emission and 0.36 for optical emission. The near-IR emission (Fig. 2) is also substantially reduced from Fe ii/H\(\beta\) = 0.326 to 0.061. EN also used a simple escape probability treatment of line overlap and a simpler treatment of Ly\(\alpha\), so significant differences with the current work are perhaps expected. Finally, we note that our atom is essentially complete in the large number of quartet and sextet Fe ii energy levels below the \(3d^3(D)5p\) configuration and that our branching ratios from the pumped levels are expected to be considerably more accurate than those used by EN.

4. CONCLUSIONS

Using precise radiative transfer and accurate atomic data for Fe ii, we demonstrate that Ly\(\alpha\) fluorescent excitation can more than double the Fe ii flux in the UV and optical regions. We also predict Fe ii emission in the 8500–9500 \&\& region as a
direct result of Lyα fluorescence. Both of these results can be viewed as theoretical confirmation of the role of Lyα fluorescence suggested by Penston (1987) on the basis of observations. New observations of the 8500–9500 Å wavelength range in strong Fe II emitters are highly desirable and would provide valuable constraints on modeling Lyα fluorescence. Potentially new information on the Lyα profile within single BLR clouds could be obtained, something that is impossible based on observations of the highly broadened Lyα profile itself.

A detailed discussion of the variation of the Fe II emission with the physical parameters defining the BLR clouds (using a much larger 827 level Fe II atom that includes the doublet spin system), and the implications for the “Fe II/Hβ” problem, will be presented by Sigut & Pradhan (1998).

We are also extending our calculations to overcome some of the limitations of the present work, in particular, to incorporate all important ions into a full solution of the non-LTE radiative transfer problem for the thermal structure of AGN BLR clouds. This will enable the Lyα–Fe II problem to be solved within a self-consistent framework.

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REFERENCES

Avrett, E. H., & Loeser, R. 1988, ApJ, 331, 211
Bautista, M. A., & Pradhan, A. K. 1998, ApJ, 492, 650
Elitzur, M., & Netzer, H. 1985, ApJ, 291, 464 (EN)
Ferland, G. J. 1991, HAZY: An Introduction to CLOUDY, OSU Internal Rep.
Fuhr, J. R., Martin, G. A., & Wiese, W. L. 1988, J. Phys. Chem. Ref. Data, 17, 1
Graham, M. J., Clowes, R. G., & Campusano, L. E. 1996, MNRAS, 279, 1349
Johansson, S. 1978, Phys. Scr., 18, 217
Johansson, S., & Jordan, C. 1984, MNRAS, 210, 239
Joly, M. 1993, Ann. Phys. Fr., 18, 241
Kingdon, J. B., & Ferland, G. J. 1996, ApJS, 106, 205
Kneer, F. 1975, ApJ, 200, 367
Kurucz, R. L. 1981, Semi-Empirical Calculation of gf-Values: Fe II, SAO Rep. 390 (Cambridge: SAO)
Kurucz, R. L. 1988, ApJ, 331, 211
Bautista, M. A., & Pradhan, A. K. 1998, ApJ, 492, 650
Elitzur, M., & Netzer, H. 1985, ApJ, 291, 464 (EN)
Ferland, G. J. 1991, HAZY: An Introduction to CLOUDY, OSU Internal Rep.
Fuhr, J. R., Martin, G. A., & Wiese, W. L. 1988, J. Phys. Chem. Ref. Data, 17, 1
Graham, M. J., Clowes, R. G., & Campusano, L. E. 1996, MNRAS, 279, 1349
Johansson, S. 1978, Phys. Scr., 18, 217
Johansson, S., & Jordan, C. 1984, MNRAS, 210, 239
Joly, M. 1993, Ann. Phys. Fr., 18, 241
Kingdon, J. B., & Ferland, G. J. 1996, ApJS, 106, 205
Kneer, F. 1975, ApJ, 200, 367
Kurucz, R. L. 1981, Semi-Empirical Calculation of gf-Values: Fe II, SAO Rep. 390 (Cambridge: SAO)