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NON-LTE MODELS AND THEORETICAL SPECTRA OF ACCRETION DISKS IN ACTIVE GALACTIC NUCLEI

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ABSTRACT

We present self-consistent models of the vertical structure and emergent spectrum of active galactic nucleus (AGN) accretion disks. The central object is assumed to be a supermassive Kerr black hole. We demonstrate that non-LTE (NLTE) effects and the effects of a self-consistent vertical structure of a disk play a very important role in determining the emergent radiation and therefore should be taken into account. In particular, NLTE models exhibit a largely diminished H I Lyman discontinuity when compared to LTE models, and the He II discontinuity appears strongly in emission for NLTE models. Consequently, the number of ionizing photons in the He II Lyman continuum predicted by NLTE disk models is 1–2 orders of magnitude higher than that following from the blackbody approximation. This prediction has important implications for ionization models of AGN broad-line regions and for models of the intergalactic radiation field and the ionization of helium in the intergalactic medium.

Subject headings: accretion, accretion disks — galaxies: active — galaxies: nuclei — radiative transfer

1. INTRODUCTION

Accretion disks around massive black holes are believed to provide the UV and soft X-ray flux observed in many active galactic nuclei (AGNs). The observational evidence is based on the "big blue bumps" seen in the UV (e.g., Shields 1978; Malkan & Sargent 1982). Other observations, however, indicate that the H I Lyman jump is weak or nonexistent (e.g., Antonucci, Kinney, & Ford 1989), which has been used to argue against the presence of a geometrically thin, optically thick accretion disk around a black hole.

To settle the argument, one has to construct realistic models of accretion disks and their emergent spectra and to check whether the predicted spectrum is consistent with observations. Several models with varying degrees of sophistication were presented in the past. The simplest approach for calculating an accretion disk spectrum is to assume that each point of the disk radiates as a blackbody at the local effective temperature. The blackbody approach is acceptable for studying the basic energetics of the system but is obviously inadequate for predicting individual spectral features. To improve the situation, Kolykhalov & Sunyaev (1984), Sun (1987), and Sun & Malkan (1989) have used model stellar atmospheres to describe the radiation from different parts of an AGN disk. This would offer a very attractive method of computing the AGN spectra, since a large pool of model stellar atmospheres exists. However, one should be cautious about using this approach because the structure of a disk and a stellar atmosphere may be significantly different.

To explore this problem, several authors (e.g., Laor & Netzer 1989; Ross, Fabian, & Mineshige 1992; Störzer & Hauschildt 1994; Coleman 1994; Shields & Coleman 1994; Blaes & Agol 1996) have constructed models of the vertical structure of AGN accretion disks, using, however, various simplifying approximations. The most realistic models computed so far are those of Störzer, Hauschildt, & Allard (1994) and Dörrer et al. (1996). The former authors (and also Coleman 1994 and Shields & Coleman 1994) specifically addressed the question of how departures from local thermodynamic equilibrium (LTE) influence the predicted H I Lyman discontinuity, and they showed that non-LTE (NLTE) effects reduce the strength of the H I Lyman jump. However, they used an approximate, semianalytical approach to solve for the physical structure of the disk. Dörrer et al. (1996) have solved the vertical structure self-consistently, using, however, two critical simplifications: (1) LTE and (2) no bound-free opacities, and a pure-hydrogen atmosphere. On the other hand, they treat the Compton scattering in detail.

In this Letter, we present some representative, self-consistent, NLTE models of the vertical structure of AGN accretion disks. The basic aim of this study is to investigate differences in the predicted spectrum between this and simpler approaches and to show that simplified models may lead to inaccurate and misleading conclusions. In order to emphasize the observable consequences of self-consistent, NLTE models, we present the predicted spectra for a few representative rings in the disk. Integrated spectra of the whole disk, taking into account general relativistic photon transfer functions (Cunningham 1975; Speith, Riffert, & Ruder 1995), will be considered in a separate paper.

2. THE MODEL

We assume a steady state, geometrically thin disk in a (general relativistic) "Keplerian" rotation. The disk is divided into a set of axially symmetric concentric rings, each ring behaving as a one-dimensional radiating slab. The relativistic radial disk structure was calculated by Novikov & Thorne (1973), Page & Thorne (1974), and recently by Riffert & Herold (1995), who have corrected the previously derived form of the vertical pressure balance equation (the correction was first worked out by Eardley & Lightman 1975). We will use the results of Riffert & Herold (1995).

The vertical structure of a single ring is computed by solving simultaneously the hydrostatic equilibrium equation, the en-

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ergy balance equation, the radiative transfer equation, and, since we do not assume LTE, the set of statistical equilibrium equations.

If we neglect self-gravity of the disk, and assume that the radial distance from the black hole, R, is much larger than the distance from the central plane, z, we can write the equation of hydrostatic equilibrium as

$$\frac{dP}{dz} = -\rho g; \quad g = \frac{GM}{R^3}\frac{C}{B}z, \tag{1}$$

where P is the total pressure, ρ is the mass density, M is the black hole mass, and G is the gravitational constant. B and C (and also A and D used later) are relativistic corrections in the notation of Dörrer et al. (1996). The total pressure is given as a sum of the gas pressure and the radiation pressure,

$$P = P_{\rm gas} + P_{\rm rad} = NkT + \frac{4\pi}{c}\int_0^\infty K_\nu \, d\nu, \tag{2}$$

where N is the total particle number density, T the temperature, k the Boltzmann constant, and K_ν the second moment of the specific intensity of radiation $I_\nu(\mu)$, i.e., $K_\nu = \int_{-1}^{1} \mu^2 I_\nu(\mu)\, d\mu/2$; μ being the cosine of the angle between direction of propagation and the normal to the disk midplane. The upper boundary condition is taken from Hubeny (1990a; see eqs. [4.19]–[4.20] there).

The energy equation expresses the balance between the mechanical energy dissipated by viscous shearing between the "Keplerian" orbits and the net radiation loss, viz.,

$$\frac{9}{4}\frac{GM}{R^3}\left(\frac{A}{B}\right)^2 \rho w = 4\pi \int_0^\infty (\eta_\nu - \kappa_\nu J_\nu)\, d\nu, \tag{3}$$

where w is the viscosity, and η_ν and κ_ν are the monochromatic absorption and emission coefficients; J_ν is the mean intensity of radiation. We parameterize the viscosity using a fixed Reynolds number (Lynden-Bell & Pringle 1974; Hubeny 1990a). We will show in a subsequent paper that this treatment yields very similar results to the traditional α–parametrization of viscosity, introduced by Shakura & Sunyaev (1973) and recently modified for AGN disks by Dörrer et al. (1996). The total energy flux from the disk surface is given through the effective temperature,

$$T_{\rm eff} = \left(\frac{3GM\dot{M}}{8\sigma\pi R^3}\frac{D}{B}\right)^{1/4}, \tag{4}$$

where $\dot{M}$ is the mass accretion rate and σ is the Stefan-Boltzmann constant.

The radiative transfer equation is written in the standard way (e.g., Mihalas 1978), viz.,

$$\mu \frac{dI_\nu(\mu)}{d\tau_\nu} = I_\nu - S_\nu, \tag{5}$$

where the monochromatic optical depth is defined through $d\tau_\nu \equiv -\chi_\nu\, dz$; $S_\nu \equiv \eta_\nu/\chi_\nu$ is the source function. Here, χ_ν is the total absorption coefficient, $\chi_\nu = \kappa_\nu + \sigma_\nu$, σ_ν being the scattering coefficient. We assume that the only scattering process is the electron (Thomson) scattering. Finally, the emission coefficient is given by $\eta_\nu = \eta_\nu^{\rm th} + \sigma_\nu J_\nu$, where $\eta_\nu^{\rm th}$ is the coefficient of thermal emission. We assume no incident radiation at the disk surface and a symmetry condition at the disk midplane, $I_\nu(\mu) = I_\nu(-\mu)$.

In LTE, the *thermal* component of the source function is given by $S^{\rm th} \equiv \eta_\nu^{\rm th}/\kappa_\nu = B_\nu$, with B_ν being the Planck function, i.e., it is a simple function of the local temperature. However, it is well known that the LTE approximation breaks down in low density, radiation-dominated media, which are precisely the conditions prevailing in the AGN disks. Therefore, we have to adopt a more general treatment, traditionally called NLTE, where the thermal source function deviates from the Planck function, because the populations of energy levels are allowed to depart from the Boltzmann-Saha distribution. These populations are determined through the equations of statistical equilibrium.

The overall system of structural equations forms a highly coupled, nonlinear set of integrodifferential equations. These are, however, very similar to the equations describing a classical NLTE stellar atmosphere (e.g., Hubeny 1990a, 1990b). We may therefore adopt numerical methods and computer programs developed for stellar atmospheres. We use here the computer program TLUSDISK, which is a derivative of the stellar atmosphere program TLUSTY (Hubeny 1988; Hubeny & Lanz 1995). We stress that no a priori assumptions about the height of the disk and its total optical thickness are made; these are determined self-consistently with other structural parameters.

An NLTE model of the vertical structure of one ring of a disk is computed in three steps. First, an LTE-gray model is constructed, as described in Hubeny (1990a). This serves as the starting solution for the subsequent step, an LTE model, computed by TLUSDISK. This in turn is used as the starting solution for the last step, an NLTE model. In the NLTE step, we assume that all bound-bound transitions are in detailed radiative balance. To stress this point, we denote these models as NLTE/C (i.e., NLTE with continua only). Since our primary interest here is to explore the continuum flux around the H I and He II Lyman discontinuities, which are formed at layers where the lines are indeed in detailed balance, this approximation is justified.

We consider here disks composed of H, He, C, N, and O, with solar abundances. The model atoms are the same as in Hubeny & Lanz (1995), with nine NLTE levels of H, one level of H^+, and 14, 14, and one levels for He, He^+, and He^{++}, respectively, and with a total of about 50 levels for C III–C V, N III–N V, and O III–O VI. The opacity sources we consider are the bound-free transitions from all considered levels of H, He, C, N, O; the free-free opacity of the considered ions; and the electron (Thomson) scattering. All the relevant cross sections and relevant collisional rates are summarized in Hubeny (1988). In this Letter, we do not consider the Compton scattering because it is only marginally important for the considered models; it will, however, be considered in a subsequent paper.

3. RESULTS

As a representative case, we take a disk around a Kerr supermassive black hole with $M = 2 \times 10^9\, M_\odot$, with a limiting stable rotation (the specific angular momentum $a/M = 0.998$; Thorne 1974). The accretion rate is taken to be $\dot{M} = 1\, M_\odot\, {\rm yr}^{-1}$. We have calculated a number of vertical structure models for rings at various distances; we present here two models for $R/R_g = 2$ and 4, where R_g is the gravitational radius, $R_g = GM/c^2$. These rings are representative for providing the emergent soft X-ray and EUV radiation of the disk. Complete results will be presented elsewhere (Hubeny & Hubeny 1997).

Our basic aim is to explore the effects of NLTE on the emergent spectra. First, we will compare the spectra computed for self-consistent models of the vertical structure of the disk as calculated in LTE and NLTE. We will also present theoretical spectra for a "partial NLTE" model, i.e., the one with the vertical structure (temperature and density) fixed by an LTE model, and where the NLTE effects are included only in solving simultaneously the radiative transfer and statistical equilibrium equations (e.g., Coleman 1994; Shields & Coleman 1994; Störzer et al. 1994). Next, we will present an emergent radiation from a classical NLTE (plane-parallel, hydrostatic) stellar atmosphere model, computed for the same effective temperature as the disk ring. The surface gravity should be taken to be the one corresponding to the local disk gravity at some characteristic layer (e.g., where the Rosseland optical depth is unity). However, such an atmosphere is usually unstable (the surface gravity is below the Eddington limit) for typical parameters of AGN disks. We then calculate a model with the lowest surface gravity for which an atmosphere is stable. Finally, for completeness, we will compare the predicted flux with a blackbody distribution corresponding to the same effective temperature.

The classical NLTE stellar atmosphere models are calculated with the program TLUSTY, using the exact same model atoms and the same opacities as for the disk models. Also, the line transitions are considered in the detailed radiative balance, in order to minimize computational differences between the disk and the atmospheric models. The differences in predicted spectra will thus reflect real differences between the physical structure of a stellar atmosphere and a disk ring. These follow from the three basic features: (1) unlike a stellar atmosphere, the total radiation flux is not constant; (2) the gravity acceleration is not constant over vertical distance, but it varies according to equation (1); (3) the total optical depth of a disk ring is not infinite.

Figure 1 displays the predicted flux for these five models. There are two striking differences between the LTE and NLTE/C disk-ring results: (1) a largely diminished Lyman discontinuity, more so in the hotter model; and (2) the He II discontinuity appears strongly in emission for NLTE models. Consequently, the number of ionizing photons in the He II Lyman continuum increases significantly for NLTE disk models, which may have profound consequences for models of intergalactic matter. This feature was first noted by Coleman (1994) and Shields & Coleman (1994), who have, however, used very approximate models. The "partial NLTE" model provides a reasonably good approximation to the consistent NLTE model; the predicted EUV flux is systematically higher by 10%–20%.

A comparison between the NLTE/C stellar atmosphere and the NLTE/C disk models reveals significant differences: The flux in the He II Lyman continuum is systematically lower, while the flux in the H Lyman limit is systematically higher, in the stellar atmosphere models. Finally, the blackbody approximation is very inaccurate, giving much too high a flux in the UV region ($\nu \approx 3-4 \times 10^{15}$ Hz), while giving too low a flux in the EUV and the soft X-ray region. In particular, the number of ionizing photons in the He II Lyman continuum for the blackbody model is by factor 15 and 75 lower than that for the NLTE disk model, for the $R/R_g = 2$ and 4 models, respectively!

Since several studies in the past used a stellar atmosphere approximation, we plot in Figure 2 the predicted flux for NLTE/C model atmospheres with $T_{\rm eff} = 53{,}078$ K (corresponding to the ring at $R/R_g = 4$), and with various gravities. Since the presence of metals (CNO) does not change the emergent spectrum significantly, we consider H-He models for simplicity. The Lyman jump goes from a strong absorption for $\log g > 3.9$ to the emission at $\log g = 3.8$. At $\log g = 3.85$, the discontinuity practically disappears.

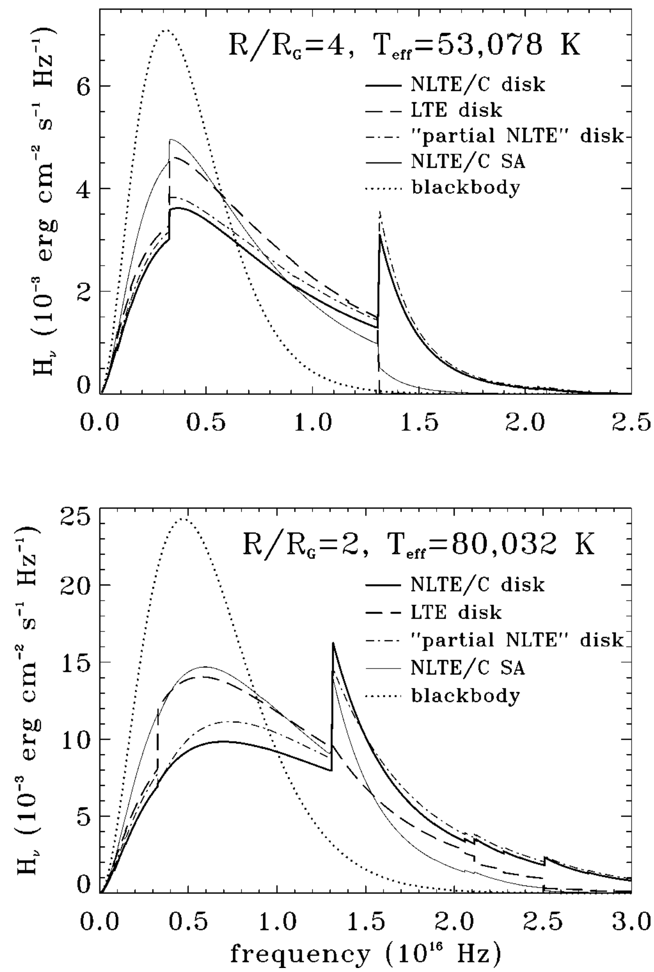

FIG. 1.—Comparison of the predicted spectra for an AGN disk model with a black hole mass, $M = 2 \times 10^9\ M_\odot$, a limiting stable rotation (the specific angular momentum $a/M = 0.998$), and an accretion rate, $\dot{M} = 1\ M_\odot\ {\rm yr}^{-1}$, for two radial distances $R/R_g = 2$ (*bottom*) and 4 (*top*). The corresponding effective temperature $T_{\rm eff}$ is given in each panel. Five different predicted spectra are displayed for each ring; see the text for explanation. The displayed model stellar atmospheres were computed for the indicated effective temperature and for $\log g = 3.8$ (*top*) and 4.5 (*bottom*), which represent the lowest gravities for which the respective hydrostatic model atmospheres can be constructed.

The behavior is easily understood by invoking the Eddington-Barbier relation, $F_\nu(\tau = 0) \approx S_\nu(\tau_\nu = 2/3)$. For all models, the hydrogen ground state is underpopulated, while the $n = 2$ state is overpopulated in the region of formation of the Lyman continuum. The thermal source function blueward of the discontinuity is roughly given by $S^{\rm th}(\nu > \nu_{\rm L}) \approx B_\nu(T_b)/b_1$, b_1 being the departure coefficient for the $n = 1$ level, while at the redward side it is roughly given by $S^{\rm th}(\nu < \nu_{\rm L}) \approx B_\nu(T_r)/b_2$. Here, T_b and T_r are the local temperatures at the depth where the monochromatic optical depth just blueward and redward of the Lyman discontinuity, respectively, is equal to 2/3. Since the opacity blueward of the jump is larger, the depth of $\tau_\nu \approx 2/3$ is located higher up in the atmosphere, where the local temperature is lower. Consequently, $T_b < T_r$. This leads to the

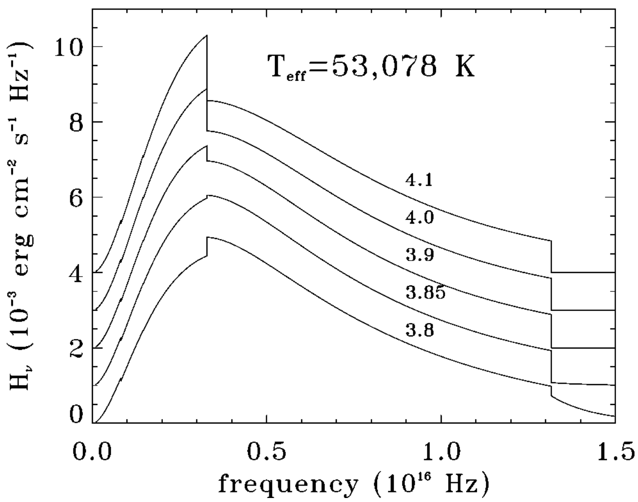

FIG. 2.—Behavior of the H I and He II Lyman discontinuity for various NLTE/C H-He model stellar atmospheres with $T_{\rm eff}$ = 53,078 K and for various values of the surface gravity. The curves are labeled by the values of log *g*. The scale on the ordinate applies for the log g = 3.8 model; the subsequent models are each offset by 1 unit for a clearer display.

presence of an absorption jump in LTE, where $b_1 = b_2 = 1$. In NLTE, the magnitude of the Lyman jump is reduced, or it may even be reversed. When going to lower gravities, the portion of electron scattering increases, which finally becomes the dominant opacity source throughout the atmosphere. Both sides of the Lyman discontinuity are now formed in almost the same region, so that $T_b \approx T_r$. Since $b_1 < b_2$, the thermal source function blueward of discontinuity is larger than that redward of the jump. Moreover, the portion of electron scattering is lower for $\nu \geq \nu_{\rm L}$, which further increases the total source function blueward of the jump. Consequently, the jump appears in emission. The explanation of the He II Lyman jump is similar. The behavior of the Lyman jump for a disk ring model is analogous; the effect is larger because the effective gravity is even lower than in the case of a classical stellar atmosphere.

4. CONCLUSIONS

We have calculated several representative models of vertical structure of an accretion disk around a supermassive Kerr black hole. The interaction of radiation and matter is treated self-consistently, taking into account departures from LTE for calculating both the disk structure and the radiation field.

We have demonstrated that NLTE effects, as well as the effects of self-consistent vertical structure of a disk, play a very important role in determining the emergent radiation. We have shown that NLTE models exhibit a largely diminished H I Lyman discontinuity when compared to LTE disk models, in agreement with the results of Störzer et al. (1994), and Shields & Coleman (1994). The most interesting result is that the He II discontinuity appears strongly in emission for NLTE models, which confirms previous exploratory calculations by Shields & Coleman (1994). Consequently, the number of ionizing photons in the He II Lyman continuum increases significantly for NLTE disk models. For the two representative models considered here, the number of He II ionizing photons predicted by NLTE disk models is larger by factor 15 and 75 than that following from the blackbody approximation. This feature may have very important implications for ionization models of the AGN broad-line region (e.g., Baldwin et al. 1995) and for models of intergalactic radiation field and the ionization of helium in the intergalactic medium.

We have also compared the models of a disk ring with the NLTE stellar atmosphere models computed for the same effective temperature. We conclude that using stellar atmosphere models for approximating the AGN disk emergent radiation is not recommended because the predicted flux in the vicinity of the H I and He II Lyman discontinuities is very sensitive to the assumed value of the surface gravity. Moreover, even the "best" stellar atmosphere model, i.e., the one with the lowest surface gravity possible, yields too low a flux in the He II Lyman continuum and too high a flux in the H Lyman continuum.

Our results show that in order to be able to test observationally the AGN accretion disk paradigm, it is necessary to construct sophisticated NLTE models of the vertical disk structure, taking into account all relevant opacity sources. It is dangerous to use simplified models, based on the LTE approximation, on a vertically constant gravity acceleration, or on approximating the disk radiation by that of a stellar atmosphere or even a blackbody. Such simplified models may lead to an incorrect predicted spectrum and thus to erroneous conclusions about the existence and properties of accretion disks in AGN.

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