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THEORETICAL ATMOSPHERES OF STARS IN THE BROAD LINE REGIONS OF ACTIVE
GALAXIES

Scott, John Franklin, Ph.D.
The Ohio State University, 1987
THEORETICAL ATMOSPHERES OF STARS IN THE BROAD LINE REGIONS OF
ACTIVE GALAXIES

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the
Graduate School of The Ohio State University

By

John Franklin Scott, B.S., M.S.

* * * * *

The Ohio State University
1987

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Adviser
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To my parents,

Franklin Simon Scott
and
Martha Lou Earley Scott
ACKNOWLEDGEMENTS

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CHAPTER I
INTRODUCTION

The spectra of Seyfert I galaxies and QSO's are characterized by the extreme breadth of their permitted emission lines relative to their forbidden emission lines. Typically, the permitted lines have a FWHM of about 1-10 thousand km/sec while the forbidden lines exhibit widths of several hundred km/sec. The usual explanation of this division is that the broad permitted lines arise in a compact region of high velocity and density, while the narrower forbidden lines are formed in a much larger surrounding volume of lower densities and velocities. Support for this general picture comes, in part, from the early and continued success of detailed photoionization models in predicting the observed intensities of the broad lines (e.g. Davidson and Netzer 1979; Weisheit, Shields and Tartar 1981; Kwan and Krolik 1981; Collin-Souffrin, Dumont, and Tully 1982; Mushotzky and Ferland 1984; Kwan 1984). These models, in which a finite slab of gas is subjected to non-thermal continuum radiation from the central energy source, are parameterized by electron density, radiation parameter, and column density. The electron density, \( N_e \), is bounded from below by the absence of any observed broad [OIII] emission and from above by the presence of observed CIII] emission. The
radiation parameter, $\Gamma$, is constrained by the observed CIII]/CIV line ratio. Extremely high values of column density, $N$, are ruled out since this would cause lines that form deep in the cloud (e.g. CII] $\lambda 2326$) to exceed their observed strengths relative to the other lines. Photoionization models therefore yield reasonable broad line spectra for electron densities $N_e \approx 10^8$-$10^{10}$ cm$^{-3}$, column densities $N \approx 10^{22}$-$10^{23}$ cm$^{-2}$, and radiation parameter $\Gamma \approx .01$-.03. The resulting temperature of the gas is somewhat dependent on the other model parameters but $T \approx 10^4$K is a nominal value. The physical size of the slab of gas is $r = N/N_e \approx 10^{12}$-$10^{13}$ cm. If the emitting gas is assumed to be in the form of spherical clouds, this can be taken as an approximate cloud radius.

Generic photoionized cloud models of this type are inadequate in several respects when used as a basis for understanding the structure and dynamics of the broad-line region (BLR). For the typical model parameters given above, the thermal energy of the clouds far exceed their gravitational energy. As a result, it is necessary to assume the presence of a hot, tenuous confining medium if the clouds are to survive (Mathews 1974; Krolik, McKee, and Tartar 1981). This inter-cloud medium leads to a number of subsequent theoretical complications; for example, the addition of a drag force term in the equation of motion for the emitting clouds. Even with the introduction of an inter-cloud medium, the question of cloud stability persists (see, for example, Mathews 1986; Elitzur and Ferland 1986; Mathews and Ferland 1987). Another shortcoming of the standard cloud model is the overly large BLR sizes which they predict. One of the input parameters of these models, the
radiation parameter $\Gamma$, sets the ratio of the number of incident ionizing photons to the electron density in the cloud at a distance $r$ from the source,

$$\Gamma = \int_{\nu_0}^{\infty} \frac{L_\nu}{4\pi r^2 h \nu N_e c} d\nu .$$

By combining standard cloud model values of $N_e$ and $\Gamma$ with the observed luminosity, $L_\nu$, of the ionizing continuum, an estimate of the size of the BLR is obtained. This size is usually an order of magnitude larger than BLR sizes deduced from line variability studies (Peterson et al 1985; Gondhalekar, O'Brien and Wilson 1986; Gaskell and Sparke 1986; Zheng et al 1987). Finally, whether optically thick or thin, these clouds experience an outward radial acceleration due to radiation pressure that is capable of explaining the widths and profile shapes of the broad lines (for an extensive review, see Mathews and Capriotti 1985). While it has been pointed out that other mechanisms are capable of reproducing the broad line profiles such as gravitational infall, ballistic outflow (Capriotti, Foltz, and Byard 1980) or infall along randomly oriented parabolic orbits (Kwan and Carroll 1982; Carroll and Kwan 1985), it is the radial outflow model that has attracted the most attention. In such a situation, however, it is difficult to understand how optically thick clouds can be prevented from introducing an asymmetry into the Ly$\alpha$ lines (Ferland, Netzer, and Shields 1979) which is absent in observations (e.g. Wilkes and Carswell 1982). Further, outflow models require a volume source of emitting clouds which is not well understood. Mathews (1983) has proposed, however, that stars orbiting into the BLR supply the emitting gas via ablation. If this is
the case, stars play a fundamental role in the BLR. In fact, the intense ionizing continuum of this region should be capable of driving stellar absorption lines into emission. If the emission line spectrum of these illuminated stars can mimic the line intensities and line intensity ratios commonly observed in Seyfert I galaxies and QSO's, then they could provide simple solutions to the difficulties encountered with the standard photoionized cloud models. Since stars are gravitationally bound, the need for an inter-cloud medium is eliminated. Though it may still be present as a result of gas ablated or lost by thermal winds from stellar surfaces, any resulting drag force on stellar motions would be negligible due to their much larger mass and smaller size. While radiation pressure is insufficient to accelerate stars to the observed BLR velocities, the smaller BLR sizes indicated by line variability studies suggest that these velocities could be produced by random Keplerian orbits without the requirement of an overly large central mass. Further, line profiles would be symmetric regardless of the fact that the star is optically thick. Finally, since the stars are in orbit, rather than outflow, no source of emitting material is required.

In this dissertation we examine the emergent radiation field of main sequence stars subjected to incident power law radiation characteristic of the BLR. The emergent stellar radiation is computed using the ATLAS 6 stellar atmospheres code (Kurucz 1979; hereafter simply ATLAS) for wavelengths between 229 and 200,000 angstroms. Effects of incident radiation at wavelengths longward of this wavelength range dominate the temperature structure of the upper atmosphere. An
approximation technique is employed to model the atmosphere in this regime. The results for the emission line spectra of these stars presented here indicate that not all of the observed line intensity ratios can be accounted for by stellar emission alone. The calculated H\textsubscript{\alpha} line flux is comparable to observed values for reasonable covering factors. The number of stars needed to achieve these covering factors, due to their small sizes, is very large.

The balance of this dissertation is divided as follows. In chapter II, an overview of the radiative transfer used in the code is given along with modifications to the temperature correction scheme and a description of the approximation technique involved in modeling the upper layers of the atmosphere. Results for various model calculations are given in chapter III, together with an analysis of the convergence properties of the atmospheres. In chapter IV, we summarize and discuss the significance of these results for BLR models and compare them to observations.
CHAPTER II
THEORY

ATLAS models plane parallel atmospheres with line opacities calculated by the ODF method of Kurucz (1979). The atomic level populations for these calculations are assumed to be in local thermodynamic equilibrium (LTE) with the exception of hydrogen for which a full non-LTE calculation is done for the first six energy levels. The radiative transfer theory was modified by Collins (1972) to handle the transport of polarized radiation and radiation incident on the surface. The general procedure used in calculating a model is iterative. A starting approximation to the atmosphere is supplied. ATLAS then calculates improved opacities for the atmosphere and solves the equation of transfer for the diffuse (emergent) radiation field. In general this solution will not meet the convergence criteria (described below) and the errors are used to improve the temperature distribution and structure for the atmosphere. The improved atmospheric structure is then used to recalculate the opacities and radiation field. This process is repeated until the convergence criteria are suitably well met.

This strategy fails for the uppermost layers of an atmosphere illuminated by incident power law flux. In this situation, the outer
layers are kept ionized by incident radiation at short wavelengths and the primary opacity source is therefore hydrogen free-free absorption which increases toward the infrared as $1/\nu^3$. Since the incident flux also rises toward the infrared, the result is that a staggering amount of energy is deposited in the uppermost layers, leading to extreme temperature gradients for which the iteration scheme in ATLAS does not converge. On the other hand, these outer layers are optically thin to shorter wavelength radiation, most of the opacity being in the infrared. This allows the re-radiated thermal flux from the atmosphere to pass through it relatively unaffected. It is therefore possible to use ATLAS to model the deeper stellar layers where opacity at shorter wavelengths becomes important, while ignoring incident infrared flux which never reaches these depths. Similarly, it is possible to approximate the temperature structure of the upper atmosphere by converting the incident infrared flux absorbed there to re-radiated black body flux, while ignoring the interaction of the higher layers with radiation coming from deeper layers. The result is a hybrid atmosphere where the primary features at shorter wavelengths originate deep in the atmosphere and are calculated by ATLAS while the outer layers act as little more than an IR screen.

2.1) Radiative Transfer in ATLAS

The diffuse field source function for thermal emission plus coherent isotropic scattering in the case of incident radiation from a distant point source of illumination is (Buerger 1972)
where $\alpha_\nu$ is the fraction of scattering to total opacity, $J_\nu^d$ is the mean intensity of the diffuse field, $J_\nu^{in}$ is the mean intensity of the incident field, and $B_\nu$ is the Planck function. The temperature which gives rise to the $B_\nu$ field is maintained by energy input from nuclear sources in the stellar core and from the fraction of the incident flux that is absorbed by the stellar material. The scattering term is divided into incident and diffuse parts as a necessary consequence of the assumption of coherent scattering. In general, the diffuse and incident frequency distributions may be different, and since no redistribution in frequency occurs upon scattering, this leads to two correspondingly different sources of radiation. If the frequency distribution of the incident flux at the stellar surface is $H^{in}_\nu$, then the incident flux as a function of monochromatic optical depth in the atmosphere is

$$H^{in}_\nu(\tau_\nu) = \mu_0 H^{in}_\nu \exp \left( - \frac{\tau_\nu}{\mu_0} \right),$$

(2.2)

where $\mu_0$ is the cosine of the angle that the parallel incident rays make with the normal to the atmosphere and $\tau_\nu$ is the optical depth at frequency $\nu$. The angular moments of the incident radiation field collapse in this situation, so that

$$J^{in}_\nu = H^{in}_\nu \exp \left( - \frac{\tau_\nu}{\mu_0} \right).$$

(2.3)

Using (2.3), the source function can be rewritten as

$$S_\nu = (1-\alpha_\nu)B_\nu + \alpha_\nu J^d_\nu + \alpha_\nu J^{in}_\nu,$$

(2.1)
Substituting the Schwarzschild equation (e.g. Mihalas 1978) for the diffuse radiation field into the above gives the following integral equation for $S_\nu$,

$$S_\nu = (1 - \alpha_\nu) B_\nu + \alpha_\nu J^d_\nu + \alpha_\nu H^{in}_\nu \exp \left(- \frac{r_\nu}{\mu_o}\right). \quad (2.4)$$

This integral equation is solved by replacing the integral with a gaussian sum (Collins 1970; Collins and Buerger 1974). The resulting expression is evaluated at the gaussian divisions to yield a system of linear equations in $S_\nu$ at these points. Written as a matrix equation, this system is then solved for $S_\nu$ by a Gauss-Seidel iteration technique. Once the source function is known, $J^d_\nu$ and $H^{d}_\nu$ can be found from the Schwarzschild-Milne equations for the diffuse field.

### 2.2) Convergence Criteria

In theory, the convergence criteria for the code are those of flux constancy; i.e. the total flux integrated over frequency must be constant with depth and its derivative with depth must be zero. In practice the numerical solution of (2.5) yields $H^d_\nu$, the diffuse flux only, so that the convergence criteria must be modified. We first define a frequency independent optical depth, $r_o$, such that

$$\frac{dr_\nu}{dr_o} = \kappa_\nu \quad , \quad (2.6)$$
where $\kappa_\nu$ is the total opacity at frequency $\nu$. For the total integrated flux to be constant with depth, the (outbound) diffuse flux at $r_o$ must be equal to the flux originating in the stellar core plus all incident flux absorbed or scattered below $r_o$. Therefore we require that the diffuse flux integrated over frequency,

$$H^d(r_o) = \int_0^\infty H^d_\nu(r_o) \, d\nu,$$

be equal to

$$H(r_o) = \frac{1}{4\pi} \sigma T_{\text{eff}}^4 + \int_0^\infty \mu_o H^{in}_\nu \exp \left( -\frac{\tau_\nu(r_o)}{\mu_o} \right) \, d\nu.$$  \hspace{1cm} (2.8)

Here, $T_{\text{eff}}$ is not the effective temperature of the resultant illuminated atmosphere, but rather a model input parameter that corresponds to the effective temperature the star would have if there were no incident radiation. This model parameter therefore sets the amount of flux due to energy generation in the core, since this is the only energy source for an unilluminated atmosphere.

Similarly, the derivative of the diffuse flux is not zero, but must equal the derivative of (2.8) above;

$$\frac{dH(r_o)}{dr_o} = -\int_0^\infty \mu_o \kappa_\nu H^{in}_\nu \exp \left( -\frac{\tau_\nu(r_o)}{\mu_o} \right) \, d\nu.$$  \hspace{1cm} (2.9)

On each iteration a new approximation to the correct radiation field, $(H_\nu^d$ and $J_\nu^d)$, is calculated. The flux error for the iteration is given by
\[ \Delta H^d = H - H^d \]  \hspace{1cm} (2.10)

and the derivative flux error by

\[ \Delta H' = \frac{dH}{dr_o} - \frac{dH^d}{dr_o} \]  \hspace{1cm} (2.11)

Since the zeroth moment (e.g. Mihalas 1978) of the diffuse equation of transfer integrated over frequency is

\[ \frac{dH^d}{dr_o} = \int_0^\infty \kappa_\nu (J_\nu^d - S_\nu) d\nu, \]  \hspace{1cm} (2.12)

(2.10) and (2.11) form separate constraints on the numerical calculation of \( H^d_\nu \) and \( J_\nu^d - S_\nu \), respectively. The flux and flux derivative errors are then used to determine a correction to the run of temperature in the atmosphere (see below). Two features of the convergence criteria should be noted at this point. First, both \( H \) (2.8) and its derivative with depth (2.9) are not absolute quantities. Each depends upon \( \kappa_\nu \), the total opacity with depth in the atmosphere. The value of \( \kappa_\nu \) changes from iteration to iteration as the opacities are brought into line with the updated temperature structure of the atmosphere. Second, the goal of the iteration scheme is to converge \( H^d_\nu \) to the point where both the flux and flux derivative errors are zero. This requires that two frequency integrals be numerically computed, one over a power law spectral distribution (for \( H \)), the other over a basically thermal distribution (for \( H^d \)). In the end, these two numbers must exactly cancel for the errors to be zero. Both of these points lead to numerical difficulties that are more fully discussed in chapter III.
The primary purpose of the temperature correction algorithm is to convert the errors made in calculating the diffuse flux into corresponding errors in the temperature profile (and hence the structure) of the atmosphere. These temperature errors are then used to correct the temperature profile for use in the next iteration. The iteration technique employed by ATLAS requires a starting guess at the atmospheric structure and radiation field. Since no models illuminated by power law spectra are available, previously calculated unilluminated atmospheres are used as a starting approximation. Once incident radiation is added, however, the energy of the absorbed incident photons goes directly into the thermal field. The temperature correction scheme must assume the additional task of adjusting the temperature structure of the initial unilluminated atmosphere to account for this extra source of heating. Since the temperature correction scheme is only accurate to first order, the very large temperature modifications needed when an unilluminated atmosphere is subjected to the large amounts of power law flux encountered in the BLR cause radical numerical instabilities. This problem can be avoided if incident flux is added very slowly, so that ATLAS need not correct for excessively large temperature jumps due to heating by the incident radiation. Each time a model converges, it can be used as a starting approximation for an atmosphere with slightly higher incident radiation levels. In this way, models with very high levels of incident flux can eventually be produced.
The temperature correction scheme given here is a variation of the double perturbation method of Avrett and Krook (1963). To converge atmospheres subject to large amounts of non-thermal incident flux, it was necessary to abandon some of the simplifying assumptions made in the original derivation.

2.3.1) The differential equation for \( \Delta \tau_0 \)

To derive the temperature correction for the atmosphere, we start with the first moment of the transfer equation for the diffuse field:

\[
\frac{dK_\nu}{d\tau_0} = \kappa_\nu H_\nu ,
\]

where the superscript \( d \) has been omitted for brevity. Following Avrett and Krook, we perturb both the temperature, \( T \), and \( \tau_0 \) variables. If \( \tau_0 \) and \( T \) denote the final optical depth and temperature distributions in the converged atmosphere, they can be expressed in terms of the current approximations and a correction term,

\[
\tau_0 = \tau_0^0 + \Delta \tau_0 - \tau + \Delta \tau_0
\]

and

\[
T = T^0 + \Delta T .
\]

Here, a superscript zero has been used to denote the current approximation to the true values, and a \( \Delta \) indicates a first order correction to this estimate. Since this notation is somewhat awkward
for $\tau_0^0$, we replace it with $t$. Other quantities become, in terms of these perturbed variables,

\begin{align}
\kappa_{\nu} &= \kappa_{\nu}^0 + \frac{d\kappa_{\nu}^0}{dt} \Delta \tau_0^0, \\
I_{\nu} &= I_{\nu}^0 + \Delta I_{\nu}, \\
J_{\nu} &= J_{\nu}^0 + \Delta J_{\nu}, \\
H_{\nu} &= H_{\nu}^0 + \Delta H_{\nu}, \\
K_{\nu} &= K_{\nu}^0 + \Delta K_{\nu}, \\
S_{\nu} &= S_{\nu}^0 + \Delta S_{\nu}, \\
H &= H^0 + \Delta H - H^0 + \frac{dH^0}{dt} \Delta \tau_0^0,
\end{align}

and the differential of $\tau_0$,

\begin{equation}
d\tau_0 = d(t + \Delta \tau_0) - dt + d(\Delta \tau_0) = \left[1 + \frac{d\Delta \tau_0}{dt}\right] dt. \tag{2.23}
\end{equation}

Substituting equations (2.23), (2.20), (2.19), and (2.16) into equation (2.13), expanding, dropping all second order terms, using equation (2.13) to eliminate zero order terms, and dividing through by $\kappa_{\nu}^0$, we obtain

\begin{equation}
\frac{1}{\kappa_{\nu}^0} \frac{d\Delta K_{\nu}}{dt} = H_{\nu}^0 \frac{d\Delta \tau_0}{dt} + \frac{1}{\kappa_{\nu}^0} \frac{d\kappa_{\nu}^0}{dt} H_{\nu}^0 \Delta \tau_0 + \Delta H_{\nu}. \tag{2.24}
\end{equation}

Integrating over frequency and using equation (2.7) together with the definition of the flux error, (2.10), we obtain a differential equation for $\Delta \tau_0$. 


At this point, Avrett and Krook set the left hand side of the above equation to zero, while Karp (1972) uses the diffusion approximation, $\Delta K_\nu = 1/3 \Delta J_\nu$, followed by the assumption $\Delta J_\nu = 3^k \Delta H_\nu$ to replace $\Delta K_\nu$ on the LHS of (2.25). We also use the diffusion approximation, which should be reasonably valid for the diffuse field, but once $\Delta K_\nu$ is replaced, we numerically estimate $\Delta J_\nu$. The method used to accomplish this is

$$\int \frac{1}{\kappa_\nu^0} \frac{d\Delta K_\nu}{dt} d\nu = H^0 \frac{d\Delta r_0}{dt} + \left( \int \frac{1}{\kappa_\nu^0} \frac{d\kappa_\nu^0}{dt} H_\nu^0 d\nu \right) \Delta r_0 + (H - H^0). \quad (2.25)$$

Since this estimation technique involves knowing the temperature correction, $\Delta T$, a first pass is made at finding $\Delta T$ with the LHS of equation (2.25) set to zero (standard Avrett-Krook). The Avrett-Krook value of $\Delta T$ is then used to estimate $\Delta J_\nu$, which is in turn used in equation (2.25) to get more refined results for $\Delta T$. Subsequent passes though the routine can be made until the estimates of $\Delta J_\nu$ and $\Delta T$ settle down at every depth in the atmosphere. One pass, however, is generally good enough considering the extra computer time multiple passes take.

In addition to $\Delta T$, the temperature derivative of $J_\nu^0$ must be found. A discussion of estimating temperature derivatives is deferred until section 2.3.3 below. Once $\Delta J_\nu$ has been estimated, however, the differential equation (2.25) can be solved for $\Delta r_0$. 

$$\Delta J_\nu = \frac{dJ_\nu^0}{dT} \Delta T. \quad (2.26)$$
2.3.2) Temperature perturbation from the flux derivative.

We now turn to the zeroth moment of the diffuse equation of transfer,

\[
\frac{dH^\nu}{dr_o} = \kappa^o (J^\nu - S^\nu). \tag{2.27}
\]

As before, all superscript d's are omitted. Substituting equations (2.23), (2.21), (2.19), (2.18), and (2.16) into the above, expanding, deleting second order terms, and using (2.27) to eliminate zero order terms, we obtain the perturbed zeroth moment of the transfer equation:

\[
\frac{d\Delta H^\nu}{dt} = \kappa^o (\Delta J^\nu - \Delta S^\nu) + \left\{ \kappa^o \frac{d\Delta r_o}{dt} + \frac{d\kappa^o}{dt} \Delta r_o \right\} (J^o - S^o). \tag{2.28}
\]

Integrating over frequency and using equation (2.10) we have

\[
\frac{d}{dt} (H - H^o) = \int \kappa^o (\Delta J^\nu - \Delta S^\nu) d\nu + \frac{d\Delta r_o}{dt} \frac{dH^o}{dt}
+ \Delta r_o \int \frac{d\kappa^o}{dt} (J^o - S^o) d\nu. \tag{2.29}
\]

Following Kurucz (1970) we approximate

\[
\Delta J^\nu - \Delta S^\nu = \left[ \frac{d}{dT} (J^o - S^o) \right] \Delta T. \tag{2.30}
\]

Substituting (2.30) into (2.29), and rearranging we have

\[
\Delta T \int \kappa^o \frac{d}{dT} (J^o - S^o) d\nu = - \left\{ 1 + \frac{d\Delta r_o}{dt} \right\} \frac{dH^o}{dt} + \frac{dH}{dt}
\]
Before solving equation (2.31) for $\Delta T$, the temperature correction to the atmosphere, an effort is made to account for the fact that in any given iteration, $H$ and its derivative are not known exactly. The depth derivative of $H$ in equation (2.31) above can be re-written using equation (2.22) as

$$\frac{dH}{dt} = \frac{dH^0}{dt} + \frac{d}{dt} \left( \frac{dH^0}{dt} \Delta r_o \right), \quad (2.32)$$

or

$$\frac{dH}{dt} = \frac{dH^0}{dt} + \frac{d^2H^0}{dt^2} \Delta r_o + \frac{dH^0}{dt} \frac{d\Delta r_o}{dt}. \quad (2.33)$$

Substituting equation (2.33) into (2.31), dropping second order terms, and rearranging gives

$$\Delta T \int \kappa_\nu^0 \frac{d}{dT} (J_\nu^0 - S_\nu^0) \, d\nu = - \left( 1 + \frac{d\Delta r_o}{dt} \right) \left( \frac{dH^0}{dt} - \frac{dH^0}{dt} \right)$$

$$- \Delta r_o \left( \int \frac{d\kappa_\nu^0}{dt} (J_\nu^0 - S_\nu^0) \, d\nu \right), \quad (2.34)$$

which can be solved for $\Delta T$, once equation (2.25) has been solved for $\Delta r_o$, and the temperature derivative of $J_\nu^0 - S_\nu^0$ has been estimated (see section 2.3.3 below).

2.3.3) Temperature derivatives of $J_\nu^0$ and $J_\nu^0 - S_\nu^0$

In order to estimate the left hand side of equation (2.25) and to solve (2.34) for the temperature correction to the atmosphere, temperature
derivatives of $J^\nu_\nu$ and $J^\nu_\nu - S^\nu_\nu$ must be found. Following Kurucz (1970), equation (2.5) can be rewritten as a matrix equation and easily solved for $S^\nu_\nu$ in terms of $B^\nu_\nu$ if only the diagonal elements of the matrices are considered,

$$S^\nu_\nu = (1 - \alpha^\nu_\nu \Lambda^\nu_\nu)^{-1} \left[ (1 - \alpha^\nu_\nu) B^\nu_\nu + \alpha^\nu_\nu H^{\text{in}}_\nu \exp \left( - \frac{\tau^\nu_\nu}{\mu^0_\nu} \right) \right], \quad (2.35)$$

where $\Lambda^\nu_\nu$ are the diagonal elements of the matrix operator for the $E_1$ integral. The expression for $S^\nu_\nu$ above can be substituted into the Schwarzschild equation, $J^\nu_\nu = \Lambda^\nu_\nu S^\nu_\nu$, which is differentiated with respect to temperature to yield

$$\frac{dJ^\nu_\nu}{dT} = \Lambda^\nu_\nu (1 - \alpha^\nu_\nu \Lambda^\nu_\nu)^{-1} \left[ (1 - \alpha^\nu_\nu) \frac{dB^\nu_\nu}{dT} - \alpha^\nu_\nu H^{\text{in}}_\nu \exp \left( - \frac{\tau^\nu_\nu}{\mu^0_\nu} \right) \right] \kappa^\nu_\nu \frac{dt}{dT}, \quad (2.36)$$

assuming that $\alpha^\nu_\nu$ and $\Lambda^\nu_\nu$ are at most weak functions of temperature. Similarly, equation (2.35) can be substituted into $J^\nu_\nu - S^\nu_\nu = \Lambda^\nu_\nu S^\nu_\nu - (\Lambda^\nu_\nu - 1) S^\nu_\nu$ to yield

$$\frac{d(J^\nu_\nu - S^\nu_\nu)}{dT} = (\Lambda^\nu_\nu - 1)(1 - \alpha^\nu_\nu \Lambda^\nu_\nu)^{-1} \left[ (1 - \alpha^\nu_\nu) \frac{dB^\nu_\nu}{dT} - \alpha^\nu_\nu H^{\text{in}}_\nu \exp \left( - \frac{\tau^\nu_\nu}{\mu^0_\nu} \right) \right] \kappa^\nu_\nu \frac{dt}{dT}, \quad (2.37)$$

after differentiation with respect to temperature. In principle, the temperature derivatives of $J^\nu_\nu$ and $J^\nu_\nu - S^\nu_\nu$ could be calculated from the full $\Lambda^\nu_\nu$ matrix operator in the same way that $S^\nu_\nu$ is found when determining the radiation field (Collins 1970), rather than using the diagonal elements of $\Lambda^\nu_\nu$ only. This procedure is costly since it involves the solution of a matrix equation at every frequency point (the majority of ATLAS run time is spent in calculating $S^\nu_\nu$) and does not
improve convergence inside of five iterations when used to replace the estimation scheme for the temperature derivatives outlined above.

2.3.4) Implementation of the temperature correction in ATLAS

ATLAS divides the temperature correction given by equation (2.34) into two parts corresponding to the two terms on the right hand side of this equation. The first term is proportional to the flux derivative error (see eq. 2.11) and the second is proportional to \( \Delta r_o \). The temperature correction that is proportional to the flux derivative error (\( \text{DTLAMB in the code} \)) is calculated directly as given in equation (2.34), i.e.,

\[
\text{DTLAMB} \cdot \int \kappa_{\nu}^c \frac{d}{dT} (J_{\nu}^c - S_{\nu}^c) \, d\nu = \left( 1 + \frac{d\Delta r_o}{dt} \right) \Delta \nu, \quad (2.38)
\]

when use is made of equation (2.11).

The correction term proportional to \( \Delta r_o \) is handled differently. Rather than calculating the second term on the right hand side of (2.34), an alternative correction term that is directly proportional to \( \Delta r_o \) is substituted, namely,

\[
\Delta T = \frac{dT^c}{dt} \Delta r_o. \quad (2.39)
\]

This correction term (\( \text{DTFLUX in the code} \)) together with DTLAMB make up the total temperature correction for the atmosphere. DTLAMB tends to be more important near the surface, while DTFLUX is more important at deep depths. In the region of the atmosphere where the two terms overlap the total temperature correction is numerically smoothed out by a third
term, DTSURF; a constant temperature shift applied to the entire atmosphere based on the flux error at the surface.

2.4) Approximation of the Temperature Structure of the Outer Layers

The upper atmosphere is kept ionized by high energy incident photons and the opacity is therefore dominated in the IR by hydrogen free-free absorption. Since the absorbed infrared radiation goes directly into the thermal field and since both the incident flux and hydrogen free-free opacity increase toward the red, large temperatures and temperature gradients can result if the incident power law spectrum is extended into the IR beyond 20\(\mu\)m. Since ATLAS is dependent on the temperature gradient for the DTFLUX temperature correction, large values for this quantity in the upper atmosphere make convergence of models with extended incident IR flux difficult, if not impossible there. The solution to the problem of modeling these atmospheres is splitting them into two parts. ATLAS is used to converge an atmosphere without incident flux longward of 20\(\mu\)m. This yields a realistic lower atmospheric structure since the incident IR flux beyond this limit does not penetrate to these depths. The upper atmosphere that ATLAS calculates with this cutoff is too cool, since absorption of the additional IR radiation dominates the temperature structure in this region. At shorter wavelengths, the upper atmosphere is optically thin, the primary contribution to total opacity being electron scattering. Therefore, radiation from the lower atmosphere, as well as thermally re-radiated flux from the upper atmospheric layers passes through the outer
layers unhindered. Under these conditions, the temperature structure of the outer atmosphere can be approximated by balancing (IR) flux absorbed with thermal radiation re-emitted at each depth, \( t \). We have, therefore, in the outer atmosphere,

\[
\int \kappa^{es} B_{\nu}(T(t)) \, d\nu = \int_0^{\nu_c} \kappa_{\nu}^{ff}(t) H_{\nu} \, \text{in} \, \exp \left[-r_{\nu}(t)\right] \, d\nu, \tag{2.40}
\]

where \( \kappa^{es} \) is the opacity due to electron scattering, \( \kappa_{\nu}^{ff} \) is the opacity due to hydrogen free-free absorption, and \( \nu_c \) is a cutoff frequency past which significant amounts of radiation make it to the lower atmosphere. In this case, \( \nu_c \) corresponds to a wavelength of 20\( \mu \)m. Since \( \kappa^{es} \) is independent of frequency, the integral of \( B_{\nu} \) can be evaluated,

\[
\kappa^{es} \sigma T^4 = \int_0^{\nu_c} \kappa_{\nu}^{ff}(t) H_{\nu} \, \text{in} \, \exp \left[-r_{\nu}(t)\right] \, d\nu, \tag{2.41}
\]

giving the following integral equation for \( T \),

\[
T(t) = \left[ \frac{1}{\kappa^{es} \sigma} \int_0^{\nu_c} \kappa_{\nu}^{ff}(t) H_{\nu} \, \text{in} \, \exp \left[-r_{\nu}(t)\right] \, d\nu \right]^{\frac{1}{4}}. \tag{2.42}
\]

While electron scattering is the dominate source of opacity for the emergent radiation, some absorption due to line blanketing is also present. It is neglected in this approximation, since it is frequency dependent and would prevent the easy integration of the \( B_{\nu} \) integral above. Some extra heating of the outer layers is to be expected, however, due to this additional source of opacity.
In equation (2.42) above, the hydrogen free-free opacity as given by Kurucz (1970) is,

\[ \kappa_{\nu}^{ff} = \frac{N(\text{HII}) N_e}{\rho} F_{\nu}(T) \frac{3.6919 \times 10^8}{\nu^3 T^4} \left[ 1 - \exp \left( \frac{-\nu}{kT} \right) \right] . \] (2.43)

The gaunt factor, \( F_{\nu}(T) \), is interpolated from data given in Karsas and Latter (1961). The electron scattering is also given as

\[ \kappa^{es} = 6.653 \times 10^{-25} \frac{N_e}{\rho} . \] (2.44)

In addition to the integral equation, (2.42), the temperature satisfies the equation of state

\[ P = \frac{\rho kT}{\mu m_H} . \] (2.45)

The gas pressure, \( P \), must in turn satisfy the equation of hydrostatic equilibrium modified for an incident radiation acceleration,

\[ \frac{dP}{dt} = g + \frac{dP_{\text{rad}}^{\text{in}}}{dt} . \] (2.46)

This form of the equation of hydrostatic equilibrium results from the fact that

\[ \frac{d \tau_{\nu}}{dt} = \kappa_{\nu}^{o} , \] (2.47)

and therefore

\[ d \tau_{\nu} = \kappa_{\nu}^{o} dt = -\kappa_{\nu} \rho dx , \] (2.48)

which implies
\[ t = - \int \rho dx, \quad (2.49) \]

where \( x \) is the physical height (shown in the structure plots of the next chapter) of the depth in question measured inward from the surface of the star. The variable \( t \) is the independent variable for depth used by ATLAS (called RHOX in the code). The integration of the equation of hydrostatic equilibrium is therefore trivial,

\[ P = gt + P_{\text{rad}}^{\text{in}}. \quad (2.50) \]

Values returned for \( P_{\text{rad}}^{\text{in}} \) and for \( t \) by ATLAS for the outer atmosphere are used in equation (2.50) above to obtain a first approximation of \( P \) for the upper atmosphere. Once this first guess at \( P \) is obtained, the equation of state is used, together with values of \( T \) returned from ATLAS, to find the density and subsequently the electron density via the formula (for the completely ionized region)

\[ N_e = \frac{\rho}{2m_H} (1+X), \quad (2.51) \]

where \( X \) is the mass fraction of hydrogen. Enough information is now available to calculate first approximations to the electron scattering and hydrogen free-free opacities using equations (2.43) and (2.44), and assuming that \( N(\text{HI}) \) is approximately \( N_e \) for the completely ionized upper atmosphere. Once this is done, the monochromatic optical depths are computed by integrating equation (2.48). With the values of \( T, N_e, \kappa_{\nu}^{ff}, \kappa_{\nu}^{es}, \) and \( \tau_{\nu} \) now known the right hand side of the integral equation for temperature, (2.42) can be evaluated to obtain a new approximation for the temperature distribution for the upper atmosphere. A better
approximation to the incident radiation pressure can also be calculated by integrating

$$\frac{dP_{\text{rad}}^{\text{in}}}{dt} = \frac{4\pi}{c} \int_0^\nu \kappa_\nu f(t) H_\nu^{\text{in}} \exp \left(-\tau_\nu(t)\right) d\nu, \quad (2.52)$$

over depth. The new value of $P_{\text{rad}}^{\text{in}}$ is used in the equation of hydrostatic equilibrium (2.50) to get refined values of $P$, which are used together with the new values of $T$ to re-estimate the density. This iterative procedure continues until the temperature stabilizes throughout the upper atmosphere. The temperature stabilizes to less than a one percent change at any depth point after about ten of these iterations.

This approximate structure for the outer atmosphere is joined to the converged ATLAS model at the depth where the temperature drops to the same value as predicted by ATLAS. This point is always at or near the ionization front, since other opacity sources become important at this point, and the approximation is no longer valid. The hybrid atmosphere is then fed back into ATLAS, along with an extended frequency set to include the IR frequencies, for a final calculation of the total radiation field.
3.1) Input Parameters

Illuminated atmospheres are characterized by the input parameters of incident flux spectral distribution and intensity, surface gravity, chemical composition, and effective temperature of the "seed" star. The incident radiation was assumed to be given by

\[ H_\nu^{in} = \beta \nu^{-\alpha}. \]  

(3.1)

The observed continua of Seyfert I galaxies and QSO's are not exactly described by a simple power law of spectral index \( \alpha \). There exists, for example, a broad excess of blue radiation above a simple power law spectrum. The most common explanation for this excess is that it is due to thermal emission from an accretion disk at about 30,000°K (Malkan and Sargent 1982). This continuum feature was not included in the radiation incident on the atmosphere models since it was a possibility that the heated atmospheres themselves might produce enough thermal emission in this wavelength range to explain the blue bump. The spectral index \( \alpha \) was set to be 1.2. The constant \( \beta \) sets the strength of the incident radiation at the stellar surface. This
constant is determined both by the distance of the star from the
central source of radiation and by the intrinsic luminosity of the
central source itself. An increase in $\beta$ can therefore be viewed as a
decrease in the distance of the star from the central source, or for a
fixed stellar distance, an increase in the luminosity of the central
source being modeled. An estimate of $\beta$ can be obtained from the
equation

$$\frac{L}{4\pi r^2} = 4\pi \beta \int_{\nu_1}^{\nu_f} \nu^{-\alpha} \, d\nu,$$

(3.2)

where $L$ is the total luminosity of the central source, $r$ is the
distance of the star from this source, and $(\nu_1, \nu_f)$ is the frequency
range over which the power law describes the continuum of the central
source. Assuming that the power law is valid from 1keV to 100$\mu$m, $\log\beta$
= 12.5 gives values of $r$ (see table 3.1) that correspond to those

**TABLE 3.1**

Approximate BLR Radii (light days) from $\beta$ and Luminosity of the Central Source

<table>
<thead>
<tr>
<th>logL</th>
<th>44</th>
<th>45</th>
<th>46</th>
<th>47</th>
<th>48</th>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
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<td>203.8</td>
<td>664.6</td>
<td>2038.</td>
</tr>
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<td>36.24</td>
<td>114.6</td>
<td>362.4</td>
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</tr>
<tr>
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<td>20.38</td>
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</tr>
<tr>
<td>12.5</td>
<td>3.624</td>
<td>11.46</td>
<td>36.24</td>
<td>114.6</td>
<td>362.4</td>
</tr>
</tbody>
</table>
deduced from line variability studies. The actual numerical
integration in ATLAS is performed over a restricted frequency range,
from 229 angstroms to 20μm. The code does not include adequate opacity
sources for wavelengths shortward of 229Å. While these high energy
photons should be more accurately treated, the only real effect they
might have in the case of these model calculations is to push the
ionization front in the atmosphere to slightly deeper RHOX depths, and
warm the atmosphere somewhat.

The effective temperatures of the models (i.e. the spectral type
of the "seed" star) ranged from 10,000°K to 5000°K. Models cooler than
5000°K are difficult to converge, but may be important in the BLR.
Models hotter than 10,000°K also become increasingly difficult to
converge, but are probably not of interest in this particular instance
since they are not formed in abundance, do not fit in with the observed
stellar population of spiral bulge components, and are probably poor
line emitters.

The surface gravity of all models was log g=4, corresponding to
main sequence gravities, and solar chemical composition was always used
(see Kurucz 1979). The incident radiation was set to be parallel to
the normal to the atmosphere in all models, i.e. μ0=1.
3.2) Model Structure with Increasing $\beta$

In order to converge models at high illuminations typical of the BLR, incident radiation was added slowly to prevent numerical difficulties. This procedure left a record of the change in atmospheric structure as $\beta$ increased. This corresponds to the structure changes that a star would undergo as it orbits in closer to the central source. Figures 3.1-3.4 show the structure change in a 10,000°K atmosphere at a log$\beta$ of 9, 10, 11, and 12.5, respectively. The development of a sharp ionization front can be seen as the amount of incident ionizing flux increases relative to the stellar ionizing flux. Figures 3.5-3.8 show the corresponding $H_\beta$ profiles for these models. Remarkably little change is seen in these profiles until a log$\beta$ of about 12 is reached. Coincidently, at this distance from the central source, incident photons of 13.6 eV begin to exceed the stellar flux at this energy. Even at log$\beta$=12.5, emission is superimposed on broad, underlying stellar absorption. This absorption is due to the hydrogen in the temperature minimum region just below the ionization front. The hydrogen at these depths is partially ionized by stellar continuum flux and kept at a temperature appropriate for absorption of $H_\beta$ photons emitted by hotter, deeper layers. Both hotter and cooler stars than type A should produce less underlying stellar absorption from the temperature minimum region. Hotter stars, however, will also have stronger continua that will tend to wash out the emission lines that appear at log$\beta$=12.5. The higher temperatures should also tend to inhibit recombination. Therefore, we expect that values of log$\beta$$\gg$12.5
Figure 3.1 Atmospheric structure for \( T = 10000^\circ \) K, \( \log \beta = 9 \). First of four plots showing the effect of increasing illumination on the structure of an A star.
Figure 3.2 Atmospheric structure for \( T=10000^\circ \text{K}, \log\beta=10 \). Second of four plots showing the effect of increasing illumination on the structure of an A star.
Figure 3.3 Atmospheric structure for $T=10000^{\circ}$ K, $\log \beta=11$, Third of four plots showing the effect of increasing illumination on the structure of an A star.
Figure 3.4 Atmospheric structure for T=10000° K, logB=12.5. Last of four plots showing the effect of increasing illumination on the structure of an A star.
Figure 3.5  H$_{\beta}$ line profile $T=10000^\circ$ K, log$\beta=9$. First of four plots showing the effect of increasing illumination on an A star H$_{\beta}$ line profile.
Figure 3.6 H₂ line profile T=10000° K, logβ=10. Second of four plots showing the effect of increasing illumination on an A star H₂ line profile.
Figure 3.7 H$_B$ line profile $T=10000^\circ$ K, $\log\beta=11$. Third of four plots showing the effect of increasing illumination on an A star H$_B$ line profile.
Figure 3.8 H$_\beta$ line profile T=10000° K, logB=12.5. Last of four plots showing the effect of increasing illumination on an A star H$_\beta$ line profile.
would be necessary to drive hotter stars into significant emission, if they are even stable in these regions very close to the central source. On the other hand, cool stars should be excellent emitters. The stellar continua drop as the temperature decreases and the hydrogen in the temperature minimum region becomes a poor Balmer line absorber.

3.3) Model Structure with Decreasing Temperature, logβ = 12.5

Figures 3.9-3.12 show the effects on atmospheric structure of decreasing the effective temperature of the underlying main sequence star. Models shown are for 8000°K, 7000°K, 6000°K, and 5000°K respectively. Figures 3.13-3.16 show the corresponding Hβ profiles for these models. By the time roughly K star temperatures are reached, underlying stellar absorption has all but disappeared. This lack of absorption is important since any absorption present in the profile in an individual star will subtract from the total line emission when many profiles of different velocities are convolved together. These models at varying temperature were obtained by slowly reducing $T_{\text{eff}}$ for the 10,000°K model at logβ = 12.5 in the previous section. A similar temperature sequence was calculated at logβ = 11 and at this level of illumination, no model at any temperature showed Hβ in emission. This implies that even when using a K star as the seed type, rather than a type A star, logβ of 11.5 or higher is necessary to drive the stellar absorption into emission. The hydrogen line intensities and line ratios calculated for the ATLAS model at 5000°K and logβ = 12.5 are given in table 3.2, below.
Figure 3.9 Atmospheric structure for $T=8000^\circ$ K, $\log\beta=12.5$. First of four plots showing the effect of decreasing effective temperature of the seed star.
Figure 3.10 Atmospheric structure for T=7000° K, log$\beta$=12.5. Second of four plots showing the effect of decreasing effective temperature of the seed star.
Figure 3.11 Atmospheric structure for $T=6000^0$ K, log$\beta$=12.5. Third of four plots showing the effect of decreasing effective temperature of the seed star.
Figure 3.12 Atmospheric structure for $T=50000^\circ K$, $\log \beta=12.5$. Last of four plots showing the effect of decreasing the effective temperature of the seed star.
Figure 3.13 H$_\beta$ line profile $T=8000^\circ$ K, $\log g=12.5$. First of four plots showing the effect of decreasing the effective temperature of the seed star on the H$_\beta$ profile.
Figure 3.14 H$_{\beta}$ line profile T=7000° K, log$\beta$=12.5. Second of four plots showing the effect of decreasing effective temperature of the seed star on the H$_{\beta}$ line profile.
Figure 3.15 $\text{H}_\beta$ line profile $T=6000^\circ \text{K}$, $\log \beta = 12.5$. Third of four plots showing the effect of decreasing the effective temperature of the seed star on the $\text{H}_\beta$ line profile.
Figure 3.16 Hβ line profile $T=5000^\circ$ K, $\log\beta=12.5$. Last of four plots showing the effect of decreasing effective temperature of the seed star on the Hβ line profile.
These numbers can be used as fiducial values for judging the importance of adding IR flux to the models in the next section. Values in Table 3.2 were obtained by fitting a linear continuum to the calculated spectrum, and integrating the emergent flux minus the continuum flux over the line with a 30 to 70 point Simpson's rule.

**TABLE 3.2**

Line Fluxes and Ratios for T=5000°K, logβ=12.5, IR cutoff=20μm

<table>
<thead>
<tr>
<th>Line</th>
<th>Line Flux (ergs/sec/cm²)</th>
<th>Ratio (F_{line}/F_{Hα})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hβ</td>
<td>0.266×10⁹</td>
<td>1.0</td>
</tr>
<tr>
<td>Lyα</td>
<td>0.160×10¹⁰</td>
<td>6.02</td>
</tr>
<tr>
<td>Hα</td>
<td>0.130×10⁹</td>
<td>0.49</td>
</tr>
<tr>
<td>Pα</td>
<td>0.116×10⁸</td>
<td>0.04</td>
</tr>
</tbody>
</table>

3.4) Models with Extended IR Flux, 5000°K and logβ=12.5

Incident IR flux longward of 20μm, when added to the ATLAS atmospheres, affects the structure of the completely ionized upper layers. The dominant opacity source is hydrogen free-free absorption, which is proportional to $N_e^2/\nu^3$. Although $N_e$ increases with depth in the atmosphere, the depth at which most of the incident energy is deposited depends strongly on the frequency at which the power law spectrum cuts off. If this cutoff comes at low enough frequencies, the $1/\nu^3$ factor
dominates the opacity and the increasing density is relatively unimportant by comparison. Since the power law radiation increases toward the red, more energy is deposited in the upper layers than the lower. This leads to a steep, decreasing temperature profile as one goes to deeper depths. On the other hand, if the infrared cutoff of the incident radiation comes at shorter wavelengths, say 100\(\mu\)m, the factor of \(N_e^2\) dominates the opacity. Since density increases inward, more of the incident IR energy is absorbed deeper in the atmosphere. This leads to an increasing temperature profile with depth. It also explains, at least in part, the gentle rise in temperature seen in the outer layers of the 20\(\mu\)m cutoff, standard ATLAS model seen in figure 3.12. This increasing temperature gradient must eventually change signs once the IR cutoff moves to long enough wavelengths for the \(1/\nu^3\) term to take over. Figures 3.17 and 3.18 show the structure of hybrid atmospheres with incident flux cutoffs at 100\(\mu\)m and 3mm, respectively. Tables 3.3 and 3.4 give line fluxes and ratios for each model.

**TABLE 3.3**

Line Fluxes and Ratios, \(T=5000^\circ\)K, \(\log\beta=12.5\), IR Cutoff = 100\(\mu\)m

<table>
<thead>
<tr>
<th>Line</th>
<th>Line Flux(ergs/sec/cm(^2))</th>
<th>Ratio((F_{line}/F_{H\alpha}))</th>
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</thead>
<tbody>
<tr>
<td>(H_\beta)</td>
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<tr>
<td>(Ly_\alpha)</td>
<td>(0.825\times10^9)</td>
<td>2.36</td>
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<tr>
<td>(H_\alpha)</td>
<td>(0.167\times10^9)</td>
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<tr>
<td>(P_\alpha)</td>
<td>(0.173\times10^8)</td>
<td>0.05</td>
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</table>
Figure 3.17 Atmospheric structure, T=5000° K, logβ=12.5. Effects of extending the incident power law from 20μm to 100μm.
Figure 3.18 Atmospheric structure, T=5000° K, log $\beta$=12.5. Effects of extending the incident power law from 20$\mu$m to 3mm.
These atmospheres are standard 5000°, log β=12.5 ATLAS results with the upper layers approximated by the technique described in section 2.4. The effect of adding incident infrared to the models is primarily to decrease the amount of Lyα relative to Hβ. In figures 3.19-3.21 the monochromatic source function for Lyα, Hβ, and Hα are plotted against depth, respectively. The source function for Lyα peaks higher in the atmosphere, while Hα and Hβ both form at about the same place, and closer to the front. The upper atmosphere is the region most affected by the addition of IR flux beyond 20μm. Lyα drops relative to Hβ since the density in the outer atmosphere decreases due to the extra heating there.

**TABLE 3.4**

Line Fluxes and Ratios, 5000°K, log β=12.5, IR Cutoff = 3mm

<table>
<thead>
<tr>
<th>Line</th>
<th>Line Flux (ergs/sec/cm²)</th>
<th>Ratio (Fline/FHβ)</th>
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<tr>
<td>Hβ</td>
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<td>Lyα</td>
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<td>Hα</td>
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<tr>
<td>Pa</td>
<td>0.169x10⁸</td>
<td>0.05</td>
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</table>
Figure 3.19 The Lyα source function, $T=5000^\circ K$, $\log g=12.5$, IR cutoff=20μm.
Figure 3.20 The H\textsubscript{\beta} source function, T=5000° K, log\beta=12.5, IR cutoff=20μm.
Figure 3.21 The H$_\alpha$ source function, $T=5000^\circ$ K, $\log$$\theta=12.5$, IR cutoff=20$\mu$m.
3.5) Convergence Properties of ATLAS Models

Figures 3.22-3.24 show the convergence properties of the 5000°K, \( \log \beta = 12.5 \) standard ATLAS model. In figure 3.22, the percentage flux error and flux derivative error are plotted with depth. Figure 3.23 plots the current predicted percentage temperature changes with depth along with the temperature profile itself. Figure 3.24 shows the actual computed values of \( H^d \) and \( H \) together with the actual values of \( dH^d/dt \) and \( dH/dt \). The DTFLUX temperature correction is proportional to \( dT^d/dt \) (eq. 2.38) so that at temperature minimum, this correction becomes ambiguous, leading to an unrealistic DTFLUX temperature corrections at this depth. This is part of the explanation for the large spike seen in the predicted temperature correction near the temperature minimum in figure 3.23. Another obvious spike is found in figure 3.24, between the curves for \( dH^d/dt \) and \( dH/dr \). The flux derivatives have been scaled in this plot so that they appear closer to convergence than they are. Actual errors are more appropriately given for the flux derivative convergence in figure 3.22. Figure 3.24, however does show a spiked difference between the two at around optical depths of -2.0 to -2.5. This coincides with the position where the source functions for \( H_\alpha \) and \( H_\beta \) peak (see figures 3.20 and 3.21). Apparently, some line flux is slipping through the holes in the frequency grid. While the frequency grid used includes points in most of the major lines, better spectral coverage is probably needed in these regions due to the large amount of flux now emitted in the lines.
Figure 3.22 Percent flux error and flux derivative error for a standard 5000° K, \( \log\beta=12.5 \) atmosphere with IR cutoff=20\( \mu \)m.
Figure 3.23 Percentage temperature change predicted, along with temperature for a standard 5000° K, $\log f=12.5$, IR cutoff=20μm atmosphere.
Figure 3.24 $H'$, $H$, $d\ln \beta_1/dt$, and $d\ln \beta_0/dt$ for a standard 5000° K atmosphere with IR cutoff-20μm.
In addition to these obvious points of difficulty, there is a general lack of flux convergence throughout the atmosphere. This can be unambiguously traced to numerical inaccuracies in computing the derivative flux error. The derivative flux error is the difference between the frequency integrals of \( \kappa_\nu (J_\nu - S_\nu) \) and \( \kappa_\nu H_\nu \epsilon e^{-\tau_\nu} \) (see equations 2.12, 2.11, and 2.9). These two integrals are therefore done with two radically different frequency distributions (one a power law, the other a black body) acting as weights for the \( \kappa_\nu \) function. The opacity is a fairly discontinuous function of frequency. Severely different weighting of the opacity tends to emphasize different regions in each integral. The integration grid should therefore be very fine to do both integrals accurately. This would have required, however, far more computing time than was available. The numerical inaccuracy in the calculation of the flux derivative error has a direct effect on the DTLAMB temperature correction (see eq. 2.38). This temperature correction is directly proportional to the flux derivative error, and therefore poor temperature corrections are made to the atmosphere. These bogus corrections would tend to add up from iteration to iteration, finally causing the atmosphere to diverge if it were not for the flux correction, DTFLUX. As the atmosphere is nudged away from convergence by the DTLAMB correction, flux errors begin to rise. The DTFLUX correction is proportional to \( \Delta \tau_0 \) (eq. 2.38) which is obtained from the differential equation (2.25) which is based on \( \Delta H \). Therefore, DTFLUX rises to cancel the spurious temperature shifts caused by DTLAMB. This leads to an atmosphere that is very stable against divergence, but also (unfortunately) against further convergence. This
behavior can also explain the spike in the predicted percentage temperature change in figure 3.23. In the vicinity of the temperature minimum, the DTFLUX error becomes ill-defined, and cannot balance the erroneous temperature shifts being made by DTLAMB. The result is a larger temperature correction than average in this region.

To summarize, the numerical inaccuracy of the flux derivative error calculation leads to a counterbalancing flux error that will cause their associated temperature corrections to cancel. If the derivative flux error was more accurately computed, the artificial flux error generated to contain it should vanish. While it was not possible to raise the number of frequency points by an order of magnitude, it was possible to calculate the flux derivative errors another way. Instead of calculating the difference of the two integrals described above, a flux derivative error can be obtained instead by numerically calculating the depth derivative of the flux error,

$$\Delta H' = \frac{d\Delta H}{dt} \quad (3.3)$$

This value is then used in equation 2.38 to calculate DTLAMB. Figure 3.25 shows the percentage flux error and flux derivative error when the new flux derivative error of equation (3.3) is used. The flux convergence is now excellent, the maximum flux error is only a few percent. The independent constraint on $J_\nu - S_\nu$ has been removed, however, and the flux derivative error (still calculated as before, though not used in the temperature correction scheme) is seriously
Figure 3.25 Percent flux error and flux derivative error for a 5100° K, log\(\beta\)=12.5 atmosphere with IR cutoff=20\(\mu\)m. This model has a modified DTLAMB temperature correction to avoid numerical errors in the flux derivative.
worse. No similar process can improve the flux derivative errors at the expense of the flux errors. This clearly indicates that the derivative errors are the cause of the fairly poor flux convergence. Line fluxes and ratios for this model are given in table 3.5. It appears that the Ly\(\alpha\)/H\(\beta\) ratio is sensitive to the derivative error. Since the DTLAMB correction (based on the derivative error) is most significant to convergence in the upper atmosphere where the Ly\(\alpha\) is formed, this is not surprising. Therefore, though the flux error is greatly improved with this model, \(J_\nu - S_\nu\) has not converged and the results are probably less reliable than the standard model (table 3.2).

### Table 3.5

Line Fluxes and Ratios, 5100°K, log\(\beta\)=12.5, IR Cutoff=20\(\mu\)m, Modified DTLAMB Calculation

<table>
<thead>
<tr>
<th>Line</th>
<th>Line Flux (ergs/sec/cm(^2))</th>
<th>Ratio ((F_{\text{line}}/F_{\text{H(\beta)}}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>H(\beta)</td>
<td>0.577\times10^8</td>
<td>1.0</td>
</tr>
<tr>
<td>Ly(\alpha)</td>
<td>0.132\times10^{10}</td>
<td>22.9</td>
</tr>
<tr>
<td>H(\alpha)</td>
<td>0.420\times10^8</td>
<td>0.73</td>
</tr>
<tr>
<td>P(\alpha)</td>
<td>0.601\times10^7</td>
<td>0.10</td>
</tr>
</tbody>
</table>
4.1) Discussion of Model Structure

In determining whether stars are important in the BLR, one of the most interesting results found from these calculations is that the atmospheres go into significant emission at $\log T = 12.5$. This corresponds to measured BLR sizes very closely (see table 3.1). In addition, it is found that cool stars are the better emitters. For any given $\log T$, at lower temperatures, the stellar continuum falls away, leaving only the emission from reprocessed incident flux. Furthermore, the lines are not contaminated by broad stellar absorption from neutral hydrogen in the temperature minimum region of the atmosphere. Bulge component stars of spiral galaxies are old and metal rich, implying that the line emitting cool stars are more likely to be found in abundance near the BLR.

All the plane parallel models computed here are very stable. Figure 4.1 shows the ratios of emergent and incident radiation pressure to the total pressure for a standard 5000°K, $\log T = 12.5$ atmosphere with
Figure 4.1 Fractional incident and emergent radiation pressures for a 5000° K, log$\beta$=12.5 atmosphere with IR cutoff=100$\mu$m.
incident IR cutoff at 100\(\mu m\). The high ratio of incident radiation to total pressure in the upper atmosphere indicates that the incoming radiation acts as a stabilizing force, helping to hold the atmosphere together. This is chiefly due to the large infrared opacities in the upper atmosphere and the copious amount of incident IR radiation. In contrast, the emergent radiation pressure is a small fraction of the total pressure. Opacity in the upper atmosphere at shorter wavelengths is small, and the emergent flux peaks at these wavelengths (see figure 4.2 for a full spectrum plot). If these stars are to lose material it must be through a thin thermal wind. Of course these plane parallel atmospheres cannot predict what happens in an actual spherical geometry. The fact that the incident radiation pressure is so dominant, however, suggests that angular pressure gradients in a spherical star may indeed cause deformations and perhaps mass loss through ablation. Figure 4.2 also shows that the spectral distribution of the emergent radiation is approximately thermal, with a wavelength at maximum of 6000 Å. This is too far into the red to be a possible explanation for the blue excess (or big bump) that is observed in the spectra of active galactic nuclei (AGN).

Finally, the structure of the outer layers is sensitive to the IR cutoff assumed for the incident power law radiation. A recent review of continuum components of AGN by Lawrence (1987) concludes that there should be a drop off in continuum radiation in the sub-millimeter bandpass, and that the continua of broad line objects have a similar power law continuum out to roughly 100\(\mu m\). Until more complete data are
Figure 4.2 Full spectrum plot for a 5000° K, log\( \beta \)=12.5 atmosphere with IR cutoff=20\( \mu \)m.
available on the IR continua of these objects, 100μm will serve as a reasonable figure for the rest of this discussion.

4.2) Comparison of Calculated Line Strengths with Observations

One of the difficulties encountered in early attempts at predicting BLR spectra with photoionized cloud models was the large (around 50) \( \text{Ly}_\alpha/\text{H}_\beta \) ratio that they produced. This problem was overcome with the addition of a soft x-ray component to the incident flux (see Ferland and Shields 1985 for a review). For the standard atmosphere model with an IR cutoff of 20μm, \( \text{Ly}_\alpha/\text{H}_\beta \approx 6 \). This is close to the average value of 7 adopted by Netzer (1985). The same atmosphere with an IR cutoff of 100μm has \( \text{Ly}_\alpha/\text{H}_\beta \approx 2.36 \). This is not far from the value found by Baldwin (1977) of 3. Lacy et al (1982) find a similar range of values (2.7 to 6) that also agree quite well with the atmosphere calculations. The reason these ratios are so low in comparison with photoionization model values is very probably a density gradient effect. \( \text{Ly}_\alpha \) is formed higher in the atmosphere where lower density means fewer emitting atoms. \( \text{H}_\beta \) forms deeper, near the front, where the density is higher. While the computed values for the \( \text{Ly}_\alpha/\text{H}_\beta \) ratio for atmospheres with extended IR flux may be somewhat dependent on the approximation technique used to model the upper atmosphere, \( \text{Ly}_\alpha/\text{H}_\beta \) seems to be correlated with the IR cutoff of the incident flux. Lower cutoff frequencies correspond to lower \( \text{Ly}_\alpha/\text{H}_\beta \) ratios. \( \text{H}_\alpha/\text{H}_\beta \) for the standard model, regardless of the IR cutoff wavelength is roughly 0.5. Commonly observed values for this ratio are around 3 to 4 (Ferland and
Shields 1985). Stellar atmosphere models fall short of this figure by a significant amount, and values of $\text{H}_\alpha/\text{H}_\beta = 0.5$ are never observed. On the other hand, photoionization models have had some difficulty in predicting a ratio as small as 3, unless the electron densities of the models are raised to higher values than the standard $10^9 \text{ cm}^{-3}$ needed to produce the correct amount of CIII] emission. A two component model with high and low density clouds has been suggested as a reasonable solution. Similarly, if $\text{H}_\alpha/\text{H}_\beta$ is too large in photoionization models, addition of stellar emission as an alternative high density component will bring the values down. At this point, however, it seems that main sequence stars alone cannot reproduce the hydrogen line ratios of the BLR spectrum on their own. The $\text{P}_\alpha/\text{H}_\beta$ ratio for the standard atmosphere model with 100$\mu$m IR cutoff is .05. Lacy et al (1982) show a majority of objects have $\text{P}_\alpha/\text{H}_\beta \approx .28$ or values along a reddening line from .28. The $\text{P}_\alpha/\text{H}_\beta$ ratio of the stellar model is quite low by comparison. One reason for the small calculated values is that the $\text{P}_\alpha$ line is strongly self absorbed. Figure 4.3 shows the $\text{P}_\alpha$ profile for this model. In summary, while $\text{Ly}_\alpha/\text{H}_\beta$ is in good agreement with the observations, the other hydrogen line ratios are too small. One way of helping both the high line ratio values of some photoionized models and the low values of stellar models is to assume that the observed spectrum is a combination of both.

The flux in the $\text{H}_\beta$ line for the standard model with 100$\mu$m IR cutoff is $3.5 \times 10^9 \text{ ergs/sec/cm}^2$. If we want approximately half of the observed $10^{42}$ ergs emitted in the $\text{H}_\beta$ line to be supplied by stellar
Figure 4.3 Paschen-α line profile for a 5000° K, logβ=12.5 atmosphere with IR cutoff=20μm.
atmospheres, then at a distance of log$\beta$=12.5 (i.e., assuming a luminosity of $10^{46}$, a radius of 36.24 ly days), one needs a covering factor of about 0.013. This is assuming that all the radiating stars are at log$\beta$=12.5 and that each star has a standard K dwarf radius of .85 solar. The radius of the star is not seriously affected by the incident radiation. The incident radiation pressure helps to increase the effective gravity in the same region it acts to increase the stellar temperature (see Fig. 4.1). Due to the small size of these stars, this covering factor implies an unreasonably high space density of stars of about $10^{16}$/pc$^3$. One way to lower this space density is to increase the stellar radius by lowering the surface gravity. Illuminated stellar atmospheres at low gravity, however, have not been wholly successful yet. In addition, stars at higher log$\beta$ should emit more line radiation. This would also tend to reduce the space density of stars needed to supply the line flux, although log$\beta$ cannot be increased to the point where the BLR is too small (i.e. less than a light day).

4.3) Directions for Further Studies

The results presented in Chapter III indicate some very promising directions for further investigation. Primarily, convergence of the models will no doubt improve if the number of frequency points is increased by an order of magnitude, from the current 400 to 4000. Vectorizing the ATLAS code for a parallel processor should provide time savings that would allow for this expansion of the frequency set. The
flux derivative calculation should become more accurate, and barriers to further flux convergence should be removed.

Illuminated low gravity models should come within reach of the code once convergence is improved. If stars are to play a significant role in the BLR, they must supply the line radiation at smaller space densities. A more realistic model of the BLR stellar population and distribution should be made. This should include a study of the change in H$_\beta$ line flux as log$\beta$ gets larger, as well as how it changes for low gravity models. Both of these factors might reduce the number of stars necessary to produce the observed line emission. Further, a more realistic incident spectrum should be employed rather than a simple power law.

It would be interesting to calculate other line strengths as well, especially for the CIII] $\lambda$1909/CIV $\lambda$1550 ratio. No main sequence model should be capable of CIII] emission, however, since electron densities for these models were always greater than $10^{11}$ cm$^{-3}$. The CIII] line is collisionally quenched at $N_e \approx 10^{10}$ cm$^{-3}$. This situation highlights another reason for investigating low gravity atmospheres, where lower densities might lead to CIII] emission. All elements except for hydrogen have level populations treated as LTE by ATLAS. Table 4.1 shows the run of hydrogen departure coefficients (for levels 1-6) with depth for the standard atmosphere with 100$\mu$m cutoff. Clearly departure from equilibrium is very strong for hydrogen and the inclusion of non-
<table>
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<th>RHOX</th>
<th>$b_1$</th>
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<th>$b_3$</th>
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<td>7.19</td>
<td>2.5971</td>
<td>1.4754</td>
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<tr>
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<td>7.19</td>
<td>2.5971</td>
<td>1.4754</td>
<td></td>
</tr>
</tbody>
</table>

**TABLE 4.1**

Departure Coefficients for Hydrogen

$T=5000^\circ K$, $\log \beta = 12.5$, IR cutoff = 100\,\mu m
LTE effects may be important for line ratios of other atomic species as well.

4.4) Summary and Conclusion

Model atmospheres with incident power law flux have been computed for main sequence stars at a variety of seed star temperatures. The models predict that line emission is produced for stars in the BLR and that the Ly\alpha/H\beta ratio is in good agreement with observations. The other line ratios predicted by the models are lower than the observed values, however. Nevertheless, the observed spectra may contain a stellar component, since photoionization models tend to predict values that are higher than observed. It appears, however, that the stellar component will only be significant if there are large space densities of stars. Cool stars are the best line emitters, but even assuming that the entire stellar population in the BLR is cool, either a large number of stars or larger stars will be needed to provide a significant amount of emission.

Although the ATLAS models suffer from fairly large flux errors, the temperature corrections being predicted by these errors are much smaller (see figure 3.23). This would imply that the structure of these atmospheres is not far from the completely converged case. The atmospheres tend to be stable, due to the importance of the incident radiation pressure and the very small emergent radiation pressure. The outer atmospheric structure is sensitive to the incident IR cutoff.
This most strongly affects the Ly$_\alpha$ line, which is formed in higher atmospheric layers. Therefore the Ly$_\alpha$/H$_\beta$ ratio is a function of the incident IR cutoff frequency. Results of this study are very intriguing and further investigation of the problem on a large computer is warranted.
LIST OF REFERENCES


Davidson, K. and Netzer, H. 1979, Rev. Mod. Phys., 51, 715.


