Chapter 11

Non-LTE Atmospheres

In the approximation of LTE we assumed that all occupation numbers for matter are given by the equilibrium values at the local temperature. The extinction coefficient and the emissivity can then be calculated in a straightforward manner using the techniques of Chapter 6, and this considerably simplifies the solution of the equation of radiative transfer.

In this chapter we will consider the consequences of not adopting the approximation of LTE and of instead calculating the ocupation numbers for the excitation and ionization distributions using techniques from statistical mechanics. The extinction coefficient and the emissivity then follow from the ocupation numbers. However, we will continue to assume the atmosphere is in steady state, we will continue to assume that we have a static atmosphere in hydrostatic equilibrium, and we will continue to assume that the distribution of massive particle velocities is given by a Maxwellian at the local temperature. (An example of a non-LTE problem in which we have to consider the time dependence explicitly is the cooling and recombination region behind a shock.)[*Need to explain somewhere why Maxwell is good even in non-LTE conditions.*]

Excitation Distribution

The general LTE problem calculates both the excitation and ionization distributions explicitly, without assuming that they are given by the Boltzmann and Maxwell distributions. However, let us consider first a special case of non-LTE problems, in which we will assume that the ionization distribution is still given by the Saha distributions, and investigate the implications of attempting to solve explicitly for the excitation distribution. We will consider the more general case subsequently.

In order to maintain a steady state on a macroscopic scale, we must have statistical equilibrium, which means that the total rates of population and depopulation of each level must be equal. Levels can be populated or depopulated by either radiative or collisional processes. The radiative processes we must consider are absorption and stimulated emission,

$$X \rightleftharpoons X' + \gamma, \tag{11.1}$$

and spontaneous emission,

$$X + \gamma \to X' + 2\gamma. \tag{11.2}$$

In both, there is an exchange of between the internal energy of particle X or X' and the photon. Recalling the definition of the Einstein coefficients, the rate per unit volume of radiative transitions from level i to level i' is

$$n_i R_{ii'} \equiv \begin{cases} n_i[A_{ii'} + B_{ii'} \int_0^\infty d\nu\ J_\nu(\nu)\psi(\nu)], & \text{for desexcitations,} \\ n_i B_{ii'} \int_0^\infty d\nu\ J_\nu(\nu)\psi(\nu), & \text{for excitations,} \end{cases} \tag{11.3}$$

in which n_i is the density of particles in level i. The collisional processes we must consider are and collisional excitation and deexcitation between states X and X',

$$X + Y \rightleftharpoons X' + Y, \tag{11.4}$$

Here there is an exchange between the internal energy of the "target" particle X or X' and and the kinetic energy of the "colliding" particle Y. The rate per unit volume of collisional transitions between level i and level i' involving a colliding particle Y is

$$n_i n_Y C_{ii'} \equiv n_i n_Y \int_0^\infty dv_Y\ f_Y(v_Y)\sigma_{ii',Y}(v_Y)v_Y, \tag{11.5}$$

in which v_Y is the speed of the colliding particle, f_Y the distribution function of speed, and $\sigma_{ii',Y}$ the differential cross-section for the transition. We can write this as

$$n_i n_Y C_{ii'} \equiv n_i n_Y \left\langle \sigma_{ii',Y} v_Y \right\rangle, \tag{11.6}$$

in which $\left\langle \sigma_{ii',Y} v_Y \right\rangle$ is the mean product of the cross-section and the speed integrated over the distribution of speeds.

Possible colliding particles include electrons, ions, and neutral atoms. Electrons always dominate ions, because although ions and electrons have similar cross-sections, the mean speed of the electrons is $(m_{\text{ion}}/m_e)^{1/2} \approx 43A_{\text{ion}}^{1/2}$ larger than that of the ions. Electrons often dominate collisions with neutral atoms, both because neutral atoms are also much slower than electrons and because the Coulomb force of an electron leads to a much higher cross-section than the Van der Waals force of a neutral atom. However, in very cool atmospheres, electrons can become very scarce, and collisions with hydrogen atoms might become important. In what follows, though, we will assume that electrons dominate collisions; including collisions with hydrogen atoms modifies the details of the non-LTE calculation, but does not change its essence (see Problem **??**).

In statistical equilibrium, the net rates of population and depopulation of a level balance, and we have

$$\sum_{i' \neq i} n_i (R_{ii'} + n_e C_{ii'}) = \sum_{i' \neq i} n_{i'} (R_{i'i} + n_e C_{i'i}). \tag{11.7}$$

or, more concisely,

$$\sum_{i' \neq i} [n_i (R_{ii'} + n_e C_{ii'}) - n_{i'} (R_{i'i} + n_e C_{i'i})] = 0. \tag{11.8}$$

We can see straight away that we have one familiar and two new complications:

1. The collisional coefficients $n_e C_{ii'}$ depend on the temperature and electron density. More precisely, $C_{ii'}$ depends on the distribution of velocities, but as we are still assuming that we have a Maxwell distribution of velocities, this reduces to a dependence on temperature. Thus, the excitation distribution depends on density and temperature. This dependence also occurs in a different form in LTE.

2. The radiative coefficients $R_{ii'}$ depends on the mean specific intensity J_ν at the frequencies $\nu_{ii'}$ given by $h\nu_{ii'} = |E_i - E_i'|$. This tight coupling between matter and radiation is new. In LTE, the interaction between matter and radiation is normally required to satisfy radiative equilibrium (or more generally thermal equilibrium), and this results in a much looser coupling through the temperature.

3. The population of each state depends on the populations in all of the states that can populate or depopulate that state. Again, this is not present in LTE.

Thus, non-LTE atmospheres have a local coupling between matter and radiation, a local coupling between states, a local coupling involving thermal equilibrium, and one non-local coupling from the transfer of radiation, whereas LTE problems have only the latter two. The additional tight local couplings make non-LTE atmospheres more difficult to understand and to model than LTE atmospheres.

Excitation-Ionization Distribution

Now let us relax the assumption that the ionization distribution is given by the Saha distribution and consider the general non-LTE problem. We now must consider not only processes that can change the excitation state, but also those that can change the the ionization state. These includes photoionization and spontaneous radiative recombination,

$$X^+ + e^- \rightleftharpoons X + \gamma, \tag{11.9}$$

along with the stimulated radiative recombination,

$$X^+ + e^- + \gamma \rightarrow X + 2\gamma, \tag{11.10}$$

and collisional ionization and three-body collisional recombination,

$$X^+ + 2e^- \rightleftharpoons X + e^-. \tag{11.11}$$

If the density of state i of ionization state j is n_{ij}, the net radiative and collisional rate coefficients for transitions from state ij to state $i'j$ (excitation and de-excitation) are $R_{ii'j}$ and $n_e C_{ii'j}$, the net radiative and collision rate coefficientes for transitions from state ij to state $i'j+1$ (ionization) are $R^+_{ii'j}$ and $n_e C^+_{ii'j}$, and the net radiative and collisional rate coefficients for transitions from state ij to state $i'j-1$ (recombination) are $n_e R^-_{ii'j}$ and $n_e^2 C^-_{ii'j}$ the equation of statistical equilibrium is

$$\sum_{i' \neq i} \left[n_{ij} (R_{ii'j} + n_e C_{ii'j}) - n_{i'j} (R_{i'ij} + n_e C_{i'ij}) \right] + \tag{11.12}$$

$$\sum_{i'} \left[n_{ij} (R^+_{ii'j} + n_e C^+_{ii'j}) - n_{i'j+1} (n_e R^-_{i'ij+1} + n_e^2 C^-_{i'ij+1}) \right] + \tag{11.13}$$

$$\sum_{i'} \left[n_{ij} (n_e R^-_{ii'j} + n_e^2 C^-_{ii'j}) - n_{i'j-1} (R^+_{i'ij-1} + n_e C^+_{i'ij-1}) \right] = 0. \tag{11.14}$$

We can see that this introduces a yet more severe form of the tight coupling that we had when we considered only the excitation distribution. Now, each level is coupled to every excitation level of every ionization state and matter is coupled to the radiation field at any frequency that can produce a transition between any two excitation levels of any two ionization states.

[*Discuss autoionization and dielectronic recombination. Charge exchange?*]

Recovering LTE

The equations of statistical equilibrium, with their high degree of coupling, are sufficiently awful that a natural reaction is to wonder if assuming LTE is really *that* bad. So let us consider under what conditions LTE is likely to be a good approximation, and under what conditions we need to worry about non-LTE effects.

We will once again begin by considering the restricted non-LTE problem in which we solve explicitly only for the excitation distribution. In perfect thermodynamic equilibrium we have detailed balance, so the radiative and collisional transition rates between two states balance, and we have

$$n_i^* R_{ii'}^* = n_{i'}^* R_{i'i}^* \tag{11.15}$$

and

$$n_i^* n_e^* C_{ii'}^* = n_{i'}^* n_e^* C_{i'i}^*. \quad (11.16)$$

Recall that we use a superscript $*$ for quantities in thermodynamic equilibrium. Summing over all states gives

$$\sum_{i' \neq i} n_i^* R_{ii'}^* = \sum_{i' \neq i} n_{i'}^* R_{i'i}^* \quad (11.17)$$

and

$$\sum_{i' \neq i} n_i^* n_e^* C_{ii'}^* = \sum_{i' \neq i} n_{i'}^* n_e^* C_{i'i}^*. \quad (11.18)$$

Multiplying the second of these by n_e / n_e^* and adding we obtain,

$$\sum_{i' \neq i} n_i (R_{ii'} + n_e C_{ii'}) = \sum_{i' \neq i} n_{i'} (R_{i'i} + n_e C_{i'i}) \quad (11.19)$$

$$\sum_{i' \neq i} n_i^* (R_{ii'}^* + n_e C_{ii'}^*) = \sum_{i' \neq i} n_{i'}^* (R_{i'i}^* + n_e C_{i'i}^*). \quad (11.20)$$

Comparing this to Equation (11.8), the equation for statistical equilibrium, we see that LTE will be good approximation, and we will have $n_i \approx n_i^*$, to the extent that

$$R_{ii'} + n_e C_{ii'} \approx R_{ii'}^* + n_e C_{ii'}^* \quad (11.21)$$

is a good approximation. Let's consider $C_{ii'}$. This will be the result of integrating a differential cross-section for excitation or de-excitation over the distribution of electron velocities. The distribution of velocities is still given by a Maxwell distribution, and so

$$C_{ii'} = C_{ii'}^*. \quad (11.22)$$

Armed with this, we see that Equation (11.21) reduces to

$$R_{ii'} + n_e C_{ii'}^* \approx R_{ii'}^* + n_e C_{ii'}^*. \quad (11.23)$$

This is a good approximation when either $R_{ii'} \approx R_{ii'}^*$ or both $R_{ii'} \ll n_e C_{ii'}$ and $R_{ii'}^* \ll n_e C_{ii'}$. Since the radiative rate coefficient $R_{ii'}$ depends on J_ν, the first case corresponds to $J_\nu \approx B_\nu$. The second case corresponds to collisions being dominant both in thermal equilibrium and in the conditions being considered.

We can apply exactly the same arguments to the general non-LTE case in which we solve for both the excitation and ionization distribution. Once again, we discover that LTE is a good approximation when either $J_\nu \approx B_\nu$ or when collisions are dominant.

Looking back to Chapter 4, we can now justify using LTE in the diffusion approximation for the transfer of radiation in the interior of a star. The density and temperatures are high, which tends to make collisions dominant, and furthermore $J_\nu \approx B_\nu$. We satisfy both of our criterion for LTE being a good approximation.

However, we can now see that LTE will *never* be a truely good approximation in an atmosphere. Here, the J_ν departs significantly from B_ν, because of the temperature gradients and the presense of the outer boundary, and the densities are low enough that radiative transition rates become important for suffiently strong lines. We might think that if only a few transitions in an atom fail to satisfy the conditions for LTE, we can still treat the other levels as is they satisfied LTE. Unfortunately, because of the coupling between levels in non-LTE problems, this is dangerous; it only needs one transition to fail to satisfy the conditions for LTE to perturb an entire atom or species out of LTE.

On the other hand, we can at least identify those situations in which LTE is a worse approximation. These will be those in which the radiation field is far from Planckian and in which radiative rates are not negligible compared to collisional rates. As we have just mentioned, being in an atmosphere, or more generally outside of the optically thick interior, guarantees that there are significant departures from Planckian radiation. Furthermore, high effective temperatures (higher J_ν and hence higher radiative rates), strong lines (higher radiative rates), and lower densities (lower collisional rates) all conspire to make LTE a worse approximation. We can then see that we should be most suspicious of LTE in winds, in the atmospheres of hot stars, and in the atmospheres of supergiant stars. Conversely, we might expect LTE to be a reasonable approximation in dwarf or degenerate stars and in cool stars.

NLTE Model Atmospheres

Introduction

Here we will discuss two applications of NLTE model atmospheres, in O stars and in solar type stars.

Before discussing the specifics, it is worth considering the two general ways in which NLTE models are different to LTE models. First, NLTE model atmospheres can have a different structure to LTE model atmospheres. That is, the temperature and density as a function of depth in the atmosphere (measured as an optical depth at a given wavelength or as the column density) can be different in LTE and NLTE models which otherwise include the same physics. Second, the emissivity and opacity in NLTE model atmospheres can be different to those in LTE model atmospheres. Thus, the emergent flux (which is an integral function of the emissivity and opacity) can be different.

These considerations give rise to "restricted NLTE" models. In these, typically the structure of the atmosphere (the temperature, total density, and perhaps the electron density as a function of depth) are calculated assuming LTE. Then, the emissivities and opacities are recalculated explicitly in NLTE and are used to produce an emergent flux. Such a procedure is not self-consistent, but it can be a reasonable approximation if the structure of the real atmosphere is indeed adequately approximated by an LTE model. In restricted NLTE models, the only NLTE effects are those of the second kind.

On the other hand, in "full NLTE" models both the structure and the emergent flux are calculated taking into account NLTE effects. These models are self-consistent, although as we shall see this does not mean they are necessarily correct. NLTE Models of O Stars

Lanz & Hubeny (2003)

We will consider the NLTE models of Lanz & Hubeny (2003; ApJS, 146, 417). These authors present a grid of models with effective temperatures from 27,500 K to 55,000 K, surface gravities log g from 3.0 to 4.75, and chemical compositions from metal free to twice the metallicity of the Sun. These ranges of parameters are appropriate for O stars in environments from the early universe to the center of massive galaxies. Their models are full NLTE models with hydrostatic equilibrium and radiative equilibrium.

The authors discuss the validity of their models. They comment that complete models of the atmospheres of O stars require consideration on NLTE effects, line blanketing, and the stellar wind. Their models include NLTE effects and line blanketing, but are conventional hydrostatic models and as such do not include the stellar wind. Given this, it is natural to ask if their models are relevant. The authors strongest argument in favor of their models is that, with the exception of strong UV resonance lines, most lines in the spectrum of a normal O star are formed in the photosphere rather than the wind. These lines are used to determine the basic stellar parameters: the effective temperature, the surface gravity (and hence the mass), and the chemical composition. This statement does not apply to stars with extremely strong winds, like Wolf-Rayet stars and extreme Of supergiants. Therefore, their models are relevant and useful, but one needs to be careful not to apply them to lines or continua that are formed in the wind.

The authors include 40 ions of H, He, C, N, O, Ne, Si, P, Fe, and Ni. Their model atoms have a total of about 100,000 levels, and treating this number of levels explicitly would be computationally difficult. Therefore, they adopt the concept of "superlevels" originally suggested by Anderson (1989; ApJ, 339, 558). A superlevel is a grouping of levels that are assumed to have the same departure coefficient. Effectively, within a superlevel the levels are assumed to have a Boltzmann distribution, but the total population of the superlevel is calculated explicitly in NLTE. They group levels into superlevels when they have the same parity and are close in energy. The parity criterion ensures that there are no radiative transitions between levels in the same superlevel. The energy criterion favors collisional transitions between levels in the same superlevel. Together, the criteria ensure that collisions determine the relative populations within a level, and we have seen that when collisions dominate we tend to regain LTE. This validates the assumption of a Boltzmann distribution within a superlevel. The authors typically treat the lower levels individually and group the higher levels into superlevels. Overall, they treat almost 1000 levels and superlevels in NLTE.

Figure 11 shows the temperature as a function of the Rosseland mean opacity for models with effective temperatures of 30,000 K, 40,000 K, and 50,000 K and ten metallicities from metal-free to twice-solar. In each case, the metal-free model has the highest surface temperature. These diagrams show two effects. One is that NLTE metal-free models show a temperature inversion: the temperature decreases through the photosphere until an optical depth of about 0.01, and then rises towards the surface by several thousands of K. An LTE model would show a monotonic decrease in temperature towards the surface. This rise is an due to indirect heating by Lyman and Balmer lines of hydrogen (Auer & Mihalas 1969; ApJ, 156, 681). However, as the metallicity increases, the surface temperature drops but the photospheric temperature at optical depths of order 0.1 increases. This called "back-warming", and is caused by the additional opacity contributed by metal lines, especially those of iron and other iron-peak elements. At solar metallicity, back-warming dominates.

One would expect that the change in temperature would cause a change in the ionization fraction, in the sense that hotter temperatures would favor higher degrees of ionization. This is certainly the case, but there is a second effect that is a pure NLTE effect. Figure **??** compares the ionization fractions of helium and carbon in models with effective temperatures of 30,000 K, 40,000 K, and 50,000 K and solar metallicity. The solid lines show the ionization fractions from the NLTE models. The dashed lines show the ionization fraction calculated in LTE using the electron density and temperature taken from the NLTE models. One can see that the dominant ionization state behaves quite similarly in NLTE and LTE. However, there are important differences in the other states. We see that the ionization states that are lower than the dominant state are typically less common and ionization states that are higher than the dominant state are typically more common. For example, in the 30,000 K model, the dominant state of carbon is C III, and we see that C II is suppressed and C IV is enhanced with respect to LTE. This shift in ionization is attributable to the contribution of photo-ionization in these atmospheres. Ions can be photo-ionized by the intense radiation coming from hotter, deeper layers, but recombined with electrons at the local temperature. This imbalance shifts the ionization to higher states.

The authors present a comparison of the emergent fluxes in their NLTE models and in the LTE models of Kurucz (1993). At low resolution in the optical and near-ultraviolet, the two sets of models are in relatively good agreement. However, the authors suggest that at the higher resolutions typically used to determine stellar parameters, their models are more reliable. The authors also consider the photon fluxes q0 and q1 in the H I (Lyman) and He I ionizing continua below 912 Å and 504 Å. They do not consider the photon flux q2 in the He II ionizing continuum below 228 Å as this is typically formed in the wind (Gabler, Kudritzki, & Mendez 1991; A&A, 245, 587). This is an example of a limitation of their hydrostatic models. The values of q0 calculated from their models and from LTE models were in systematic agreement, but individual models differed by factors of up to 1.5 higher or lower. However, the NLTE values of q1 were systematically higher by a factor of 1.8 compared to the LTE models, with individual models differing by up to a factor of 3. The value of q1 is important for models of H II regions. The authors consider that, within the limitations of a plane-parallel atmosphere in radiative equilibrium,

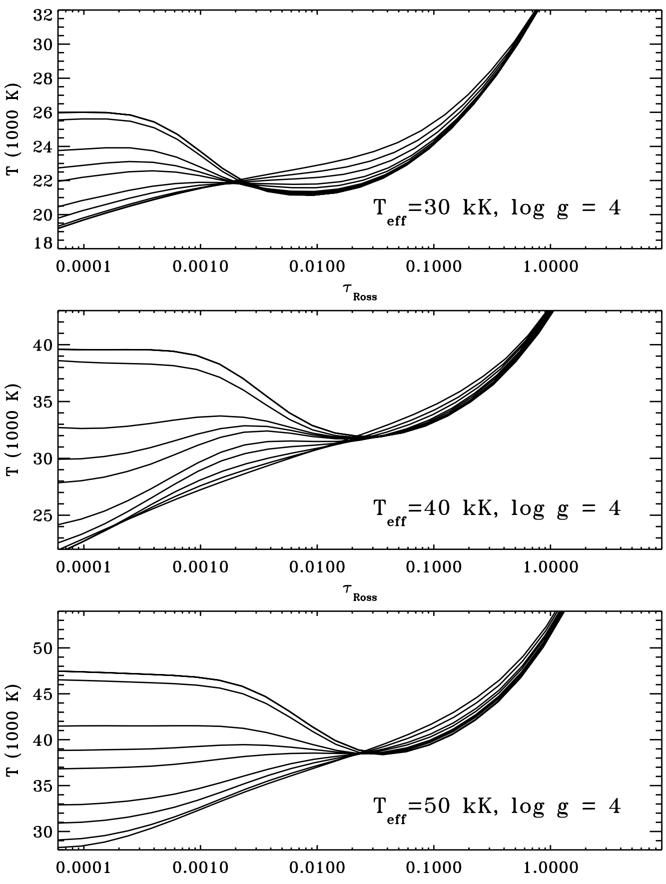

Figure 11.1: Temperature as a function of optical depth in the NLTE models of Lanz & Hubeny (2003). Three effective temperatures and ten metallicities are shown. In each case, the surface gravity is log g = 4.0. The metalicites range from metal-free to twice solar. At each effective temperature, the metal-free models have the highest surface temperature and the solar metallicity models have the second lowest surface temperatures.

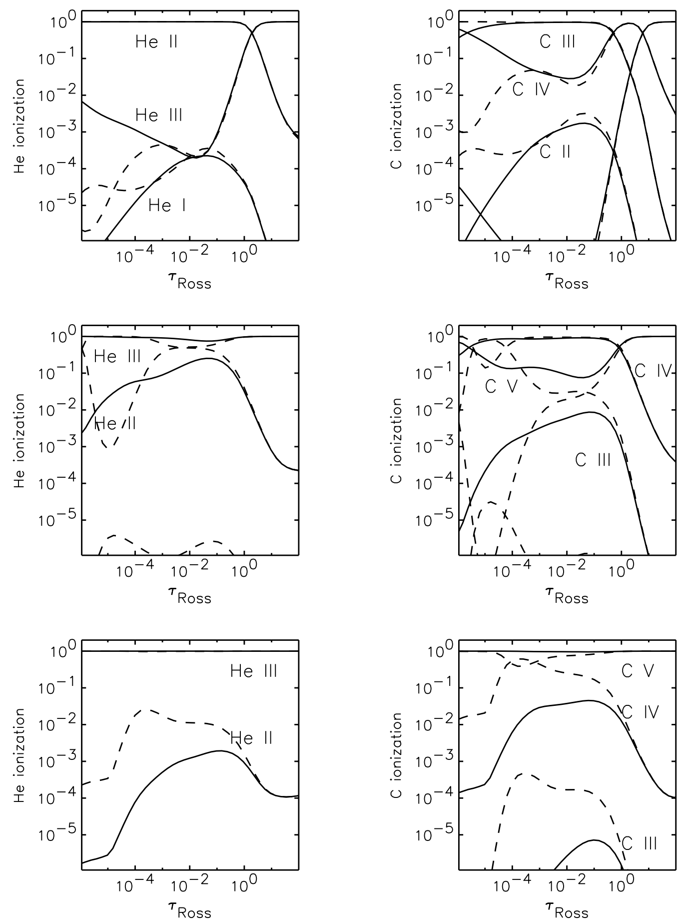

Figure 11.2: Ionization fractions of helium and carbon as a function of optical depth in the NLTE models of Lanz & Hubeny (2003). Three effective temperatures are shown. In each case, the surface gravity is log g = 4.0 and the metallicity is solar. The ionization fraction from the NLTE models are shown as solid lines. The ionization fraction in LTE calculated using the Saha distribution using the electron density and temperature from the NLTE model are shown as dashed lines.

the most serious shortcomings in their models a crude treatment of collisional rates for forbidden transitions of iron and nickel and their neglect of higher states of light elements such as carbon.

Short & Hauschildt (2005)

Here we will consider the LTE and NLTE models of the Sun presented by Short & Hauschildt (2005; ApJ, 618, 926). Their NLTE models are "full NLTE" models in which both the atmospheric structure and emergent flux are calculated under NLTE. In comparison, the earlier models of Allende Prieto, Hubeny, & Lampard (2003; ApJ, 591, 1192) were "restricted NLTE" models, in which the atmospheric structure was calculated in LTE and only the emergent flux using NLTE.

The solar atmosphere is obviously cooler than the atmosphere of an O star and more species contribute to the structure and opacity. The models of Short & Hauschildt include H, He, Li, C, N, O, Ne, Na, Mg, Al, Si, P, S, K, Ca, Ti, Mn, Fe, Co, and Ni, twice as many elements as in the O star models of Lanz & Hubeny (2003).

These authors do not adopt "superlevels". Instead, they treat levels connected by relatively strong transitions (those with log gf greater than -3) in NLTE and all others in LTE (i.e., using the Boltzmann distribution with the local temperature and electron density). They treat a total of about 6500 levels in NLTE.

The authors begin by showing that the temperature differences between LTE and NLTE models are less than 250 K. The NLTE model is 200 K warmer close to the surface (above optical depths of 0.01) and 150 K cooler at the base of the photosphere (at optical depths above 10). These changes are much less than in the case of O stars, in which we observed changes of thousands of K. This is expected; LTE is a better approximation in the photosphere of the Sun because the radiation field is weaker and collisions are more dominant.

However, despite the similarity in temperature between the LTE and NLTE models, there are significant differences between the emergent fluxes in the UV. The reason for this is that Fe I provides significant opacity in the UV, although Fe II is the dominant ionization state. The NLTE model show enhanced ionization of Fe I resulting from photo-ionization from the hotter, deeper layers. As can be seen in Figure 11, this reduces the abundance of Fe I and lowers the opacity in the UV.

The bad news is the NLTE model provides a worse fit to the observed flux than the LTE model. This is shown in Figure reffigure:short-hauschild-flux. In the UV, below about 4200 Å, the LTE model over-predicts the flux by about 10% whereas the NLTE model over predicts the flux by about 30%. The authors suggest that this "may indicate that the adoption of LTE masks some other inadequacy in the models". They suggest that it is likely that there is a significant source of opacity that is still missing from the models.

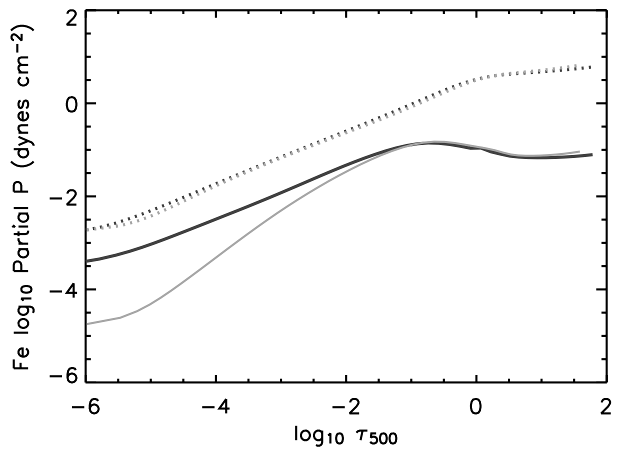

Figure 11.3: Partial pressures of Fe I (solid lines) and Fe II (dotted lines) in the LTE (thick lines) and NLTE (thin lines) models of Short & Hauschildt (2005).

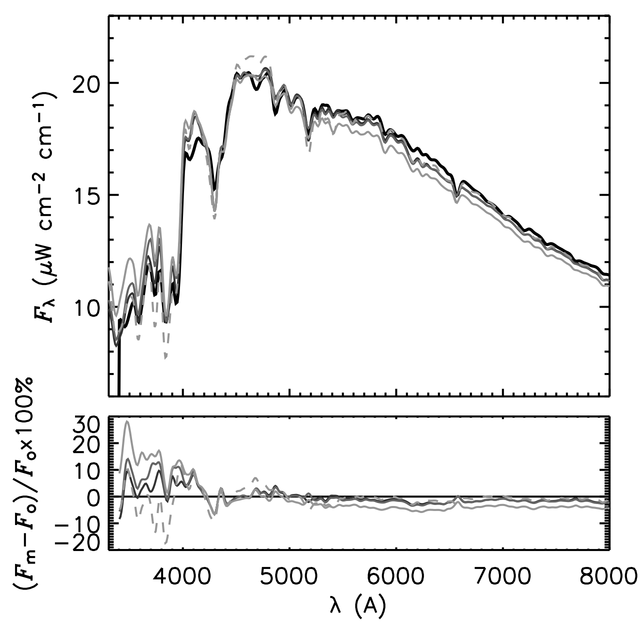

Figure 11.4: Comparison of the absolute flux of the Sun measured by Neckel & Labs (1984) and the LTE and NLTE models of Short & Hauschildt (2005). The thick black line is the measured flux. The thin black line is the flux from the LTE model. The light gray line is the NLTE model. The lower panel shows the difference between the model fluxes and the observed flux.

Summary

As we have seen, NLTE effects are important in stars as diverse as O stars and solar-type stars. However, we have also seen that NLTE models are not magically correct in all respects. They suffer from uncertainties in atomic data and from the omission of important physics such as winds, chromospheric heating, and inhomogeneities. Nevertheless, NLTE is an important step towards more realistic models.