

# 2 Stellar Atmospheres

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**Abstract:** Basic concepts of the stellar atmospheres theory are briefly outlined. After discussing essential assumptions, approximations, and basic structural equations describing a stellar atmospheres, emphasis is given to describing efficient numerical methods developed to deal with the stellar atmosphere problem, namely the method of complete linearization and its recent variants, and the whole class of methods known by name Accelerated Lambda Iteration. The existing computer codes, and some of the most useful grids of model atmospheres that are publicly available, are briefly summarized. Some interesting properties of newly computed NLTE models atmospheres and their comparison to LTE models are shown. Finally, it is briefly shown how the model atmospheres are used to determine basic stellar parameters.

## 1 Introduction

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The term stellar atmosphere refers to any medium connected physically to a star from which the photons escape to the surrounding space. In other words, it is a region where the radiation, observable by a distant observer, originates. Since in the vast majority of cases the radiation is the only information about a distant astronomical object that can be obtained (exceptions being a direct detection of solar wind particles, neutrinos from the Sun and SN1987a, or gravitational waves), all the information that is gathered about stars is derived from analysis of their radiation.

It is therefore of considerable importance to develop reliable methods which are able to decode the information about a star contained in its spectrum with confidence. Having understood the physics of the problem and being able to carry out detailed numerical simulations makes it possible to construct theoretical models of a stellar atmosphere and predict a stellar spectrum. Model stellar atmospheres are one of the building blocks of our understanding of the radiating objects in the Universe. Modeling stellar atmospheres is one of the most mature fields that deals with analysis and spectroscopic diagnostics of astronomical bodies. Being a mature field, one might not expect any significant new developments. But such a view is completely wrong. The last decade brought a renewed interest in modeling stellar atmospheres. There are several reasons for that. The first, more or less obvious, reason is a significantly increased quality and quantity of observational data that bring new challenges for modelers. For instance, thanks to *Hipparcos*, the accurate distances are now known for many stars, which means that the normalization factor to convert the predicted fluxes at the stellar surface to observed fluxes at the Earth is no longer a free parameter.

The last decade also brought an introduction, after almost a century, of completely new stellar spectral types – L and T dwarfs (sometimes referred to as brown dwarfs; Burgasser et al. 1999; Delfosse et al. 1997). At present, there is a vigorous debate about the name for a spectroscopic class of objects cooler than the coolest T-dwarfs; likely candidate being “Y-dwarfs”, essentially because there are not many more remaining letters of the alphabet available.

The second reason, or motivation, for a progress in modeling stellar atmospheres is an ever-increasing computer power, both the memory available, as well as the computer speed. Consequently, much more sophisticated model atmospheres of unprecedented degree of realism may now be constructed in a reasonable amount of computer time.

However, even with most powerful computers and largest memory chips available, one would still not be able to compute sophisticated models without employing clever and powerful numerical methods. Therefore, the third basic reason for a recent progress in modeling stellar atmospheres is a development of new, very efficient numerical methods for solving the highly nonlinear and nonlocal problem, which the solution of the structural equations for stellar atmosphere requires.

Besides being a crucial diagnostic tool for analyzing stellar spectra, the stellar atmospheres theory provides a guide to the methodology of astrophysical quantitative spectroscopy. Stellar atmospheres are the best-studied example of a medium where radiation is not only a *probe* of the physical state, but is in fact an *important constituent*. In other words, radiation in fact *determines* the structure of the medium, yet the medium is probed *only* by this radiation. Unlike laboratory physics, where one can change a setup of the experiment in order to examine various aspects of the studied structures separately, one does not have this luxury in astrophysics: all what is available is an observed spectrum, so the information encoded in it should be extracted as completely as possible. This is exactly what the stellar atmosphere theory is doing for almost a century now. Consequently, it is developed to such an extent that it provides an excellent methodological guide for other situations where the radiation has the dual role of a probe and a constituent. Examples of such astronomical objects are planetary atmospheres, interstellar medium, H II regions, and accretion disks, to name just few.

The main goal of this chapter is to provide a brief introduction to the basic concepts needed to understand the fundamental physics of stellar atmospheres, as well as the leading principles behind recent developments. Particular emphasis will be devoted to the classical plane-parallel atmospheres in hydrostatic and radiative equilibrium. Much more material on stellar atmospheres is presented in several monographs and conference proceedings. The fundamental textbook of the field, Mihalas (1978), is still a highly recommended text, although it does not cover important recent developments, like, for instance, modern numerical methods. The third edition of the book is now in preparation, but it will take some time before it is available. There is a textbook by Rutten (1995), distributed electronically, which covers both the basic concepts as well as some of the modern developments and is recommended to the beginner in the field. There are two books edited by Kalkofen which present a collection of reviews on various mathematical and numerical aspects of radiative transfer (Kalkofen 1984, 1987). A good textbook that covers both the theoretical and observational aspects of the stellar atmospheres is that by Gray (1992). Other related textbooks include Rybicki and Lightman (1979), Shu (1991), and an elementary-level textbook by Böhm-Vitense (1989). An old but excellent textbook on radiative transfer is Jefferies (1968), an even older but classical one by Chandrasekhar (1960), and a newer book by Cannon (1985). There are two excellent books on the topic of radiation hydrodynamics, which contain several chapters related to the present topic, namely Mihalas and Mihalas (1984), and Castor (2004). Besides these monographs, two recent Proceedings (Hubeny et al. 2003, 2009) contain a number of excellent review papers covering various topics in theory and modeling of stellar atmospheres.

## 2 Basic Physics of Stellar Atmospheres

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From the physical point of view, a stellar atmosphere is generally a plasma composed of many kinds of particles, namely atoms, ions, free electrons, molecules, or even dust grains. In an early-type stellar atmospheres, because of the high temperature and strong radiation field, there are typically no molecules nor dust grains present, at least in the layers that are traditionally considered as an atmosphere. Molecules are present in the atmospheres of solar-type stars and cooler, and dust grains (cloud particles) are present in very cool stars and subsolar-mass objects (brown dwarfs and giant planets).

Typical values of temperature range from  $10^3$  K (or even much less in atmospheres of planets and brown dwarfs; say down to 50 K) to a few times  $10^5$  K in the hottest stars. Temperature is even higher,  $10^6$ – $10^7$  K, in stellar coronae. The total particle density ranges from, say,  $10^6$  to  $10^{16}$   $\text{cm}^{-3}$ . Under such conditions, the natural starting point for the physical description is the kinetic theory. The physical state of the system is then fully described by a set of kinetic (Boltzmann) equation for the distribution functions,  $f_i$ , of all kinds of particles that exist in the atmosphere (generally, not only for the individual atoms, ions, free electrons, and possibly molecules, but also for individual excitation states of the atoms/ions),

$$\frac{\partial f_i}{\partial t} + (\mathbf{u} \cdot \nabla) f_i + (\mathbf{F} \cdot \nabla_p) f_i = \left( \frac{Df_i}{Dt} \right)_{\text{coll}} , \quad (2.1)$$

where  $\nabla$  and  $\nabla_p$  are the usual nabla differential operators with respect to position and momentum components, respectively;  $\mathbf{u}$  is the particle velocity, and  $\mathbf{F}$  is the external force. The term  $(Df/Dt)_{\text{coll}}$  is the so-called collisional term, which describes creations and destructions of particles of type  $i$  with the position  $(\mathbf{r}, \mathbf{r} + d\mathbf{r})$  and momentum  $(\mathbf{p}, \mathbf{p} + d\mathbf{p})$ .

However, the full distribution functions are usually not needed, and in any case the number of unknowns to be determined would be enormous. The standard procedure to reduce the problem is to form moments of the kinetic equation that lead to the usual hydrodynamic equations. The procedure is described in any textbook of kinetic theory or hydrodynamics; in the astrophysical context, the excellent textbooks are Mihalas and Mihalas (1984) and Castor (2004).

The standard set of hydrodynamic equations are the continuity equation,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 , \quad (2.2)$$

the momentum equation,

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla P + \mathbf{f} , \quad (2.3)$$

and the energy balance equation,

$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho v^2 + \rho \epsilon \right) + \nabla \cdot \left[ \left( \frac{1}{2} \rho v^2 + \rho \epsilon + P \right) \mathbf{v} \right] = \mathbf{f} \cdot \mathbf{v} - \nabla \cdot (\mathbf{F}_{\text{rad}} + \mathbf{F}_{\text{con}}) . \quad (2.4)$$

Here,  $\mathbf{v}$  is the macroscopic velocity,  $\rho$  the total mass density,  $P$  the pressure,  $\mathbf{f}$  the external force,  $\epsilon$  the internal energy,  $\mathbf{F}_{\text{rad}}$  the radiation flux, and  $\mathbf{F}_{\text{con}}$  the conductive flux. **Equations 2.2–2.4** represent moment equations of the kinetic equation (**2.1**), summed over all kinds of particles.

In addition to classical hydrodynamics, one also considers a zeroth-order moment equation for the individual kinds of particles in the individual degrees of freedom (excitation states), i.e., the conservation equation for particles of type  $i$ ,

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v}) = \left( \frac{Dn_i}{Dt} \right)_{\text{coll}} , \quad (2.5)$$

which are used for the so-called non-LTE (or NLTE) description – see below. Here,  $n_i$  is the number density (population) of the state  $i$ .

These equations provide the most general description of the dynamics of a stellar atmosphere. They are still extremely complex to solve in full generality; therefore, one has to resort to various simplifying approximations, which are briefly discussed next.

## 2.1 Overview of Basic Equilibrium Conditions: Atmospheric Layers

Traditionally, a stellar atmosphere is divided into several basic layers, depending on what kind of equilibrium conditions can be reasonably assumed to hold there. In the case of early-type stars (early A-type and hotter), the two basic layers are the photosphere and the stellar wind. In the case of solar-type stars and cooler, the layers are somewhat different. Typically, there is again a photosphere, then chromosphere and corona, and finally a (typically weak) wind.

The *photosphere* is the innermost part of the atmosphere. The mass outflow velocities are very small there, smaller than the local sound speed, so that they can be neglected. The photosphere is assumed to be an essentially *static* region. The radial extent of the photosphere is typically very small compared to the stellar radius, even for hot massive stars. This region is very important because most of the observed spectral features originate there. Therefore, it is fair to say that the photosphere is crucial for determining basic stellar parameters, such as effective temperature, gravity acceleration, and chemical composition. Stellar photospheres are characterized by the condition of hydrostatic and radiative equilibrium.

The **hydrostatic equilibrium** stipulates that the gradient of the total pressure is balanced by the local gravity acceleration. Because the radial extent of the photosphere is small compared to the stellar radius, the gravity acceleration is essentially constant. The explicit form of this equation is (for a spherically-symmetric star):

$$\frac{dP}{dR} = -\rho GM_*/R^2 \approx -\rho GM_*/R_*^2 \equiv -\rho g, \quad (2.6)$$

where  $P$  is the total pressure,  $R$  is the radial coordinate,  $M_*$  and  $R_*$  are the stellar mass and radius, respectively,  $g$  is the gravity acceleration at the stellar surface, and  $\rho$  the mass density. Notice that (2.6) follows from the general momentum equation (2.3) by setting  $\partial/\partial t = 0$  (a stationary situation),  $\mathbf{v} = 0$  (static case), and  $f = -\rho g$  (external force being given by the gravity force; the minus sign reflects the fact that the gravity acts inward, while the radial coordinate increases outward).

The **radiative equilibrium** simply states that the total radiation flux is conserved. As follows from the energy equation (2.4), its reduction to the static case and neglecting conduction leads to

$$\nabla F_{\text{rad}} = 0 \implies F_{\text{rad}} = \text{const} \equiv \sigma T_{\text{eff}}^4, \quad (2.7)$$

where  $\sigma$  is the Stefan–Boltzmann constant and  $T_{\text{eff}}$  is the so-called effective temperature.

As follows from (2.6) and (2.7), the gravity acceleration  $g$  and the effective temperature  $T_{\text{eff}}$  are two basic parameters of the stellar photosphere problem.

The atmospheres of cool stars (late A-type and cooler) contain regions that are unstable against convection; the unstable regions are those that satisfy the *Schwarzschild criterion*, (e.g., Mihalas 1978),

$$\nabla_R \equiv \left( \frac{d \ln T}{d \ln P} \right)_R > \left( \frac{d \ln T}{d \ln P} \right)_A \equiv \nabla_A, \quad (2.8)$$

where  $\nabla_R$  is the logarithmic gradient of temperature with respect to the total pressure assuming radiative equilibrium, while  $\nabla_A$  is the adiabatic gradient. The latter can be easily evaluated as a function of temperature and density of the stellar material.

Convection is a transport of energy by rising and falling bubbles of material with properties (e.g., temperature) different from the ambient medium. It is therefore, by its very nature, a non-stationary and nonhomogeneous phenomenon. Putting  $\mathbf{v} = 0$  and assuming a 1D medium

means, strictly speaking, that convection is a priori neglected in the hydrodynamic equations. However, most modeling approaches use simplified descriptions, such as the mixing-length theory (see any standard textbook, e.g., Mihalas 1978), which recasts the problem in the form of a 1D stationary equation, viz.

$$F_{\text{rad}} + F_{\text{conv}} = \sigma T_{\text{eff}}^4, \quad (2.9)$$

where the convective flux  $F_{\text{conv}}$  is a specified function of basic state parameters (temperature, density, etc.)

The *stellar wind* is the region where the outflow velocities are comparable or larger than the local sound speed. The radial extent of this region may be comparable to or, in some cases, significantly larger than, the radius of the stellar photosphere.

Stellar winds, as well as stellar chromospheres and coronae, are covered in another chapters. This chapter concentrates mainly on the stellar photospheres.

## 2.2 Interaction of Radiation with Matter

From the very nature of stellar atmospheres, it is clear that a detailed description of the processes of interaction between radiation and matter is a crucial ingredient of the stellar atmospheres theory. These processes determine (1) how the radiation is transported in the atmosphere and (2) what is the distribution of the microscopic degrees of freedom of the massive particles (e.g., the excitation and ionization states of the individual atomic species, etc.).

The interaction between radiation and matter is described through the radiative transfer equation, which is generally written as

$$\left( \frac{1}{c} \frac{\partial}{\partial t} + \mathbf{n} \cdot \nabla \right) I(\nu, \mathbf{r}, \mathbf{n}, t) = \eta(\nu, \mathbf{r}, \mathbf{n}, t) - \chi(\nu, \mathbf{r}, \mathbf{n}, t) I(\nu, \mathbf{r}, \mathbf{n}, t). \quad (2.10)$$

Here,  $I$  is the *specific intensity* of radiation, defined such that it is the energy transported by radiation in a unit frequency range at the frequency  $\nu$ , across a unit area perpendicular to the direction of propagation,  $\mathbf{n}$ , into a unit solid angle, and in a unit time interval. The specific intensity provides a complete description of the unpolarized radiation field from the macroscopic point of view. This description can be generalized to an arbitrarily polarized light by introducing the *Stokes vector* instead of the scalar intensity (e.g., Chandrasekhar 1960). This case will not be considered here.

Quantities  $\chi$  and  $\eta$  are the *absorption* and *emission* coefficients, respectively. They are defined analogously to the specific intensity, namely as the energy removed or added to a beam of radiation at unit frequency range, solid angle, area, and time.

It is known from the quantum theory of radiation that there are three types of elementary processes that give rise to an absorption or emission of a photon: (1) induced absorption – an absorption of a photon accompanied by a transition of an atom/ion to a higher energy state; (2) spontaneous emission – an emission of a photon accompanied by a spontaneous transition of an atom/ion to a lower energy state; and (3) stimulated emission – an interaction of an atom/ion with a photon accompanied by an emission of another photon with identical properties. In the astrophysical formalism, the stimulated emission is usually treated as negative absorption.

In thermodynamic equilibrium, the microscopic detailed balance holds, and therefore the radiation energy absorbed in an elementary volume in an elementary frequency interval is

exactly balanced by the energy emitted in the same volume and in the same frequency range, i.e.,  $\chi I = \eta$ . Moreover, in thermodynamic equilibrium, the radiation intensity is equal to the Planck function,  $I = B$ , where

$$B(\nu, T) = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}. \quad (2.11)$$

In thermodynamic equilibrium, one has, therefore,  $\eta/\chi = B$ , which is called the *Kirchhoff's law*.

The absorption coefficient (or opacity) is given by

$$\chi_\nu = \kappa_\nu + \sigma_\nu, \quad (2.12)$$

where  $\kappa_\nu$  is the coefficient of true absorption (or extinction coefficient) and  $\sigma_\nu$  is the scattering coefficient. The extinction coefficient is given by

$$\begin{aligned} \kappa_\nu = & \sum_i \sum_{j>i} [n_i - (g_i/g_j)n_j] \sigma_{ij}(\nu) + \sum_i (n_i - n_i^* e^{-h\nu/kT}) \sigma_{ik}(\nu) \\ & + \sum_\kappa n_e n_\kappa \sigma_{\kappa\kappa}(\nu, T) (1 - e^{-h\nu/kT}), \end{aligned} \quad (2.13)$$

where the three terms represent, respectively, the contributions of bound-bound transitions (i.e., spectral lines), bound-free transitions (continua), and free-free absorption (also called *brehmstrahlung*).

Here,  $n_i$  is the occupation number (population) of an atom in the energy level labeled  $i$ ,  $g_i$  the corresponding statistical weight, and  $n_i^*$  denotes an equilibrium population of level  $i$  corresponding to temperature  $T$ , and electron density  $n_e$ .  $\sigma(\nu)$  are the corresponding cross sections; subscript  $\kappa$  denotes the “continuum,” and  $n_\kappa$  the ion number density. The negative contributions represent the stimulated emission. The relation between the bound-bound cross section  $\sigma_{ij}(\nu)$  and the well-known Einstein coefficients for the photoexcitation is  $\sigma_{ij}(\nu) = (h\nu_0/4\pi)B_{ij}\phi(\nu)$ , where  $\nu_0$  is the frequency of the line center, and  $\phi(\nu)$  the *absorption profile coefficient*, normalized to unity,  $\int \phi(\nu) d\nu = 1$ . It represents the conditional probability density that if a photon is absorbed in the transition  $i \rightarrow j$ , it is absorbed in the frequency range  $(\nu, \nu + d\nu)$ .

In hot stars, a photon scattering on free electrons – *electron scattering*, is the dominant scattering process. Moreover, it is to a good approximation coherent, i.e., without a change of frequency – Thomson scattering. In this case,

$$\sigma_\nu = n_e \sigma_e, \quad (2.14)$$

where  $\sigma_e$  is the Thomson cross section. A more general, incoherent case is called Compton scattering. The effects of Compton scattering are negligible in the atmospheres of most stars, with a possible exception of extremely hot subdwarfs, white dwarfs, and pre-white dwarfs. For cooler stars, the Rayleigh scattering becomes important, and for very cool objects (M dwarfs and substellar mass-objects) where clouds are formed, the Mie scattering on clouds particles is important. There is no stimulated emission correction for the coherent scattering, because this contribution exactly cancels with ordinary absorption.

The absorption coefficient defined by (2.13) has the dimension  $\text{cm}^{-1}$ , and its inverse has a meaning of the photon mean free path. This coefficient is also called *opacity per length*, in contrast to *opacity per mass* which is defined as  $\chi_\nu/\rho$ . The advantage of the latter is that it is typically much less dependent on mass density, because the atomic level populations and the electron density roughly scale with mass density, so that these dependencies almost cancel.

Analogously, the emission coefficient is given by

$$\eta_\nu = \eta_\nu^{\text{th}} + \eta_\nu^{\text{scat}}, \quad (2.15)$$

where the thermal emission coefficient is given by

$$\eta_\nu^{\text{th}} = (2h\nu^3/c^2) \left[ \sum_i \sum_{j>i} n_j (g_i/g_j) \sigma_{ij}(\nu) + \sum_i n_i^* \sigma_{i\kappa}(\nu) e^{-h\nu/kT} + \sum_\kappa n_e n_\kappa \sigma_{\kappa\kappa}(\nu, T) e^{-h\nu/kT} \right]. \quad (2.16)$$

The three terms again describe the bound-bound, bound-free, and free-free emission processes, respectively.

The scattering part of the emission coefficient is more complex. Generally, it is given by

$$\eta_\nu^{\text{scat}}(\mathbf{n}) = \int d\nu' \oint d\Omega' / (4\pi) R(\nu', \mathbf{n}', \nu, \mathbf{n}) I(\nu', \mathbf{n}'), \quad (2.17)$$

where  $R(\nu', \mathbf{n}', \nu, \mathbf{n})$  is the *redistribution function* that represents a probability density that a photon in the frequency range  $(\nu', \nu' + d\nu')$  and in an element of solid angle  $d\Omega'$  around direction  $\mathbf{n}'$  is absorbed, and a photon in the frequency range  $(\nu, \nu + d\nu)$  and in an element of solid angle  $d\Omega$  around direction  $\mathbf{n}$  is emitted in the scattering process. The redistribution function is usually assumed to be separable into the frequency and the angular part,

$$R(\nu', \mathbf{n}', \nu, \mathbf{n}) = R(\nu', \nu) g(\mathbf{n}', \mathbf{n}), \quad (2.18)$$

where  $R(\nu', \nu)$  is called frequency redistribution function, and  $g$  the phase function. In the case of electron (Thomson) scattering,  $R(\nu', \nu) = n_e \sigma_e \delta(\nu' - \nu)$ , and assuming isotropic scattering,  $g(\mathbf{n}', \mathbf{n}) = 1$ , the scattering emission coefficient is simply given by

$$\eta_\nu^{\text{scat}} = n_e \sigma_e J_\nu, \quad (2.19)$$

where  $J$  is the mean intensity of radiation – see (► 2.29).

The absorption and emission coefficients are thus described through the corresponding cross sections, given by the atomic physics, the local thermodynamic parameters,  $T$  and  $n_e$ , and the atomic level populations for all the levels involved in the microscopic processes that give rise to an absorption and emission at frequency  $\nu$ ; such a number may be enormous. The scattering emission coefficient moreover depends explicitly the radiation field. Besides that, the main difficulty of the stellar atmospheres theory is that the level populations generally depend (in a NLTE situation) on other state parameters and the radiation field.

It should also be realized that the number of cross sections and other parameters to be supplied by atomic physics is enormous. In fact, once efficient numerical methods for solving the coupled problem of radiation transport and hydrodynamics are developed, the main limiting factor in producing realistic model stellar atmospheres is the availability of necessary atomic data. The most popular large-scale source of data for bound-bound transitions, lines, are the Kurucz line lists (Kurucz 1993; the latest additions described in Kurucz 2009). In the last two decades, two major collaborative projects – Opacity Project (OP – OP Team 1995, 1997; Seaton 1987) and its continuation the Iron Project (Hummer et al. 1993; Pradhan et al. 1996), and the OPAL Project (Iglesias and Rogers 1991, 1996) – have produced accurate atomic data on a large scale. There have also been a significant progress on the molecular data; for a review, see Jørgensen (2003) and Sharp and Burrows (2007).



### 2.3 LTE Versus Non-LTE

It is well known from statistical physics that a description of material properties is greatly simplified if the thermodynamic equilibrium (TE) holds. In this state, the particle velocity distributions as well as the distributions of atoms over excitation and ionization states are specified uniquely by two thermodynamic variables. In the stellar atmospheres context, these variables are usually chosen to be the (kinetic) temperature ( $T$ ), and the total particle number density ( $N$ ), or the electron number density ( $n_e$ ). From the very nature of a stellar atmosphere, it is clear that it cannot be in thermodynamic equilibrium – a star is detectable by a distant observer, so photons must be escaping from it. Because photons carry significant momentum and energy, the elementary fact of photon escape has to give rise to significant *gradients* of the state parameters in the stellar outer layers.

However, even if the assumption of TE cannot be applied to a stellar atmosphere, one may still use the concept of *local thermodynamic equilibrium* – LTE. This assumption stipulates that one may employ the standard thermodynamic relations not globally for the whole atmosphere, but *locally*, for local values of  $T(\mathbf{r})$  and  $N(\mathbf{r})$  or  $n_e(\mathbf{r})$ , despite the gradients that exist in the atmosphere. This assumption simplifies the problem enormously, for it implies that all the particle distribution functions may be evaluated locally without reference to the physical ensemble in which the given material is found. Notice that the equilibrium values of distribution functions are assigned to *massive particles*; the radiation field is allowed to depart from its equilibrium, Planckian, distribution function (i.e.,  $I = B$  is valid only in strict TE).

Specifically, LTE is characterized by the following three distributions:

- Maxwellian velocity distribution of particles

$$f(\mathbf{v})d\mathbf{v} = (m/2\pi kT)^{3/2} \exp(-mv^2/2kT) d\mathbf{v} , \quad (2.20)$$

where  $m$  is the particle mass and  $k$  the Boltzmann constant.

- Boltzmann excitation equation,

$$(n_j/n_i) = (g_j/g_i) \exp[-(E_j - E_i)/kT] , \quad (2.21)$$

where  $g_i$  is the statistical weight of level  $i$ , and  $E_i$  the level energy, measured from the ground state.

- Saha ionization equation.

$$\frac{N_I}{N_{I+1}} = n_e \frac{U_I}{U_{I+1}} C T^{-3/2} \exp(\chi_I/kT) , \quad (2.22)$$

where  $N_I$  is the total number density of ionization stage  $I$ ,  $U$  is the partition function, defined by  $U = \sum_1^\infty g_i \exp(-E_i/kT)$ ;  $\chi_I$  is the ionization potential of ion  $I$ , and  $C = (h^2/2\pi mk)^{3/2}$  is a constant. It should be stressed that in the astrophysical LTE description, the *same* temperature  $T$  applies to all kinds of particles, and to all kinds of distributions, (☉ 2.20–2.22).

☛ Equations 2.20–2.22 define the state of LTE from the macroscopic point of view. Microscopically, LTE holds if all atomic processes are in *detailed balance*, i.e., if the number of processes  $A \rightarrow B$  is exactly balanced by the number of inverse processes  $B \rightarrow A$ .  $A$  and  $B$  refer to any particle states between which there exists a physically possible transition. For instance,  $A$  is an atom in an excited state, and  $B$  the same atom in another state (either of the same ion, in which

case the process is an excitation/de-excitation; or of the higher or lower ion, in which case the term is an ionization/recombination).

In contrast, the term non-LTE (or NLTE) characterizes any state that departs from LTE. In practice, this usually means that populations of some selected energy levels of some selected atoms/ions are allowed to depart from their LTE values, while the velocity distributions of all particles are assumed to be Maxwellian, all at the same local kinetic temperature,  $T$ .

In this case, the number densities (populations) of all energy levels of all atoms and ions that are important in the atmosphere have to be determined. Equations that describe how the level populations behave are the *statistical equilibrium equations* (or rate equations), which are (2.5) reduced to a static case,  $(Dn_i/Dt)_{\text{coll}} = 0$ . More explicitly, they express the fact that under stationary situation, the total number of transitions *into* a given level  $i$  is equal to the total number of transitions *out* of level  $i$ ,

$$n_i \sum_{j \neq i} (R_{ij} + C_{ij}) = \sum_{j \neq i} n_j (R_{ji} + C_{ji}) \quad , \quad (2.23)$$

where  $R_{ij}$  and  $C_{ij}$  are the radiative and collisional rates, respectively, for the transition from level  $i$  to level  $j$ . The left-hand side of (2.23) represents the total number of transitions *out* of level  $i$ , while the right-hand side represents the total number of transitions *into* level  $i$  from all other levels.

One of the important issues of the stellar atmospheres theory for the last three decades was whether, and if so to what extent, departures from LTE should be included in numerical modeling. Generally, to understand why and where one may expect departures from LTE, it is best to turn to the microscopic definition of LTE. It is clear that LTE breaks down if the detailed balance in at least one transition  $A \rightarrow B$  breaks down. There are two types of transitions: the *collisional transitions* (arising due to interactions between two or more massive particles) and *radiative transitions* (interactions involving particles and photons). Under stellar atmospheric conditions, collisions between massive particles tend to maintain the local equilibrium (because velocities are Maxwellian). Therefore, the validity of LTE hinges on whether the radiative transitions are in detailed balance or not.

The fact that the radiation escapes from a star implies that LTE should eventually break down at a certain point in the atmosphere. Essentially, this is because detailed balance in radiative transitions generally breaks down at a certain point near the surface. Because photons escape (and more so from the uppermost layers), there must be a lack of them there. Consequently, the number of photoexcitations (or any atomic transition induced by absorbing a photon) is less than a number of inverse processes, spontaneous de-excitations (neglecting here, for simplicity, the stimulated emission).

These considerations explain that departures from LTE are expected if the following two conditions are met: (1) radiative rates in some important atomic transition dominate over the collisional rates; and (2) radiation is not in equilibrium, i.e., the intensity does not have the Planckian distribution. Because the collisional rates are proportional to the particle density, the departures from LTE tend to be small for high densities. Likewise, deep in the atmosphere, photons do not escape, and so the intensity is close to the equilibrium value. Departures from LTE are therefore small, even if the radiative rates dominate over the collisional rates. On the other hand, departures from LTE are important for low-density media immersed in a strong radiation field, which are precisely the conditions met in the atmospheres of hot stars.

### 3 Model Atmospheres

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Model stellar atmospheres are basic tools to analyze observed stellar spectra. By fitting the observed spectrum by a grid of theoretically predicted spectra, one can derive the basic parameters used for constructing the models, i.e., the effective temperature, surface gravity, chemical composition, and, in the general case, the mass loss rate. From those parameters, one can derive the fundamental stellar parameters, like the mass, radius, and luminosity. Besides these, there are a number of secondary parameters, such as the rotational velocity, or auxiliary parameters describing the nature of atmospheric velocity fields, etc.

By the term *model stellar atmosphere*, it is understood a specification of all the atmospheric state parameters as functions of position. These parameters are obtained by solving appropriate structural equations, which, in the case of stellar photospheric models, are the equations of hydrostatic equilibrium, radiative equilibrium, radiative transfer equation, and the set of statistical equations (rate equations) for the atomic level populations. In the case of LTE models, the rate equations are not needed because the level populations are given by the Saha–Boltzmann distribution. Because the problem is very complex, it is impossible to find analytical solutions. Therefore, one has to resort to numerical simulations. In order to make the overall problem tractable, it is necessary to make a number of simplifications by invoking various approximations. The quality of an appropriate model, and consequently its applicability to the individual stellar types, is closely related to the degree of approximation used in the construction of the model. Needless to say, the degree of approximation critically influences the amount of computational effort to compute it. It is fair to say that the very art of computing model stellar atmospheres is to find such physical approximations that allow the model to be computed with a reasonable amount of numerical work, yet the model is sufficiently realistic to allow its use for a reliable interpretation of observed stellar data. The adopted approximations are therefore critical. There are several types of approximations that are typically made in the model construction, which are summarized below.

#### 3.1 Hierarchy of Approximations

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##### 3.1.1 Approximations of the Geometry

What is meant by the geometrical simplification is that either some prescribed geometrical configuration is assumed or some special kind of overall symmetry is invoked. The goal of those simplifications is to reduce the dimensionality of the problem from a spatially 3D problem to 1- or 2D problem. The most popular approximations are (from simplest to more complex):

- Plane-parallel geometry, with an assumption of horizontally homogeneous layers. This decreases the number of dimensions to one: the depth in the atmosphere. This approximation is typically quite reasonable for stellar photospheres, which indeed are by several orders of magnitude thinner than the stellar radius, so the curvature effects are negligible. The assumption of horizontal homogeneity is made for the sake of simplicity – there is no plausible verification of this approximation, and, moreover, observational evidence mostly shows that stellar surfaces are far from being homogeneous (a notorious example being detailed pictures of the solar surface). Nevertheless, even in the presence of inhomogeneities,

1D models still have their value since, in many cases, one may construct different 1D models for the individual “patches” on the surface.

- Spherical symmetry. Again, the problem is one-dimensional. The approach is used for extended atmospheres, for which the atmospheric thickness is no longer negligible with respect to the stellar radius. Typically, one has to consider such models for giants and supergiants, as well as for earliest types of main-sequence O stars.
- Multidimensional geometry. This field is at its infancy. A numerical solution is extremely demanding on computer time and memory, and only very recently has the computer power reached a stage that calculating such models is becoming feasible. Model atmospheres with a 2D and 3D geometry have been constructed for solar-type atmospheres; for a recent review, see Carlsson and Stein (2003), Stein and Nordlund (2003), and Nordlund and Stein (2009).

### 3.1.2 Approximations of the Presence of External Forces

In a typical stellar atmospheres, the only external force that is taken into account is the force of gravity of the star, and its effect (in the case of a photosphere) is described through the hydrostatic equilibrium (● 2.6). Other forces are sometimes taken into account, depending above all on the nature of the studied object.

- Centrifugal force. If the star rotates very fast, close to breakup rotation rate, the whole star becomes distorted. A star is still assumed to be cylindrically symmetric, but the overall atmosphere is no longer described by a single model, but instead it is assumed to be composed of a set of latitudinal belts, each described by a unique model atmosphere. This approach implicitly assumes that the physical properties of the atmosphere vary much faster in the vertical direction (toward the stellar center) than in the horizontal direction. This is usually an excellent approximation. The centrifugal force thus does not enter the model construction directly, but only indirectly through the need of constructing several models for a stellar atmosphere instead of one.
- Magnetic force. Some objects (magnetic Ap stars, magnetic white dwarfs, neutron stars) possess a strong magnetic field, which needs to be taken into account in model construction. This topic will not be discussed in this chapter.

### 3.1.3 Approximations of the Dynamical State of the Atmosphere

This is basically a specification of the realism of the treatment of the macroscopic velocity fields. From the simplest to the most complex, the approaches are the following:

- Static models, in which the macroscopic velocity field is set to zero. As discussed above, these models describe a *stellar photosphere*.
- Models with an a priori-given velocity field. In these models, the velocities are taken into account explicitly, and their influence upon other state parameters, in particular the emergent radiation, is studied in detail. In these models, one can either consider only a dynamical region (i.e., the wind) and take an incoming radiation from the photosphere as given a priori – the so-called core-halo model; or a model which treats the photosphere and the wind on the same footing. Such models are called *unified models*. The most successful computer

- programs for computing such models are CMFGEN (Hillier 2003; Hillier and Miller 1998), Hoeflich's suite of programs (Hoeflich 1995, 2003), PHOENIX (Hauschildt et al. 1997), Munich codes (FASTWIND – Santolaya-Rey et al. 1997; WM-BASICS – Pauldrach et al. 2001), and the Kiel-Potsdam code (Hamann 1985; Koesterke et al. 2002).
- Models where the velocity field is determined self-consistently by solving the appropriate hydrodynamical equations. This problem is very complicated because the wind driving force is given by the absorption of photons in thousands to millions of metal lines, so the hydrodynamical equations should be solved together with at least an approximate treatment of radiative transfer in spectral lines.

### 3.1.4 Approximations of the Opacity Sources

In real stellar atmospheres, there is an enormous number of opacity sources. It is essentially impossible (or, at least, impractical) to take all of them into account in full detail. The light elements (H, He, C, N, O) have comparatively a small number of lines per ion (say  $10^2$ – $10^4$ ) because of a relatively simple atomic level structure. The number of lines generally increases with increasing atomic number, and for the iron-peak elements (Fe and Ni being the most important ones), there are of the order of  $10^6$ – $10^7$  spectral lines per ion! Therefore, the opacity (and emissivity) may be an enormously complicated function of frequency. For cool stars, the problem is even worse because the number of molecular lines is even larger (for instance, water has of the order of  $10^9$  lines that should be taken into account).

There are several approximations that are meant to reduce this complexity considerably:

- Models constructed using certain frequency-averaged opacities; these models are called *grey* models. The approach is based on the implicit assumption that the behavior of the frequency-averaged intensity of radiation is well described by means of some frequency-averaged opacities. There are several possible mean opacities, depending on how exactly the averaging is done. The most used averaged opacity is the *Rosseland mean* opacity, defined by

$$\frac{1}{\chi_R} \equiv \frac{\int_0^\infty (1/\chi_\nu)(dB_\nu/dT) d\nu}{\int_0^\infty (dB_\nu/dT) d\nu}, \quad (2.24)$$

where  $\chi_\nu$  is the opacity (per gram of stellar material). Because averaging is done for  $1/\chi$ , the largest weight is given to regions of lowest opacity, which are the most efficient regions for the energy flux transport. This explains why the Rosseland mean opacity is well suited for describing the total radiation flux, and why it is the most appropriate mean opacity to be used for modeling stellar interiors.

The grey model atmospheres are no longer used for spectroscopic analysis, but they are useful for providing an initial estimate in any iterative method for constructing more realistic model atmospheres, and they are very useful for pedagogical purposes because they allow one to understand a rough behavior of temperature and radiation field as a function of depth in the atmosphere.

- A possibility is to use stepwise frequency averages for a number of subintervals (frequency bins), called sometimes multifrequency/multi-grey method. This approach was used in constructing model stellar atmospheres only rarely (Anderson 1985, 1987, 1989) but is more used in other branches of astrophysical and laboratory radiative transfer.

- A completely different approach is to construct a model atmosphere neglecting the line opacity completely. Although this may seem very crude, such models may actually provide reasonable results for very metal-poor stars because, as was pointed out above, H and He possess only a small number of lines, which occupy only a very small frequency range and therefore have a small influence on the model structure. (Strictly speaking, this is not completely true because just three of the most important hydrogen lines –  $L\alpha$ ,  $L\beta$ , and  $H\alpha$  – may already have an important indirect effect upon the temperature structure in the outer layers of early-type photospheres (Auer and Mihalas 1969). In any event, this approximation was introduced at the early stages of development of the non-LTE model atmospheres and was motivated by limitations of then available computers and numerical techniques.
- An obvious next level of approximation is to consider a small number of lines (typically tens to hundreds) explicitly while neglecting the bulk of metal lines; the selected lines are those which presumably have the largest effect upon the atmospheric structure. This approach was used in early days of NLTE model atmospheres (Auer and Mihalas 1969).
- Finally, one can take into account, by one way or another, “all” metal lines. Such models are traditionally called *metal line-blanketed model atmospheres*. The problem of constructing such models is computationally very demanding. Under the assumption of LTE, it is, however, considerably simplified because the opacity and emissivity is a function of only local temperature and electron density; the only problem is the complicated frequency dependence of the opacity. Without the approximation of LTE, the problem is significantly more difficult because one has to determine all the atomic level populations and temperature self-consistently with the radiation field.

There are essentially two possibilities:

- *Opacity Distribution Functions* (ODF). In LTE, the use of ODFs is straightforward (Kurucz 1970). In NLTE, this method is used in conjunction with the concept of superlevels. A *superlevel* is a set of individual energy levels with close energies, and with identical or similar quantum numbers (e.g., the same spin quantum number  $S$ , the same parity) that share the common NLTE departure coefficient, that is, they are in Boltzmann equilibrium within each other (Anderson 1985). Transitions between superlevels are called superlines. The idea is to resample a complicated frequency dependence of the superline cross section to form a monotonic function of frequency; this function is then represented by a smaller number of frequency quadrature points (Anderson 1989; Dreizler and Werner 1993; Hubeny and Lanz 1995).
- *Opacity Sampling* (OS). The idea is a simple Monte Carlo-like sampling of frequency points of the superline cross sections (Anderson 1989; Dreizler and Werner 1993). The advantage of this approach is that it can easily treat line blends and overlaps; the disadvantage is that considering too few frequency points may easily lead to missing many important line cores. On the other hand, the “exact” method is in fact a variant of the OS with a sufficiently high frequency resolution.

An explicit comparison between results using the ODF and the OS approaches, and with various frequency resolutions in the latter, is presented, e.g., in Lanz and Hubeny (2003). With increasing computational power, both memory and speed, the Opacity Sampling scheme with high-frequency resolution becomes the method of choice.

### 3.1.5 Approximations Concerning the Thermodynamic Equilibria

As was discussed above, the issue here is whether the approximation of LTE is adopted or not. If one assumes LTE, the resulting model atmospheres are called LTE models. Two state parameters, the temperature,  $T$ , and density,  $\rho$  (or electron density,  $n_e$ ), suffice to describe the physical state of the atmosphere at any given position. In practice, LTE models may be useful only for stellar photospheres because for extended atmospheres and/or stellar winds, this approximation breaks down completely and its application would yield erroneous and misleading results.

The models that take some kind of departure from LTE into account are called non-LTE (or NLTE) models. This term is rather ambiguous because it is not a priori specified what is actually allowed to depart from LTE in a given model. In early models, the populations of only few low-lying energy levels of the most abundant species, like H and He, were allowed to depart from LTE; the rest were treated in LTE. During the development of the field, progressively more and more levels were allowed to depart from LTE. The situation is similar for stellar photospheres (static models), as well as for stellar winds and for unified models.

## 3.2 Basic Equations of Classical Stellar Atmospheres

The basic equations of stellar atmospheres for the case of horizontally-homogeneous, plane-parallel, static atmospheres, that is, stellar photospheres) are summarized below.

### 3.2.1 Radiative Transfer Equation

For a 1D, static, planar atmosphere, the general transfer (2.10) can be considerably simplified to read

$$\mu \frac{dI(\nu, \mu, z)}{dz} = \eta(\nu, \mu, z) - I(\nu, \mu, z) \chi(\nu, \mu, z), \quad (2.25)$$

where the intensity of radiation is now only a function of the geometrical coordinate  $z$ , frequency  $\nu$ , and the directional cosine  $\mu$ . Here,  $\mu = \cos \theta$ , where  $\theta$  is the angle between the direction of photon propagation and the normal to the surface. Defining the *optical depth* through

$$d\tau_\nu = -\chi_\nu dz, \quad (2.26)$$

and the *source function* as

$$S_\nu = \eta_\nu / \chi_\nu, \quad (2.27)$$

(the functional dependence of position and direction was omitted for notational simplicity, and a dependence on frequency is expressed through subscript  $\nu$  which is customary in astrophysical literature), the transfer is rewritten to a usual form

$$\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu. \quad (2.28)$$

It is customary to introduce moments of the specific intensity as

$$\begin{pmatrix} J_\nu \\ \mathbf{H}_\nu \\ K_\nu \end{pmatrix} = \frac{1}{4\pi} \oint \begin{pmatrix} 1 \\ \mathbf{n} \\ \mathbf{nn} \end{pmatrix} I_\nu d\omega \longrightarrow \frac{1}{2} \int_{-1}^1 \begin{pmatrix} 1 \\ \mu \\ \mu^2 \end{pmatrix} I_\nu(\mu) d\mu, \quad (2.29)$$

where the last term corresponds to the 1D plane-parallel approximation. In this case, the only nonvanishing component of vector  $\mathbf{H}$  is the  $H_z$ -component, which is written simply as  $H$ ; analogously the only nonvanishing component of tensor  $\mathbf{K}$  is the  $K_{zz}$ -component, denoted as  $K$ . The moment equations of the radiative transfer equation, in a plane-parallel approximation, are written as

$$\frac{dH_v}{d\tau_v} = J_v - S_v \quad , \quad (2.30)$$

and

$$\frac{dK_v}{d\tau_v} = H_v \quad . \quad (2.31)$$

The system of moment equations is not closed, i.e., the equation for  $n$ -th moment contains the  $(n + 1)$ -th moment, etc. It is therefore necessary to come up with some kind of closure relation. In the stellar atmospheres theory, one defines the Eddington factor,  $f^K$ , by (Auer and Mihalas 1970)

$$f_v^K \equiv K_v/J_v \quad . \quad (2.32)$$

It is clear from the definition of moments that in the case of isotropic radiation,  $I_v(\mu) = I_v$  being independent of angle, the Eddington factor  $f^K = 1/3$ . Assuming the Eddington factor to be specified, one may combine the two moment (2.30) and (2.31) together,

$$\frac{d^2(f_v^K J_v)}{d\tau_v^2} = J_v - S_v \quad . \quad (2.33)$$

This equation is very useful. It effectively eliminates one independent variable, the angle  $\mu$ , from the problem. Numerically, it replaces the original transfer equation, which is a first-order linear differential equation for the specific intensity,  $I_{v\mu}$ , by a second-order but still linear differential equation for the mean intensity,  $J_v$ . However, it cannot be used alone because the Eddington factor is unknown unless the full solution of the transfer equation is known. However, it can be used to advantage in iterative methods in which the current values of  $J$  and  $K$  are used to determine the current Eddington factor  $f^K$ , which is then kept fixed during the subsequent iteration step. This form is usually used in constructing model stellar atmospheres.

### 3.2.2 Hydrostatic Equilibrium Equation

Recalling (2.6), this equation reads

$$\frac{dP}{dz} = -\rho g \quad , \quad (2.34)$$

where  $P$  is the total pressure. Introducing the Lagrangian mass  $m$ , defined as the mass in the column of a cross section of  $1 \text{ cm}^2$  above a given point in the atmosphere,

$$dm = -\rho dz \quad , \quad (2.35)$$

the hydrostatic equilibrium equation is rewritten as

$$\frac{dP}{dm} = g \quad , \quad (2.36)$$

which, since  $g$  is constant in a plane-parallel atmosphere, has a trivial solution,  $P(m) = mg + P(0)$ . In fact, this is the reason why one usually chooses  $m$  as the basic depth variable of the



1D plane-parallel atmospheres problem. Nevertheless, it should be kept in mind that the total pressure is generally composed of three parts, the gas pressure,  $P_{\text{gas}}$ , the radiation pressure,  $P_{\text{rad}}$ , and the turbulent pressure,  $P_{\text{turb}}$ , i.e.,

$$P = P_{\text{gas}} + P_{\text{rad}} + P_{\text{turb}} = NkT + \frac{4\pi}{c} \int_0^\infty K_\nu d\nu + \frac{1}{2} \rho v_{\text{turb}}^2, \quad (2.37)$$

where  $v_{\text{turb}}$  is the microturbulent velocity. The hydrostatic equilibrium equation may then be written as (neglecting the turbulent pressure)

$$\frac{dP_{\text{gas}}}{dm} = g - \frac{4\pi}{c} \int_0^\infty \frac{dK_\nu}{dm} = g - \frac{4\pi}{c} \int_0^\infty \frac{\chi_\nu}{\rho} H_\nu d\nu. \quad (2.38)$$

The right-hand side of this equation can be interpreted as the *effective gravity acceleration* since it expresses the action of the true gravity acceleration (acting downward, i.e., toward the center of the star), reduced by the radiative acceleration (acting outward).

### 3.2.3 Radiative Equilibrium Equation

This expresses the fact that the total radiation flux is conserved – (☛ 2.7),

$$\int_0^\infty H_\nu d\nu = \text{const} = \frac{\sigma}{4\pi} T_{\text{eff}}^4. \quad (2.39)$$

This equation may be rewritten, using the radiative transfer equation, as

$$\int_0^\infty (\kappa_\nu J_\nu - \eta_\nu) d\nu = \int_0^\infty \kappa_\nu (J_\nu - S_\nu) d\nu = 0, \quad (2.40)$$

Notice that (☛ 2.40) contains the *thermal* absorption coefficient  $\kappa_\nu$ , not the total absorption coefficient  $\chi_\nu$ . This is because the scattering contributions cancel out. To illustrate this mathematically, let us take an example of electron scattering. The absorption coefficient for the process (see ☛ 2.13) is given by  $n_e \sigma_e$ ;  $\sigma_e$  being the electron scattering (Thomson) cross section. The emission coefficient is then given by  $n_e \sigma_e J_\nu$ . As it is seen from (☛ 2.40), these two contributions cancel. This is also clear physically because an absorption followed immediately by a reemission of a photon does not change the energy balance of the medium, and therefore cannot contribute to the radiative equilibrium equation. The situation is different for noncoherent, Compton, scattering. This case will not be discussed here; the interested reader is referred to Rybicki and Lightman (1979).

### 3.2.4 Statistical Equilibrium Equations

They are also sometimes called the *rate equations*. These are given by (☛ 2.23),

$$n_i \sum_{j \neq i} (R_{ij} + C_{ij}) = \sum_{j \neq i} n_j (R_{ji} + C_{ji}). \quad (2.41)$$

The collisional rates are given functions of temperature and electron density (since collisions with electrons are usually most efficient), assumed to be known from atomic physics (e.g., Mihalas 1978). The radiative rates are given by:

1. For bound-bound (line) transitions between levels  $i$  and  $j$ , assuming that  $E_i < E_j$  (that is,  $i$  is the lower level and  $j$  the upper level of the transition)

$$R_{ij} = B_{ij} \int_0^\infty J_\nu \phi_{ij}(\nu) d\nu \equiv B_{ij} \bar{J}_{ij} , \quad (2.42)$$

$$R_{ji} = A_{ji} + B_{ji} \int_0^\infty J_\nu \psi_{ji}(\nu) d\nu \rightarrow A_{ji} + B_{ji} \bar{J}_{ij} , \quad (2.43)$$

where  $A$  and  $B$  are the Einstein coefficients. Quantity  $\bar{J}$  is called the *frequency-averaged mean intensity* of radiation.  $\phi_{ij}(\nu)$  is a normalized *line profile coefficient for absorption*, often called shortly “absorption profile”. It represents a probability density that if a photon is absorbed in the transition  $i \rightarrow j$ , it is absorbed at an elementary frequency range  $(\nu, \nu + d\nu)$ . Analogously,  $\psi_{ji}$  is the profile coefficient for emission, which is generally different form  $\phi$ . However, if one assumes *complete frequency redistribution*, which is a common approximation in the stellar atmospheres theory, both profiles are equal,  $\phi_{ij}(\nu) = \psi_{ji}(\nu)$ . In other words, absorbed and reemitted photons are not correlated. A more general situation where the correlation between an absorbed and an emitted photon is taken into account is usually referred to in astrophysical literature as *partial frequency redistribution*. This case will not be considered here; a review can be found, e.g., in Mihalas (1978), Hubeny (1985), and Uitenbroek (2003). The last part of (2.43) corresponds to the complete redistribution.

In the case of a pure Doppler profile, i.e., no intrinsic broadening of the spectral line, which is broadened only due to the thermal motion of radiators, the absorption profile is given by

$$\phi(x) = \exp(-x^2)/\sqrt{\pi} . \quad (2.44)$$

where  $x$  is a dimensionless frequency displacement from the line center,  $\nu_0$ , measured in unites of Doppler widths,

$$x \equiv \frac{\nu - \nu_0}{\Delta\nu_D} , \quad (2.45)$$

where  $\Delta\nu_D$  is the Doppler width, given by  $\Delta\nu_D = (\nu_0/c)v_{\text{th}}$ , with the thermal velocity  $v_{\text{th}} = (2kT/m)^{1/2}$ ,  $m$  being the mass of the radiating atom.

In a more general case where there is an intrinsic broadening of lines described by a Lorentz profile in the atomic rest frame (the most common types of intrinsic broadening being the natural, Stark, and Van der Waals broadening – see Mihalas 1978, or monograph by Griem 1974), the profile function is given by

$$\phi(x) = H(a, x)/\sqrt{\pi}, \quad (2.46)$$

where  $H(a, x)$  is the Voigt function,

$$H(a, x) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(x-y)^2 + a^2} dy . \quad (2.47)$$

The Voigt function is a convolution of the Doppler profile (i.e., the thermal motions) and the Lorentz profile (intrinsic broadening). The parameter  $a$  is a damping parameter expressed in unites of Doppler width,  $a = \Gamma/(4\pi\Delta\nu_D)$ , where  $\Gamma$  is the atomic damping parameter. For instance, for the natural broadening of a line originating in a two-level atom,  $\Gamma = A_{21}$ .

2. The radiative rates for bound-free transitions (continua) are given by

$$R_{ij} = 4\pi \int_{\nu_0}^{\infty} \sigma_{ij}(\nu)/(h\nu) J_{\nu} d\nu, \quad (2.48)$$

where  $\sigma(\nu)$  is the corresponding cross section, supplied again by the atomic physics.

The set of rate equations for all levels of an atom would form a linearly dependent system. Therefore, one equation of the set has to be replaced by another equation. Usually, this is the *total number conservation* equation (or abundance definition equation),  $\sum_i n_i = N_{\text{atom}}$ , where the summation extends over all levels of all ions of a given species.

### 3.2.5 Charge Conservation Equation

This equation expresses the global electric neutrality of the medium,

$$\sum_i n_i Z_i - n_e = 0, \quad (2.49)$$

where  $Z_i$  is the charge associated with level  $i$  (i.e., equal to 0 for levels of neutral atoms, 1 for levels for once ionized ions, etc.). The summation now extends over all levels of all ions of all species.

## 3.3 Numerical Methods

The resulting set forms a highly coupled, highly nonlinear system of equations. Even in a classical case of plane-parallel, horizontally homogeneous, static atmospheres, this presents a considerable numerical challenge. The basic numerical strategies are described below.

### 3.3.1 Complete Linearization

The physical state of a 1D plane-parallel, horizontally-homogeneous atmosphere in hydrostatic and radiative (or radiative + convective) equilibria is fully described by the set of vectors  $\psi_d$  for every depth point,  $d, d = 1, \dots, ND$ ,  $ND$  being the number of discretized depth points. The state vector  $\psi_d$  is given by

$$\psi_d \equiv \{J_1, \dots, J_{NF}, N, T, n_e, n_1, \dots, n_{NL}\}, \quad (2.50)$$

where  $J_i$  is the mean intensity of radiation in the  $i$ -th frequency point,  $N$  the total particle number density,  $n_e$  the electron density, and  $n_i$  the atomic level populations. The structural equations are discretized, and the resulting set of nonlinear algebraic equations is solved by linearization, i.e., by an application of the Newton-Raphson method. This approach was first used in the context of stellar atmosphere models in a seminal paper by Auer and Mihalas (1969), who coined the term *Complete Linearization* (CL).

Writing the complete set of equations schematically as  $P(\mathbf{x}) = 0$ , where  $\mathbf{x}$  is a vector composed of all state vectors  $\psi_d$  at all depths, the iteration scheme is written as

$$\delta \mathbf{x}^{(n)} \equiv \mathbf{x}^{(n+1)} - \mathbf{x}^{(n)} = -J(\mathbf{x}^{(n)})^{-1} P(\mathbf{x}^{(n)}), \quad (2.51)$$

where  $J$  is the Jacobi matrix (Jacobian),  $J_{ij} = \partial P_i / \partial x_j$ , i.e., the  $ij$ -element of the Jacobian is the derivative of the  $i$ -th equation with respect to the  $j$ -th unknown. Since the system (2.51) represents a *finite difference* solution of at most second-order differential equations, the Jacobian  $J$  has a particularly simple structure, namely a block-tridiagonal form, and (2.51) reduces to,

$$-A_d \delta \psi_{d-1} + B_d \delta \psi_d - C_d \delta \psi_{d+1} = L_d. \quad (2.52)$$

Here  $A$ ,  $B$ ,  $C$  are  $NN \times NN$  matrices, and  $L_d = P_d(\mathbf{x}^{(n)})$  is the residuum vector (of dimension  $NN$ ) at depth  $d$ ; the total number of unknown per depth is given by  $NN = NF + NL + NC$ ;  $NC$  is the number of constraint equations, in this case  $NC = 3$ .

Equation 2.52 is solved as a block-tridiagonal system, which means that one is left with inverting one  $NN \times NN$  matrix per depth point. Therefore, the total computer time for ordinary complete linearization scales roughly as

$$t \propto (NF + NL + NC)^3 \times ND \times N_{\text{iter}}, \quad (2.53)$$

where  $N_{\text{iter}}$  is the number of iterations needed to obtain a converged solution, defined through a suitably selected convergence criterion. It is immediately clear that the original complete linearization, despite its inherent power and robustness, cannot be used as a general numerical scheme because in realistic calculations, one needs a very large number of frequency points  $NF$  to describe the radiation field with a sufficient accuracy – of the order of  $10^5$ – $10^6$  points. Likewise, a number of energy levels  $NL$  may also be quite large ( $10^4$ – $10^5$  levels). Therefore, one has to seek less global, but faster schemes. The basic options are (1) reducing the size of the problem keeping the general framework of CL intact, (2) avoiding repeated inversions of a Jacobian (examples are the Broyden scheme implemented in this context by Koesterke et al. 1992; or Kantorovich scheme – Hubeny and Lanz 1992), or (3) using an idea of the so-called approximate Newton–Raphson method (e.g., Hillier 1990; Hillier and Miller 1998).

The first category of approaches achieve a reduction of computer time by reducing the size and/or the number of matrices to be inverted, and/or the number of iterations needed. Taking (2.53) as a guide, in order to reduce the computer time in the most efficient way, one has to reduce  $NF$  or  $NL$ . One can trivially reduce these numbers by considering less frequencies (levels), and thus constructing less accurate models, but this ruled out since the goal is to construct as accurate and reliable models as possible. So, the way to go is keep the necessary (large) numbers of these quantities, but only to eliminate them from matrices to be inverted. Since  $NF$  is typically the largest contributor to the size of the linearization matrices, reducing  $NF$  is most important. This can be achieved by using an idea of Accelerated Lambda Iteration (ALI) method, which will be briefly described below. For a detailed discussion of other possible improvements and modifications of the Complete Linearization scheme, see Hubeny and Lanz (2003).

For LTE models, an interesting possibility is to linearize radiation intensities in all frequency points. but to reorganize matrices as first suggested by Rybicki (1971) in the context of two-level atom. Mihalas (1978) has reformulated the scheme to be applied for constructing LTE model atmospheres. The scheme was implemented in a stellar atmosphere code TLUSTY (Hubeny 1988; Hubeny and Lanz 1995) by Burrows et al. (2006) and Hubeny and Burrows (2007b) and was used to construct comprehensive grids of model atmospheres for L and T dwarfs. It should be noted that in order to make this scheme practical, all the structural parameters have to be expressed as functions of a single parameter, the temperature.

The idea consists in the following: The original complete linearization organizes the master Jacobi matrix in a block-tridiagonal structure, that is, as an  $ND \times ND$  grand block matrix, with inner  $(NF + 1) \times (NF + 1)$  matrices. The inner matrices are composed of a diagonal  $NF \times NF$  upper left corner (because the individual frequency points are not explicitly coupled), plus a full last row and column (arising from the linearization of the energy equation). The Rybicki scheme reverses the order of the inner and outer structure: The grand matrix is an  $(NF + 1) \times (NF + 1)$  blocks matrix with inner blocks being  $ND \times ND$  matrices. The outer block structure corresponds to structural parameters (radiation intensities and temperature), and the inner structure to depth points. The upper part of the  $NF \times NF$  blocks is a block-diagonal matrix, with each block being an  $ND \times ND$  tridiagonal matrix, and the last row and column of blocks are full matrices. The bulk of work consists in inverting  $NF$  tridiagonal  $ND \times ND$  matrices, which scales only as  $ND^2 \times NF$ , that is linearly with the number of frequency points. The very unfavorable cubic scaling of computer time with the number of frequencies is now completely avoided and is replaced by a linear scaling. The only cubic scaling is now with the number of depth points, which is always kept quite low (up to about 100). The method is most efficient with just one constraint equation; with more constraints the scaling would involve a term with  $(NC \times ND)^3$ .

### 3.3.2 Accelerated Lambda Iteration

Soon after the advent of Complete Linearization, another crucial ingredient of the modern numerical stellar atmospheres and radiation transfer was introduced, namely the first astrophysical application of an iteration scheme that later became known as Accelerated Lambda Iteration, or ALI for short. It was introduced by Cannon (1973a, b) by the name “Operator Perturbation” technique. Although recognized for its potential, the method was not widely used until its reformulation by Scharmer (1981). The first application of the method to NLTE model stellar atmospheres was worked out by Werner (1986), and the term ALI itself was coined by Hamann (1985). A historical review is given by Hubeny (1992) and a more recent review by Hubeny (2003).

The idea of the method is usually explained on a simple case of two-level atom with complete frequency redistribution. Very briefly, the source function is written as

$$S = (1 - \epsilon)\bar{J} + \epsilon B, \quad (2.54)$$

where  $\bar{J}$  is a frequency-averaged mean intensity of radiation,  $\epsilon$  is the photon destruction parameter, and  $B$  the Planck function. In this problem,  $\epsilon$  and  $B$  are viewed as specified parameters. The unknown quantity  $\bar{J}$  is given by

$$\bar{J} \equiv \int J_\nu \phi_\nu d\nu = \Lambda[S], \quad (2.55)$$

where  $\phi_\nu$  is the (normalized) absorption profile coefficient. The second equality in (2.55) represents the formal solution of the transfer equation, which is essentially a process of obtaining the radiation intensity from the source function. In the case of two-level atom, the Lambda operator is linear in the mean intensity. The two-level atom problem may be written as a single integral equation

$$S = (1 - \epsilon)\Lambda[S] + \epsilon B, \quad (2.56)$$

or, upon discretization, as a linear algebraic equation. Although it may be solved in a single step without a need to iterate, a matrix representing  $\Lambda$  may be large and thus expensive to invert.

From the mathematical point of view, the ALI scheme is nothing else but an application of the idea of iterative solution of large linear system by *preconditioning*, long known in numerical analysis. The matrix is split into two parts,  $\Lambda = \Lambda^* + (\Lambda - \Lambda^*)$ , and the iterative procedure is set up as

$$S^{(n+1)} = (1 - \epsilon)\Lambda^*[S^{(n+1)}] + (1 - \epsilon)(\Lambda - \Lambda^*)[S^{(n)}] + \epsilon B. \quad (2.57)$$

The action of the exact  $\Lambda$  operator is thus split into two contributions: an approximate  $\Lambda^*$  operator that acts on the new iterate of the source function, and the difference  $\Lambda - \Lambda^*$  that acts on the old, known, iterate of the source function. The latter contribution may be easily obtained by a formal solution of the transfer equation. With the choice  $\Lambda^* = \Lambda$ , one recovers the exact, non-iterative scheme, while with  $\Lambda^* = 0$ , one obtains the classical Lambda iteration (e.g., Mihalas 1978) which is known to converge extremely slowly. Thus, in order that  $\Lambda^*$  operator brings an essential improvement over both schemes, it has to incorporate all the essential properties of the exact  $\Lambda$  but, at the same time, be easy and cheap to invert. During the development of the field, several approximate operators were suggested (for a historical review see Hubeny 1992). In a seminal paper, Olson et al. (1986) performed a rigorous numerical analysis of the problem and demonstrated that a nearly optimum operator is the diagonal (local) part of the exact  $\Lambda$  operator. This makes the corresponding matrix inversions particularly easy because they are reduced to simple algebraic divisions. Such a choice of approximate operator is equivalent to the Jacobi method.

Finally, it should be noted that the convergence properties of the ALI scheme can be significantly enhanced by applying various acceleration techniques, such as the Ng acceleration (Auer 1987; Hubeny and Lanz 1992; Ng 1974), or methods based on Krylov subspace scheme such as the Generalized Minimum Residual (GMRES) scheme (Auer 1991; Hubeny and Burrows 2007a; Klein et al. 1989).

In the context of model stellar atmospheres, one does not use the ALI scheme as a means of evaluating the source function; instead, it is used as a means of expressing current mean intensities, namely

$$J_\nu = \Lambda_\nu^* S_\nu + (\Lambda_\nu - \Lambda_\nu^*) S_\nu^{\text{old}}, \quad (2.58)$$

where the second term represents a “correction” which is known from the previous iteration. The source function is a function of other structural parameters (temperature, electron density, atomic level populations). In the context of a linearization scheme, the first term of (2.58) is easy to linearize in terms of these structural parameters, and the second term is known and need not be linearized at all. The mean intensities of radiation are thus effectively eliminated from the state vector. This is essentially the procedure used by Werner and collaborators (Dreizler and Werner 1993; Werner 1986; Werner et al. 2003).

### 3.3.3 Hybrid CL/ALI Method

Hubeny and Lanz (1995) developed a variant of this approach, in which one uses (2.58) to eliminate the mean intensities in most, but not all, frequency points, while the intensities in a few, most important, frequencies are treated as in original Complete Linearization (cores of the strongest lines; frequencies just above the ionization thresholds of most important continua).

The method is called *hybrid CL/ALI method* and offers a wide spectrum of options ranging from full Complete Linearization to a full ALI scheme. It was demonstrated that the method combines essential advantages of its both constituents: the computer time per iteration is essentially the same as in the case of full ALI scheme, while the number of iterations needed to get a converged model is essentially the same as in the original Complete Linearization, i.e., quite small.

### 3.4 Available Modeling Codes

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There are several publicly available codes for computing model stellar atmospheres. The following list is by no means exhaustive.

For LTE models, the most popular code is Kurucz's *ATLAS* (Kurucz 1970, 1993) and *MARCS* (Gustafsson et al. 1975). It should be noted that most of the NLTE codes listed below can be used to calculate LTE models as well. Appropriately modified versions of *PHOENIX* and *TLUSTY* were actually used for generating grids of LTE models – see [Sect. 3.5.1](#).

In the context of NLTE static models, the first publicly available NLTE model atmosphere code was the “NCAR code” (Mihalas et al. 1975). More recently, popular and widely used codes are *TMAP* – Tuebingen Model Atmosphere Package (Dreizler and Werner 1993; Werner 1986, 1989; Werner et al. 2003), and *TLUSTY* (Hubeny 1988; Hubeny et al. 1994; Hubeny and Lanz 1992, 1995). Static models are also being constructed by codes originally designed for expanding atmospheres (by setting the expansion velocity to a very low value), such as *CMFGEN* (Hillier and Miller 1998) or *PHOENIX* (Hauschildt et al. 1997, 1999a).

It should be noted that besides the codes that solve for the complete NLTE model atmosphere structure, there are several codes that take an atmospheric structure (temperature, density) given and fixed, and solve for statistical equilibrium + radiative transfer for a selected chemical element – the so-called restricted NLTE problem. Although recently these codes lost much of their former appeal because the modern codes are capable of solving the structure plus detailed NLTE rate equations for many species, they are still being used for analyzing stellar spectra. The most popular codes of this sort are *PANDORA* (Avrett and Loeser 2003); *DETAIL/SURFACE* (Butler and Giddings 1985), and, perhaps the most widely used, *MULTI* (Carlsson 1986).

### 3.5 Existing Model Atmosphere Grids

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#### 3.5.1 LTE Models

The most extensive grid of LTE plane-parallel line-blanketed models is that of Kurucz (1979, 1993), widely used by the astronomical community. The grid covers effective temperatures between 3,500 and 50,000 K,  $\log g$  between  $-1$  and  $5$ , and for several metallicities. The term “metallicity” traditionally means that all the chemical species heavier than helium share a common ratio of their abundance to the solar abundance; this ratio is called metallicity. Numerically, the metallicity is often taken as a logarithm of the metal abundance ratio.

Using the *MARCS* code, Gustafsson et al. (1975) generated their original grid of models for cool stars, with  $T_{\text{eff}}$  between 3,750 and 6,000 K;  $\log g$  between 0.75 and 3.0 and metallicities

$-3.0 \leq [M/H] \leq 0$ . Recently, Gustafsson et al. (2008) made public a new, very extensive grid of MARCS model atmospheres, with  $T_{\text{eff}}$  between 2,500 and 8,000 K,  $\log g$  between  $-1$  and  $5$ , and metallicities  $-5 \leq [M/H] \leq 1$ . They also include “CN-cycled” models with  $C/N = 4.07$  (solar),  $1.5$  and  $0.5$ , and  $C/O$  from  $0.09$  to  $5$ , which represents stars of spectral types R, S, and N.

Hauschildt et al. (1999a, b) used their code PHOENIX to generate a grid LTE spherical models for cool stars, called NextGen, with  $T_{\text{eff}}$  between 3,000 and 10,000 K, with step 200 K;  $\log g$  between  $3.5$  and  $5.5$ , with step  $0.5$ , and metallicities  $-4.0 \leq [M/H] \leq 0$ . Another grid (Allard et al. 2000) is for pre-main-sequence cool stars with  $T_{\text{eff}}$  between 2,000 and 6,800 K,  $\log g$  between  $2$  and  $3.5$  with step  $0.5$ , stellar mass  $M = 0.1M_{\odot}$ , and metallicities  $-4.0 \leq [M/H] \leq 0$ . The models are available online at [www.hs.uni-hamburg.de/EN/For/ThA/phoenix/index.html](http://www.hs.uni-hamburg.de/EN/For/ThA/phoenix/index.html). A detailed comparison between the ATLAS and NextGen models was performed by Bertone et al. (2004).

### 3.5.2 NLTE Models

During the last three decades, it was amply demonstrated that departures from LTE are crucial for spectroscopic studies of early-type stars, even the photospheric layers. Early NLTE models were constructed already in the late 1960s and in the first half of the 1970s by Mihalas and coworkers (Mihalas 1972; Mihalas and Auer 1972). Nevertheless, the numerical problems and sheer amount of computer time and memory needed for computing non-LTE metal line-blanketed model atmospheres have precluded computing such models until the late 1980s. Thanks to the development of a very efficient numerical methods such as ALI or the hybrid CL/ALI scheme, this last barrier of the classical stellar atmosphere problem was broken and non-LTE metal line-blanketed model, including literally millions of spectral lines in NLTE, are now being constructed more or less routinely.


There are several partial grids of NLTE models for various stellar types mostly of hot stars. The models constructed by the TMAP code for very hot white dwarfs, subdwarfs, and pre-white dwarfs (also known as the PG 1,159 stars) are available online at <http://astro.uni-tuebingen.de/~rauch/TMAP/TMAP.html>. Rauch and Werner (2009) describe the so-called *Virtual Observatory*, which is a web-based interface that enables a user either to extract already computed models, or generate specific model using TMAP, for very hot objects (hottest white dwarfs; super-soft X-ray sources).

The effort of the developers of TLUSTY culminated in the construction of a grid of NLTE fully blanketed models atmospheres for O stars (OSTAR2002; Lanz and Hubeny 2003) and early B stars (BSTAR2006; Lanz and Hubeny 2007). It is believed that these grids, which each took several years of computer time of several top-level workstations, represent a more or less definitive grids of models in the context of 1D plane-parallel geometry, with hydrostatic and radiative equilibrium, and without any unnecessary numerical approximations.



The basic characteristics are as follows: The OSTAR2002 grid contains 680 individual model atmospheres for 12 values of  $T_{\text{eff}}$  between 27,500 and 55,000 K, with a step of 2,500 K, and 8 values of  $\log g$ , and for 10 metallicities: 2, 1,  $1/2$ ,  $1/5$ ,  $1/10$ ,  $1/30$ ,  $1/50$ ,  $1/100$ ,  $1/1000$ , and 0 times the solar metal composition. The following species are treated in NLTE: H, He, C, N, O, Ne, Si, P, S, Fe, Ni, in all important stages of ionization; which means that there are altogether over 1,000 (super)levels to be treated in NLTE, and about  $10^7$  lines, and about 250,000 frequency points to describe the spectrum.







The BSTAR2006 grid is similar. It contains 1,540 individual models for 16 values of  $T_{\text{eff}}$  between 15,000 and 30,000 K, with a step of 1,000 K, and for 6 metallicities: 2, 1, 1/2, 1/5, 1/10, and 0 times solar. The species treated in NLTE are the same as in OSTAR2002, adding Mg and Al, but removing Ni, which is less important for B stars. There are altogether about 1,450 (super)levels treated in NLTE, about  $10^7$  lines, and about 400,000 frequency points. The models for both grids are available online at <http://nova.astro.umd.edu>.

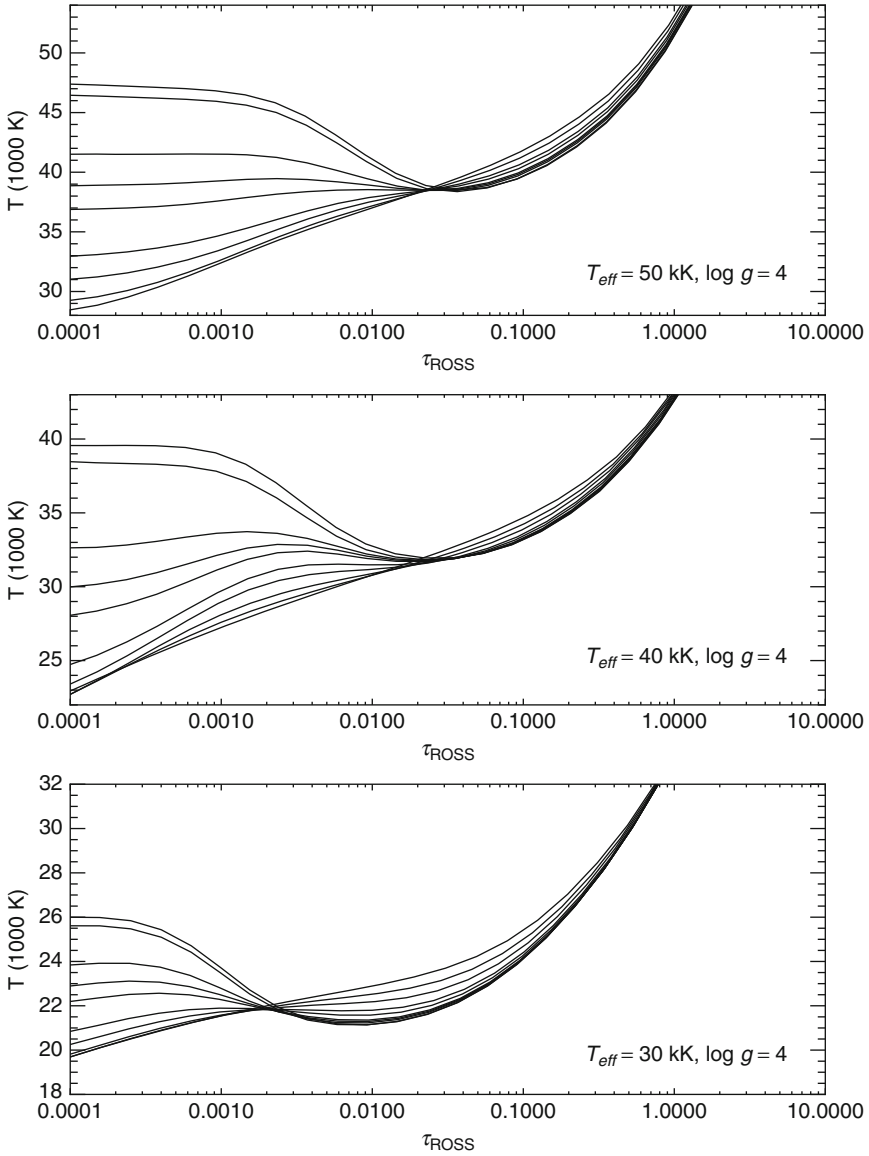
Several representative results from the grids are shown below.  *Figure 2-1* displays the temperature structure for three representative effective temperatures of the OSTAR2002 grid. The temperature distribution nicely illustrates the basic features of line blanketing, namely the so-called back-warming (line blanketing leads to a heating of moderately deep atmospheric layers between Rosseland optical depths 0.01 and 1), and a surface cooling. The zero-metallicity and low metallicities models exhibit a temperature rise at the surface, a typical NLTE effect discovered by Auer and Mihalas (1969) and explained as an indirect heating effect of the hydrogen Lyman and Balmer lines. This effect competes with surface cooling caused by metal lines, and these effects nearly cancel at metallicities 1/50 (for hotter models) to 1/10 (cooler models). Interestingly, the temperature curves for all metallicities cross in a very narrow range of optical depths.

From the practical point of view, the most important result of model atmospheres is the prediction of emergent radiation, which is then compared to the observed spectrum in order to determine the basic stellar parameters. Also, theoretical predictions are indispensable for estimating the radiation in unobservable spectrum regions, in particular in the hydrogen Lyman continuum (wavelength less than 912 Å), which produces ionizing photons, but which cannot be directly detected for early-type stars because of the absorption by interstellar hydrogen. (Only two early-type stars,  $\epsilon$  and  $\beta$  CMa, which are relatively close, and which lie in the direction of a “tunnel” of low density in the local interstellar medium, have detectable Lyman continuum flux as observed by the *EUVE* satellite.)

A sensitivity of the predicted spectra to the effective temperature is depicted in  *Fig. 2-2*, which shows (from top to bottom) emergent spectra for 50, 45, 40, 35, and 30 kK. Notice a diminishing Lyman jump at 912 Å when going to higher temperatures; this is a consequence of increased ionization of hydrogen. A similar sensitivity to metallicity is shown in  *Fig. 2-3*. The models with higher metallicities exhibit deeper lines but higher continuum flux.

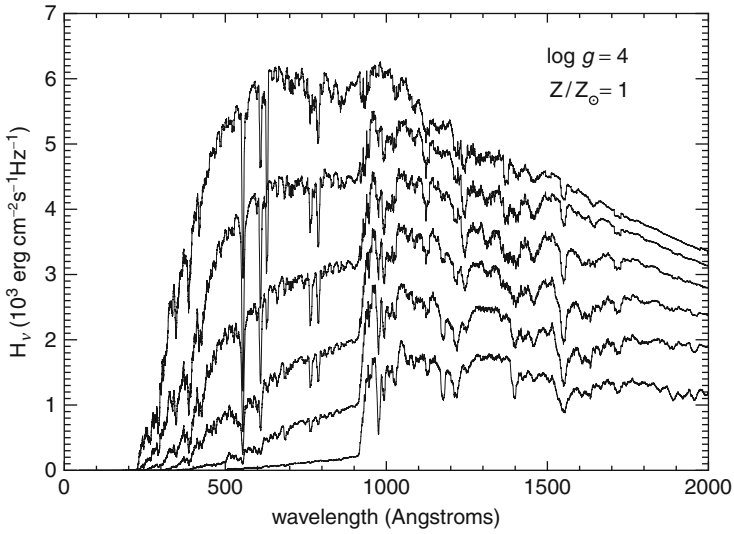
 *Figure 2-4* shows the predicted flux from the OSTAR2002 grid for three solar composition model atmospheres with  $T_{\text{eff}} = 30,000$  K, 40,000 K, and 50,000 K, for  $\log g = 3$ , degraded to a lower resolution (about 5 Å), compared to Kurucz model fluxes. Differences both in the continuum level, as well as in the individual line features, are clearly seen. An analogous comparison of the predicted flux from the BSTAR2006 grid for three solar composition model atmospheres with  $T_{\text{eff}} = 25,000$  K, 20,000 K, and 15,000 K, for  $\log g = 3$ , degraded to a lower resolution (about 5 Å), compared to Kurucz model fluxes, is presented in  *Fig. 2-5*. A similar comparison of high-resolution spectra in several wavelength intervals is presented in  *Fig. 2-6*.

As an actual example of a fit of OSTAR2002 models to observations,  *Fig. 2-7* displays a sample of the predicted flux for a model for  $T_{\text{eff}} = 33,500$  K,  $\log g = 3.85$ , and a high-resolution, high signal-to-noise observation of a late-O main-sequence star 10 Lac secured by the *Goddard High Resolution Spectrograph* (GHRS) aboard the *Hubble Space Telescope* (Hubeny et al. 1998; Lanz et al., in preparation). The agreement between observations and predictions is excellent and demonstrates a power of the present-day model atmospheres of early-type stars.



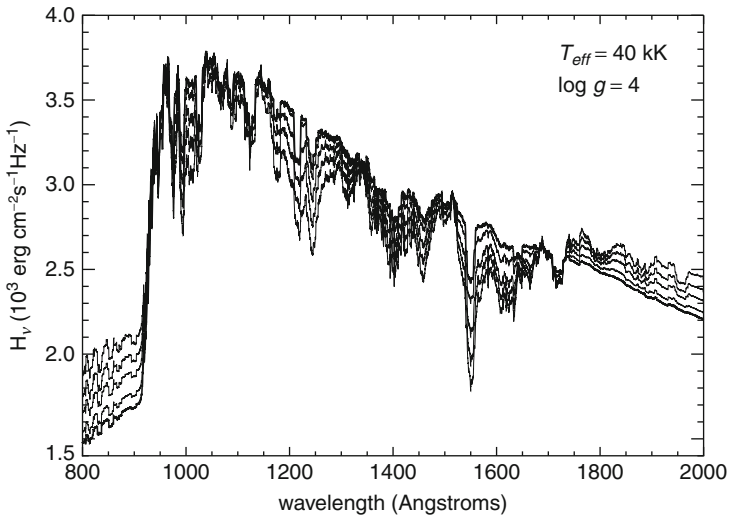
■ Fig. 2-1

Temperature as a function of Rosseland optical depth for OSTAR2002 model atmospheres with  $T_{\text{eff}} = 50,000$  K (*top*),  $40,000$  K (*middle*), and  $30,000$  K (*bottom*);  $\log g = 4.0$ , and various metallicities. At low optical depths ( $\tau_{\text{Ross}} < 10^{-3}$ ), the top curves are for a pure H-He model, and temperature is progressively lower when increasing the metallicity, while the reverse applies in deep layers ( $\tau_{\text{Ross}} > 10^{-2}$ ) (From Lanz and Hubeny 2003)



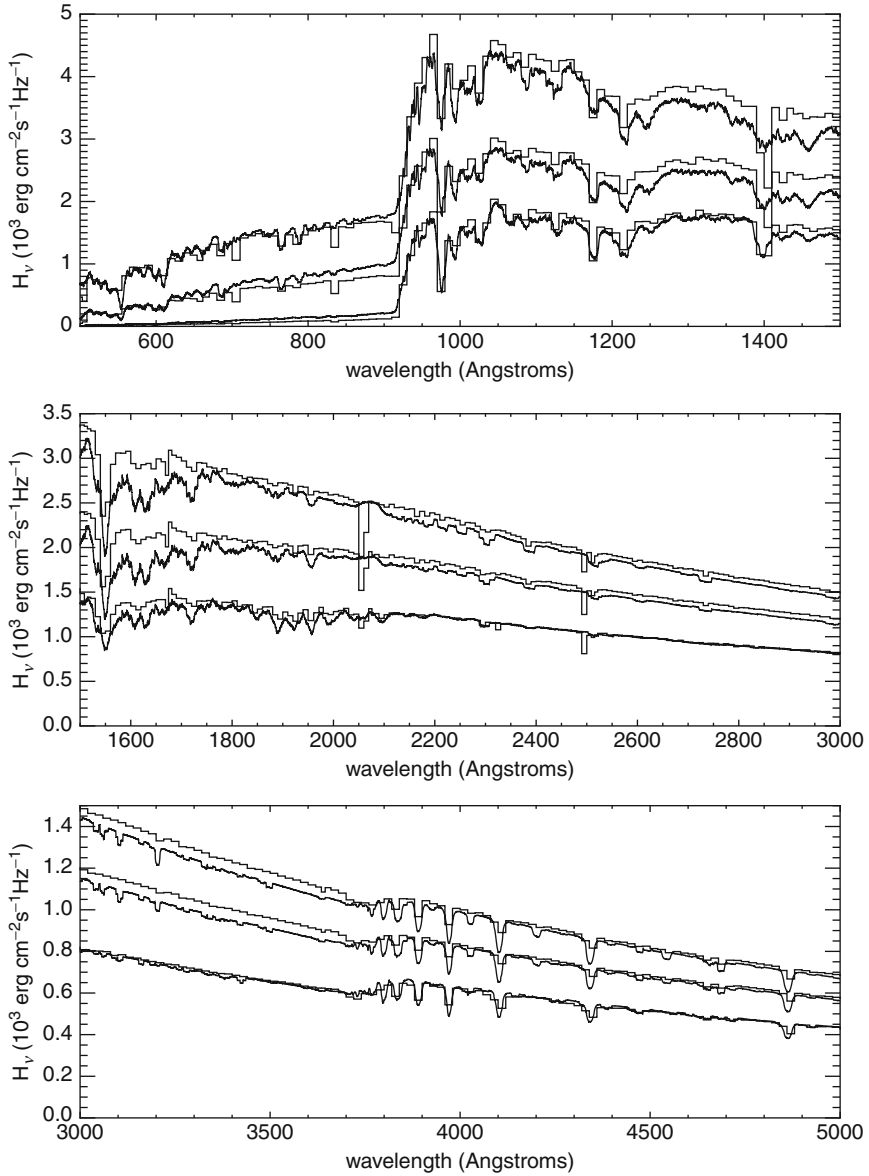
■ Fig. 2-2

Predicted flux for six solar composition OSTAR2002 model atmospheres with  $T_{\text{eff}}$  between 55 and 30 kK, with a step of 5 kK, and for  $\log g = 4$  (From Lanz and Hubeny 2003)



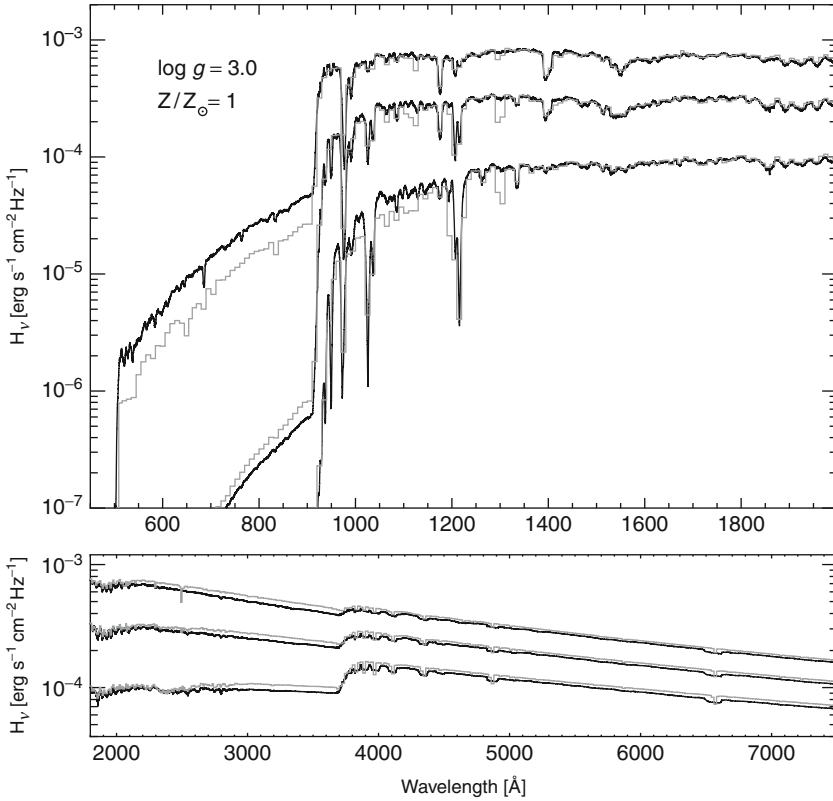
■ Fig. 2-3

Predicted flux for five model atmospheres with  $T_{\text{eff}} = 40 \text{ kK}$  and  $\log g = 4$ , for five different metallicities (From Lanz and Hubeny 2003)



■ Fig. 2-4

Predicted flux for three solar composition mode atmospheres with  $T_{\text{eff}} = 50,000 \text{ K}$ ,  $40,000 \text{ K}$ , and  $30,000 \text{ K}$ , for  $\log g = 4$  (black lines), compared to Kurucz models with the same parameters (gray histograms). The OSTAR2002 model fluxes were degraded to lower resolution to roughly match the resolution of the Kurucz grid (From Lanz and Hubeny 2003)



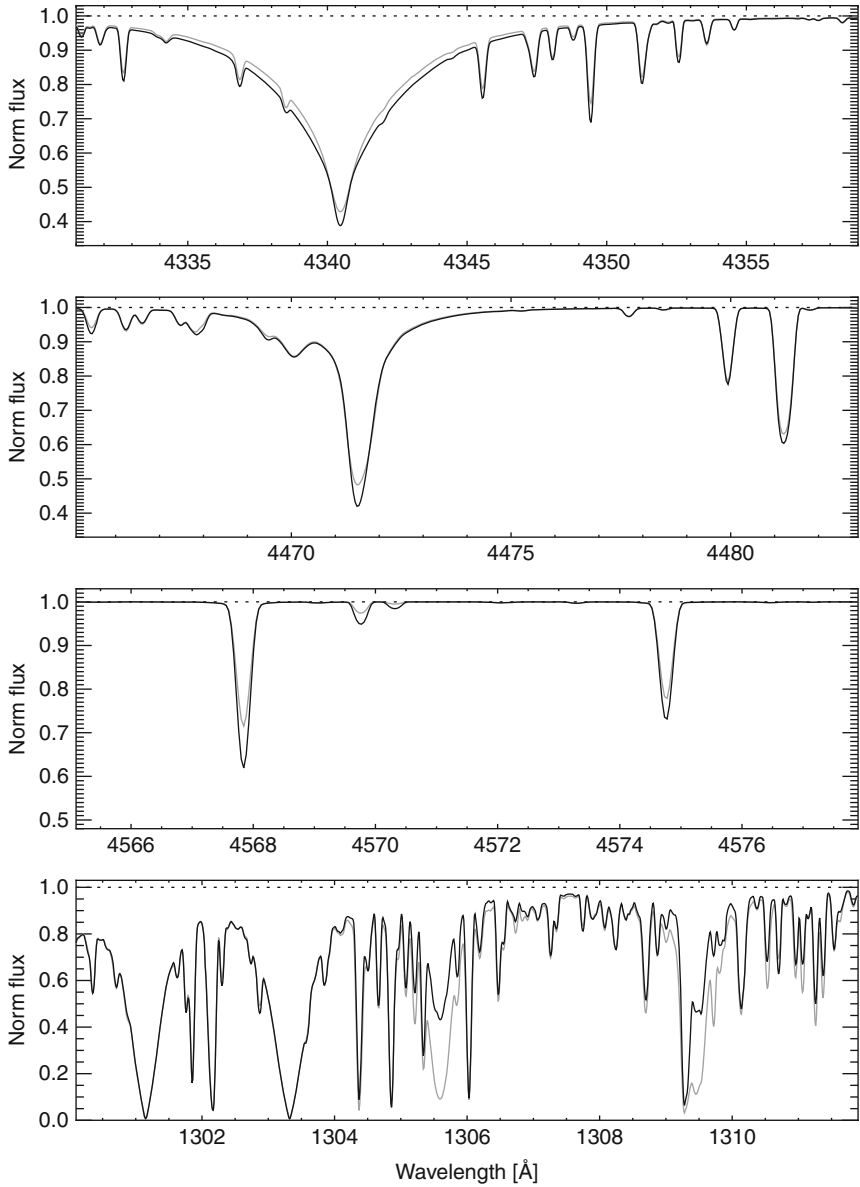
■ Fig. 2-5

Predicted flux for three solar composition model atmospheres with  $T_{\text{eff}} = 25,000$  K,  $20,000$  K, and  $15,000$  K, for  $\log g = 3$  (black lines), compared to Kurucz models with the same parameters (gray histograms). The BSTAR2006 model fluxes were degraded to lower resolution to roughly match the resolution of the Kurucz grid (From Lanz and Hubeny 2007)

## 4 Using Model Stellar Atmospheres to Determine the Fundamental Stellar Parameters

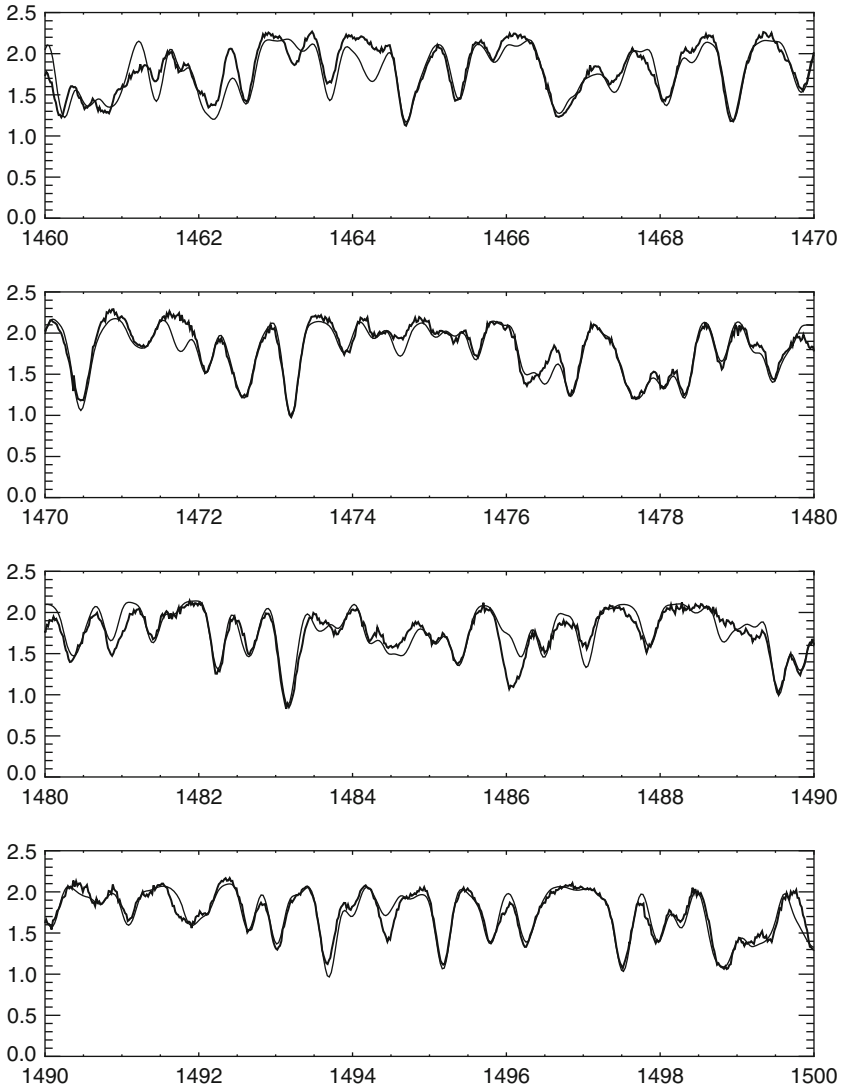
The fundamental stellar parameters to be determined are the stellar mass,  $M_*$ , radius,  $R_*$ , luminosity,  $L_*$ , and the chemical composition, i.e., the set of abundances (ratios of the total number of particles of species  $A$  with respect to hydrogen). If the distance to the star,  $d$ , is not known, it is added to the list of fundamental parameters to be determined, even if it does not represent an intrinsic stellar property.

A determination of chemical composition is a subject of a vast volume of literature so that there is no need to repeat it here. Essentially, they are determined by comparing the observed line profiles (or integrated quantities, like equivalent widths) with those predicted from model atmospheres.



■ Fig. 2-6

Predicted line profiles for solar-composition model atmospheres with  $T_{\text{eff}} = 20,000 \text{ K}$ ,  $\log g = 3.0$ , and  $v_{\text{turb}} = 2 \text{ km s}^{-1}$  (black lines); compared to the Kurucz model with the same parameters (gray lines) (From Lanz and Hubeny 2007)



■ Fig. 2-7

A comparison of the observed HST/GHRS flux for 10 Lac (*heavy line*) and the predicted flux from the fully blanketed NLTE model atmosphere with  $T_{\text{eff}} = 33,500 \text{ K}$ ,  $\log g = 3.85$ , and for the solar abundances of all species (*thin line*). The abscissa is the wavelength in  $\text{\AA}$ , and the ordinate is the flux in  $10^{-9} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$ . Most spectral features are lines of Fe IV, Fe V, Ni IV, and Ni V. A difference between theory and predictions is hardly seen on the plots

There are, obviously, other stellar parameters, like the rotational velocity and others, but for the purposes of this chapter, it is assumed that these additional parameters and the chemical abundances are determined independently of the fundamental parameters listed above.

The parameters which can be determined directly from observations are the effective temperature,  $T_{\text{eff}}$ , and surface gravity,  $g$ . In addition, one has the measured magnitude,  $m_{\text{obs}}$ , that

reflects the whole observationally accessible wavelength range. If the flux in the unobservable region is negligible, then this magnitude represents the total, *bolometric*, magnitude,  $m_{\text{bol}}$ . If not, one has to apply the bolometric correction, which follows from the model atmosphere.

In any case, one ends up with three “measured” quantities,  $T_{\text{eff}}$ ,  $g$ , and  $m_{\text{bol}}$ , but there are four unknown fundamental parameters,  $M_*$ ,  $R_*$ ,  $L_*$ , and  $d$ . The governing relations between them are

$$\sigma T_{\text{eff}}^4 = L_*/(4\pi R_*^2) , \quad (2.59)$$

$$g = GM_*/R_*^2 , \quad (2.60)$$

$$L_* = L_* [m_{\text{bol}} (m_{\text{obs}}, T_{\text{eff}}), d] , \quad (2.61)$$

The last relation expresses the conversion of the observed magnitude to the stellar luminosity.

There are thus three relations for four unknowns. In fact, in some cases, the stellar evolution theory may supply an independent additional relation between the fundamental parameters, for instance, the mass–radius relation for white dwarfs (Hamada and Salpeter 1961) or the mass–luminosity relation for central stars of planetary nebulae (Paczynski 1971). However, in the general situation one does not have such a relation, and, even if so, one may want to check the theoretically predicted relations observationally.

Therefore, from the photospheric analysis only, one cannot derive all four parameters simultaneously. This is easily understood from the physical point of view. A plane-parallel hydrostatic atmosphere is just a thin layer located on the top of a spherical star. The only information about a dimension of the underlying star is contained in the surface gravity  $g$  which depends also on the stellar mass. Since the atmosphere is thin, the emergent spectrum does not carry any independent information about the atmospheric extent.

To remove the radius–mass degeneracy, either an independent geometrical information (knowing the radius or the distance) or an independent knowledge of the mass is needed. A typical situation is that the distance  $d$  is known (e.g., from Hipparchos parallaxes); then the other parameters are determined as follows:

1. From known  $m_{\text{obs}}$  and  $d$  (and, possibly,  $T_{\text{eff}}$ ), the absolute bolometric magnitude,  $M_{\text{bol}}$  and, therefore, luminosity,  $L_*$ , is determined.
2. From  $L_*$  and  $T_{\text{eff}}$ , the stellar radius,  $R_*$ , is determined.
3. From  $R_*$  and  $g$ , the stellar mass,  $M_*$ , is determined.

As it turns out, if the mass of an early-type O stars is determined in this way, the so-called spectroscopic mass, and if the mass is also determined by comparing the evolutionary tracks and the position of the star in the H-R diagram, the so-called evolutionary mass, one finds a significant discrepancy (e.g., Herrero et al. 1992). The sense of discrepancy is that the spectroscopic masses are systematically lower than the evolutionary masses. The discrepancy arises either by inaccuracies of the stellar atmospheres theory, or the stellar evolution theory, or, most likely, both. From the stellar atmospheres side, there has been a progress in understanding the reasons for the discrepancy (e.g., Lanz et al. 1996), namely as an effect of a previously neglected effects of metal line blanketing on the atmospheric structure. However, the problem is not yet fully solved.



## 5 Summary and Outlook

Thanks to the concentrated effort of several groups of researchers, starting with pioneering work of Mihalas and Auer in the late 1960s and early 1970s, and a continuing effort during the last three decades, the problem of constructing 1D stationary model atmospheres, even with full metal line blanketing and in NLTE, is now conceptually solved, although a significant amount of new models still need to be computed.

Even in the domain of LTE models, new discoveries led to new challenges. In particular, the rapidly evolving field of modeling atmospheres of substellar-mass objects, such as brown dwarfs and extrasolar giant planets, provides a natural extension of the traditional stellar atmosphere theory to new and exciting domains, and contributes to a revival of stellar atmospheres theory in general.

The next big step will be to go to 3D radiation hydrodynamic models, which will undoubtedly be one of the main themes of theoretical astrophysics in the next decade. The effort in this area is under way, but much remains to be done. The future of the stellar atmospheres theory thus seems quite bright and exciting.

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