METHOD FOR CALCULATING THE OPACITY OF THE ATOMIC LINES IN STELLAR ATMOSPHERES

O. Cardona[1], E. Simonneau[2], and L. Crivellari[3]
[1] Instituto Nacional de Astrofísica, Óptica y Electrónica, L. E. Erro 1, M72840 Tonantzintla, Puebla, Mexico; ocardona@inaoep.mx
[2] Institut d'Astrophysique de Paris, CNRS, 98 bis Boulevard Arago, F-75014 Paris, France
[3] Osservatorio Astronomico di Trieste and Instituto de Astrofísica de Canarias, Vía Lactea s/n, E-38200 La Laguna, Tenerife, Spain; luc@iac.es
Received 2008 March 14; accepted 2008 September 11; published 2008 December 12

ABSTRACT

A new approximate method for calculating the opacity of the atomic lines in the computation of stellar model atmospheres is presented. Transforming the sums in the equation of the opacity of the lines into integrals and considering the Kramers equation for the oscillator strengths for level transitions in the hydrogenic atoms as a continuous function of frequency, we can apply the mean value theorem for integrals in order to describe the variation of the global opacity of the lines of all the chemical elements. The high-lying levels in nonhydrogenic atoms as well as their hydrogen-like transitions can also benefit from this method. For the case of stellar atmospheres not in local thermodynamic equilibrium, we can apply our method directly. The compact analytic expressions obtained are easy to use. The application of the method to the hydrogen lines shows the classical line-blanketing effects.

Key words: atomic processes – line: formation – stars: atmospheres

1. INTRODUCTION

The emergent energy spectra of stars show a great number of atomic and molecular spectral lines superposed on a continuum background. One of the objectives of modeling stellar atmospheres is to reproduce the variation of the continuum as well as that of the spectral lines through the construction of numerical models. Another objective is to obtain the structure and physical characteristics of the stellar atmosphere, i.e., the model atmosphere. This work is principally addressed to the latter objective. For this objective, the models constructed until now generally include few explicit lines with their correct frequency and depth variation in the atmosphere, and most of the lines are only represented approximately. The former are generally the most important lines or resonance lines and the latter are the so-called secondary lines. Due to problems with computational capacity and the prohibitive computing time, approximate procedures are necessary for treating all the lines. The secondary, and sometimes all, the lines are taken into account using approximate statistical methods as are the means of calculating the opacity using procedures such as the Picket-Fence, the opacity distribution function (ODF), the opacity sampling (OS) method, and their generalizations. Alternative procedures must be found for calculating the opacities of the lines using the basic concepts of atomic quantum physics applied to the bound–bound transitions in order to find approximate nonstatistical methods for introducing the effects of the secondary lines.

In this work we propose a method for calculating the contribution of the secondary lines to the opacity in a deterministically approximate way that is nonstatistical and from the Kramers formula corrected by Gaunt for the oscillator strengths for hydrogenic atoms with the objective of producing realistic stellar atmospheric models efficiently and expeditiously. These results permit us to maintain a globally controlled vision of the calculations and to record when and how the inclusion of certain lines or groups of lines would affect the structure of the atmosphere as well as the emergent spectrum; this is because we can systematically select what elements and states of ionization enter into the calculations, make a systematic analysis of the numerical procedures, and select the results to compare with the observations. The physical structure of the models calculated in this form is more reliable and can be used for the calculation of the emergent spectra of stars and can fulfill observational needs that include, for example, the ultraviolet emergent flux of stars, the identification of spectral lines for stellar classification in order to obtain theoretical color indices for all types of stars, and for studies of stellar populations and galactic structure, among others.

The procedures used until now require, among other things, the construction of tables of the opacities of the lines for certain particular physical conditions of the atmospheric structure and then to interpolate the values in those tables when they are required for the calculation of the atmosphere under consideration, like in the ODF (Kurucz 1979). Others require many frequencies for defining the intervals necessary to cover the complete spectrum with the intention of obtaining a good approximation of the opacity of the lines, as for the OS model (Peytremann 1974). As these procedures are statistical in nature, they lose the direct information of the behavior of the lines or groups of lines in the calculation of the structure of the stellar atmosphere and of its emitted spectrum.

In what follows, Section 2 presents a revision of the methods used to introduce the opacities of the lines in stellar atmospheres. The basic physical processes are introduced in Section 3 as well as a brief description of the statistical methods. The assumptions and mathematical development to find the opacity of the lines in local (LTE) and nonlocal thermodynamic equilibrium (NLTE) in an analytic form are presented in Sections 4.1 and 4.2, respectively. Section 5 describes the procedures for applying our formulation in the evaluation of the line opacity with an example using hydrogen. Some results that show the effects of the inclusion of the three first series of hydrogen plus their respective pseudo-continua are shown in Section 6. Finally, Section 7 presents our conclusions.

2. BACKGROUND

The first stellar atmosphere models were the so-called gray models, which assumed that the opacity did not vary with frequency. Later, only the effects of the continuum processes were included due to the inherent difficulty of the numerical calculation with manual calculating machines and with low-capacity computers. From the construction of the first stellar

atmosphere models (Stromgren 1940), the inclusion of the lines in the calculation of stellar atmosphere models has been a fundamental problem for reproducing the emergent spectra of the stars. The effects that the lines produce in the structure of the calculated atmosphere using only the continuum opacities and in the emergent spectrum are called Line Blanketing (Milne 1928). The effects of the inclusion of the lines in an approximate form were carried out by Chandrasekhar (1936) using the Picket-Fence Method and refined by Munch (1948) and Labs (1951). A series of stellar atmosphere models was obtained using the ODF method (Strom & Kurucz 1965; Kurucz 1979). The ODF and the OS methods are now normally used to calculate stellar atmospheres of all types in LTE as well as those in NLTE. The fundamental idea of the ODF method is to sample the dependencies of the line opacities on frequency in order to form a monotonic function of the opacity with respect to frequency. Then this function is represented by a small number of frequencies in the model calculation. The main idea of the OS method is to statistically sample the real opacities of the lines averaged using very many frequencies within narrow bins to form again a monotonic function of the opacity. In the more recent methods for NLTE, the main idea is to group together several states close enough in energy to form a so-called "superlevel." Considering that the individual levels forming a superlevel are in Boltzmann equilibrium with each other (Anderson 1989; Hauschildt 1993; Hubeny & Lanz 1995), the transitions between individual superlevels, called "superlines", are treated by means of the ODF or the OS.

Our objective is to develop a method for calculating the opacity of the spectral lines in stellar atmosphere models using the fundamental principles of the interaction of the radiation field with atoms and molecules in gaseous media in LTE as well as in NLTE. The lines are produced when the radiation absorbed by the particles that compose the gaseous media causes a transition between bound levels taking energy away from the background or continuum radiation. The lines are characterized by their intensities, its form or frequency profiles, and their central position in frequencies. These characteristics are obtained from atomic and molecular physics using quantum mechanics. The form of the lines reveals the interactions of the atoms with the thermal medium that surrounds them. The intensities of the lines are expressed through the oscillator strengths for the transitions between bound states. These oscillator strengths were obtained in an analytically closed form for the hydrogenic atoms using a semiclassic treatment by Kramers and corrected by Gaunt multiplying by a factor called the Gaunt factor that depends on the principal quantum numbers of the levels that participate in the transition and that reproduces the more elaborate calculations of quantum mechanics. Using the expression of the oscillator strength of Kramers–Gaunt we develop the mathematical procedure for obtaining the opacity of the lines in an approximately closed analytical form.

3. BASIC CONCEPTS

The frequency variation of the opacity in stellar atmospheres plays a very important role in understanding the structure and emergent energy spectra of stars. The opacity of the continuum must be considered because it introduces the coarse characteristics of the energy distribution in the calculated emergent spectrum; for more refined work, of course, one must include the effect of the lines. The effect of the lines in stellar atmospheres is the superposition of the intensities of the lines onto the continuum. Therefore, the lines change the physical structure of the atmosphere and the emergent spectrum compared to those obtained with only the continuum opacity. The opacity contains the contributions of all the possible processes produced by the interaction of the radiation with the material that composes the atmosphere, such as the bound–bound processes (the spectral lines), the bound–free and free–free processes of all the chemical species plus the scattering processes that form the continuum. The absorption coefficient for the transition from level i, lower in energy, to the higher level j considering all the levels, in LTE, for the frequency ν of the radiation is obtained from (Mihalas 1978)

$$\chi(\nu) = \sum_i \sum_{j>i} n_i^* \alpha_{ij}(\nu)\left(1 - e^{-\frac{h\nu}{kT}}\right). \tag{1}$$

The term in parentheses is the correction for stimulated or induced emission. In Equation (1), α_{ij} is the effective cross-section for the transition, n_i^* are the populations of level i (number of atoms per unit volume), where the asterisk means that they are populations in LTE, T is the temperature of the medium considered, h is the Planck constant, and k is the Boltzmann constant. In addition to the continuum opacities, the opacity of the stellar material contains the contributions of thousands to millions of atomic and molecular spectral lines that make the problem difficult to solve numerically. The most natural method to introduce the lines into the calculation of the atmospheric structure is the so-called direct procedure. The lines are included explicitly, along with sufficient frequencies in order to describe the profiles of all the lines considered. Hence, the variations in frequency and in geometric depth are included in the real absorption coefficient of the lines. This direct treatment is prohibitive in terms of computer time and therefore one must employ alternative methods that include, at least approximately, the contribution of the lines to the opacity, such as the direct and the harmonic mean opacities, the Picket-Fence, and the so-called statistical methods. The first two represent the line opacity in a frequency interval only by a single number. The other methods (statistical) use a small number of parameters to describe this opacity in the interval of frequencies given. Among the statistical methods one finds the Picket-Fence (Chandrasekhar 1936; Munch 1948; Labs 1951), the ODF (Strom & Kurucz 1965; Kurucz et al. 1974; Kurucz 1979), and the OS (Peytremann 1974; Sneden et al. 1976). The direct mean, the harmonic mean, and the Picket-Fence are now only of historical interest. The comparisons between some of the methods, their advantages, and disadvantages have been presented in different papers (Carbon 1974, 1979, 1984). There are a number of generalizations of the last two methods for different types of problems, including NLTE problems as mentioned above.

In the normal modeling of stellar atmospheres, very often some of the statistical methods are used for all the lines generating a false continuum that is superposed over the true continuum, producing a blurred representation of the general opacity. With the model thus obtained the spectrum is generated using only the equation of radiative transport, considering the many more frequencies that represent all the possible lines that are allowed by the computational capacity. Other models consider some important lines with the direct method and all the others with one of the statistical methods to generate the model. The calculation of the model defines the structural characteristics of the atmosphere using all the necessary physics and equations that describe the radiative transport, the state of the gas, the material opacity, and energy conservation. These equations form a

nonlinear, nonlocal system of equations difficult to solve numerically, thus restricting the number of frequencies and therefore the number of explicit lines included in the calculation. On the other hand, one must account for the spatial variation of the most intense lines up toward the most external regions of the atmosphere far beyond the region of its formation. For example, the Lyman lines play an important role in determining the temperature structure in stars of the solar type and cooler. Therefore, one must calculate the models considering the most external layers of the atmospheres, corresponding to a Rosseland mean of $\tau_R = 10^{-14}$. So when one does not consider the most important lines explicitly in the calculation, one will produce an incorrect variation of the temperature and a wrong flux in the ultraviolet (Crivellari et al. 2007). Therefore, approximate methods must include the effects of the secondary lines.

4. MATHEMATICAL METHOD

4.1. LTE Case

Taking only the contribution of the lines to the absorption coefficient, and disregarding the stimulated emission for the sake of simplicity, Equation (1) is represented as

$$\chi_l(\nu) = \sum_i \sum_{j>i} n_i^* \alpha_{ij}(\nu). \tag{2}$$

Dividing the sum into two parts results in the following formula:

$$\chi_l(\nu) = \sum_i \left[\sum_{j>i}^{u-1} n_i^* \alpha_{ij}(\nu) + \sum_{j=u}^{\infty} n_i^* \alpha_{ij}(\nu) \right], \tag{3}$$

where the first sum takes into account the few lines that will be treated explicitly and directly. The second sum considers the lines from the level u up to infinity or to a maximum level in the atom that could exist due to the interaction with other atoms in the gas (Cardona et al. 2005 and references therein). The second summation in Equation (3) is the basic expression for the development of our procedure:

$$\chi_l = \sum_i n_i^* \sum_{j=u}^{\infty} \alpha_{ij}(\nu). \tag{4}$$

The effective cross-section for the transition is given by

$$\alpha_{ij}(\nu) = \frac{\pi e^2}{mc} f_{ij} \phi_i(\nu), \tag{5}$$

where f_{ij} is the oscillator strength, and $\phi_{ij}(\nu)$ is the normalized absorption profile of the line, c is the speed of light, e is the charge and m the mass of the electron. Using the classic result of Kramers (1923) for the hydrogenic atoms together with the quantum correction of Gaunt (1935), and the developments of Menzel & Pekeris (1935), we have the following expression for the oscillator strength of the transition in absorption between levels i and j:

$$f_{ij} = \frac{32}{3\sqrt{3}\pi} \frac{g_{ij}}{\left(\frac{1}{i^2} - \frac{1}{j^2}\right)^3 i^5 j^3}, \tag{6}$$

where g_{ij} is the Gaunt factor. Substituting Equations (5) and (6) into Equation (4) we have

$$\chi_l = \frac{\pi e^2}{mc} \frac{32}{3\sqrt{3}\pi} \sum_i n_i^* \sum_{j=u}^{\infty} \frac{g_{ij}\phi_{ij}(\nu)}{\left(\frac{1}{i^2} - \frac{1}{j^2}\right)^3 i^5 j^3}. \tag{7}$$

The profiles are normalized; therefore

$$\int_{-\infty}^{\infty} \phi_{ij}(\nu) = 1. \tag{8}$$

When the levels are close enough to each other to effectively form a continuum, we can approximate the sum of Equation (7) by an integral producing

$$\chi_l = C \sum_i \frac{n_i^*}{i^5} \int_u^{\infty} \frac{g_{ij}\phi_{ij}(\nu) dy}{\left(\frac{1}{i^2} - \frac{1}{y^2}\right)^3 y^3}, \tag{9}$$

where

$$C = \frac{e^2}{mc} \frac{32}{3\sqrt{3}}. \tag{10}$$

To obtain analytic expressions we use the mean value theorem of calculus for integrals resulting in

$$\chi_l = C \sum_i \frac{n_i^*}{i^5} \bar{g}_{ij} \bar{\phi}_{ij}(\nu) \int_u^{\infty} \frac{dy}{\left(\frac{1}{i^2} - \frac{1}{y^2}\right)^3 y^3}, \tag{11}$$

where $\bar{g}_{ij}$ and $\bar{\phi}_{ij}(\nu)$ are evaluated in the closed interval (u,∞). We can take the Gaunt factor and the profile with the value for the transition from level i to level u; that is, $\bar{g}_{ij} = g_{iu}$ and $\bar{\phi}_{ij}(\nu) = \phi_{iu}$. Expression (11) must be divided into the frequency intervals that cover the summed lines, wherein the absorption coefficient is constant within each interval. The value within each interval does not reflect the real variation that would occur within that interval. Therefore, an expression must be found that accounts for the variation of the lines' absorption coefficient and that simultaneously reproduces the integrated value of Equation (11). That expression is found by transforming Equation (7) from a discreet function into a continuous function of frequency with a Gaunt factor and profile like that in Equation (11), but with a different starting value, u, for each spectral series; that is, Lyman, Balmer, Paschen, etc., in the hydrogen atom. We will use the value of the Gaunt factor and line profile for the transition $(i \to u)$. Expressing the frequencies as functions of the principal quantum numbers of the transition for the hydrogenic atoms, we have the Balmer equation

$$\nu = RZ^2 \left(\frac{1}{i^2} - \frac{1}{j^2} \right), \tag{12}$$

where R is the Rydberg frequency and Z is the atomic number of the hydrogenic atom. Substituting into Equation (11) and integrating, we obtain

$$\chi_l = C \sum_i \frac{n_i^* g_{iu} \phi_{iu}}{i^2} x^3 \left(1 - \frac{1}{x} \right)^{\frac{3}{2}}, \tag{13}$$

where we have defined

$$x = \frac{RZ^2}{i^2 \nu}. \tag{14}$$

Equation (13) is a continuous function reproducing a pseudo-continuum running from the frequencies of the first to last lines in the summation, or from the first line to the bound–free continuum of the series. Equation (13) must now be divided into the frequency interval of width $\Delta \nu_i$. Equation (13) when integrated over the interval of frequencies mentioned above

reproduces the value of Equation (11). This Equation (13) must be substituted into Equation (3) to obtain the opacity of all the lines of the given chemical element, yielding

$$\chi_l(\nu) = \sum_i n_i^* \left[\sum_{j>i}^{u-1} \alpha_{ij}(\nu) \ + \ C \frac{g_{iu}\phi_{iu}}{i^2} x^3 \frac{\left(1 - \frac{1}{x}\right)^{\frac{3}{2}}}{\Delta \nu_i} \right], \quad (15)$$

an equation for each hydrogenic chemical species that is included in the calculation of the stellar atmosphere. This equation must be multiplied by the stimulated emission factor to obtain the absorption coefficient for the hydrogenic atoms. For the profile ϕ_{iu} we take the intensity of the whole line. Therefore, by (8) it is equal to one. Equation (15) for the hydrogenic ions is our main result.

For the case of atoms different from the hydrogenic ones, we can generalize our results for transitions to very high levels in the atom, because the higher and higher levels more and more closely resemble the levels of the hydrogenic atoms as the continuum is approached (Sobelman 1992). For this case, one must deal with the nonhydrogenic behavior of the atoms using effective charge as well as effective quantum number of the lower level of the transition, because the lowest levels are those that less resemble hydrogenic behavior. Accordingly, Equation (13) becomes

$$\chi_l = C \sum_i \frac{n_i^* g_{iu}\phi_{iu}}{i_{\text{eff}}^2} x^3 \left(1 - \frac{1}{x}\right)^{\frac{3}{2}}, \quad (16)$$

and then Equation (14) becomes

$$x = \frac{R Z_{\text{eff}}^2}{i_{\text{eff}}^2 \nu}. \quad (17)$$

The effective quantum number is obtained from the tables of experimental energy levels of the atoms (NIST 2007) and is represented by

$$i_{t\text{eff}} = Z \sqrt{\frac{R_y}{E_i}}, \quad (18)$$

where E_i is the energy of the level with respect to the continuum in Rydbergs (R_y) obtained from the tables. The effective charge is obtained considering that the electron making the transition is in a field produced by the screened atomic nucleus by the inner or core electrons. For very high levels, we can take into account the screening using as the effective charge $Z_{\text{eff}} = J + 1$, where J is the state ionization of the chemical element with $J = 0$ for neutral atoms, $J = 1$ for atoms once ionized, etc. Substituting Equation (16) into Equation (3), we find

$$\chi_l(\nu) = \sum_i n_i^* \left[\sum_{j>i}^{u-1} \alpha_{ij}(\nu) \ + \ C \frac{g_{iu}\phi_{iu}}{i_{t\text{eff}}^2} x^3 \frac{\left(1 - \frac{1}{x}\right)^{\frac{3}{2}}}{\Delta \nu_i} \right]. \quad (19)$$

This equation must be multiplied by the stimulated emission correction factor as before to obtain the absorption coefficient for the nonhydrogenic atoms.

4.2. NLTE Case

For stellar atmospheres where the conditions of NLTE prevail, we can generalize our results using the absorption coefficient for the lines (Mihalas 1978), instead of Equation (2), as

$$\chi_l(\nu) = \sum_i \sum_{j>i} \left(n_i - \frac{g_i}{g_j} n_j\right) \alpha_{ij}(\nu), \quad (20)$$

where now we have the populations of the upper levels j of the transition, the statistical weights of the levels g_i and g_j of the states i and j respectively, and the NLTE populations. We can deal with the first term in the same form as we have done before for the similar case in LTE. We will study the the second term dividing the sum of Equation (20) into two parts, as follows:

$$\sum_i g_i \left[\sum_{j>i}^{u-1} \frac{n_j}{g_j} \alpha_{ij}(\nu) \ + \ \sum_{j=u}^{\infty} \frac{n_j}{g_j} \alpha_{ij}(\nu) \right]. \quad (21)$$

The first sum is over the first few inferior levels and as we previously said its evaluation is explicit. We can treat the second term just as we did when we used the mean value theorem for integrals. If we want to integrate using this theorem we would have to use a value within the interval of integration for all the variables that are taken out of the integral, then we can take the lower limit of integration directly to evaluate the populations, the Gaunt factors, and profiles in what follows. As an alternative to integrating, we are going to use the Kramers–Gaunt function directly as we did before for the case in LTE. Starting from the second sum within the square brackets of Equation (21) and substituting the formula for the oscillator strengths, we obtain

$$\sum_{j=u}^{\infty} \frac{n_j}{g_j} \alpha_j(\nu) \ = \ C \sum_{j=u}^{\infty} \frac{n_j}{g_j} \frac{g_{ij}\phi_{ij}(\nu)}{\left(\frac{1}{i^2} - \frac{1}{j^2}\right)^3 i^5 j^3}. \quad (22)$$

As for the hydrogenic atoms the statistical weights are given by $g_j = 2j^2$, and for the nonhydrogenic ones we can consider that the very high levels behave hydrogenically permitting the hydrogenic approximation $g_j = m_{jk} j^2$ (Fischel & Sparks 1971). The m_{jk} is the structure factor that accounts for the structure of the levels of the atom under study. For example, for neutral He $m_{j\text{He}} = 4$. Now we have from Equation (22)

$$\sum_{j=u}^{\infty} \frac{n_j}{g_j} \alpha_{ij}(\nu) \ = \ \frac{C n_u m_{uk}}{g_{iu}} \phi_{iu} \sum_{j=u}^{\infty} \frac{1}{\left(\frac{1}{i^2} - \frac{1}{j^2}\right)^3 i^7 j^3}, \quad (23)$$

where we have taken the populations evaluated in the first level of the sum as well as the profiles and Gaunt factor, as mentioned before. Following the method used for LTE, we convert the sum to a continuous function with frequency as a variable,

$$\sum_{j=u}^{\infty} \frac{n_j}{g_j} \alpha_{ij}(\nu) \ = \ C \frac{n_u}{m_{uk}} \frac{g_{iu}\phi_{iu}}{i^4} x^3 \left(1 - \frac{1}{x}\right)^{\frac{3}{2}}. \quad (24)$$

This expression when integrated over the given frequency interval must reproduce the value of Equation (21). Substituting into Equations (15) or (19), depending on whether it is hydrogenic or not, but in NLTE, and Equation (24) into Equation (20) and simplifying results in

$$\chi_l(\nu) = \sum_i \left[\sum_{j>i}^{u-1} \left(n_i - \frac{g_i}{g_j} n_j\right) \alpha_{ij}(\nu) + C \left(n_i - \frac{g_i}{g_u} n_u\right) \right.$$
$$\left. \times \frac{g_{iu}\phi_{iu}}{i^2} x^3 \frac{\left(1 - \frac{1}{x}\right)^{\frac{3}{2}}}{\Delta \nu_i} \right], \quad (25)$$

where one must consider the values of x given by Equations (15) and (18), the values of the statistical weights $g_u = 2u^2$ and

$g_u = m_{uk}u^2$ as well as the lower quantum numbers i and i_{eff} for the hydrogenic and the nonhydrogenic ions, respectively. We have divided the last term of Equation (25) by the interval of frequencies $\Delta\nu_i$ that covers the included lines of the respective series. This is the result for the case of an NLTE atmosphere.

5. APPLICATION OF THE METHOD

Now we show how to use the equations of our method taking hydrogen as an example, because it is simpler and shows all the peculiarities of the procedure; it has well known physical properties and is the most abundant in stellar atmospheres. Apparently, it is simple in structure but difficult to calculate up to the most external regions of the atmospheres. The methods that use the Feautrier techniques for solving the transfer equation cannot handle this problem. Hydrogen has groups of spectral lines that converge to a common continuum. Each group of lines is called a spectral series. The first series is called the Lyman series that for absorption begins in the lowest or ground level with $i = 1$, the second is the Balmer series with $i = 2$, followed by Paschen, Brackett, and Pfund with $i = 3, 4$, and 5, respectively. The initial frequency of the relevant interval in Equation (13) comes from Equation (12), where

$$\nu_i = R\left(\frac{1}{i^2} - \frac{1}{u^2}\right), \qquad (26)$$

with u as the lowest level from where all the lines are added together. The final frequency is given by the ionization frequency of level i, that is,

$$\nu_f = \frac{R}{i^2}. \qquad (27)$$

When the atoms are known to have a maximum level n_{max}, Equation (27) is instead

$$\nu_f = R\left(\frac{1}{i^2} - \frac{1}{n_{\text{max}}^2}\right). \qquad (28)$$

The relevant interval of computation is given by

$$\Delta\nu_u = R\left(\frac{1}{u^2} - \frac{1}{n_{\text{max}}^2}\right), \qquad (29)$$

where the maximum number n_{max} can be equal to infinity, when it happens that the atom is isolated. In hydrogen if two consecutive lines of the same series are separated by a distance (in frequency) equal to the distance between their centers they are not resolved. From Equation (12)

$$\nu_{JK+1} - \nu_{JK} = RJ^2\left[\frac{1}{K^2} - \frac{1}{J^2}\right], \qquad (30)$$

for high lines of each series, $K^2 \gg J^2$, then

$$\nu_{JK+1} - \nu_{JK} = RJ^2\frac{2}{K^2}. \qquad (31)$$

The lines are not resolved for a critical value of $K = K_c$. Also

$$\nu_{JK+1} - \nu_{JK} = 2\sigma, \qquad (32)$$

where σ is the Doppler HFWHM of the lines. Therefore, from Equations (31) and (32), we obtain

$$K_c^3 = J^2\frac{R}{\sigma}. \qquad (33)$$

For the Balmer series, for example, with $J = 2$, for the line that corresponds to $K = 10$, we have $\nu_{JK} = 7.895 \times 10^{14}$ Hz, $R = 8.218 \times 10^{14}$ Hz, and $R - \nu_{JK} = 3.23 \times 10^{13}$ Hz, giving $\sigma \simeq 3.23 \times 10^{12}$ Hz $\sim 9 \times 10^{-3} R$. That may be the line width for the corresponding line. Practically, due to other broadening effects like microturbulence, one can set $u = 7$.

For hydrogen with $u = 7$, we have $\Delta\nu_u = 6.7118 \times 10^{13}$ Hz and the initial frequencies for each series are 3.22098×10^{15}, 7.55131×10^{14}, and 2.98319×10^{14} Hz, for the Lyman, Balmer, and Paschen series, respectively. The final frequencies are given by the previous numbers for the initial frequencies and applying the above given frequency intervals to them. All these values can also be taken from the tables of levels for hydrogen and for all the hydrogenic atoms to be included in the calculation.

For the nonhydrogenic atoms we follow the same procedure used for hydrogen: for each series we choose $u = 7$ for calculating Equation (16). Because we are using the expression obtained above where we have applied the hydrogenic approximations, the levels above this value are very close to the levels of the respective hydrogenic atoms. The lowest terms of lower angular momentum are farther away from the hydrogenic behavior (Sobelman 1992). Therefore, one must use an effective quantum number that accounts for that physical situation. The behavior of the higher levels with respect to the hydrogenic ones is taken into account using effective charge and, in addition, the quasihydrogenic structure factor, which considers the weighted sum of the statistical weights of the levels to form this factor. The alkali atoms have four series of levels where one must apply our formulation to each of them. The helium and the alkaline atoms have four series for the singlets and four series for the triplets; the equations developed here apply to each of the four series. For other atoms and ions, their Grotrian diagrams (NIST 2007) and their tables of energy levels must be consulted in order to define to which series the equations would apply. For all the series, one must find the initial and final frequencies that define the pseudo-continuum that will be included in the calculation of the atmosphere. One can also take all the levels of the nonhydrogenic atoms as if they were hydrogenic, degenerate in energy, and therefore the spectroscopic terms are reduced, thereby decreasing the number of series to calculate. For the case of atmospheres in NLTE, we must follow the same procedure, that is, find the initial and final frequencies, and therefore the interval where Equation (25) will be evaluated.

6. RESULTS

To show the application of the method for the hydrogen lines, we have calculated plane–parallel models in hydrostatic, radiative–convective equilibrium and LTE for the temperatures $T_{\text{eff}} = 5 \times 10^3$, 10^4, and 2×10^4 K with the logarithm of gravity $\log g = 4.5$ and solar abundance of the elements. The models contain the continua and discontinuities of the principal chemical elements and their ions (Cardona et al. 2002). To include the effects of the Lyman lines, we have calculated the models up to the optical depths 10^{-14}, 10^{-12}, and 10^{-10} for the different temperatures given above. The models were calculated using the Integral Implicit Method (IIM; Simonneau & Crivellari 1993), and considering the procedures described in different papers (Crivellari et al. 1994, 2003, 2004). Figure 1 shows the calculated emergent flux of the models where five Lyman, four Balmer and three Paschen lines can be seen plus the pseudo-continua for those series (equivalent to millions of lines). The Paschen lines are barely visible on the scale of this figure. Figure 1 shows the lines that are calculated individually with
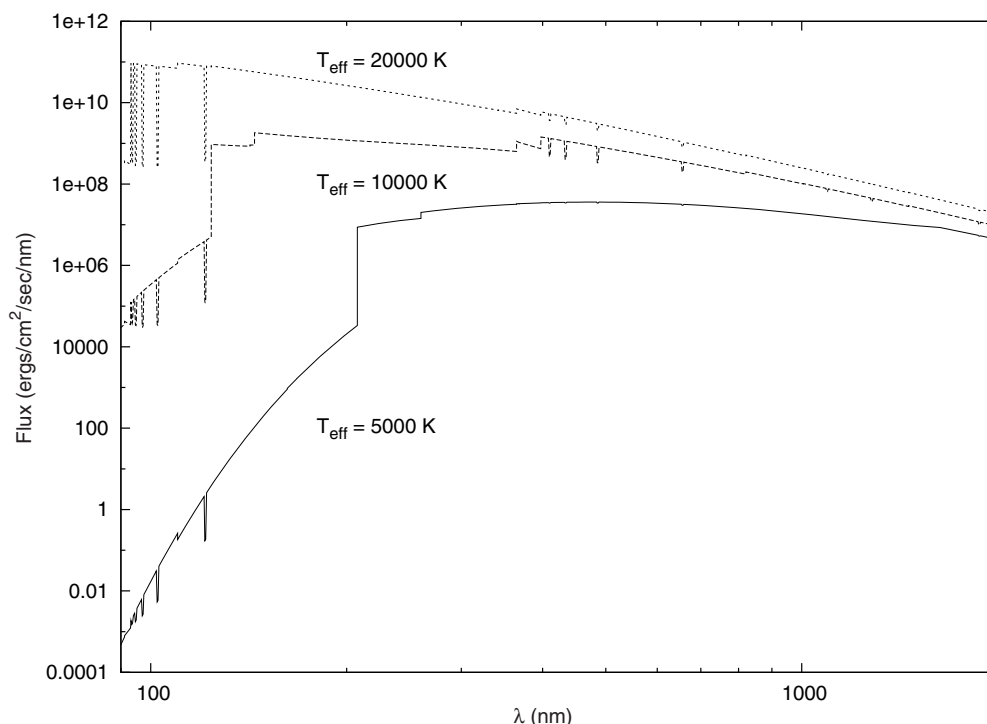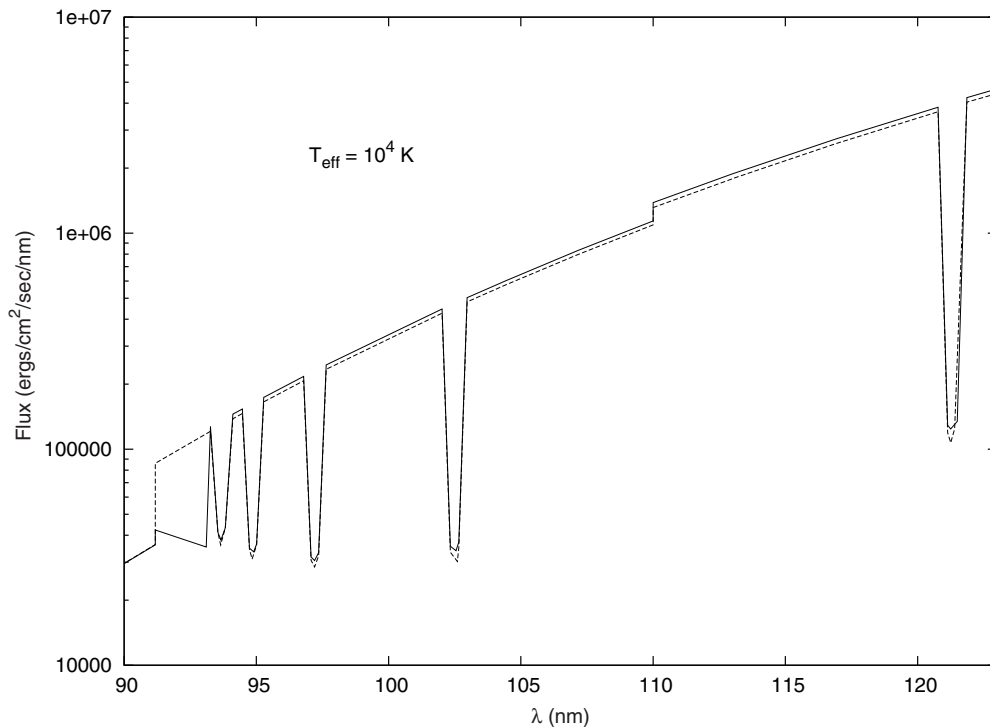
Figure 1. Calculated emergent fluxes for three models with temperatures of 5×10^3, 10^4, and 2×10^4 K; with $\log g = 4.5$. From left to right the lines and pseudo-continua of Lyman, Balmer, and Paschen are shown.

the direct method plus the pseudo-continuum for each series generated by our method and all of them superposed on the true general continuum. This result shows the real input to the model, the number of explicit lines that in our case are 12 hydrogen lines and the continua. The structure obtained using the nonlinear, nonlocal system of equations of stellar atmospheres for hundreds of frequencies, the model of the atmosphere, can be used by anyone to calculate the spectrum using the transfer equation for millions of frequencies. The flux obtained in the model calculation defines the real continuum of the emergent energy distribution, very important in photometry.

This analysis is based on the validity of the Kramers–Gaunt function for the hydrogenic atoms and mainly to transitions to higher levels in the atoms. Therefore, for those atoms and ions the most important approximation is converting the sum over all the transitions above the level u to a continuous function of frequency using the equation of Kramers–Gaunt. We have used the integrated profile of the first line included in the given pseudo-continuum. Each line is spread out to form its part of a pseudo-continuum. Therefore, there are no longer any levels, and we can integrate up to maximum level for each atom or ion that we include. Hence, what we have done is valid for all the hydrogenic atoms and ions when one uses the approximations introduced for the transitions to the high-lying level in the atoms. From numerical experiments for nonhydrogenic atoms over transitions to the quasihydrogenic higher levels of the atoms, we have found that the Kramers–Gaunt equation produces fair results in comparison with the values reported in the literature for the oscillator strengths as well as from other sources (Cowan 1981; Sobelman 1992); therefore, we can apply this equation in our procedure. The equations obtained can be applied to all types of atoms and ions. For atoms different from the hydrogenic atoms, effective quantum numbers of the spectroscopic terms of lower angular momentum and lower in energy as well as the effective charge sensed by the valence electron must be used.

For the case of atoms that are in NLTE, for the hydrogenic atoms the expressions derived above are applied directly and for nonhydrogenic atoms the statistical weights can be obtained from the hydrogenic approximation using the structure factor. The results are simple and easy to apply, and they are reasonable given that an exact expression for the oscillator strengths is used that is valid for transitions to high levels in the atoms. The results are not trivial because they show the behavior that each single line would have within the relevant frequency range. In addition, we have to remark that the opacities of the lines in our approach directly contain all the physical information at each depth in the atmosphere through the atomic populations, which is missing in other methods. There are no similarities with the previous methods for calculating the opacities of the lines because this is not an average opacity, nor is it a statistical method. The main difference is that our results show the variation that the pseudo-continuum would have within the frequency range of the calculations following the real variation of the individual lines over the whole atmosphere. If one uses other values for u, the only thing that changes is the length of the pseudo-continua and therefore the distribution of the flux.

It is difficult to compare the applications of our procedures with other methods because in general the calculations of the structure are carried out to optical depths greater than 10^{-7} where the effects of the lines of Lyman begin to appear in stars of the solar type and cooler, thereby ignoring the great changes in the structure of the atmosphere and of the emergent ultraviolet flux (Crivellari et al. 2007). The hotter models are calculated to the same optical depths as above ignoring the effects of the lines of Lyman also. We have made a comparison between models with and without the inclusion of the secondary lines of hydrogen for a temperature of 10^4 K and $\log g = 4.5$ and solar abundance. Figure 2 shows the calculated flux. The continuous line is the model calculated with our approximations and the dotted line is the model without the secondary lines. The

Figure 2. Calculated emergent fluxes for models with (continuous line) and without (dotted line) the effects of the secondary lines of our procedure for the effective temperature 10^4 K; with $\log g = 4.5$. From left to right the pseudo-continuum and lines of Lyman are shown.

main change is in the Lyman jump at the left of Figure 2. We can see the slope of the Lyman pseudo-continuum that our method produces. The effects are important because the Lyman jump is decreased more than eight times and the pseudo-continuum is decreased even more compared with a model without the secondary lines. The energy taken away is distributed over all frequencies and also the flux is increased over all the frequency range of the calculation by the back-warming effect produced by the blocking effect of the secondary lines, the so-called line-blanketing effects of the lines. If one integrates over all the frequencies the increase in energy is really great. The hydrogen jumps are very important for the classification of stars and can be measured with any photometric system. For example, the *U* filter is centered in the Balmer jump in the *UBV* photometric system. All the models calculated by the groups mentioned above include the secondary lines using any of the methods exposed before and our results show that they are very important in the calculation of the model atmospheres.

The synthetic emergent spectra calculated from statistical methods that use millions of lines do not show the real continuum of the models for the case at hand. Further, the comparison with the direct spectroscopic observations of the stars is very difficult because all the lines of all the elements are visible in the spectra, thereby rendering it very difficult to define a continuum for comparison with the current work.

Our method can also be used to treat all the lines as secondary when the computational constraints are a serious issue. Doing this requires the oscillator strength given in the tables for the first line. Strictly speaking, setting $u = 1$ violates the main assumption that the upper levels are hydrogenic and roughly form a continuum to apply the equations. Hence we would produce a blurred continuum different from that produced by the statistical methods, because our procedure accounts for the intensities and frequencies in each atomic series.

7. CONCLUSIONS

We present a method for introducing the effects of the opacities of the lines into the calculation of stellar atmosphere models in an analytically approximate way. The method uses the behavior of the oscillator strengths of the bound–bound transitions between the atomic levels. This was carried out using the Kramers–Gaunt formula for the oscillator strengths for the hydrogenic atoms. Supposing that we can transform the sum that represents the opacities of the lines into a continuous function of frequency, we obtain an analytical expression for the contribution of the lines to the general opacity. The equations thus obtained are functions of frequency and are an extension of the equation of Kramers–Gaunt that was originally developed for discreet transitions. For the hydrogenic atoms this is the main assumption of our method. For the other atoms, this assumption is accompanied by the possibility that we can use the Kramers–Gaunt function for nonhydrogenic atoms considering that the oscillator strengths for the atomic transitions to the higher levels are similar enough to the values obtained from the published tables of oscillator strengths. Also in these developments, we have considered as an example the use of the mean value theorem of calculus for integrals for evaluating the quantities that are taken out of the integral; this has allowed us to evaluate the populations, statistical weights, the profiles, and the structure factor for the first level of the sum of the opacities of the lines. These results are important for stellar atmosphere calculations because they reflect the behavior of atmospheres and the emergent spectrum with the inclusion of the lines directly.

REFERENCES

Anderson, L. S. 1989, ApJ, 339, 558
Carbon, D. F. 1974, ApJ, 187, 135
Carbon, D. F. 1979, ARA&A, 17, 513

Carbon, D. F. 1984, in Methods in Radiative Transfer, ed. W. Kalkofen (Cambridge: Cambridge Univ. Press), 395

Cardona, O., Crivellari, L., & Simonneau, E. 2005, Rev. Mex. Fis., 51, 476

Cardona, O., Simonneau, E., & Crivellari, L. 2002, in New Quests in Stellar Astrophysics, ed. M. Chavez, A. Bressan, A. Buzzoni, & D. Mayya (Dordrecht: Kluwer), 29

Chandrasekhar, S. 1936, MNRAS, 96, 21

Cowan, R. D. 1981, The Theory of Atomic Structure and Spectra (Berkeley: Univ. California Press)

Crivellari, L., Cardona, O., & Simonneau, E. 2007, in Proc. of IAU 241, Stellar Populations as Building Blocks for Galaxies, ed. A. Vazdekis & R. F. Peletier (Cambridge: Cambridge Univ. Press), 91

Crivellari, L., & Simonneau, E. 1994, ApJ, 429, 331

Crivellari, L., Simonneau, E., & Cardona, O. 2003, Mm SAI, 3, 97

Crivellari, L., Simonneau, E., & Cardona, O. 2004, Mm SAI, 75, 154

Fischel, D., & Sparks, W. 1971, ApJ, 164, 359

Gaunt, J. A. 1935, Proc. R. Soc., A126, 654

Hauschildt, P. 1993, JQSRT, 50, 301

Hubeny, I., & Lenz, T. 1995, ApJ, 439, 875

Kramers, H. 1923, Phil. Mag., 46, 836

Kurucz, R. 1979, ApJS, 40, 1

Kurucz, R., Peytremann, E., & Avrett, E. 1974, Blanketed Model Atmospheres for Early-Type Stars (Washington, DC: Smithsonian Institutions)

Labs, D. 1951, Z. Astrophys., 29, 199

Menzel, D., & Pekeris, C. 1935, MNRAS, 96, 77

Mihalas, D. 1978, Stellar Atmospheres (San Francisco, CA: Freeman)

Milne, E. A. 1928, Observatory, 51, 88

Munch, G. 1948, ApJ, 104, 87

NIST 2007, http://physics.nist.gov/PhysRefData/

Peytremann, E. 1974, A&A, 33, 203

Simonneau, E., & Crivellari, L. 1993, ApJ, 409, 830

Sneden, C., Johnson, H., & Krop, B. 1976, ApJ, 204, 281

Sobelman, I. I. 1992, Atomic Spectra and Radiative Transitions (Berlin: Springer)

Strom, S. E., & Kurucz, R. L. 1965, J. Quant. Spectros. Rad. Transfer, 6, 591

Stromgren, B. 1940, Pub. Mind. Med. Kobenhavns Obs., 1, 127