Semiempirical LTE modelling of solar photospheric layers

I. Theoretical background

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Abstract. The calculation of the physical parameters of photospheric layers using the LTE approximation is described. The main algorithm for calculating photospheric lines is given. The corrections of the Saha and Boltzman equations for the upper layers are discused and the effect of the magnetic field is taken into account. The actual computational code and detailed description of how to use it will be published in Part II of this paper.

Key words: solar atmosphere - LTE modelling - spectral lines calculations

1. Introduction

The study of line profiles, the comparison of observed and calculated profiles is one of the most effective methods of investigating active formations of the solar atmosphere. A number of special programs has been created for calculating line profiles. These programs are rather complicated and time-consuming. Approximate methods are therefore being used in some cases. The LTE-approximation is good enough for investigating the photospheric layers of solar formations. This means that the ionization can be determined from the Saha equation and the level population from the Boltzman equation. These two equations do not provide good accuracy for upper photospheric layers. For this reason we have used the ionization equilibrium equation which is different from the Saha equation, but nevertheless is simple for calculations. Beside that the corrections to the Bolzman equation are made for the most external photospheric layers $(\tau_{0.5} < 0.01)$. These corrections are derived using the approximate method of the source function calculation by Ivanov et al. (1984). The main algorithm for calculating the profiles of these lines originating in photospheric layers is described. The LTE conditions are assumed to be satisfied, but the corrections to the Saha and Bolzman equations are used in the program. All parameters necessary for beginning the calculations are also described. We do not restrict the choice of models by requiring hydrostatic equilibrium. It may not exist in an active atmosphere where the magnetic field (i.e. magnetic pressure), velocity field and turbulence are present.

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2. Line intensity and absorption coefficient

The radiation intensities at line frequencies ν are given by the expressions:

$$I_{\nu}(\mu) = \int_0^{\infty} \left[S(\tau) \varphi_{\nu}(\tau) + r(\tau) B(\tau) \right] e^{-\int_0^{\tau} \left[\varphi_{\nu}(\tau) + r(\tau) \right] \frac{d\tau}{\mu}} \frac{d\tau}{\mu}, \tag{1}$$

where

$$\tau = \int_0^h K^L \varphi_{\nu_0} dh \tag{2}$$

is the optical depth in the line centre $(\nu = \nu_0)$ at depth h [cm], and

$$K^{L} = \frac{h\nu_0}{4\pi} \frac{1}{\sqrt{\pi}\Delta\nu_D} n_l B_{l_m} \left(1 - \frac{g_l}{g_m} \frac{n_m}{n_l} \right). \tag{3}$$

Here l, m are the numbers of the lower and upper levels in the atom model (the line originates when transition l-m is realized); n_l, n_m are the number densities (per cm^3) of atoms excited at levels $l, m; g_l, g_m$ are statistical weights of levels $l, m; B_{lm}$ are Einstein coefficients.

The Doppler width

$$\Delta\nu_D = \frac{1}{\lambda} \sqrt{\frac{2kT}{A_t m_H} + V_t^2},\tag{4}$$

where $\lambda = c/\nu$; k is the Bolzman coefficient; A_t atomic weight; m_H the weight of the hydrogen atom; V_t the turbulent velocity; T temperature. The Einstein coefficients A_{ml} , B_{lm} and oscillator strength f_{lm} for the same transition are related as

$$\frac{h\nu_0 B_{lm}}{4\pi^{\frac{3}{2}}} = \frac{g_m}{q_l} \frac{A_{ml}}{8\pi^{\frac{3}{2}}} \lambda^2 = 0.01495 f_{lm}. \tag{5}$$

Now

$$K^{L} = 0.01495 f_{lm} \left(\frac{n_l}{\Delta \nu_0}\right) \left(1 - \frac{g_l}{g_m} \frac{n_m}{n_l}\right) \tag{6}$$

For lines in the visible spectrum the value of $\left(1 - \frac{g_l}{g_m} \frac{n_m}{n_l}\right)$ is nearly unity. Function φ_{ν} (in eq.2) reads

$$\varphi_{\nu} = \sqrt{\pi}\phi_{\nu},\tag{7}$$

where ϕ_{ν} is the Voigt profile normalised as

$$\int \varphi_{\nu} d\nu = \Delta \nu_{D}. \tag{8}$$

The form of ϕ_{ν} depends on two parameters: $\phi_{\nu}(x,a)$, where $x = \Delta \lambda / \Delta \lambda_D$,

$$\Delta \lambda_D = \frac{\lambda}{c} \sqrt{\frac{2kT}{A_t m_H} + V_t^2},\tag{9}$$

 $\Delta\lambda$ is the distance from the line centre, $a=\delta^{'}/\Delta\nu_{D},\,\delta^{'}=\Gamma/$ $4\pi,$

$$\Gamma = \sum_{i=1}^{m-1} A_{mi} + \gamma_{vw} + \gamma_{st}, \tag{10}$$

where A_{mi} are Einstein coefficients, *i* denoting all levels lower than m. A_{mi} can be calculated from equation

$$A_{mi} = 0.665 \; \frac{g_i f_{im}}{\lambda_{im}^2 g_m}. \tag{11}$$

The Van-der-Waals broadening γ_{vw} has the form $\gamma_{vw} = C_{vw} n_H$, where n_H is the number density of hydrogen atoms. For hydrogen lines

$$C_{vw} = \frac{g_m}{g_l} \frac{A_{ml} \lambda_{cm}}{32\pi}.$$
 (12)

For other elements there is a number of different methods of calculating γ_{vw} . Irwin (1979) approximated γ_{vw} by equations:

$$\gamma_{vw} = n_H A(l) T^{B(l)}(n^*)^{C(l)}, \qquad n^* = \sqrt{\frac{RZ^2}{\chi_{ion} - \chi_{exc}}}$$
 (13)

where n^* is the quantum number of upper level; Rydberg constant $R=1.097 \times 10^5~cm^{-1}$; Z - ion charge (Z=1 for neutrals); χ_{ion} , χ_{exc} are ionization and excitation potentials for the upper level given in cm^{-1} ($\varepsilon_{cm^{-1}}=\varepsilon_{e.v}\times 10^4/1.235$). Quantities A(l), B(l), C(l) are presented in Table I.

Table 1. Van-der-Waals coefficients

ī	$A(l)\times 10^{10}$	B(l)	C(l)	range of n*
0	2.34	0.365	2.48	1.5-3.50
1	1.84	0.362	2.68	1.5 - 3.50
2	0.843	0.356	3.25	2.5 - 3.75
3	0.236	0.340	4.07	3.5 - 4.00

For FeI lines the equation for γ_{vw} is presented in Edmunds (1975) where

$$\gamma_{vw} = 1.54 \times 10^{-8} n_H \ T^{0.3} / (7.88 - \chi_{exc})^{1.5}$$
 (14)

and χ_{exc} is the excitation potential of the upper level in electronvolts. Parameter γ_{st} (in eq. 10) denotes the Stark broadening. This form of including the Stark broadening is an approximation. For a precise account of the Stark effect it is necessary to combine the Voigt and Stark profiles. There is a special subroutine for this procedure in the program, but in most cases the approximate method provides sufficient accuracy. We express γ_{st} as $\gamma_{st} = C_{st} n_e$; n_e is the electron number density. Several forms of C_{st} have been proposed. For hydrogen lines L_{α} , L_{β} , H_{α} C_{st} is as follows:

$$C_{st}(for L_{\alpha}) = 4.25 \times 10^{-5} T^{-\frac{1}{2}} \log(1.96 \ 10^{12} T^2 / n_e),$$
 (15)

$$C_{st}(for L_{\beta}) = 2.22 \times 10^{-4} T^{-\frac{1}{2}} \log(3.76 \ 10^{11} T^2 / n_e),$$
 (16)

$$C_{st}(for H_{\alpha}) = 2.0 \times 10^{-4} T^{-\frac{1}{2}} \log(4.81 \ 10^{11} T^2 / n_e). \tag{17}$$

 C_{st} for Balmer lines are given in Hirayama (1963):

$$C_{st} = 3.81 \times 10^{-6} (mn)^2 (m^2 - n^2)^{1/2} R(n_e, T), \tag{18}$$

$$R(n_e, T) = 9.5 \times 10^3 \frac{\left[m(m-1) + 2\right]^{0.5}}{\lambda \sqrt{T}} \times$$

$$\times [9.012 + \log T - 1/2 \log n_e - \log (m(m-1) + 2)], \tag{19}$$

where n,m are the main quantum numbers for the lower and upper levels. The halfwidths for Stark broadening w_{λ} for some lines are given by Griem (1974). Parameter C_{st} is connected with w_{λ} by equation

$$C_{st} = 3.77 \times 10^3 \lambda_{\stackrel{\circ}{(A)}}^{-2} w_{\lambda},$$
 (20)

The Voigt function ϕ_{ν} is calculated using special programs (see for example Avrett and Loeser 1969). Oscillator strengths f_{lm} can be found in Kurucz and Peytreman (1975). Quantity n_l in (3) depends on the plasma condition characterized by such parameters as temperature T, density n_H , and the density of radiation field. Usually n_l is presented in the form:

$$n_l = \frac{n_l}{n_{el}} \frac{n_{el}}{n_H} n_H = \frac{n_l}{n_{el}} A n_H \tag{21}$$

where n_{el} is the total number of atoms and ions of the element being considered (at all stages of ionization and excitation), $A = n_{el}/n_H$ is the abundance. The calculation of n_l/n_{el} (level populations) in a general case presents a rather complicated problem which reduces at the end to a system of radiative transfer and equilibrium equations. Quantities n_l/n_{el} can easily be found, however, for the case of LTE conditions. n_l/n_{el} can be then calculated by using the equations of Bolzman (22) and Saha (24)

$$\frac{n_m}{n_l} = \frac{g_m}{g_l} e^{-(\varepsilon_m - \varepsilon_l)/kT}, \qquad \frac{n_m}{n_r} = \frac{g_m}{u_r} e^{-\varepsilon_m/kT}, \qquad (22)$$

 $\varepsilon_m, \varepsilon_l$ are excitation potentials for levels m, l and

$$u_r = g_1 + g_2 e^{-\epsilon_2/kT} + g_3 e^{-\epsilon_3/kT} + \dots$$
 (23)

is the partition function.

$$\frac{n_{r+1}}{n_r}n_e = \frac{2u_{r+1}}{u_r}2.46 \times 10^{15}T^{3/2}e^{-\chi_r/kT},\tag{24}$$

where n_r, n_{r+1} are the numbers of ions in the r, r+1 ionization states: χ_r is the ionization potential of the ion in state r.

3. Continuous absorption coefficient

The function $r(\tau)$ in (eq.1) is the ratio of continuous absorption K_{ν}^{c} to line absorption:

$$r(\tau) = K_{\nu}^{c}/K_{\nu_{\alpha}},\tag{25}$$

$$K_{\nu_o} = K^L \varphi_{\nu_o}. \tag{26}$$

The continuous absorption coefficient K_{ν}^{c} reflects the absorption of neutral hydrogen, of ions H^{-} , of atoms SiI, MgI, CI, AlI, FeI and a scattering of electrons and neutral hydrogen. The continuous absorption was calculated as described in Vernazza *et al.* (1976). Some of the equations are given below:

The absorption coefficients of neutral hydrogen (bound-free) and of other elements are as follows:

$$K(\lambda) = \sum_{l} n_{l} \left(1 - \frac{1}{b_{l}} e^{-h\nu/kT} \right) \sigma_{l}(\lambda) \times 10^{-18}, \tag{27}$$

 n_l is the number of atoms excited to level l; b_l are departure coefficients (equal to unity in the LTE approximation).

 $\sigma_l(\lambda)$ has the following forms (for $\lambda \leq \lambda_l$ where λ_l denotes the wavelength of the ionization treshold) for different elements:

$$\sigma_l(\lambda) = 7.93 \ l\left(\frac{\lambda}{\lambda_l}\right)^3 \ g_l(\lambda), \quad (for H)$$
 (28)

where $g_l(\lambda)$ - Gaunt factor; $\lambda_l = 0.091176 l^2$

$$\sigma_1(\lambda) = a_1; \quad (\lambda_1 \geq \lambda \geq 0.135 \,\mu)$$

$$= a_1 \left(\frac{\lambda}{0.135}\right)^5; \qquad (\lambda < 0.135 \,\mu) \qquad (for SiI) \qquad (29)$$

$$\sigma_3(\lambda) = 16 \left(\frac{\lambda}{\lambda_3}\right)^{2.1} - 7.8 \left(\frac{\lambda}{\lambda_3}\right)^{9.5} \qquad (for MgI)$$
 (30)

$$\sigma_1(\lambda) = 40.4 \left(\frac{\lambda}{\lambda_1}\right)^2 - 28.2 \left(\frac{\lambda}{\lambda_1}\right)^3$$

$$\sigma_2(\lambda) = 28.7 \left(\frac{\lambda}{\lambda_2}\right)^{1.5} - 18.4 \left(\frac{\lambda}{\lambda_2}\right)^{2.5}$$

$$\sigma_3(\lambda) = 33.6 \left(\frac{\lambda}{\lambda_3}\right)^{1.5} - 24.0 \left(\frac{\lambda}{\lambda_3}\right)^{2.5} \qquad (for CI)$$
 (31)

For other values of l we adopt the formula

$$\sigma_l(\lambda) = a_l(\lambda/\lambda_l)^{S_l}. \tag{32}$$

The a_l, λ_l, S_l values can be found in Vernaza et al. (1976).

The bound-free absorption coefficient for H^- is:

$$K(\lambda) = n_{H^{-}} \sigma(\lambda) \times 10^{-17} \left(1 - \frac{e^{-h\nu/kT}}{b_{H^{-}}} \right),$$
 (33)

$$n_{H^{-}} = 1.0354 \times 10^{-16} b_{H^{-}} n_{e} n_{HI} T^{-3/2} e^{8762/T}, \tag{34}$$

where $\sigma(\lambda)$ is tabulated in Doughty *et al.* (1966). The free-free absorption coefficient for H and H^- is as follows:

$$K(\lambda) = 1.3705 \times 10^{-35} n_e n_p T^{-1/2} \lambda^3 \left(1 - e^{-h\nu/kT} \right) g_{ff}(\lambda, T), \qquad (35)$$

 n_p stands for the proton number density; $g_{ff}(\lambda, T)$ is the Gaunt factor,

$$K(\lambda) = 4.5791 \times 10^{-40} n_e n_{HI} \lambda \left[1 + 10.631 \lambda \left(1 - 594.15/T \right) \right]. \tag{36}$$

Gaunt factors $g_l(\lambda)$ and $g_{ff}(\lambda, T)$ were published by Karsas and Latter (1962).

 $S(\tau)$ and $B(\tau)$ in (1) are the source functions for line and continuum. In our approximation we take the Planck function for $B(\tau)$, i.e.

$$B(\tau) = \frac{2h\nu^3}{c^2} e^{-h\nu/kT} / (1 - e^{-h\nu/kT}). \tag{37}$$

Source function $S(\tau)$ may also be taken to be equal to the Planck function, but $S(\tau)$ can be calculated more accurately using the method proposed by Ivanov and Serbin (1984).

4. Correction to the Saha equation

To derive the correction to the Saha equation the ionization equilibrium equation is used:

$$\sum_{l=1}^{N} n_l \left(R_{lk}^{\cdot} + C_{lk} \right) = n_k \sum_{l=1}^{N} \left(R_{kl} + C_{kl} \right)$$
 (38)

where n_l is the number of atoms excited to level l; n_k is the number of ions at the next ionization stage; R_{lk} , C_{lk} , R_{kl} , C_{kl} are coefficients that dependent on the ionization radiation field density and on electron density (see Avret and Loeser 1969, p 106). If we insret the obvious expressions of R and C into (38) and carry out the necessary transformations, we obtain the following equation:

$$rac{n_k n_e}{n_1} = rac{2u_k}{g_1} \left(rac{2\pi m_e kT}{h^2}
ight)^{3/2} e^{-rac{h
u_{k1}}{kT}} imes 0$$

$$\times \frac{\sum_{l=1}^{N} \left(w \frac{8\pi}{c^2} \int_{\nu_{kl}}^{\infty} \alpha_l(\nu) \nu^2 e^{-h\nu/kT_l} d\nu + C_{lk} \right) \frac{g_l}{g_1} e^{-h\nu_{1l}/kT}}{\sum_{l=1}^{N} \left(\frac{8\pi}{c^2} \int_{\nu_{kl}}^{\infty} \alpha_l(\nu) \nu^2 e^{-h\nu/kT} d\nu + C_{lk} \right) \frac{g_l}{g_1} e^{-h\nu_{1l}/kT}}, \tag{39}$$

where T_l is the effective temperature of the radiation field for ionization from the l-level; T is the local temperature; $\alpha_l(\nu)$ is the continuous absorption coefficient for l level; w is the dilution of radiation. The intensity of ionizing radiation for level l was taken as

$$J_{\nu} = w \frac{2h\nu^3}{c^2} e^{-h\nu/kT_l} \tag{40}$$

(This radiation comes from all photospheric layers.) Dilution w is a function of optical depth $\tau_{0.5}$: w = 1/2 for $(\tau_{0.5} = 0)$, and w = 1 for $(\tau_{0.5} \ge 1)$.

If the LTE condition is fulfilled, then $T_l = T$; w = 1 and (39) transforms to the Saha equation.

For continuous absorption coefficients expressed as

$$\alpha_l(\nu) = a_l \left(\frac{\nu_{kl}}{\nu}\right)^3,\tag{41}$$

equation (39) takes the form:

$$\frac{n_k n_e}{n_1} = \frac{2u_k}{g_1} \left(\frac{2\pi m_e kT}{h^2}\right)^{3/2} e^{-\frac{h\nu_{k1}}{kT}} \times
\times \frac{\sum_{l=1}^{N} \left(w \frac{8\pi}{c^2} a_l \nu_{kl}^3 E_1 \left(\frac{h\nu_{kl}}{kT_l}\right) + C_{lk}\right) \frac{g_l}{g_1} e^{-h\nu_{1l}/kT}}{\sum_{l=1}^{N} \left(\frac{8\pi}{c^2} a_l \nu_{kl}^3 E_1 \left(\frac{h\nu_{kl}}{kT}\right) + C_{lk}\right) \frac{g_l}{g_1} e^{-h\nu_{1l}/kT}}$$
(42)

(In (39) and (42) the condition $h\nu_{11} = 0$ has been applied. The quantities $a_l, \nu_{kl}, T_l, C_{lk}$ and others in (39) and (42) for different elements are inserted into the program and the user need not worry about them

5. Calculations with magnetic field

The program provides the possibility of calculating the profiles of magnetosensitive lines for longitudinal or for transverse magnetic fields. The magnetic field is assumed to be a function of depth in the photosphere. These calculations for a longitudinal field yield either the σ -components of left (or right) polarization, or all the σ components. The first alternative corresponds to observations with polarizing optics, which eliminate the σ -components of right (or left) polarization, the second alternative is to interprete observations without polarizing optics. For the transverse field three alternative calculated profiles are possible:

1) only σ -components; 2) only π -components; 3) all components. The third alternative corresponds to observations without polarizing optics.

The algorithm for calculating line profiles in a magnetic field have been derived from the Unno equations for Stokes parameters I, Q, V (see Stenflo 1985):

$$\cos \Theta \frac{dI}{d\tau} = (1 + \eta_I)I + \eta_Q Q + \eta_V V - (1 + \eta_I)B$$

$$\cos \Theta \frac{dQ}{d\tau} = \eta_Q I + (1 + \eta_I)Q - \eta_Q B$$

$$\cos \Theta \frac{dV}{d\tau} = \eta_V I + (1 + \eta_I)V - \eta_V B$$
(43)

where B, τ are the source function and the optical depth in continuum;

$$\eta_{I} = \frac{1}{2}\eta_{p}\sin^{2}\gamma + \frac{1}{4}(\eta_{l} + \eta_{r})(1 + \cos^{2}\gamma)$$

$$\eta_{Q} = \left[\frac{1}{2}\eta_{p} - \frac{1}{4}(\eta_{l} + \eta_{r})\right]\sin^{2}\gamma$$

$$\eta_{V} = \frac{1}{2}(-\eta_{l} + \eta_{r})\cos\gamma,$$
(44)

with $\eta_p = \kappa_p/\kappa, \eta_l = \kappa_l/\kappa$, $\eta_r = \kappa_r/\kappa$ where $\kappa_p, \kappa_l, \kappa_r$ are absorption coefficients for the π - and σ - components; κ is the absorption coefficient for continuum; Θ, γ are angles between the normal to the solar surface and the magnetic field vector, and the direction to the observer, respectively. The shape and magnitude of absorption coefficients $\kappa_p, \kappa_l, \kappa_r$ depend on the temperature, density, magnetic field and magnetic pattern of line splitting.

For $\gamma = 0$ (longitudinal field) $\eta_Q = 0$, and if we add the first and third equations in (43) we arrive at

$$\cos\Theta \frac{d(I+V)}{d\tau} = (1+\eta_I + \eta_V) I + (1+\eta_I + \eta_V) V - (1+\eta_I + \eta_V) B \quad (45)$$

For $\gamma = 0$

$$\eta_I + \eta_V = \frac{1}{2} (\eta_l + \eta_r) - \frac{1}{2} (\eta_l - \eta_r) = \eta_r$$
(46)

so that (20) becomes

$$\cos\Theta\frac{d(I+V)}{(1+\eta_r)d\tau} = I + V - B \tag{47}$$

But $(I+V)/2 = I_{\sigma_r}$ (intensity of the right σ -component, see Stenflo 1985) and (47) becomes

$$\cos\Theta \frac{dI_{\sigma_r}}{dt} = I_{\sigma_r} - \frac{1}{2}B,\tag{48}$$

 $dt = d\tau + \eta_r d\tau$. Equation (48) has the solution

$$I_{\sigma_r} = \frac{1}{2} \int_0^\infty B(t) e^{-t \sec \Theta} \sec \Theta dt. \tag{49}$$

The same equation is valid for the σ -component of left polarization, but in this case $dt = d\tau + \eta_l d\tau$. In a similar way the combination of the first and second equations in (43) for $\gamma = 90^{\circ}$ yields the expressions for I_{π} and I_{σ} for this case. To this end we must keep in mind that $I_{\pi,\sigma} = 1/2(I \pm Q)$. Thus equation (49) is valid for I_{π} and I_{σ} with $dt = d\tau + \eta_p d\tau$ or $dt = d\tau + 1/2(\eta_l + \eta_r) d\tau$.

6. Model parameters and properties of atom ions and lines

The model photosphere is defined by a series of temperatures T[K], number densities n_H , turbulent velocities V_t [km/s], radial velocities V_r [km/s] for a set of optical depths in continuum for $\lambda = 5000$ Å $(\tau_{0.5})$. The values $\tau_{0.5}$ are distributed uniformly from $\sim 10^{-5}$ to ~ 6 . If the magnetic field is present, the set of field values [Gauss] is also to be fixed for all points in the model atmosphere.

For calculating continuous absorption the number densities of Mg, Si, C, Al, Fe, (relative to hydrogen) have to be fixed; all other necessary quantities are inserted in the program block.

The following parameters have to be given for every spectral line:

- 1) The number density (relative to hydrogen) of element A, and atomic weight A_t ;
- 2) The ionization potential of the atom (or ion) and of the ion in the next ionization step;
- 3) Statistical weights g_i and excitation potentials ε_i of the ten lowest terms of the ion and of the ion in the next ionization step. If the terms are situated very close together, they should be combined into one term with an aggregate statistical weight and weighted average of the excitation potential. Thus, e.g., for VI (vanadium) we can take the terms a^4F , a^6D , a^4D , a^4P , a^2G as the first five terms and then we can combine all the terms a^2P , a^2D , a^4H , b^4P , a^2H , b^4F to one term, which will be the sixth term with $g_6 = 108$, and $\varepsilon_6 \simeq 1.90$.
- 4) The excitation potential and statistical weight for the lower level of the line transition.
 - 5) Oscilator strengths $g_l f_{lm}$.
- 6) The sum $\sum_{i=1}^{m-1} A_{mi}$ and constants C_{vw} and C_{st} in equation (10) for Γ . These parameters determine the broadening of the line. The Einstein coefficients are usually calculated through oscillator strengths after eq.(11). Equations for C_{vw} and C_{st} have alredy been described above.

Stark broadening should be calculated for all hydrogen and helium lines. For metal lines, Stark broadening in most cases is smaller than the Van-der-Waals broadening and can be ignored.

Now it is necessary to mention one very important circumstance. Calculations of the Van-der-Waals broadening by means of existing equations do not provide reliable results. Therefore, the first step in the profile calculations is to calculate the profiles for the standard, undisturbed model photosphere. The comparison of theoretical undisturbed with observed "undisturbed" profiles could be a check of the broadening constants. The same remark also applays to the values of oscillator strengths.

- 7) Wavelength of calculated spectral line [Å].
- 8) The values of effective temperature of ionizing radiation T_l for each level of the atom $(T_l$ enter equations (39),(42)). Values T_l depend on the ionization potentials from levels $h\nu_{kl}$ and on the wavelength distribution of ionizing radi-

ation. Thus, e.g., T_l for FeI and 15 levels can be found in the paper of Athay and Lites (1972).

If a magnetic field is present, the following parameters should be added:

- 1) Lande-factor g for simple triplets.
- 2) For lines with many σ and π components the following parameters are required: Quantum numbers S,L,J for both levels of the line transition. Values S,L,J can be found in the tables published by Moore (1945). For example, take the line of FeI $\lambda_{5198.7}$, multiplet N66. Transitions of these multiplets are denoted by symbols $a^5P y^5P^o$. The digit '5' stands for multiplicity and is connected with S by equation 5=2S+1, thus S=2. Digit L is connected with the letters of multiplet symbols as follows:

Letter:	S	P	D	F	G	H	Ī
<u>L</u> =	0	1	2	3	4	5	6

Thus in our case L=1 for both the lower and upper terms. J is given in (Moore 1945) tables in the 6th column. For line $\lambda_{5198.7}$ J=1 and 2 for the lower and upper levels. We thus have six values: \$1=2, \$2=2, L1=1, L2=1, J1=1, J2=2.

3) Angle γ between the line of sight and the magnetic field vector is equal to 0° or 90° for longitudinal or transverse fields, respectively.

The text of the program, the detailed code and a description of how to enter all the necessary parameters into the data files will be given in the second part of this paper.

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