

COMPUTATION AND OBSERVATION OF ZEEMAN MULTIPLY POLARIZATION IN FRAUNHOFER LINES

II: *Computation of Stokes Parameter Profiles*

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Abstract. A self-contained summary of the generalized Unno theory of LTE line formation in solar magnetic fields and its application to the numerical computation of Stokes parameter profiles is given. Within this context, computational details of general interest are described and numerical results for sunspot fields are given. Finally, a new method of computing the height of line formation is presented.

1. Introduction

The theoretical interpretation of polarization in magnetoactive Fraunhofer lines provides the necessary basis for the measurement of solar magnetic fields by means of magnetographs and other kinds of polarimeters. As was pointed out in an earlier paper of this series (Wittmann, 1973b; hereafter called Paper I), the polarization properties of Fraunhofer lines are conveniently treated in terms of Stokes parameters S . The theory of magnetoactive line formation in terms of Stokes parameters was initially developed by Unno (1956) for the simplified case of triplet formation in an homogeneous magnetic field embedded in a Milne-Eddington atmosphere with linear Planck source function and in the absence of scattering (true absorption). In his review, Stenflo (1970) has described the further development of the theory, credit for which is shared among several authors, which has led to a generalization to arbitrary atmospheres and the inclusion of inhomogeneous fields, arbitrary multiplet splitting, scattering and magneto-optical effects. More recently, a quantum-theoretical derivation has been given (Landi Degl'Innocenti and Landi Degl'Innocenti, 1972) and non-LTE effects have been treated as well (Domke and Staude, 1973a, b). The pertinent equations are quite involved and have to be solved by numerical integration (Beckers, 1969a). Because of the complexity of the equations, which in general leads to a prohibitive amount of computing time, some of the aforementioned simplifications are still retained with actual computations. Accordingly, most of the hitherto published numerical results have been obtained for arbitrary LTE atmospheres in the absence of scattering (e.g. Beckers, 1969a; Staude, 1970; Wittmann, 1971a, b).

As pointed out in Paper I, simultaneous profiles $S(\lambda)$ of the Stokes parameters in a sunspot have been obtained with a photographic polarimeter. For the interpretation of such profiles as well as for investigations concerned with the performance and calibration of magnetographs, a modular program named ZEEMANLINES has been developed which performs the numerical integration of the transfer equations. The program is self-contained to a large extent, in the sense that physical parameters

entering the differential equations (absorption coefficients, damping constants, Zeeman multiplet patterns, Voigt function etc.) are not solicited from input in the form of interpolation tables, but actually computed as needed. This provides the prerequisites for efficient updating techniques. It is the purpose of the present paper to give an account of the generalized Unno theory for LTE underlying the current version of ZEEMANLINES and to report on those computational details which are of general interest. Some applications of results are described, and a new method of computing the height of line formation is presented.

2. The Equations of Transfer

The definition of the Stokes parameters $S = (I, Q, U, V)$ which unequivocally determine a partially elliptically polarized beam of light was given in Paper I. In brief, I is the total intensity of the beam, Q and U are the intensities of linearly polarized components in two directions which differ by 45 deg, and V is the intensity of the circularly polarized component. Orthogonal polarizations are distinguished by the sign of the parameters Q , U and V . If, for instance, the magnetic field vector \mathbf{H} makes an angle $\gamma \leq 90^\circ$ with the line of sight, left-hand circular polarization results in the red wing of an absorption triplet, and hence $V \geq 0$ for $\Delta\lambda > 0$.

On the assumption of LTE, a single temperature can be introduced for which both Kirchhoff's law, Boltzmann's law, the Maxwellian velocity distribution, the Saha-Eggert equation and true absorption are locally valid. Let τ be the continuous optical depth along the outward normal z . In the absence of a magnetic field, $Q = U = V = 0$ and the formation of the line profile is governed by the equation of transfer

$$\cos \vartheta \frac{dI}{d\tau} = \eta \times (I - B), \quad (1)$$

where ϑ is the angle between the z -direction and the line of sight, $d\tau = -\kappa_c dz$ with the continuous absorption coefficient κ_c (per g), and B is the Planck function. The quantity η is the total absorption coefficient in units of κ_c , with the line absorption coefficient κ_L it may be expressed as

$$\eta = 1 + \frac{\kappa_L}{\kappa_c} = 1 + \eta_0 H(a, v). \quad (2)$$

The quantities η_0 , $H(a, v)$, a , v have their usual meaning, but as they are further needed below, their definitions are briefly recalled:

Voigt function:

$$H(a, v) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-(y+v)^2}}{a^2 + y^2} dy, \quad (3)$$

damping parameter:

$$a = \Gamma \lambda_0^2 / (4\pi c \Delta\lambda_D), \quad (4)$$

specific wavelength:

$$v = \Delta\lambda / \Delta\lambda_D, \quad (5)$$

line absorption parameter:

$$\eta_0 = \frac{\kappa_L(a=0, v=0)}{\kappa_c}, \quad (6)$$

and Doppler width:

$$\Delta\lambda_D = \frac{\lambda_0}{c} \sqrt{\frac{2RT}{M} + \xi_t^2}. \quad (7)$$

In case of a magnetoactive line and in the presence of a magnetic field an equation of transfer similar to Equation (1) holds for each Stokes parameter (Unno, 1956), and Equation (1) is replaced by a coupled system of ordinary differential equations which may be written in matrix notation:

$$\cos \vartheta \frac{d\mathbf{S}}{d\tau} = \boldsymbol{\eta} \times (\mathbf{S} - \mathbf{B}), \quad (8)$$

where

$$\mathbf{B} = \begin{pmatrix} B \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (9)$$

The components of matrix $\boldsymbol{\eta}$ will be explained in Sections 3 and 4, they represent the substantial part of the theory of magnetoactive line formation:

$$\boldsymbol{\eta} = \begin{pmatrix} \eta_U & \eta_Q & \eta_V & \eta_I \\ \eta_Q & \eta_I & \varrho_R & \varrho_W \sin 2\varphi \\ \eta_V & -\varrho_R & \eta_I & -\varrho_W \cos 2\varphi \\ \eta_I & \varrho_W \sin 2\varphi & -\varrho_W \cos 2\varphi & \eta_V \end{pmatrix}. \quad (10)$$

Expressions for the components of matrix (10), including magneto-optical effects, have been given by Beckers (1969a, b) following earlier treatments of these effects by Rachkovsky (1962) and Kai (1968). Beckers (1969b) also indicated, how to extend the theory to magnetic dipole and electric quadrupole (cf. Rubinowicz and Blaton, 1932) transitions. However, his results contained several mistakes, as was notified by Staude (1971). Subsequently the matter was discussed by Rachkovsky (1972) and Wittmann (1972) and the discrepancies were eliminated from his report by Stenflo (1971). The above-mentioned papers are concerned but with several aspects of the theory, whereas a self-contained summary of its context is still missing in the literature and may not be out of place at this point. Hence for the sake of completeness, in what follows a short account will be given providing the relevant formulas in a fashion suitable for practical applications.

3. Absorption Matrix Elements

For sufficiently weak fields and Russell-Saunders coupling, the absorption line arising from an electric dipole transition $1 \rightarrow 2$ between lower and upper atomic states characterized by quantum numbers J_k, L_k, S_k ($k=1, 2$) is split into components in accordance with the selection rule $\Delta M = M_2 - M_1 = 0, \pm 1$ for the magnetic quantum number $M_k = -J_k, \dots, J_k$. Let the line be split into N_p linearly polarized π -components ($\Delta M = 0$), N_r right-hand circularly polarized σ_r -components ($\Delta M = +1$) and N_l left-hand circularly polarized σ_l -components ($\Delta M = -1$). Further let the individual components be distinguished by subscripts

$$\begin{aligned} i_p &= 1, \dots, N_p \\ i_r &= 1, \dots, N_r \\ i_l &= 1, \dots, N_l \end{aligned} \quad (11)$$

The Zeeman wavelength shift (in cm) of each component is then determined by

$$\Delta\lambda_{ij} = 4.6685 \times 10^{-5} (M_1 g_1 - M_2 g_2)_{ij} \times H \times \lambda_0^2, \quad (j = p, r, l) \quad (12)$$

where the bracket is evaluated for transition i_j , λ_0 is the unshifted wavelength (in cm) and H the magnetic induction (in G). The g_k are the Landé factors of lower and upper level:

$$g_k = \frac{3}{2} + \frac{S_k(S_k + 1) - L_k(L_k + 1)}{2J_k(J_k + 1)} \quad (k = 1, 2). \quad (13)$$

The line absorption coefficients η_j ($j=p, r, l$) for the π - and σ -components are equal to the sum of the individual contributions:

$$\eta_j(v) = \eta_0 \sum_{i_j=1}^{N_j} S_{i_j} H(a, v - v_{i_j}) \quad (j = p, r, l), \quad (14)$$

where $v_{i_j} = \Delta\lambda_{i_j}/\Delta\lambda_D$. The S_{i_j} are the strengths of the components which must be normalized to unity:

$$\sum_{i_j=1}^{N_j} S_{i_j} = 1. \quad (15)$$

Unnormalized strengths are given in Table I, they depend on both ΔJ and ΔM .

TABLE I
Unnormalized strengths of Zeeman components

$\begin{array}{c} M_2 \\ \swarrow \\ J_2 \end{array}$	$M_1 + 1$	M_1	$M_1 - 1$
$J_1 + 1$	$(J_2 + M_2)(J_1 + M_2)$	$2(J_2^2 - M_2^2)$	$(J_2 - M_2)(J_1 - M_2)$
J_1	$(J_2 + M_2)(J_2 - M_2 + 1)$	$2M_2^2$	$(J_2 - M_2)(J_2 + M_2 + 1)$
$J_1 - 1$	$(J_1 - M_2)(J_2 - M_2 + 2)$	$2(J_1^2 - M_2^2)$	$(J_1 + M_2)(J_2 + M_2 + 2)$

Now, if φ denotes the apparent azimuth of the magnetic field vector \mathbf{H} at optical depth τ , reckoned counter-clockwise from the fixed direction defined by $U=0$, the symmetric elements of matrix (10) are determined by the relations

$$\eta_I = \frac{1}{2} \left(\eta_p - \frac{\eta_l + \eta_r}{2} \right) \sin^2 \gamma + \frac{1}{2} (\eta_l + \eta_r) + 1, \quad (16)$$

$$\eta_Q = \frac{1}{2} \left(\eta_p - \frac{\eta_l + \eta_r}{2} \right) \sin^2 \gamma \cos 2\varphi, \quad (17)$$

$$\eta_U = \frac{1}{2} \left(\eta_p - \frac{\eta_l + \eta_r}{2} \right) \sin^2 \gamma \sin 2\varphi, \quad (18)$$

$$\eta_V = \frac{1}{2} (\eta_r - \eta_l) \cos \gamma, \quad (19)$$

where γ is the angle between \mathbf{H} and the direction of propagation. If, for instance, φ is reckoned from the N-S direction and the position under consideration is at heliocentric angle ϑ on the N-S meridian in the northern hemisphere of the Sun, one has:

$$\cos \gamma = \cos \psi \cos \vartheta - \sin \psi \sin \vartheta \cos \varphi \quad (20)$$

and

$$\sin \varphi = \sin \psi \sin \varphi_0 / \sin \gamma, \quad (21)$$

where ψ is the magnetic field inclination with respect to the outward normal z , and φ_0 is the true field azimuth reckoned counter-clockwise in the x, y -plane at depth τ . For example at the northern limb, if $\psi = 90^\circ$, one has $\gamma = 180^\circ - \varphi_0$ and $\varphi = 90^\circ$ for $0 < \varphi_0 < 180^\circ$.

4. Magneto-Optical Effects

Magneto-optical effects are taken into account by the antisymmetric elements of matrix (10). The Faraday effect (induced circular birefringence) leads to a rotation of the electric vector of linearly polarized light through an angle which depends on the refractive index n of the medium for the two orthogonal modes of circularly polarized light. The differential rotation angle is given by

$$\cos \vartheta \frac{d\varphi}{dz} = \frac{\pi}{\lambda_0} (n_r - n_l) \cos \gamma. \quad (22)$$

Thus counter-clockwise rotation results if $\gamma < 90^\circ$ and $n_r > n_l$. The refractive index of a single unshifted component is given by (cf. Born, 1972):

$$n(v) = 1 + \frac{N f e^2 \lambda_0^3}{2 \sqrt{\pi} m c^2 \Delta \lambda_D} F(a, v). \quad (23)$$

As Beckers (1969a) has shown, a comparison with the line absorption coefficient per unit volume

$$\kappa_L(v) = \frac{\sqrt{\pi} e^2 N f \lambda_0^2}{m c^2 \Delta \lambda_D} H(a, v) \quad (24)$$

yields the expression

$$n(v) = 1 + \frac{\kappa_L(0) \lambda_0}{2\pi H(a, 0)} F(a, v). \quad (25)$$

With definition (6) one obtains

$$n(v) = 1 + \frac{\eta_0 \kappa_c \lambda_0}{2\pi} F(a, v). \quad (26)$$

In the above equations, the function

$$F(a, v) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{y e^{-(y-v)^2}}{a^2 + y^2} dy \quad (27)$$

is the plasma or line dispersion function which will be discussed together with the related Voigt function in Section 6. The contributions of the individual σ -components have to be added (cf. Corney *et al.*, 1966), and from Equation (22) one finally obtains

$$\cos \vartheta \frac{d(2\varphi)}{d\tau} = \varrho_R = -\eta_0 \cos \gamma \left[\sum_{i_r=1}^{N_r} S_{i_r} F(a, v - v_{i_r}) - \sum_{i_l=1}^{N_l} S_{i_l} F(a, v - v_{i_l}) \right]. \quad (28)$$

The Voigt effect (induced linear birefringence, also known as Cotton-Mouton effect) leads to a phase retardation between linear polarizations parallel and perpendicular to the magnetic field which depends on the corresponding refractive index difference. The differential retardation is given by

$$\cos \vartheta \frac{d\delta}{dz} = \frac{2\pi}{\lambda_0} (n_{\parallel} - n_{\perp}) \sin^2 \gamma. \quad (29)$$

For the corresponding matrix elements one gets

$$\begin{aligned} \cos \vartheta \frac{d\delta}{d\tau} = \varrho_W = -\eta_0 \sin^2 \gamma & \left[\frac{1}{2} \sum_{i_r=1}^{N_r} S_{i_r} F(a, v - v_{i_r}) + \right. \\ & \left. + \frac{1}{2} \sum_{i_l=1}^{N_l} S_{i_l} F(a, v - v_{i_l}) - \sum_{i_p=1}^{N_p} S_{i_p} F(a, v - v_{i_p}) \right]. \end{aligned} \quad (30)$$

5. The Continuous Absorption Coefficient

In the visible and near-infrared region of the solar spectrum the major contribution to the continuous opacity arises from the negative hydrogen ion, but many other sources contribute significantly to the continuous absorption coefficient κ_c (e.g.

molecules in the case of sunspots). For practical computations, the number of cross-sections being evaluated has to be kept within reasonable limits unless it is preferred to make use of extensive, precomputed interpolation tables (like Bode's tables, 1965). The latter evidently have the disadvantage that each implementation of updated atomic data makes a recomputation of the tables necessary (which for the user's part may even be impossible). For these reasons, an independent subroutine (program module) called KAPPAC has been developed for use within the ZEEMAN LINES or other programs, which computes κ_c as function of wavelength λ , temperature T , and electron pressure p_e . The partial pressures of some of the atmospheric constituents contributing to the opacity are evaluated in a separate subroutine called GAS, they are then made available to KAPPAC through a COMMON block.

Practical methods of computing continuous absorption coefficients are treated in many texts (e.g. Mihalas, 1967). I shall therefore restrict the discussion of this section to a few remarks of specific interest.

(a) The bound-free and free-free absorption of the negative hydrogen ion (H^-) is computed with the aid of polynomial approximations to Geltman's (1962) and John's (1964) data, the former have been derived by Gingerich (cf. Gingerich *et al.*, 1967). A comparison of the bound-free cross-sections with the tabulated more recent results of Doughty *et al.* (1966) and Krogdahl and Miller (1967) shows agreement within 10% or better. The question of whether LTE conditions dominate in maintaining the H^- equilibrium is of some importance in this connexion. As was pointed out by Praderie (1971), charge exchange as well as associative detachment reactions (Schmeltekopf *et al.*, 1967; Dalgarno and Browne, 1967) do not play a significant role in the photosphere and lower chromosphere. Ionization by electron impact is also of minor importance (Peart *et al.*, 1970; Walton *et al.*, 1971; John and Williams, 1973). Tarafdar and Vardya (1970) have considered the effect of interparticle interaction which for solar conditions is rather small as compared to the intrinsic accuracy of the H^- cross-sections. Recently, Adelman (1973) has determined the two-photon detachment cross-section of H^- which may be of some importance in the infrared.

(b) The absorption coefficient of neutral hydrogen (H) is evaluated according to Mihalas (1967). The first 12 levels (averaged over substates) are treated explicitly, the corresponding bound-free Gaunt factors are conveniently approximated by polynomials (Carbon and Gingerich, 1969 for $n \leq 6$; Chapman, 1970 for $n \geq 7$). Free-free Gaunt factors are obtained from Strom's fit (cf. Carbon and Gingerich, 1969).

(c) Absorption by neutral helium (He) is computed as indicated by Mihalas (1967). The first 12 bound-free transitions for $n=1, 2, 3$ are treated explicitly, for $n \geq 4$ the hydrogenic approximation (Vitense, 1951) is used. Cross-sections for the 12 transitions are taken from Hunger and van Blerkom (1967), it should be noted that similar approximations by Strom as reproduced by Mihalas (1967) for 7 transitions contain a few misprints.

(d) Absorption by the negative helium ion (He^-) is approximated by a polynomial fit (Carbon *et al.*, 1969) which represents the values given by John (1968).

(e) A convenient fit to the absorption coefficient of the negative hydrogen molecule (H_2^-) has been given by Somerville (1964). According to Carbon *et al.* (1969) his expression should be multiplied by a correction factor of about 2.

(f) The absorption coefficient of the ionized hydrogen molecule (H_2^+) is approximated by an expression due to Kurucz (1970). Because of the large magnitude of the polynomial coefficients it has to be evaluated in double precision.

(g) For wavelengths in the UV, absorption by metals, especially C, Na and Mg, gives non-negligible contributions. In this case, the absorption coefficients are determined from tabulated quantum defect results (Peach, 1970) by interpolation.

(h) Scattering coefficients are computed for Rayleigh scattering by neutral hydrogen (Dalgarno, 1962), molecular hydrogen (Dalgarno and Williams, 1962) and neutral helium (Dalgarno, 1962, quoted by Kurucz, 1970) as well as grey Thomson scattering by free electrons.

(i) Other negative ions (like C^- ; Ne^- ; Li^- , Na^- , K^- , Rb^- , Cs^- ; Cl^-) have large photoabsorption cross-sections (cf., respectively, Myerscough and McDowell, 1966; McDowell, 1971; John and Williams, 1972; Vardya, 1966a), but with the exception of Cl^- their electron affinities and solar abundances are too small to yield significant contributions.

6. Damping Parameter, Voigt- and Dispersion Function

A description of pressure broadening mechanisms has been given by Traving (1959). For the lines investigated within the current project, van der Waals damping Γ_6 is the predominant broadening mechanism (cf. Holweger, 1967) which is augmented by radiation damping Γ_{rad} , so that for the damping constant one has:

$$\Gamma = \Gamma_{\text{rad}} + \Gamma_6. \quad (31)$$

Deviations from predictions by Unsöld's theory (Unsöld, 1955) have often been detected (e.g. Kusch, 1958). Therefore a semi-empirical approach is being used for the computation of Γ , which consists of introducing some correction factor Z^* into the theoretical expression. This is tantamount to increasing the effective nuclear charge of the perturbed particle. Z^* is treated as a free parameter which is determined by fitting the computed photospheric line profile with observed profiles of high accuracy (e.g. Delbouille and Roland, 1971; Kochan and Pechinskaya, 1973). Neutral hydrogen, helium and hydrogen molecules are taken into account as perturbers, the collision parameter C of the latter two particles should be proportional to their polarizability α to a certain approximation (Table II).

TABLE II
Polarizability α for perturbers

particle	$\alpha(\text{cm}^3)$
H	6.6–25
H_2	8.0–25
He	2.1–25

One thus finally obtains:

$$\Gamma_6 = 17.0 \times C_H^{0.4} \times n_H \times \sum_{\text{H, He, H}_2} \left(\frac{\alpha_i}{\alpha_H} \right)^{0.4} \times \frac{n_i}{n_H} \times v_i^{0.6}, \quad (32)$$

$$v_i = \left[\frac{8RT}{\pi} (M^{-1} + M_i^{-1}) \right]^{1/2}, \quad (33)$$

$$C_H = 10^{-30.5325} \times Z^{*2} \times [\Delta E_2^{-2} - \Delta E_1^{-2}], \quad (34)$$

where n_i is the particle number density (cf. Section 7), v_i the collision velocity, M the molecular weight of the radiating atom, and ΔE_k ($k=1, 2$) the effective ionization energy of level k , which in case of neutral atoms with unperturbed ionization energy E_{ion} (eV) is approximately given by (Drawin and Felenbok, 1965)

$$\Delta E_k = E_{\text{ion}} - 9.96 \times 10^{-7} \times n_e^{1/3} - E_k \quad (k=1, 2). \quad (35)$$

After Γ has been computed, one immediately obtains the damping parameter a from Equations (4) and (7). By virtue of the empirical correction, a is typically augmented by a factor of 3 or 4.

The damping parameter a increases with increasing depth, and at those optical depths where the integration starts it may well be of the order of 2 or 3. For $a \gtrsim 1$ the computation of the Voigt function $H(a, v)$ and the dispersion function $F(a, v)$ is somewhat complicated, since the Taylor series expansions of both functions (Harris, 1948; Rachkovsky, 1962) converge but for $a \ll 1$. Since $a > 0$, the functions H and $2F$ are equal to the real and imaginary parts of the complex error function of argument $z = (v + ia)$, respectively:

$$w(z) = e^{-z^2} \left(1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{y^2} dy \right). \quad (36)$$

Many different algorithms have been proposed for evaluating H or F or both (e.g. Hummer, 1965; Chiarella and Reichel, 1966; Reichel, 1968; Harstad, 1972; Gerbilschij, 1972; Kielkopf, 1973). Numerical tables have also been calculated (e.g. Hjerting, 1938; Fried and Conte, 1961; Faddeyeva and Terent'ev, 1961; Davies and Vaughan, 1963; Hummer, 1965; Finn and Mugglestone, 1965) and reviews of existing methods have been given by e.g. Mitchell and Zeemansky (1961), Corney *et al.* (1966), Armstrong (1967) and Armstrong and Nicholls (1973). For a high accuracy evaluation of both H and F , a subroutine ERRFCT has been written which is based on the method proposed by Reichel (1968). This method is found very satisfactory, as it is reasonably fast and yields at least 10 significant digits. For the productive computation of solar line profiles, however, a few digits accuracy are completely sufficient, and very fast methods should be preferred at the expense of accuracy. For the Voigt function, a very convenient algorithm due to Rybicki (quoted by Armstrong and Nicholls, 1973) is used. It is based on a complex series expansion which converges after 31 terms. A function subprogram VOIGT for Rybicki's al-

gorithm has been published by Avrett and Loeser (1969), this is used with slight modifications.

For small a , the dispersion function $F(a, v)$ is computed by means of its Taylor series expansion (Rachkovsky, 1962):

$$F(a, v) = F_0 + a(F_1 + a(F_2 + aF_3)), \quad (37)$$

where

$$F_0(v) = \frac{1}{\sqrt{\pi}} D(v), \quad (38)$$

$$D(v) = e^{-v^2} \int_0^v e^{y^2} dy, \quad (39)$$

$$F_1(v) = -ve^{-v^2}, \quad (40)$$

$$F_2(v) = \frac{v}{\sqrt{\pi}} + (1 - 2v^2) F_0(v), \quad (41)$$

$$F_3(v) = \frac{1}{3}(3 - 2v^2) F_1(v). \quad (42)$$

Dawson's function $D(v)$ is found from precomputed values by interpolation. For $a \geq 0.4$ the polynomial approximation (Wittmann, 1973a)

$$\log F(a, v) = G_0 + a(G_1 + a(G_2 + aG_3)) \quad (43)$$

is used, where the coefficients $G_i(v)$ have been pretabulated.

7. Partial Pressures, Molecule Formation

The atmospheric models yield T and p_e as function of τ . On the assumption of LTE and chemical equilibrium, one may compute the various partial pressures including molecule formation. If only hydrogen molecule formation is taken into account (which is necessary since hydrogen is the dominant constituent), the computation can be done directly, and time-consuming iterations are avoided. Even in sunspots, other molecules are less important for the gas pressure balance, and the current version of GAS neglects molecules other than H_2 and H_2^+ . However, a subroutine MOLEC is presently used which computes the dissociation constants $K(\Theta)$ with $\Theta = 5040/T$ for up to 91 different molecules from data given by Tsuji (1965), Tatum (1966), Vardya (1966b) and Tarafdar and Vardya (1973). A third-degree polynomial fit in powers of Θ has been determined for those cases where a representation was not supplied by the above-cited authors. Since a collection of polynomial representations is of considerable interest for many kinds of applications, a listing of hitherto unpublished fitting coefficients A_i is reproduced in Table III. Let the chemical symbol of the molecule under consideration be $X_l Y_m Z_n$, then the expression for $K(\Theta)$ is

$$\log K(\theta) = \log \left(\frac{p_{x_l y_m z_n}}{p_x^l \cdot p_y^m \cdot p_z^n} \right) \approx A_0 + \theta(A_1 + \theta(A_2 + \theta A_3)) \quad (44)$$

TABLE III
Fitting coefficients for molecular dissociation constants

molecule	A_0	A_1	A_2	A_3
NaH	$-1.1457500 + 01$	$3.108092 + 00$	$-3.31598 - 01$	$4.3149 - 02$
KH	$-1.0964723 + 01$	$2.270225 + 00$	$-7.66888 - 02$	$6.5192 - 03$
BeH	$-1.0807839 + 01$	$2.744854 + 00$	$5.75802 - 02$	$3.3154 - 03$
ŠrH	$-1.0491008 + 01$	$2.051217 + 00$	$-7.64373 - 02$	$6.4254 - 03$
SrO	$-1.1019290 + 01$	$3.138290 + 00$	$1.21497 + 00$	$-1.7708 - 01$
BaH	$-1.0446909 + 01$	$2.024548 + 00$	$-7.68074 - 02$	$6.4714 - 03$
BaO	$-1.0921254 + 01$	$3.847116 + 00$	$1.18965 + 00$	$-1.6628 - 01$
ScO	$-1.3561415 + 01$	$7.528355 + 00$	$-5.03181 - 01$	$6.7874 - 02$
YO	$-1.4107593 + 01$	$1.222632 + 01$	$-1.01915 + 00$	$1.0205 - 01$
LaO	$-1.4231303 + 01$	$1.128907 + 01$	$-1.10855 + 00$	$1.2741 - 01$
Si ₂	$-1.2031930 + 01$	$3.012432 + 00$	$1.79889 - 01$	$-1.7924 - 02$
LiH	$-1.1344906 + 01$	$2.836732 + 00$	$-1.13412 - 01$	$1.9966 - 02$
VO ₂	$-2.5913244 + 01$	$1.185632 + 01$	$1.05407 + 00$	$-1.5411 - 01$
SiO ₂	$-2.6934577 + 01$	$1.342119 + 01$	$2.67133 - 01$	$-3.4752 - 02$
SiH ₂	$-2.3225499 + 01$	$4.820973 + 00$	$6.72212 - 01$	$-5.9034 - 02$
Si ₃	$-2.5079417 + 01$	$7.196588 + 00$	$1.19671 - 01$	$1.0484 - 02$
C ₂ H	$-2.6331315 + 01$	$1.250039 + 01$	$6.53101 - 01$	$-1.1626 - 01$
BH	$-1.1673776 + 01$	$3.245147 + 00$	$1.33429 - 01$	$-1.5241 - 03$
BO	$-1.2972588 + 01$	$7.809830 + 00$	$-6.26338 - 02$	$4.7633 - 03$

which equals the sum of the $\log K$'s (in dyne cm^{-2}) for those reactions which successively build up the molecule.

The computation of partial pressures $f=p/p_{H'}$, scaled to the fictitious hydrogen pressure

$$p_{H'} = p_H + p_{H^+} + p_{H^-} + 2p_{H_2} + 2p_{H_2^+} \quad (45)$$

is done in 3 steps as outlined by Mihalas (1967). For the sake of completeness, his method, with slight modifications, will be briefly recalled. Its first step is to compute quantities g_k defined by

$$\begin{aligned}
 g_1 &= \sum_{i=2}^{18} \left[\varepsilon_i \sum_{j=1}^2 j \left(\frac{n_j}{n} \right)_i \right] \\
 g_2 &= n_{H^+}/n_H \\
 g_3 &= n_{H^-}/n_H \\
 g_4 &= p_e \times \left(\frac{p_{H_2^+}}{p_H \cdot p_{H^+}} \right) \\
 g_5 &= p_e \times \left(\frac{p_{H_2}}{p_H^2} \right).
 \end{aligned} \quad (46)$$

Here g_1 is the contribution to the electron pressure by singly and doubly ionizing the 18 most abundant elements i (except hydrogen, $i=1$), and $\varepsilon_i = n_i/n_{H'}$ is the abundance

by number. The number densities n and n_j are those of the total number of atoms (regardless of ionization) and the number of j -fold ionized atoms of element i , respectively. The degree of ionization n_j/n is determined by Saha-Eggert's equation, e.g. $n_2/n = (n_2/n_1)(n_1/n)$ and

$$\frac{n_{r+1}}{n_r} = 0.66749 \frac{U_{r+1}}{U_r} T^{2.5} 10^{-\theta E_r} p_e^{-1}. \quad (47)$$

In Equation (47), E_r is the (effective) ionization energy (in eV) for $r \rightarrow r+1$, and U_r , U_{r+1} are the partition functions of the corresponding ions. The temperature dependence of the latter is approximated by polynomials (Bolton, 1970; Aller and Everett, 1972). Abundances, ionization energies and partition functions are supplied for 83 elements by subroutine ATMDAT.

The second step is simply to define:

$$\begin{aligned} a &= 1 + g_2 + g_3 \\ b &= 2(1 + g_2 g_4 / g_5) \\ c &= g_5 \\ d &= g_2 - g_3 \\ e &= g_2 g_4 / g_5 \end{aligned} \quad (48)$$

and

$$\begin{aligned} c_1 &= cb^2 + adb - ea^2 \\ c_2 &= 2ae - db + abg_1 \\ c_3 &= -(e + bg_1) \end{aligned} \quad (49)$$

and

$$\begin{aligned} f_1 &= p_H / p_{H'} \\ f_2 &= p_{H^+} / p_{H'} \\ f_3 &= p_{H^-} / p_{H'} \\ f_4 &= p_{H_2^+} / p_{H'} \\ f_5 &= p_{H_2} / p_{H'} \\ f_6 &= p_e / p_{H'}. \end{aligned} \quad (50)$$

Then the final step directly yields the desired quantities:

$$\begin{aligned} f_1 &= -\frac{c_2}{2c_1} \pm \sqrt{\left(\frac{c_2}{2c_1}\right)^2 - c_3/c_1} \\ f_5 &= (1 - af_1)/b \\ f_2 &= g_2 f_1 \\ f_3 &= g_3 f_1 \\ f_4 &= ef_5 \\ f_6 &= f_2 - f_3 + g_1 + f_4 \\ p_{H'} &= p_e / f_6. \end{aligned} \quad (51)$$

In the first equation, the minus sign applies if $c_1 < 0$. In the extreme outer layers, a numerical instability not mentioned by Mihalas may occur if f_5 is small (say, $f_5 < 10^{-4}$). In this case a solution can be obtained from a few subsequent iterations:

$$\begin{aligned} f_5 &= p_{H'} \times (g_5 f_1^2 / p_e) \\ f_4 &= e f_5 \\ f_6 &= (f_2 - f_3 + g_1) + f_4 \\ p_{H'} &= p_e / f_6 \\ f_5 &= \dots \text{etc.}, \end{aligned} \quad (52)$$

where the quantities in brackets remain unchanged. Finally, the gas pressure is found from

$$p_g = p_e \left[1 + \frac{\sum_{i=2}^{83} \varepsilon_i + \sum_{i=1}^5 f_i}{f_6} \right]. \quad (53)$$

8. Numerical Integration and Tests

On the basis of a model solar atmosphere the numerical integration can be carried out by e.g. the Runge-Kutta-Merson technique (cf. Göttsche, 1965), starting with appropriate boundary conditions at some large optical depth τ_0 . A discussion of possible boundary conditions has been given by Katz (1972). Tests have shown that the most simple set of boundary conditions

$$S_0 = B(\tau_0) \quad (54)$$

can be used for $\tau_0 > 10$. Since the computing time increases strongly with increasing τ_0 , it is desirable to start the integration at some compromise depth, say, $\tau_0 = 5$. In this case slightly more elaborate boundary conditions should be used, as was pointed out by Beckers (1969a):

$$\begin{aligned} I_0 &= B' \eta_I / \eta^2 + B \\ Q_0 &= -B' \eta_Q / \eta^2 \\ U_0 &= -B' \eta_U / \eta^2 \\ V_0 &= -B' \eta_V / \eta^2, \end{aligned} \quad (55)$$

where $B' = dB/d\tau$ and $1/\eta^2 = \cos \vartheta / (\eta_I^2 - \eta_Q^2 - \eta_U^2 - \eta_V^2)$. The integration is most conveniently carried out with respect to the variable $x = \log \tau (5000 \text{ \AA})$ instead of $\tau(\lambda)$ itself, since the atmospheric models usually give T , p_e , etc. versus x . The models used at present are the Holweger photosphere (Holweger, 1967), the HSRA model (Gingerich *et al.*, 1971), the Hénoux umbra model (Hénoux, 1969) and the penumbra model by Kjeldseth Moe and Maltby (1969).

A number of test calculations have been made in an early stage of this investigation in order to ensure the correct performance of the entire program. In brief, the Runge-Kutta integration by means of the RKMN subroutine (Göttsche, 1965), which was slightly modified and renamed RUNGE, was tested with systems of differential equations

with known solutions, and comparisons of numerical results for restricted Unno models with the corresponding analytical solutions were made.

An example of Stokes parameter profiles computed with the ZEEMANLINES program has been given earlier (Wittmann, 1971b). In what follows another application will be described, showing that measurements of sunspot fields have to be interpreted very carefully.

9. Application to Sunspots

A very complex problem is the determination of magnetic field configurations in sunspots which will be treated in more detail elsewhere. A variety of relations exist

TABLE IV
Parameters for Zeeman triplets

Line	E_1 (eV)	transition	$gf\ \varepsilon$	$\Delta\lambda_H$ (mÅ kG ⁻¹)
FeI 5250.216	0.122	$a^5D_0 - z^7D_1$	3.0056-10	38.606
FeI 6173.341	2.220	$a^5P_1 - y^5D_0$	3.4609-08	44.479
VI 6256.887	0.280	$a^6D_{2.5} - z^6D_{2.5}$	7.9455-11	30.284
FeI 6302.499	3.690	$z^5P_1 - e^5D_0$	1.2306-06	46.360

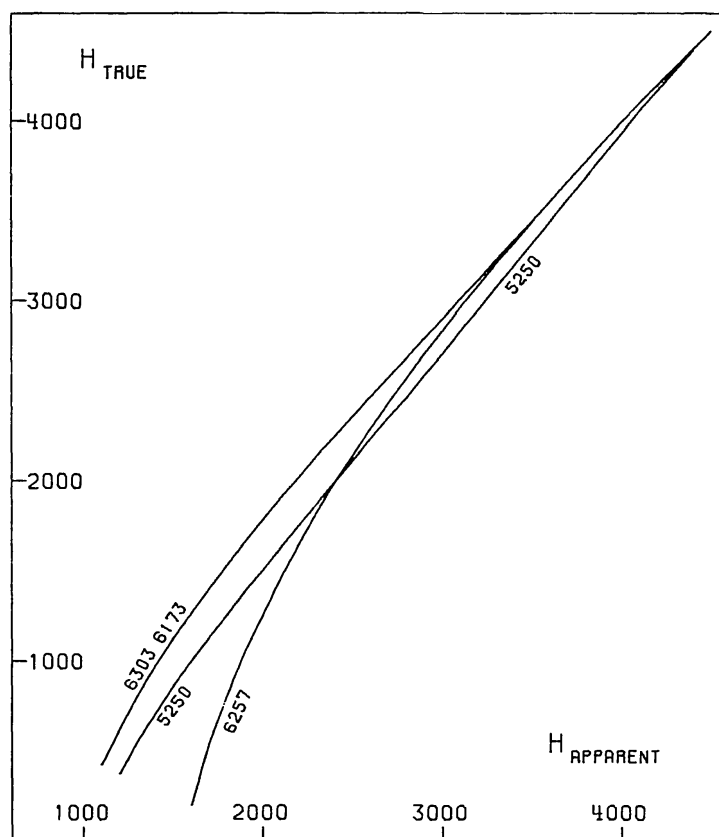


Fig. 1. Computed relation between apparent and true magnetic field strength for the umbra model

which in principle reflect the physical conditions in a sunspot umbra and, if properly interpreted, may serve as a means of determining the magnetic field properties. For instance, in case of a triplet and a quasi-homogeneous field, the observed wavelength shift of the sigma components (usually designated $\Delta\lambda_H$) is related to the magnetic field strength H , and the maximum amplitude of the V parameter V_{\max} is related to both field strength H and inclination γ . Computations show that due to the overlap-

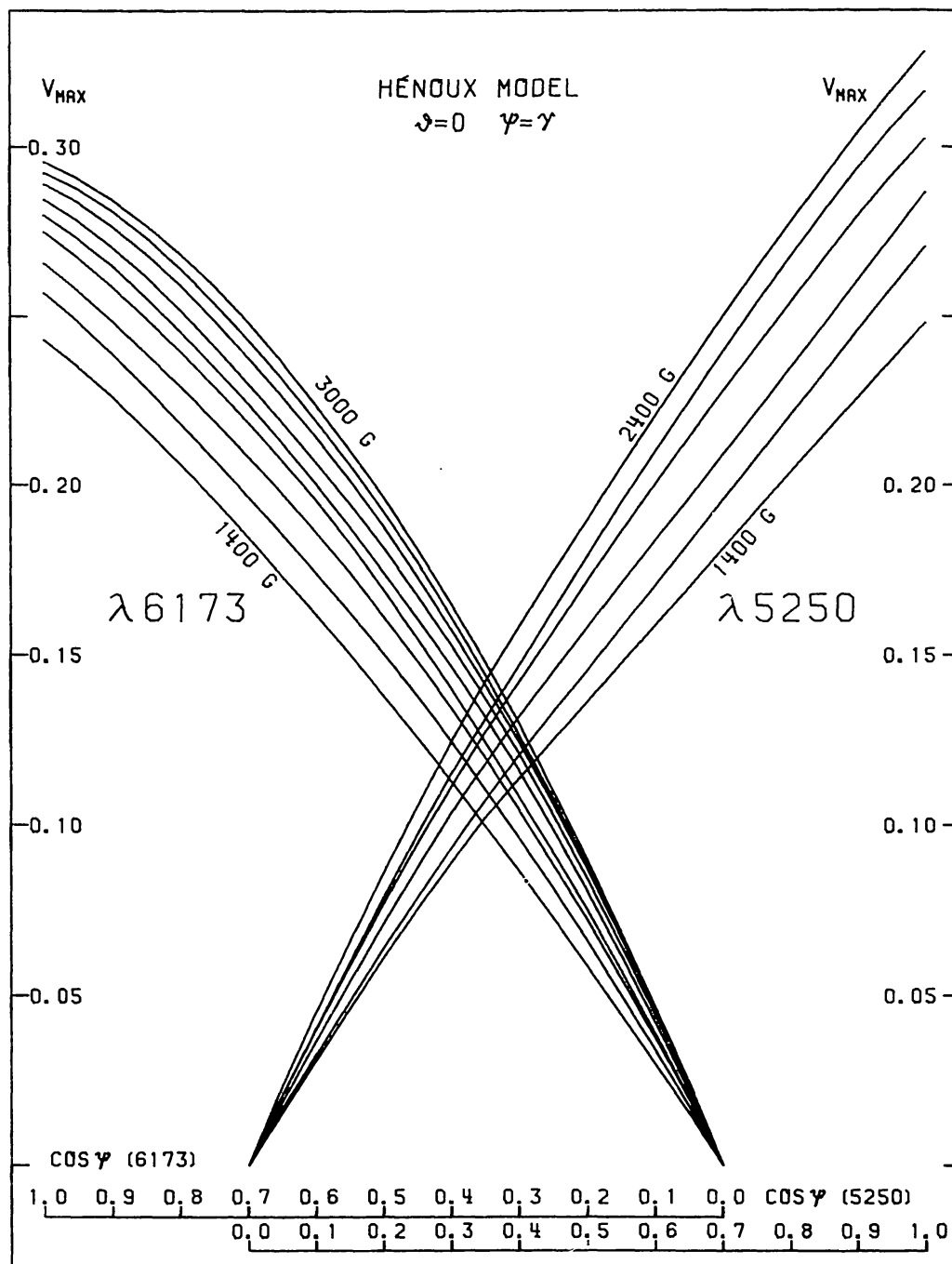


Fig. 2. Computed relation between magnetic field inclination and maximum amplitude of the V parameter.

ping of broadened components and, less important, due to magneto-optical effects these relations are not linear (i.e. $\Delta\lambda_H \sim H$, and $V_{\max} \sim \cos \gamma$ for constant H , do not hold), and hence corrections must be applied. For the strong triplets listed in Table IV I have computed the relation between the apparent field strength (as found from Equation (12) and Table IV) and the true field strength in case of Hénoux's umbra model. The result is shown in Figure 1. It can be seen that substantial errors arise if this correction is neglected for field strengths less than 3 kG. For two of the lines the computed relation between V_{\max} and $\cos \gamma$ is shown in Figure 2 which refers to a spot umbra at the centre of the disc (where $\gamma = \psi$).

10. The Height of Line Formation

Though Fraunhofer line formation actually occurs throughout an extended layer of the solar atmosphere, it is often desirable to associate a certain height of formation with a specific line. The usual procedure then is to calculate the run of analytical contribution functions versus optical or geometrical depth. However, the somewhat artificial concept of analytical contribution functions and the question of their appropriate definition has led to quite different approaches and to controversial results as well (cf. Gussmann, 1967; Staude, 1972). A more rigorous probabilistic approach has been proposed by Staude (1972), a specific advantage of which is its ability to include magnetoactive line formation. In particular, Staude has shown that generally each of the Stokes parameters originates at a different height in the atmosphere. If, for instance, profiles of the Stokes parameters of diverse lines are investigated, one might gain some insight into the height-dependence of the magnetic field vector, provided that realistic heights of origin can be determined for those lines.

Now, in close connexion with the numerical integration described above, a very straightforward method of computing the height of line formation suggests itself:

Imagine a model atmosphere with vanishing magnetic field $H(z)=0$ everywhere except for a very thin layer of thickness Δx at height z_H . Then, from a set of Stokes parameter profiles computed for various heights z_H , the relative contribution to these profiles by the magnetic layer at height z_H can be obtained if a suitable measure for that contribution is introduced. For instance, if the magnetic field strength H is to be measured from the splitting $\Delta\lambda_H$ of the sigma components, the maximum amplitude V_{\max} apparently would be an appropriate measure.

This method has been applied to the V parameter for the triplets of Table IV with the results for the umbra model shown in Figure 3.

The full-drawn curves are for $\cos \vartheta = 1$, whereas the broken curves are for $\cos \vartheta = 0.438$ in order to show the centre-to-limb effect. Of course Figure 3 once again demonstrates the fact that in principle it is impossible to define a single height of formation, but the height where V_{\max} attains its maximum may be said to represent the height of formation of the V parameter z_V . In this way the quantity z_V is unequivocally defined for each line. The computed results for photosphere, penumbra and umbra are given in Table V for each line.

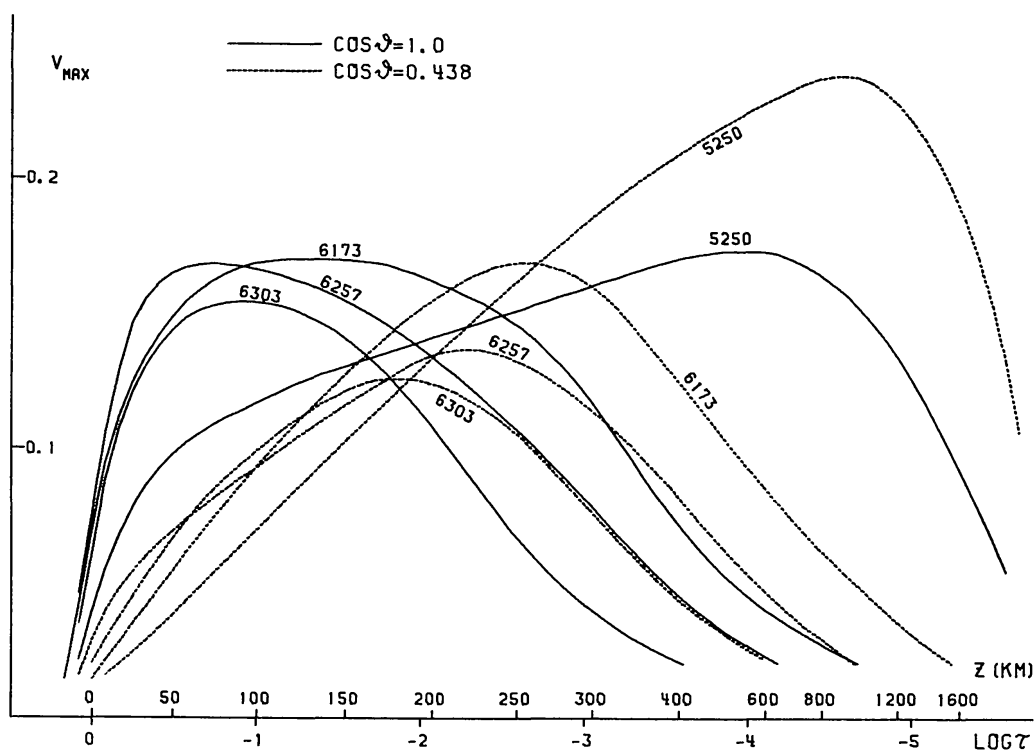


Fig. 3. Maximum amplitude of the V parameter versus geometrical height z_H (labeled Z) and optical depth τ for the Hénoux umbra model, computed with $H=2$ kG in the magnetic layer at z_H .

TABLE V
Heights of origin z_V (km) of the V Stokes parameter

λ_0 (Å)	Umbra	Penumbra	Photosphere
5250.216	540	230	240
6173.341	135	220	230
6256.887	65	200	175
6302.499	90	190	230

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