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ASTRONOMY AND ASTROPHYSICS

Polarized line formation by resonance scattering

I. Basic formalism

V.V. Ivanov, S.I. Grachev, and V.M. Loskutov

Astronomy Department, St.Petersburg University, St.Petersburg 198904, Russia

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Abstract. The model two-level problem of non-LTE line formation in homogeneous plane atmospheres is reconsidered with the complete account of polarization arising in resonance scattering. We use the approximation of complete frequency redistribution (CFR) and restrict our discussion to the most important case of axially symmetric radiation fields in semi-infinite atmospheres. The primary sources are assumed to be partially polarized. The problem is reduced to the 2×2 matrix Wiener-Hopf integral equation for the matrix source function $\mathbf{S}(\tau)$. The matrix kernel $\mathbf{K}_1(\tau)$ of the $\mathbf{\Lambda}$-operator appearing in this equation is represented as a continuous superposition of exponentials. As we show in Paper II of the series, this enables one to develop a matrix version of the analytical theory which, on the one hand, is a generalization of the scalar CFR theory and, on the other, is the CFR version of the theory of multiple monochromatic Rayleigh scattering. As a preparatory step for this, we discuss in detail the properties of the kernel matrix $\mathbf{K}_1(\tau)$ and the dispersion matrix $\mathbf{T}(z)$. The latter is essentially the two-sided Laplace transform of $\mathbf{K}_1(\tau)$. We consider the asymptotic behavior of $\mathbf{K}_1(\tau)$ and $\mathbf{T}(z)$ for large τ and z, respectively. For the particular case of the Doppler profile the complete asymptotic expansions of these matrices are presented. These results are at the base of the theory presented in Paper II of the series.

Key words: radiative transfer – line: formation – polarization – scattering – Sun: atmosphere – stars: atmosphere

1. Introduction

In the standard theory of non-LTE line formation in the solar and stellar spectra (see, e.g., Mihalas 1978) polarization effects are completely ignored. One may expect that this has negligible effect on the *intensity profiles* of spectral lines. However, in the last two decades it was found that near the solar limb many Fraunhofer lines show measurable polarization (Stenflo et al. 1980; Auer et al. 1980; Stenflo et al. 1983a, 1983b; Henze & Stenflo 1987; Stenflo 1996; for a review, see Stenflo 1994). Essentially, this was the discovery of the *second solar spectrum*. Evidently the interpretation of the *polarization profiles* of spectral lines needs more refined theory of line formation which incorporates polarization effects.

The problem of polarized line formation by resonance scattering has been considered in many publications. In all of them except one (Faurobert-Scholl & Frisch 1989) the approach is purely numerical (Stenflo & Stenholm 1976; Dumont et al. 1977; Rees 1978; Rees & Saliba 1982; Gopasiuk & Rachkovsky 1983; MacKenna 1985; Faurobert 1987, 1988; Nagendra 1988, 1989). One of rather unexpected results found in these publications is that, within the Doppler core of the line, the approximation of complete frequency redistribution (CFR) provides reasonable accuracy in treating both the intensity and polarization.

Is there a possibility to incorporate polarization into the well-known analytical theory of CFR radiative transfer? The positive answer to this question was given in the pioneering paper of Faurobert-Scholl & Frisch (1989), who, in particular, first formulated the Milne problem for CFR resonance scattering, i.e., the problem of finding the field of polarized line radiation in a purely scattering atmosphere with sources at infinity. They also attempted to find the asymptotic solutions of this problem, to develop the vector version of the first-order escape probability approximation etc. The paper by Faurobert-Scholl & Frisch triggered our research in this field.

The aim of the present series of papers is to develop, within the framework of the assumption of CFR, a detailed theory of multiple resonance scattering similar to the scalar CFR theory of line formation (cf. Ivanov 1973, 1991; Nagirner 1984; Frisch 1988). Recently we have published a series of papers on monochromatic Rayleigh and molecular scattering (Ivanov 1995, 1996; Ivanov et al. 1995, 1996; these papers will be referred to as GRaS.I, GRaS.III, GRaS.II and GRaS.IV, respectively; the abbreviation GRaS stands for Generalized Rayleigh Scattering). In the GRaS series it was shown that by using the appropriate matrix notation, the transfer problems with polarization may be cast in the form similar to the scalar ones, with scalars replaced by matrices. In the present series of papers we

Send offprint requests to: V.V. Ivanov

combine the methods of the scalar CFR line formation theory with the formalism developed in GRaS series. This enables us to incorporate polarization in line formation theory in quite a natural manner, so that the form of the theory remains essentially unchanged except, of course, for the fact that scalars are replaced by matrices. Along with analytical results, we shall present extensive numerical data on model problems of polarized line formation.

In the present paper we formulate the problem and develop the basic formalism which will be used in subsequent papers of the series. The paper is aimed primarily at preparation of tools rather than presentation of the results.

In Sect. 2 we present the differential and integral *vector* transfer equations for the zeroth azimuth Fourier component of the radiation field for the case of CFR resonance scattering. We assume that in the atmosphere there are embedded sources of partially polarized radiation. In Sect. 3 we show that it is possible to reformulate the problem in terms of the *matrix* transfer equation. In case of a semi-infinite atmosphere, the problem is reduced to the Wiener-Hopf integral equation for the matrix source function $\mathbf{S}(\tau)$. In Sect. 4 we discuss the properties of the kernel matrix $\mathbf{K}_1(\tau)$ of this equation closely following the approach used in GRaS.I. The crucial point here is the concept of the matrix photon destruction probability $\boldsymbol{\epsilon}$. The other important concept borrowed from GRaS series and introduced in this section is the λ-plane. This concept will be our main instrument in discussing the dependence of solutions of the radiative transfer equation, both numerical and analytical, on the parameters of single scattering — photon destruction probability $\varepsilon_{\rm I}$ and depolarization factor W. In Sect. 5 we introduce the dispersion matrix $\mathbf{T}(z)$ which will play a very important role in the analytical theory of the matrix transfer problems to be developed in subsequent papers of the series. Some simplest properties of $\mathbf{T}(z)$ are presented. After this, in Sect. 6, we formulate and briefly discuss the *standard problem* modeled after the standard scalar problem (isothermal atmosphere). The specific feature of the matrix standard problem as formulated in Sect. 6 is that depth-independent embedded primary sources are assumed to be partially polarized. Using the notion of the λ-plane, we briefly discuss some simplest properties of solutions of the standard problem. The emergent radiation is discussed in Sect. 7. It is expressed in terms of the matrix $\mathbf{I}(z)$ related to the source martix $\mathbf{S}(\tau)$ by exactly the same relation which transforms $S(\tau)$ to $I(0,\mu)$ in monochromatic scalar case. In case of the standard problem the matrix $\mathbf{I}(z)$ satisfies two integral equations, one linear, and the other non-linear. They may be used to find $\mathbf{I}(z)$ independently of $\mathbf{S}(\tau)$. The non-linear equation is the matrix generalization of the usual Chandrasekhar H-equation. In Paper II, it is solved numerically, while the linear equation for $\mathbf{I}(z)$ is used as our main instrument in obtaining the asymptotic solutions of the matrix transfer equation. These asymptotic solutions are, of course, governed by the asymptotic properties of the kernel and dispersion matrices. They are discussed in Sects. 8 and 9. Finally, in Sect. 10 a brief critical discussion of the results is given.

In Paper II we shall consider the conservative vector Milne problem, i.e., the radiation field in a purely scattering atmosphere with the source at infinite depth and report the asymptotic solutions of the matrix transfer equation for conservative scattering with the Doppler profile. In Paper III we plan to present analytical and numerical results for non-conservative scattering.

The notation is identical to that used in GRaS series. Namely, boldface type is used to denote two-component vectors (lowercase Roman characters, e.g., $\mathbf{e}$, $\mathbf{i}$, $\mathbf{s}$ etc.) and 2×2 matrices (uppercase Roman and lowercase and uppercase Greek characters, e.g., $\mathbf{I}$, $\mathbf{S}$, $\boldsymbol{\epsilon}$, $\boldsymbol{\lambda}$, $\boldsymbol{\Psi}$ etc.).

2. Vector transfer equation

Let $\mathbf{i} = (I, Q)^{\rm T}$ be the zeroth azimuth Fourier component of the Stokes vector of the diffuse radiation field in a plane-parallel atmosphere with embedded sources of partially polarized line radiation; here $^{\rm T}$ means transpose. It is assumed that the atmosphere is composed of two-level atoms, and we consider the line radiation arising in transitions between the two levels. Then the Stokes vector $\mathbf{i} = \mathbf{i}(\tau, \mu, x)$, where τ is the usual optical depth averaged over line, μ is the cosine of the zenith angle of the direction of propagation of radiation (the top of the atmosphere is at $\tau = 0$), and x is the usual dimensionless frequency measured from the center of the line. In the absence of continuum absorption, the Stokes vector $\mathbf{i}(\tau, \mu, x)$ of the diffuse, i.e., scattered, radiation obeys the transfer equation (see, e.g., Faurobert 1987; Stenflo 1994)

$$\mu \, \frac{\partial \mathbf{i}(\tau, \mu, x)}{\partial \tau} = \phi(x) \, \mathbf{i}(\tau, \mu, x) - \mathbf{s}(\tau, \mu, x) \,, \tag{1}$$

where $\mathbf{s}(\tau, \mu, x)$ is the vector source function:

$$\mathbf{s}(\tau, \mu, x) = \frac{\lambda_{\rm I}}{2} \int_{-\infty}^{\infty} dx' \int_{-1}^{1} \mathbf{R}(\mu, x; \mu', x') \, \mathbf{i}(\tau, \mu', x') \, d\mu' + \mathbf{s}^*(\tau, \mu, x) \tag{2}$$

and $\mathbf{s}^*(\tau, \mu, x)$ is the primary source function; it is assumed known. Evidently $\mathbf{s}^*(\tau, \mu, x)$ is representable as

$$\mathbf{s}^*(\tau, \mu, x) = \frac{\lambda_{\rm I}}{2} \int_{-\infty}^{\infty} dx' \int_{-1}^{1} \mathbf{R}(\mu, x; \mu', x') \, \mathbf{i}^*(\tau, \mu', x') \, d\mu' \,, \tag{3}$$

where $\mathbf{i}^*(\tau, \mu', x')$ is the Stokes vector of the direct radiation of primary sources (a given function). In Eqs. (1) – (3), $\phi(x)$ is the line absorption profile normalized to unity:

$$\int_{-\infty}^{\infty} \phi(x) \, dx = 1, \tag{4}$$

$\lambda_{\rm I}$ is the albedo of single scattering, so that photon destruction probability per scattering is $\varepsilon_{\rm I} = 1 - \lambda_{\rm I}$ (the reason why we use this rather strange notation, and not just λ and ε, will become clear later); finally, the 2×2 redistribution matrix $\mathbf{R}(\mu, x; \mu', x')$ describes the details of the angular, frequency and polarization changes in single scattering.

Since there is no diffuse radiation illuminating the atmosphere from outside, we have

$$\mathbf{i}(0,\mu,x) = \mathbf{0}, \quad \mu < 0; \qquad \mathbf{i}(\tau_0,\mu,x) = \mathbf{0}, \quad \mu > 0\,. \tag{5}$$

Here, τ_0 is the optical thickness of the atmosphere.

In the Doppler core of the line one can assume complete frequency redistribution (CFR). According to this approximation (see, e.g., Dumont et al. 1977; Faurobert 1987),

$$\mathbf{R}(\mu,x;\mu',x') = \phi(x)\,\phi(x')\,\mathbf{P}(\mu,\mu')\,, \tag{6}$$

where $\mathbf{P}(\mu,\mu')$ is the *phase matrix* of resonance scattering.

The matrix $\mathbf{P}(\mu,\mu')$ is a linear combination of the Rayleigh phase matrix $\mathbf{P}_{\mathrm{R}}$ and the phase matrix of scalar isotropic scattering $\mathbf{P}_{\mathrm{I}}$:

$$\mathbf{P} = (1-W)\,\mathbf{P}_{\mathrm{I}} + W\,\mathbf{P}_{\mathrm{R}}\,, \tag{7}$$

where

$$\mathbf{P}_{\mathrm{I}} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{8}$$

and

$$\mathbf{P}_{\mathrm{R}} = \mathbf{P}_{\mathrm{R}}(\mu,\mu') =$$
$$\mathbf{P}_{\mathrm{I}} + \frac{3}{8}\begin{pmatrix} \frac{1}{3}(1-3\mu^2)(1-3\mu'^2) & (1-3\mu^2)(1-\mu'^2) \\ (1-\mu^2)(1-3\mu'^2) & 3(1-\mu^2)(1-\mu'^2) \end{pmatrix}. \tag{9}$$

The depolarization parameter W appearing here, $W \in [0,1]$, is often denoted also as W_2 (this is the notation used, e.g., by Stenflo 1994). The value of W is determined by the quantum numbers of the total angular momentum of the upper j_u and the lower j_l states of the transition. The explicit expressions for W (denoted by E_1) in terms of j_u (denoted as j) and $\Delta j = j_u - j_l$ are given in Chandrasekhar 1950, Sect. 19. As W decreases, the polarization effects become smaller. The value $W = 1$ corresponds to dipole scattering ($j_l = 0,\ j_u = 1$); in this case the phase matrix is the same as for the usual Rayleigh scattering. In Sect. 4 we shall see that, for purely mathematical reasons, it is useful to consider not only $W \in [0,1]$, but also $W > 1$. This enables one to get deeper insight into the inner structure of solutions to vector transfer problems.

It is well known that the matrix $\mathbf{P}(\mu,\mu')$ can be factorized, i.e., the variables μ and μ' can be separated (see, e.g., van de Hulst 1980, Chap. 16). We shall use the 'natural factorization' (Rachkovsky 1983; see also GRaS.I)

$$\mathbf{P}(\mu,\mu') = \mathbf{A}(\mu)\,\mathbf{A}^{\mathrm{T}}(\mu')\,, \tag{10}$$

in which

$$\mathbf{A}(\mu) = \begin{pmatrix} 1 & \sqrt{\frac{W}{8}}\,(1-3\mu^2) \\ 0 & \sqrt{\frac{W}{8}}\,3\,(1-\mu^2) \end{pmatrix}. \tag{11}$$

Eqs. (6) and (10) imply drastic simplification: in the approximation of CFR the redistribution matrix $\mathbf{R}$, which depends on *four* variables, is representable as a product of four functions of *one* variable. This variable separation is one of the cornerstones of the analytical theory developed in the present series of papers.

Substituting Eqs. (6) and (10) into the transfer equation, Eqs. (1) – (3), we can rewrite it as

$$\mu\,\frac{\partial\,\mathbf{i}(\tau,\mu,x)}{\partial\,\tau} = \phi(x)\,\mathbf{i}(\tau,\mu,x) - \phi(x)\,\mathbf{A}(\mu)\,\mathbf{s}(\tau)\,, \tag{12}$$

where $\mathbf{s}(\tau)$ is the angular-independent reduced vector source function

$$\mathbf{s}(\tau) = \lambda_{\mathrm{I}}\,\mathbf{j}(\tau) + \mathbf{s}^*(\tau)\,, \tag{13}$$

with

$$\mathbf{j}(\tau) = \frac{1}{2}\int_{-\infty}^{\infty}\phi(x')\,dx'\int_{-1}^{1}\mathbf{A}^{\mathrm{T}}(\mu')\,\mathbf{i}(\tau,\mu',x')\,d\mu', \tag{14}$$

and $\mathbf{s}^*(\tau) = \lambda_{\mathrm{I}}\,\mathbf{j}^*(\tau)$, where $\mathbf{j}^*(\tau)$ is given by Eq. (14) with $\mathbf{i}(\tau,\mu',x')$ replaced by $\mathbf{i}^*(\tau,\mu',x')$. By formally solving the transfer Eq. (12) subject to the boundary conditions (5) and substituting the result into Eq. (14), we obtain the integral equation for the reduced vector source function $\mathbf{s}(\tau)$ (henceforth, the word 'reduced' will be omitted):

$$\mathbf{s}(\tau) = \int_0^{\tau_0}\mathbf{K}_1(\tau-\tau')\,\mathbf{s}(\tau')\,d\tau' + \mathbf{s}^*(\tau)\,, \tag{15}$$

where the *kernel matrix* $\mathbf{K}_1(\tau)$ is

$$\mathbf{K}_1(\tau) = \int_{-\infty}^{\infty}\phi^2(x)\,dx\int_0^1 \mathrm{e}^{-\phi(x)|\tau|/\mu}\,\mathbf{\Psi}(\mu)\,d\mu/\mu \tag{16}$$

and $\mathbf{\Psi}(\mu)$ is the *characteristic matrix*

$$\mathbf{\Psi}(\mu) = \frac{\lambda_{\mathrm{I}}}{2}\,\mathbf{A}^{\mathrm{T}}(\mu)\,\mathbf{A}(\mu)\,. \tag{17}$$

For the specific factorization which we use, Eqs. (10) – (11), the explicit expression of the characteristic matrix is

$$\mathbf{\Psi}(\mu) = \frac{\lambda_{\mathrm{I}}}{2}\begin{pmatrix} 1 & \sqrt{\frac{W}{8}}\,(1-3\mu^2) \\ \sqrt{\frac{W}{8}}\,(1-3\mu^2) & W\left(\frac{5}{4} - 3\mu^2 + \frac{9}{4}\mu^4\right) \end{pmatrix}. \tag{18}$$

The two components of the primary source vector $\mathbf{s}^*(\tau)$ will be denoted by $S_{\mathrm{I}}^*(\tau)$ and $S_{\mathrm{Q}}^*(\tau)$, respectively, so that

$$\mathbf{s}^*(\tau) = \left(S_{\mathrm{I}}^*(\tau),\ S_{\mathrm{Q}}^*(\tau)\right)^{\mathrm{T}}. \tag{19}$$

The vector integral transfer Eq. (15) with unpolarized primary sources, i.e., with $\mathbf{s}^* = \left(S_{\mathrm{I}}^*,\ 0\right)$, has been considered, e.g., by Faurobert-Scholl & Frisch 1989; the factorization implicitly used by these authors slightly differs from ours. Although Eq. (15) may as well be used in the case of primary sources of partially polarized radiation, we prefer a more general (and mathematically more natural) approach based on using the *matrix* rather than the *vector* transfer equation. This approach is presented in the next section.

3. Matrix transfer equation

Let us introduce the 2×2 *Stokes matrix* $\mathbf{I}(\tau, z)$, which, by definition, is the solution of the matrix transfer equation

$$z \frac{\partial \mathbf{I}(\tau, z)}{\partial \tau} = \mathbf{I}(\tau, z) - \mathbf{S}(\tau) \tag{20}$$

satisfying the boundary conditions

$$\mathbf{I}(0, z) = \mathbf{0}, \quad z < 0; \qquad \mathbf{I}(\tau_0, z) = \mathbf{0}, \quad z > 0. \tag{21}$$

The matrix source function $\mathbf{S}(\tau)$ appearing in Eq. (20) is given by

$$\mathbf{S}(\tau) = \mathbf{J}(\tau) + \mathbf{S}^*(\tau)\,, \tag{22}$$

where

$$\mathbf{J}(\tau) = \int_{-\infty}^{\infty} \phi(x')\, dx' \int_{-1}^{1} \mathbf{\Psi}(\mu')\, \mathbf{I}\big(\tau, \mu'/\phi(x')\big)\, d\mu'\,. \tag{23}$$

The matrix primary source term $\mathbf{S}^*(\tau)$ in Eq. (22) is

$$\mathbf{S}^*(\tau) = \mathrm{diag}\big(S_\mathrm{I}^*(\tau),\ S_\mathrm{Q}^*(\tau)\big), \tag{24}$$

where $S_\mathrm{I}^*(\tau)$ and $S_\mathrm{Q}^*(\tau)$ are the I- and Q-components of the vector primary source function, cf. Eq. (19). The auxiliary variable z appearing in Eqs. (20) and (21) is related to the commonly used variables μ and x by

$$z = \mu/\phi(x)\,. \tag{25}$$

To meet our immediate and further needs, we introduce the notation

$$\mathbf{e}_\mathrm{I} = (1,\ 0)^\mathrm{T}; \qquad \mathbf{e} = (1,\ 1)^\mathrm{T}\,. \tag{26}$$

Comparison of Eqs. (12) and (20) reveals that the usual Stokes vector $\mathbf{i}(\tau, \mu, x)$ is expressed in terms of the Stokes matrix $\mathbf{I}(\tau, z)$ as follows:

$$\mathbf{i}(\tau, \mu, x) = \mathbf{A}(\mu)\, \mathbf{I}\big(\tau, \mu/\phi(x)\big)\, \mathbf{e}\,, \tag{27}$$

while the vector source function $\mathbf{s}(\tau)$ is related to the matrix source function $\mathbf{S}(\tau)$ by

$$\mathbf{s}(\tau) = \mathbf{S}(\tau)\, \mathbf{e}\,. \tag{28}$$

We note that for unpolarized primary sources ($S_\mathrm{Q}^* = 0$) Eqs. (27) and (28) can also be rewritten as

$$\mathbf{i}(\tau, \mu, x) = \mathbf{A}(\mu)\, \mathbf{I}\big(\tau, \mu/\phi(x)\big)\, \mathbf{e}_\mathrm{I} \tag{29}$$

and

$$\mathbf{s}(\tau) = \mathbf{S}(\tau)\, \mathbf{e}_\mathrm{I}\,, \tag{30}$$

respectively. Hence, in this particular case, only the first columns of the matrices $\mathbf{I}$ and $\mathbf{S}$ are needed to find the complete radiation field.

Let us now introduce $z' = \mu'/\phi(x')$ instead of μ' as the integration variable in the inner integral in Eq. (23) and then interchange the order of z'- and x'-integrations. Assuming that $\phi(x)$ is an even continuous monotonically decreasing function of x, which is practically always the case, one can obtain from Eqs. (22) and (23) that the matrix source function $\mathbf{S}(\tau)$ is representable as

$$\mathbf{S}(\tau) = \int_{-\infty}^{\infty} \mathbf{G}(z')\, \mathbf{I}(\tau, z')\, dz' + \mathbf{S}^*(\tau)\,, \tag{31}$$

where

$$\mathbf{G}(z) = 2 \int_{x(z)}^{\infty} \phi^2(y)\, \mathbf{\Psi}\big(z\phi(y)\big)\, dy \tag{32}$$

and the (non-negative) function $x(z)$ is defined by

$$x(z) = 0, \qquad |z| \le 1/\phi(0);$$
$$\phi(x(z)) = 1/|z|, \quad |z| > 1/\phi(0)\,. \tag{33}$$

Essentially the same transformation is used in the scalar theory (Ivanov 1973, Sect. 5.1). We note that the matrix $\mathbf{G}(z)$ is even in z and symmetric:

$$\mathbf{G}(-z) = \mathbf{G}(z), \qquad \mathbf{G}^\mathrm{T}(z) = \mathbf{G}(z). \tag{34}$$

The most important particular case is that of the Doppler profile:

$$\phi(x) = \frac{1}{\sqrt{\pi}}\, \mathrm{e}^{-x^2}. \tag{35}$$

In this case the function $x(z)$ is

$$x(z) = 0, \qquad |z| \le \sqrt{\pi}\,;$$
$$x(z) = \sqrt{\ln \frac{|z|}{\sqrt{\pi}}}\,, \qquad |z| > \sqrt{\pi}\,. \tag{36}$$

In the usual manner, by substituting the formal solution of the transfer Eq. (20) into Eq. (31), we obtain the integral equation for the matrix source function $\mathbf{S}(\tau)$:

$$\mathbf{S}(\tau) = \int_0^{\tau_0} \mathbf{K}_1(\tau - \tau')\, \mathbf{S}(\tau')\, d\tau' + \mathbf{S}^*(\tau) \tag{37}$$

with the kernel function $\mathbf{K}_1(\tau)$ given by

$$\mathbf{K}_1(\tau) = \int_0^{\infty} \mathrm{e}^{-|\tau|/z}\, \mathbf{G}(z)\, dz/z\,. \tag{38}$$

This alternative representation of the kernel matrix (16) is highly useful. The major part of the analytical theory presented below is based on the fact that the kernel matrix $\mathbf{K}_1(\tau)$ can be written in the form (38), i.e., essentially, as Laplace-type integral.

In the present paper we confine our discussion to semi-infinite atmospheres only ($\tau_0 = \infty$). For this particular case, we shall write Eq. (37) in short operator notation as

$$\mathbf{S} = \mathbf{\Lambda}\, \mathbf{S} + \mathbf{S}^*. \tag{39}$$

The investigation of solutions to this Wiener-Hopf matrix integral transfer equation is the main subject of the present series of papers. Evidently the properties of the solutions are determined by the properties of the kernel matrix $\mathbf{K}_1(\tau)$. The latter are discussed in the next section.

4. Kernel matrix; the λ-plane

In this section we consider those general properties of the kernel matrix $\mathbf{K}_1(\tau)$ which hold for an arbitrary absorption profile $\phi(x)$. They are essentially the same as in the particular case of the rectangular profile discussed in GRaS.I, Sect. 3.2; in the present Section we shall closely follow this earlier discussion. The deep distinction between GRaS and resonance scattering appears when one considers the large-τ behavior of the corresponding kernels $\mathbf{K}_1(\tau)$. These matters are the subject of Sect. 8.

The kernel matrix $\mathbf{K}_1(\tau)$ is even in τ and symmetric:

$$\mathbf{K}_1(-\tau) = \mathbf{K}_1(\tau)\,; \qquad \mathbf{K}_1^{\mathrm{T}}(\tau) = \mathbf{K}_1(\tau)\,. \tag{40}$$

The physical significance of its diagonal and off-diagonal elements is substantially different. The elements 11 and 22 describe propagation of respectively Stokes I and Q if they were independent. The off-diagonal elements are responsible for coupling of I and Q. This difference in physics causes substantial difference in the overall behavior of the diagonal and off-diagonal elements of $\mathbf{K}_1(\tau)$: the propagation elements are positive for all τ, while the coupling terms change sign and integrate to zero. The last point is very important.

The normalization of $\mathbf{K}_1(\tau)$ is:

$$\int_{-\infty}^{\infty} \mathbf{K}_1(\tau)\,d\tau = 2\int_0^{\infty} \mathbf{G}(z)\,dz =$$
$$2\int_0^1 \mathbf{\Psi}(\mu)\,d\mu \equiv 2\,\mathbf{\Psi}_0 = \mathrm{diag}\big(\lambda_{\mathrm{I}}, \lambda_{\mathrm{Q}}\big), \tag{41}$$

where we have denoted

$$\lambda_{\mathrm{Q}} = \frac{7}{10} W \lambda_{\mathrm{I}}\,. \tag{42}$$

The parameter λ_{Q} is essentially the albedo of single scattering for the Stokes parameter Q. The two albedos, λ_{I} and λ_{Q}, may be combined into the *matrix albedo of single scattering*:

$$\boldsymbol{\lambda} \equiv \mathrm{diag}\big(\lambda_{\mathrm{I}}, \lambda_{\mathrm{Q}}\big)\,. \tag{43}$$

The matrix

$$\boldsymbol{\epsilon} \equiv \mathbf{E} - \boldsymbol{\lambda} \equiv \mathrm{diag}\big(\varepsilon_{\mathrm{I}}, \varepsilon_{\mathrm{Q}}\big) \tag{44}$$

is the matrix counterpart of the photon destruction probability; here $\mathbf{E}$ is the unit matrix.

Using the notation (42), one can rewrite the characteristic matrix (18) as

$$\mathbf{\Psi}(\mu) = \mathbf{L} \odot \mathbf{\Psi}_1(\mu)\,, \tag{45}$$

where

$$\mathbf{L} = \begin{pmatrix} \lambda_{\mathrm{I}} & \sqrt{\lambda_{\mathrm{I}}\lambda_{\mathrm{Q}}} \\ \sqrt{\lambda_{\mathrm{I}}\lambda_{\mathrm{Q}}} & \lambda_{\mathrm{Q}} \end{pmatrix}, \tag{46}$$

$$\mathbf{\Psi}_1(\mu) = \frac{1}{2}\begin{pmatrix} 1 & c\,\left(1-3\mu^2\right) \\ c\,\left(1-3\mu^2\right) & 2c^2\left(5-12\mu^2+9\mu^4\right) \end{pmatrix} \tag{47}$$

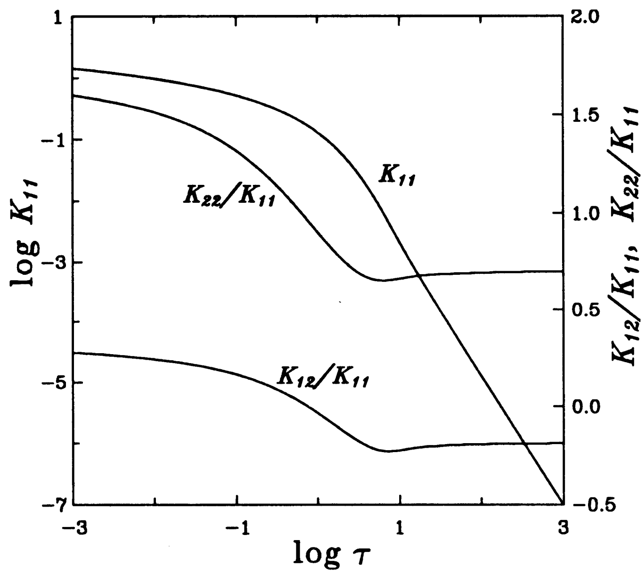

Fig. 1. Depth dependence ot the elements of the kernel matrix $\mathbf{K}(\tau)$ (Doppler profile)

and

$$c = \frac{1}{2}\sqrt{\frac{5}{7}}\,. \tag{48}$$

The operation $\odot$ on arbitrary 2×2 matrices $\mathbf{X}$ and $\mathbf{Y}$ is defined so that $\mathbf{Z} = \mathbf{X} \odot \mathbf{Y}$ if $z_{ij} = x_{ij}\,y_{ij},\ i,j = 1,2$.

Now, we can represent the kernel matrix $\mathbf{K}_1(\tau)$ as

$$\mathbf{K}_1(\tau) = \mathbf{L} \odot \mathbf{K}(\tau), \tag{49}$$

where $\mathbf{K}(\tau)$ is normalized to the unit matrix:

$$\int_{-\infty}^{\infty} \mathbf{K}(\tau)\,d\tau = 2\int_0^1 \mathbf{\Psi}_1(\mu)\,d\mu = \mathbf{E}. \tag{50}$$

The matrix $\mathbf{L}$ determines the scales of variation of the elements of $\mathbf{K}_1(\tau)$ while parameter-free matrix $\mathbf{K}(\tau)$ describes basic shape of their τ-dependence. In Fig. 1 we give the graphs of $K_{11}(\tau)$ and of the ratios $K_{22}(\tau)/K_{11}(\tau)$ and $K_{12}(\tau)/K_{11}(\tau)$; here $K_{ij}(\tau)$ is the element ij of the matrix $\mathbf{K}(\tau)$. The curves refer to the Doppler profile. We note that $K_{11}(\tau)$ is identical to the commonly used scalar kernel function $K_1(\tau)$ (Eq. (84) below). Comparison with Figs. 1 and 2 of GRaS.I which refer to monochromatic scattering, i.e., to the rectangular profile, reveals that the gross features of the dependence on τ of the elements of $\mathbf{K}$ for not too large τ are not sensitive to the shape of the absorption profile. However, there are *very important* qualitative differences in the large-τ asymptotic behavior of the kernel functions for the Doppler and for the rectangular absorption profiles (see Sect. 8 below).

The albedos λ_{I} and λ_{Q} appear in Eq. (46) rather symmetrically. The same ‘symmetry’ is present in the kernel matrix $\mathbf{K}_1(\tau)$ and hence is inherent in the basic integral Eq. (39). This naturally leads to the idea to investigate the solutions to Eq. (39) in the symmetric domain of the parameter values

$\lambda_\mathrm{I} \in [0,1]$; $\lambda_\mathrm{Q} \in [0,1]$. This domain is larger than the 'physical triangle' $\lambda_\mathrm{I} \in [0,1]$; $\lambda_\mathrm{Q} \leq 0.7\lambda_\mathrm{I}$. For the particular case of the rectangular profile, i.e., for monochromatic scattering, such an investigation was given in the GRaS series. In the present series of papers we apply the same ideology to CFR problems of resonance scattering, both physical ($\lambda_\mathrm{Q} \leq 0.7\,\lambda_\mathrm{I}$) and 'non-physical' ($1 \geq \lambda_\mathrm{Q} > 0.7\,\lambda_\mathrm{I}$). This wider class of problems will be called the *generalized resonance scattering* (GReS) problems.

As we shall see shortly, the notion of the λ-*plane*, i.e., the plane with the axes λ_I, λ_Q, and related concepts of isopols, polarization angle φ etc. discussed at length in GRaS.I and GRaS.II play an equally important role in the analysis of GReS problems. Various particular and limiting cases of GReS are quite similar to those of GRaS (see Sect. 3.3 of GRaS.II), and we shall not dwell on this. The terminology introduced in GRaS.II will be used without detailed discussion; it is more or less self-explanatory. The only difference is that Rayleigh and molecular scattering of GRaS are replaced in GReS by, respectively, dipole and resonance scattering.

5. Dispersion matrix $\mathbf{T}(z)$

In the analytical investigation of GReS problems, in particular, in the asymptotic analysis of the properties of solutions of the matrix transfer Eq. (20) – (21), a very important role is played by the *dispersion matrix* $\mathbf{T}(z)$ defined as

$$\mathbf{T}(z) = \mathbf{E} - \overline{\mathbf{K}}_1\left(\frac{1}{z}\right) - \overline{\mathbf{K}}_1\left(-\frac{1}{z}\right), \tag{51}$$

where $\overline{\mathbf{K}}_1(s)$ is the Laplace transform of the kernel matrix $\mathbf{K}_1(\tau)$:

$$\overline{\mathbf{K}}_1(s) = \int_0^\infty \mathbf{K}_1(\tau)\,\mathrm{e}^{-s\tau}\,d\tau. \tag{52}$$

If one uses the representation of the kernel matrix in the form (38), one gets the expression of $\mathbf{T}(z)$ in terms of $\mathbf{G}$-matrix:

$$\mathbf{T}(z) = \mathbf{E} - 2z^2 \int_0^\infty \frac{\mathbf{G}(z')\,dz'}{z^2 - z'^2}\,, \tag{53}$$

while by using the representation of $\mathbf{K}_1(\tau)$ in the form (16) we find that

$$\mathbf{T}(z) = \mathbf{E} + 2z^2 \int_{-\infty}^\infty \phi^3(x)\,dx \int_0^1 \frac{\boldsymbol{\Psi}(\mu)\,d\mu}{\mu^2 - z^2\phi^2(x)}\,. \tag{54}$$

For real z, the integrals in (53) and (54) are the Cauchy principal values.

Let the elements of the dispersion matrix $\mathbf{T}(z)$ be $T_{ik}(z),\ i,k = 1,2$. Using the explicit expression of the characteristic matrix $\boldsymbol{\Psi}$ given by Eqs. (45) – (48), one can show from Eq. (54) by direct calculation that (cf. Ivanov 1973, Sect. 2.7)

$$-z^2 \frac{d}{dz}\left(\frac{T_{11}(z) - \varepsilon_\mathrm{I}}{z}\right) = \lambda_\mathrm{I} \int_{-\infty}^\infty \frac{\phi(x)\,dx}{1 - z^2\phi^2(x)}\,. \tag{55}$$

There are two other useful differential relations between the elements of the dispersion matrix. By elementary, but rather cumbersome transformations one can obtain from Eq. (54)

$$\lambda_\mathrm{I}\, z^3 \frac{d}{dz}\left(\frac{T_{12}(z)}{z^3}\right) + 2c\sqrt{\lambda_\mathrm{I}\lambda_\mathrm{Q}}\,\frac{d\,T_{11}(z)}{dz} = 0\,, \tag{56}$$

$$\lambda_\mathrm{I}\, z^6 \frac{d}{dz}\left(\frac{T_{22}(z) - \varepsilon_\mathrm{Q}}{z^5}\right) + 2c\sqrt{\lambda_\mathrm{I}\lambda_\mathrm{Q}}\,\frac{1}{z^4}\,\frac{d}{dz}\left(z^5 T_{12}(z)\right) + 5\lambda_\mathrm{Q}\big(T_{11}(z) - \varepsilon_\mathrm{I}\big) = 0\,. \tag{57}$$

For the most important case of the Doppler profile, Eqs. (55) – (57) can be used to obtain the asymptotic expansion of $\mathbf{T}(z)$ for large real z (Sect. 9). This expansion plays an important role in the asymptotic analysis of the solutions of GReS problems to be given in the forthcoming papers of the present series.

6. Standard problem

Two particular cases of Eq. (39) will be considered in this series of papers. The first one,

$$\mathbf{S}(\tau) = \int_0^\infty \mathbf{K}_1(\tau - \tau')\,\mathbf{S}(\tau')\,d\tau' + \boldsymbol{\epsilon}^{1/2}, \tag{58}$$

or, in short operator notation,

$$\mathbf{S} = \boldsymbol{\Lambda}\,\mathbf{S} + \boldsymbol{\epsilon}^{1/2}, \tag{59}$$

where

$$\boldsymbol{\epsilon}^{1/2} = \mathrm{diag}\big(\varepsilon_\mathrm{I}^{1/2}, \varepsilon_\mathrm{Q}^{1/2}\big), \tag{60}$$

corresponds to uniformly distributed embedded primary sources of partially polarized radiation. It will be referred to as the *standard problem*; the corresponding source matrix will be denoted $\mathbf{S}(\tau)$.

The second case,

$$\mathbf{S} = \boldsymbol{\Lambda}\,\mathbf{S} + \mathrm{e}^{-\tau/z_0}\mathbf{E}, \tag{61}$$

where z_0 is a parameter, $z_0 \in (0,\infty)$, corresponds to primary sources exponentially decaying with depth. The solution of Eq. (61) will be denoted $\mathbf{S}(\tau, z_0)$. The two source matrices, $\mathbf{S}(\tau)$ and $\mathbf{S}(\tau, z_0)$, are related by

$$\mathbf{S}(\tau) = \mathbf{S}(\tau, \infty)\,\boldsymbol{\epsilon}^{1/2}. \tag{62}$$

The solution of the standard problem satisfies the *matrix* $\sqrt{\varepsilon}$-*law*

$$\mathbf{S}^\mathrm{T}(0)\,\mathbf{S}(0) = \mathbf{E}\,, \qquad \mathbf{S}(\infty) = \boldsymbol{\epsilon}^{-1/2}. \tag{63}$$

This result will be widely used. Its proof given in GRaS.I holds for the arbitrary displacement matrix kernel $\mathbf{K}_1(\tau - \tau')$; hence Eq. (63) holds for CFR with the arbitrary profile $\phi(x)$, and not only for monochromatic scattering. The first of the Eqs. (63), combined with the fact that $\mathbf{S}(0) = \mathbf{E}$ for $\lambda_\mathrm{I} = \lambda_\mathrm{Q} = 0$, enables

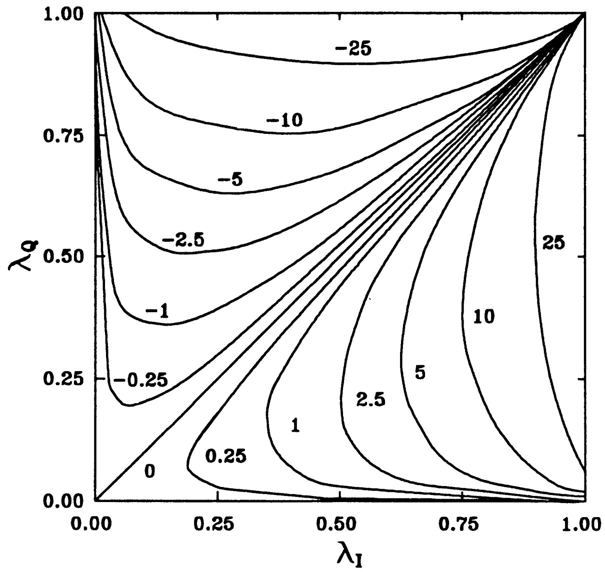

Fig. 2. Curves of constant polarization angle φ = const on the λ-plane (isopols). Curves are labeled with values of $10^3 \sin\varphi$

one to conclude that, for arbitrary $\lambda_{\rm I}$ and $\lambda_{\rm Q}$, the source matrix at the boundary $\mathbf{S}(0)$ is a rotation matrix:

$$\mathbf{S}(0) = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \equiv \mathbf{R}\,, \qquad (64)$$

so that the four elements of $\mathbf{S}(0)$ satisfy the following three relations:

$$S_{11}^2(0) + S_{21}^2(0) = 1; \qquad S_{22}^2(0) + S_{12}^2(0) = 1;$$
$$S_{21}(0) = -S_{12}(0). \qquad (65)$$

These relations proved to be a valuable check of the accuracy of numerical data. According to Eq. (64), the matrices $\mathbf{S}(0)$ form a one-parameter family.

The rotation angle φ will be referred to as the *polarization angle*. This is a very important parameter. It measures an overall strength of the 'boundary-induced' polarization, i.e., the polarization arising in a semi-infinite atmosphere solely due to the escape of radiation, and not due to the gradient of the strength of the primary source. For further details, see Sect. 3 of GRaS.II.

The curves φ = const on the λ-plane, or the *isopols*, are shown in Fig. 2. The curves refer to CFR resonance scattering with the Doppler profile; they are labeled with values of $10^3 \sin\varphi$. The general features of the isopols shown in Fig. 2 and the isopols for monochromatic scattering (cf. Fig. 1 in GraS.II) are the same. Indeed, on the scale of the figures, the two sets of the isopols are indistinguishable. In Table 1 we give the values of $10^3 \sin\varphi$ as a function of $\lambda_{\rm I}$ and $\lambda_{\rm Q}$. To get an idea of the influence of the shape of the absorption profile on the strength of the boundary-induced polarization, one may compare the value of $\sin\varphi = 0.1057$ for conservative Rayleigh scattering (rectangular profile) with $\sin\varphi = 0.0860$ for conservative dipole ($W = 1$) resonance scattering (Doppler profile). Due to frequency redistribution, the polarization effects become smaller.

The point of the λ-plane corresponding to *biconservative scattering* ($\lambda_{\rm I} = \lambda_{\rm Q} = 1$) is singular, there is no uniqueness. The possible values of $\sin\varphi$ at this point satisfy the inequalities

$$-0.14 \le \sin\varphi \le 0.12. \qquad (66)$$

The upper bound is the limit of $\sin\varphi$ as one approaches the point of biconservative scattering along the right boundary of the λ-square ($\lambda_{\rm I} = 1$, $\lambda_{\rm Q} \to 1$); the lower bound corresponds to $\lambda_{\rm Q} = 1$, $\lambda_{\rm I} \to 1$. We note also that the limit of $\sin\varphi$ as one approaches the point of biconservative scattering along the diagonal of the λ-plane ($\lambda_{\rm I} = \lambda_{\rm Q}$) is 0.00124. For the rectangular profile the same limit is 0.00422, cf. Eq. (39) of GRaS.II.

The numerical procedures used to obtain the numerical data just given will be discussed in Paper II of the present series; they are similar to those which we used earlier for monochromatic scattering (see GRaS.II and GRaS.IV).

In the limit of $\boldsymbol{\epsilon} \to \mathbf{0}$, the integral equation of the standard problem reduces to the homogeneous matrix equation

$$\mathbf{S}_{\rm h} = \boldsymbol{\Lambda}_{\rm b}\,\mathbf{S}_{\rm h}\,, \qquad (67)$$

the solution of which, according to Eq. (63), should satisfy

$$\mathbf{S}_{\rm h}^{\rm T}(0)\,\mathbf{S}_{\rm h}(0) = \mathbf{E}\,. \qquad (68)$$

The $\boldsymbol{\Lambda}$-operator in Eq. (67) refers to biconservative scattering, i.e., to $\boldsymbol{\epsilon} = \mathbf{0}$, so that the kernel of the $\boldsymbol{\Lambda}_{\rm b}$-operator is the matrix $\mathbf{K}(\tau)$ defined by Eq. (49). The subscript 'b' emphasizes this fact. Eqs. (67) and (68) define the (biconservative) *matrix Milne problem*. Its solution is evidently not unique, since if $\mathbf{S}_{\rm h}(\tau)$ is a solution of Eqs. (67) – (68), then $\mathbf{S}_{\rm h}(\tau)\,\mathbf{R}$, where $\mathbf{R}$ is an arbitrary orthogonal matrix, is also a solution. From Fig. 2 it is clear that we are interested in those solutions for which $\mathbf{R}$ is the rotation matrix (64), with $\sin\varphi$ satisfying Eq. (66). The solution of Eqs. (67) – (68) normalized to the unit matrix at $\tau = 0$ will be denoted $\mathbf{S}_0(\tau)$, so that

$$\mathbf{S}_0 = \boldsymbol{\Lambda}_{\rm b}\,\mathbf{S}_0\,; \qquad \mathbf{S}_0(0) = \mathbf{E}\,. \qquad (69)$$

The remarkable properties of $\mathbf{S}_0(\tau)$ will be discussed in a forthcoming paper.

7. Emergent radiation; the matrix $\mathbf{I}(z)$

Let $\mathbf{I}(0,z)$ be the Stokes matrix of the emergent radiation, so that

$$\mathbf{I}(0,z) = \int_0^\infty \mathbf{S}(\tau)\,{\rm e}^{-\tau/z}\,d\tau/z\,, \quad z > 0. \qquad (70)$$

According to Eq. (27), the Stokes vector of the emergent radiation $\mathbf{i}(0,\mu,x)$ is expressed in terms of $\mathbf{I}(0,z)$ by

$$\mathbf{i}(0,\mu,x) = \mathbf{A}(\mu)\,\mathbf{I}(0,\mu/\phi(x))\,\mathbf{e}\,, \quad \mu > 0. \qquad (71)$$

The particular case of $\mathbf{I}(0,z)$ corresponding to the primary source term $\mathbf{S}^* = \boldsymbol{\epsilon}^{1/2}$, i.e., the Stokes matrix of the emergent radiation of the standard problem, will be denoted by $\mathbf{I}(z)$:

$$\mathbf{I}(z) \equiv \mathbf{I}(0,z) \quad \text{for} \quad \mathbf{S}^* = \boldsymbol{\epsilon}^{1/2}\,. \qquad (72)$$

Table 1. Values of $10^3 \sin\varphi$ as a function of λ_I and λ_Q for CFR scattering with the Doppler profile

	λ_I										
λ_Q	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	0.95	1.0
1.00	−33.67	−48.67	−61.02	−72.30	−83.16	−94.06	−105.38	−117.68	−131.89	−140.29	—
0.95	−16.19	−22.70	−27.44	−31.04	−33.60	−34.92	−34.39	−30.36	−17.15	0.89	117.57
0.9	−11.71	−16.17	−19.17	−21.14	−22.09	−21.78	−19.55	−13.81	0.64	17.97	109.56
0.8	−7.12	−9.54	−10.88	−11.38	−10.97	−9.40	−6.09	0.37	14.20	29.19	96.72
0.7	−4.59	−5.95	−6.47	−6.29	−5.32	−3.32	0.22	6.50	19.05	31.99	85.99
0.6	−2.99	−3.70	−3.74	−3.20	−1.98	0.14	3.61	9.45	20.65	31.82	76.33
0.5	−1.89	−2.18	−1.95	−1.22	0.08	2.16	5.42	10.71	20.56	30.16	67.19
0.4	−1.11	−1.14	−0.75	0.04	1.33	3.28	6.22	10.89	19.39	27.54	58.20
0.3	−0.58	−0.44	0.02	0.81	1.99	3.73	6.29	10.27	17.39	24.12	48.97
0.2	−0.21	0.01	0.46	1.16	2.17	3.61	5.70	8.90	14.54	19.80	38.94
0.1	0.00	0.22	0.58	1.11	1.85	2.88	4.35	6.57	10.44	14.03	26.88

The matrix $\mathbf{I}(z)$ plays a fundamental role in model problems of resonance scattering. It is the generalization of the usual scalar H-function for the problem at hand. It satisfies the non-linear integral equation

$$\mathbf{I}(z)\left(\boldsymbol{\epsilon}^{1/2} + \int_0^\infty \mathbf{I}^{\mathrm{T}}(z')\,\mathbf{G}(z')\,\frac{z'\,dz'}{z+z'}\right) = \mathbf{E}\,, \tag{73}$$

which is the matrix version of the alternative form of the Chandrasekhar-type H-equation. Eq. (73) may be solved by iteration. The results will be presented in Paper II.

The matrix $\mathbf{I}(z)$ satisfies also the linear integral equation

$$\mathbf{T}(z)\,\mathbf{I}(z) = \boldsymbol{\epsilon}^{1/2} - \int_0^\infty \mathbf{G}(z')\,\mathbf{I}(z')\,\frac{z'\,dz'}{z-z'}\,, \tag{74}$$

where $\mathbf{T}(z)$ is the dispersion matrix defined by Eq. (53). This equation is essentially the Laplace-transformed version of the basic integral equation for the source function, Eq. (59). Eq. (74) plays the crucial role in our asymptotic analysis of GReS problems to be given in Paper II.

We note that from Eqs. (73) and (74) it follows that

$$\mathbf{I}(z)\,\mathbf{I}^{\mathrm{T}}(-z) = \mathbf{T}^{-1}(z)\,. \tag{75}$$

One can easily show that

$$\mathbf{I}(0) = \mathbf{R}, \qquad \mathbf{I}(\infty) = \boldsymbol{\epsilon}^{-1/2} \tag{76}$$

and

$$\int_0^\infty \mathbf{G}(z')\,\mathbf{I}(z')\,dz' = \mathbf{R} - \boldsymbol{\epsilon}^{-1/2}. \tag{77}$$

The matrix $\mathbf{I}(z)$ is closely related to the surface value of the source matrix $\mathbf{S}(\tau, z)$ defined by Eq. (61), namely,

$$\mathbf{I}(z) = \mathbf{S}^{\mathrm{T}}(0, z)\,\mathbf{R}\,, \tag{78}$$

where $\mathbf{R}$ is defined by Eq. (64) (cf. Sect. 3 of GRaS.III).

The Stokes matrix $\mathbf{I}(0, z, z_0)$ of the radiation emerging from an atmosphere with the exponential primary source term $\mathbf{S}^* = \mathrm{e}^{-\tau/z_0}\mathbf{E}$ is expressed in terms of $\mathbf{I}(z)$ as follows:

$$\mathbf{I}(0, z, z_0) \equiv \int_0^\infty \mathbf{S}(\tau, z_0)\,\mathrm{e}^{-\tau/z}\,d\tau/z = \frac{\mathbf{I}(z)\,\mathbf{I}^{\mathrm{T}}(z_0)}{z+z_0}\,z_0\,. \tag{79}$$

The derivation of these results is essentially the same as for monochromatic scattering; for the details, see GRaS.III.

8. Large-τ behavior of the kernel matrices

The fundamental difference between the monochromatic scattering and CFR scattering with the absorption profiles with infinitely extended wings appears when one considers the asymptotic behavior of the corresponding kernels.

For monochromatic scattering $\mathbf{K}_1(\tau) \sim \mathbf{O}(\mathrm{e}^{-|\tau|}/|\tau|)$, $|\tau| \to \infty$, while for CFR scattering with non-rectangular profiles the kernel decreases algebraically. To be more specific, for lines with infinite wings the *leading term* of the asymptotic expansion of $\mathbf{K}_1(\tau)$ is given by

$$\mathbf{K}_1(\tau) \sim \boldsymbol{\kappa}_1\,\frac{\Gamma(2\gamma+1)}{2\gamma+1}\,\frac{x'(|\tau|)}{|\tau|}\,, \qquad |\tau| \to \infty\,, \tag{80}$$

where

$$\boldsymbol{\kappa}_1 = 2\,(2\gamma+1)\int_0^1 \boldsymbol{\Psi}(\mu)\,\mu^{2\gamma}\,d\mu = \mathbf{L} \odot \begin{pmatrix} 1 & -\frac{4c\gamma}{2\gamma+3} \\ -\frac{4c\gamma}{2\gamma+3} & \frac{4c^2(4\gamma^2+4\gamma+21)}{(2\gamma+3)(2\gamma+5)} \end{pmatrix} \tag{81}$$

and $\Gamma(s)$ is the Euler gamma function. The number γ is the so-called *characteristic exponent* of the kernel function. For lines with infinite wings $\gamma \in [0,\ 1/2]$. One has

$$\lim_{z\to\infty} \frac{x'(tz)}{x'(z)} = t^{-2\gamma}. \tag{82}$$

In Eqs. (80) and (82) the function $x(z)$ is defined by Eq. (33) and x' is the derivative of x. Eq. (82) may be used as the definition of the characteristic exponent for such lines. The faster the decrease

Table 2. Coefficients for asymptotic expansions of Doppler kernel matrices $\mathbf{K}_1(\tau)$ and $\mathbf{K}_2(\tau)$

k	a_{11}	a_{12}	a_{22}	b_{11}	b_{12}	b_{22}
0	1.000000E+00	1.000000E+00	1.000000E+00	1.000000E+00	1.000000E+00	1.000000E+00
1	−3.860783E−02	3.363922E−01	−1.636078E−01	−5.386078E−01	−1.636078E−01	−6.636078E−01
2	3.378361E−01	1.537773E−01	4.304391E−01	1.145748E+00	3.991891E−01	1.425851E+00
3	−2.693384E−01	4.791411E−01	−5.574161E−01	−3.133708E+00	−5.188316E−01	−4.122043E+00
4	9.586014E−01	−4.033315E−01	1.580624E+00	1.192658E+01	1.412579E+00	1.600778E+01
5	−2.164737E+00	2.602717E+00	−4.220406E+00	−5.583435E+01	−3.753889E+00	−7.625540E+01
6	7.764689E+00	−7.720102E+00	1.481065E+01	3.148536E+02	1.292629E+01	4.342153E+02
7	−2.824690E+01	3.476875E+01	−5.688524E+01	−2.074795E+03	−4.925211E+01	−2.879285E+03
8	1.225849E+02	−1.544582E+02	2.507306E+02	1.568355E+04	2.149327E+02	2.184537E+04
9	−5.828766E+02	7.873191E+02	−1.221148E+03	−1.338930E+05	−1.039609E+03	−1.869068E+05
10	3.082210E+03	−4.325000E+03	6.561877E+03	1.275066E+06	5.551281E+03	1.782176E+06

of $\phi(x)$ for $|x| \to \infty$, the larger the value of γ. For the Doppler profile one has $\gamma = 1/2$; Voigt profile has $\gamma = 1/4$. For a more general definition of the characteristic exponent, which applies to both monochromatic scattering and lines with infinite wings, see Ivanov 1973, Sect. 2.6; Nagirner 1984.

Eq. (80) implies that

$$\mathbf{K}_1(\tau) \sim \boldsymbol{\kappa}_1 \, K_1(\tau), \qquad |\tau| \to \infty, \tag{83}$$

where $K_1(\tau)$ is the usual scalar kernel function,

$$K_1(\tau) = \frac{1}{2} \int_{-\infty}^{\infty} \phi^2(x) \, E_1(\phi(x)|\tau|) \, dx \, . \tag{84}$$

Here E_1 is the first exponential integral:

$$E_1(y) = \int_0^1 \mathrm{e}^{-y/\mu} \, d\mu/\mu \, . \tag{85}$$

According to Eq. (83), the functional forms of the *leading terms* of the asymptotic expansions of the scalar and the matrix kernel functions for large τ are identical; in the matrix case there is an extra (matrix) multiplier. This multiplier is a full matrix, i.e., none of its elements is zero.

Along with the kernel function $\mathbf{K}_1(\tau)$, it is useful to introduce also the *second kernel function*

$$\mathbf{K}_2(\tau) \equiv \int_{\tau}^{\infty} \mathbf{K}_1(t) \, dt = \int_0^{\infty} \mathrm{e}^{-\tau/z} \, \mathbf{G}(z) \, dz \, , \; \tau \geq 0. \tag{86}$$

The leading terms of the asymptotic expansions of $\mathbf{K}_1(\tau)$ and $\mathbf{K}_2(\tau)$ are related by

$$\mathbf{K}_2(\tau) \sim \frac{\tau}{2\gamma} \, \mathbf{K}_1(\tau), \qquad \tau \to \infty. \tag{87}$$

This can be easily obtained from Eqs. (86) and (80) if use is made of Eq. (82).

In case of the Doppler profile we have

$$K_1(\tau) \sim \left(4\tau^2 \sqrt{\ln \frac{|\tau|}{\sqrt{\pi}}} \right)^{-1} \equiv K_1^{\mathrm{as}}(\tau), \qquad |\tau| \to \infty, \tag{88}$$

and

$$\boldsymbol{\kappa}_1 = \mathbf{L} \odot \begin{pmatrix} 1 & -c/2 \\ -c/2 & 4c^2 \end{pmatrix} = \lambda_{\mathrm{I}} \begin{pmatrix} 1 & -\frac{1}{4}\sqrt{\frac{W}{2}} \\ -\frac{1}{4}\sqrt{\frac{W}{2}} & \frac{W}{2} \end{pmatrix} . \tag{89}$$

This is the specification of the general asymptotic forms (80) and (82) valid for the arbitrary line profile.

For the particular case of the Doppler profile, the above asymptotic results may be substantially refined. One can show that for $\tau \to \infty$

$$\mathbf{K}_1(\tau) \sim \boldsymbol{\kappa}_1 \odot \sum_{k=0}^{\infty} \frac{\mathbf{A}_k}{T^k} \, K_1^{\mathrm{as}}(\tau) \, , \tag{90}$$

$$\mathbf{K}_2(\tau) \sim \boldsymbol{\kappa}_1 \odot \sum_{k=0}^{\infty} \frac{\mathbf{B}_k}{T^k} \, \tau \, K_1^{\mathrm{as}}(\tau) \, , \tag{91}$$

where

$$T \equiv \ln \frac{\tau}{\sqrt{\pi}} \, . \tag{92}$$

The matrices $\mathbf{A}_k, \; k = 0, 1, 2, \ldots$, are given by

$$\mathbf{A}_k = \frac{(2k-1)!!}{2^{2k}} \sum_{i=0}^{k} (-1)^{k-i} \, \frac{2^i \, \Gamma^{(i)}(2)}{i!} \, \tilde{\mathbf{G}}_{k-i} \tag{93}$$

with

$$\tilde{\mathbf{G}}_n = \begin{pmatrix} 1 & 3 \cdot 2^{-n} - 2 \\ 3 \cdot 2^{-n} - 2 & \frac{1}{2}\left(5 - 3 \cdot 2^{1-n} + 3^{1-n}\right) \end{pmatrix} . \tag{94}$$

Here $\Gamma^{(i)}$ is the i-th derivative of the Euler gamma function. Finally, the matrices $\mathbf{B}_k$ appearing in Eq. (91) are given by a version of Eq. (93) in which $\Gamma^{(i)}(2)$ is replaced by $\Gamma^{(i)}(1)$.

We note that knowledge of the higher order terms of the expansions (90) and (91) is important. The reason is that the parameter of the expansions is not τ^{-1}, but T^{-1}, i.e., essentially, the inverse of the *logarithm* of τ.

In Table 2 we give the numerical values of the elements a_{ij}^k and b_{ij}^k of the (symmetric) matrices $\mathbf{A}_k$ and $\mathbf{B}_k$. We emphasize that they do *not* depend on the values of $\lambda_\mathrm{I},\ \lambda_\mathrm{Q}$.

The derivation of the asymptotic series (90) and (91) is omitted. It proceeds along the same general lines as in the scalar case (cf. Avrett & Hummer 1965; Ivanov 1973, Sect. 2.7). The expansions equivalent to (90) and (91) were found in Faurobert-Scholl & Frisch (1989). In their paper one can also find the coefficients of the Padé approximations of the elements of these matrices for $\lambda_\mathrm{I} = W = 1$.

For the Voigt profile we have $\gamma = 1/4$, and the matrix $\boldsymbol{\kappa}_1$ appearing in Eqs. (80) and (83) is

$$\boldsymbol{\kappa}_1 = \lambda_\mathrm{I} \begin{pmatrix} 1 & -\frac{1}{7}\sqrt{\frac{W}{2}} \\ -\frac{1}{7}\sqrt{\frac{W}{2}} & \frac{89}{154}\,W \end{pmatrix}, \tag{95}$$

while

$$x(z) \sim \sqrt{\frac{az}{\pi}}\,, \qquad z \to \infty, \tag{96}$$

so that

$$\mathbf{K}_1(\tau) \sim \frac{1}{2\tau}\,\mathbf{K}_2(\tau) \sim \boldsymbol{\kappa}_1\,\frac{\sqrt{a}}{6}\,\tau^{-3/2}, \qquad \tau \to \infty\,. \tag{97}$$

In these expressions, a is the usual Voigt parameter. The real domain of applicability of the Voigt asymptotic forms is $\tau \gg a^{-1}$.

Along with the asymptotic forms of the kernel functions $\mathbf{K}_1(\tau)$ and $\mathbf{K}_2(\tau)$, one often needs also the information on the behavior of $\mathbf{G}(z)$ for $|z| \to \infty$. For an arbitrary line with infinite wings, the *leading term* is given by

$$\mathbf{G}(z) \sim \boldsymbol{\kappa}_1\,\frac{1}{2\gamma+1}\,\frac{x'(|z|)}{|z|}\,, \qquad |z| \to \infty, \tag{98}$$

which may also be rewritten as

$$\mathbf{G}(z) \sim \boldsymbol{\kappa}_1\,G(z), \qquad |z| \to \infty, \tag{99}$$

where $G(z)$ is the scalar G-function, i.e., the 11 element of $\mathbf{G}(z)$ with $\lambda_\mathrm{I} = 1$.

For the particular case of the Doppler profile the complete asymptotic expansion of $\mathbf{G}(z)$ for $|z| \to \infty$ is given by

$$\mathbf{G}(z) \sim \boldsymbol{\kappa}_1 \odot \sum_{k=0}^{\infty} \frac{\mathbf{G}_k}{Z^k}\,G_\mathrm{as}(z)\,, \tag{100}$$

where

$$G_\mathrm{as}(z) = \frac{1}{4\,z^2\sqrt{Z}} \tag{101}$$

and

$$Z = \ln\frac{|z|}{\sqrt{\pi}}\,. \tag{102}$$

The matrices $\mathbf{G}_k$ appearing here are defined as follows:

$$\mathbf{G}_k = (-1)^k\,\frac{(2k-1)!!}{2^{2k}}\,\tilde{\mathbf{G}}_k\,. \tag{103}$$

Eqs. (100) – (103) are easily obtained from Eqs. (32), (18) and (36) if use is made of the well-known asymptotic expansion of the probability integral erfc(y) for $y \to \infty$. We omit the calculation which is quite straightforward.

9. Asymptotic behavior of the dispersion matrix

Evidently, the asymptotic behavior of the kernel function $\mathbf{K}_1(\tau)$ discussed in the previous Section determines the large-τ behavior of the solution $\mathbf{S}(\tau)$ of the standard problem. From the theoretical point of view, the most interesting case is that of conservative scattering ($\varepsilon_\mathrm{I} = 0$) with the Doppler profile. The problem is not easy, and it is a serious challenge to a theoretician. Paradoxically, to find the large-τ expansion of $\mathbf{S}(\tau)$ for this problem, one can completely by-pass the use of the asymptotic expansions of the kernel functions. In Paper II we show that the shortest route to asymptotic expansions of $\mathbf{S}(\tau)$ is based on using the information on the asymptotic properties of the dispersion matrix $\mathbf{T}(z)$, rather than on the kernel $\mathbf{K}_1(\tau)$ itself.

The dispersion matrix is defined by Eq. (53). In our discussion we shall assume that z is real. By rewriting Eq. (53) as

$$\mathbf{T}(z) = \boldsymbol{\epsilon} + 2\int_0^\infty \mathbf{G}(z')\,\frac{z'^2\,dz'}{z^2 - z'^2} \tag{104}$$

and substituting for $\mathbf{G}(z')$ in the integrand the asymptotic form (99), after minor rearrangements we get

$$\mathbf{T}(z) \sim \boldsymbol{\epsilon} + \boldsymbol{\kappa}_1\,T_\mathrm{as}(z), \tag{105}$$

where

$$T_\mathrm{as}(z) \equiv -\frac{\pi\,\cot\pi\gamma}{2\gamma+1}\,x'(|z|)\,. \tag{106}$$

This $T_\mathrm{as}(z)$ is the leading term of the large-$|z|$ asymptotic form of the conservative ($\lambda_\mathrm{I} = 1$) scalar dispersion function $T(z)$, which, in turn, is the 11 element of the matrix $\mathbf{T}(z)$ for conservative case.

In the particular case of the Doppler profile we have $\gamma = 1/2$, and from the general asymptotic form (106) one can only conclude that $T_\mathrm{as}(z) = o\big((|z|\sqrt{Z}\,)^{-1}\big)$. A more accurate analysis shows that in this particular case (Ivanov 1973, Sect. 2.7)

$$T_\mathrm{as}(z) = -\frac{\pi^2}{16\,|z|\,Z^{3/2}}\,. \tag{107}$$

The power of the logarithmic correction factor Z appearing here is $-3/2$, and not $-1/2$, as elsewhere, e.g., in Eq. (101). As we shall see in Paper II, this causes somewhat unexpected asymptotic behavior of the Q-component of the vector source function in purely scattering atmospheres.

The complete asymptotic expansion of $\mathbf{T}(z)$ for the Doppler profile is

$$\mathbf{T}(z) \sim \boldsymbol{\epsilon} + \boldsymbol{\kappa}_1 \odot \sum_{n=0}^{\infty} \frac{\mathbf{T}_n}{Z^n}\,T_\mathrm{as}(z)\,, \qquad z \to \infty, \tag{108}$$

where the matrices $\mathbf{T}_n$ are given by

$$\mathbf{T}_n = (-1)^n \frac{(2n+1)!!}{2^{2n}} \sum_{l=0}^{[n/2]} 2^{4l} f_{2l} \, \tilde{\mathbf{G}}_{n-2l} \, . \tag{109}$$

Here $[n/2]$ is the largest integer not exceeding $n/2$, and

$$f_n = \frac{2^{n+2}-1}{2^{n-2}(n+2)!} \, \pi^n \, |B_{n+2}| \, , \tag{110}$$

where B_k are the Bernoulli numbers:

$$B_2 = \frac{1}{6} \, , \quad B_4 = -\frac{1}{30} \, , \quad B_6 = \frac{1}{42} \ldots \, ; \tag{111}$$

finally, the matrices $\tilde{\mathbf{G}}_k$ are defined by Eq. (94). We note that for odd n one has $f_n = 0$. The first few non-zero numbers f_n are

$$f_0 = 1; \quad f_2 = \frac{\pi^2}{48}; \quad f_4 = \frac{\pi^4}{1920} \, . \tag{112}$$

The asymptotic series (108) for the Doppler dispersion matrix $\mathbf{T}(z)$ is obtained from Eq. (104). First we observe that due to the presence of the factor z'^2 in the integrand, the main contribution to the integral comes from large z'. This enables one to substitute in the integrand the expansion of $\mathbf{G}(z')$ given by Eq. (100). [Accurate mathematical justification of the possibility of this as well as of some other steps of the present derivation is omitted.] Interchanging the order of summation and integration, we get

$$\mathbf{T}(z) \sim \boldsymbol{\epsilon} + \boldsymbol{\kappa}_1 \odot \sum_{k=1}^{\infty} \mathbf{G}_k \, \frac{1}{2} \int_0^{\infty} \frac{dz'}{(Z')^{k+1/2} \, (z^2 - z'^2)} \, , \tag{113}$$

where $Z' = \ln(z'/\sqrt{\pi})$. By substituting $t = z'/z$, we can transform the integrals appearing here to

$$\int_0^{\infty} \frac{dz'}{(Z')^{k+1/2} \, (z^2 - z'^2)} = \frac{1}{z Z^{k+1/2}} \int_0^{\infty} \left(1 + \frac{\ln t}{Z}\right)^{-(k+1/2)} \frac{dt}{1-t^2} \, , \tag{114}$$

where Z is given by Eq. (102). Now we expand the bracket in the integrand and perform term-by-term integration, taking into account that

$$\int_0^{\infty} \frac{dt}{1-t^2} = 0 \tag{115}$$

and for $n = 1, 2, 3, \ldots$

$$\int_0^{\infty} \frac{(\ln t)^n \, dt}{1-t^2} = \frac{1-2^{n+1}}{n+1} \, \pi^{n+1} \, |B_{n+1}| \, . \tag{116}$$

The result of the calculation is substituted into Eq. (113). The double series appears. Collecting together its terms with equal powers of Z, we finally get Eq. (108).

There are three useful recursion relations for the elements t_{ik}^n of the matrices $\mathbf{T}_n$, $n = 1, 2, \ldots$:

$$t_{11}^n = -\frac{2n+1}{4} \, t_{11}^{n-1} + (2n-1)!! \, f_n \, , \tag{117}$$

$$t_{12}^n = t_{11}^n + \frac{2n+1}{8} \left(4 t_{11}^{n-1} - t_{12}^{n-1}\right) , \tag{118}$$

$$t_{22}^n = t_{11}^n - \frac{2n+1}{48} \left(2 t_{11}^{n-1} - t_{12}^{n-1} + 2 t_{22}^{n-1}\right) . \tag{119}$$

The initialization condition is

$$t_{ik}^0 = 1 \, , \qquad i, k = 1, 2. \tag{120}$$

These relations can be derived from Eqs. (55) – (57) in the same manner as it has been done earlier in the scalar case (Ivanov 1973, Sect. 2.7). They can also be verified using the explicit expressions for t_{ik}^n given by Eqs. (109) and (94).

10. Concluding remarks

1. The formalism developed in the present paper enabled us to recast the basic equations describing multiple CFR resonance scattering in exactly the same form as in the usual CFR scalar theory, with scalars replaced by matrices. In principle, it could have been done more than 20 years ago — but it has not happened.

2. The idea of using the matrix rather than the vector transfer equation is not new. In the theory of monochromatic Rayleigh scattering it is known at least since the sixties (see, e.g., Mullikin 1969). However, as far as we know, it has never been used in problems of polarized line formation, either magnetic or non-magnetic.

Clearly, the idea of using matrices to describe polarizing properties of an atmosphere is quite general. In particular, it has nothing to do with the assumption of CFR.

The Stokes matrix $\mathbf{I}(\tau, z)$ defined by Eqs. (20) – (23) with $\mathbf{S}^* = \boldsymbol{\epsilon}^{1/2}$ is essentially the Mueller matrix of the atmosphere with uniformly distributed primary sources of partially polarized radiation.

3. Having in mind the identity of the forms of the matrix and the scalar transfer equations, it is natural to ask to what extent do the matrix *solutions* resemble their scalar counterparts.

At least one exact result of the scalar theory is easily generalized to the matrix case. This is the $\sqrt{\varepsilon}$-law, Eq. (63). On the other hand, closed-form exact solutions of half-space scalar CFR problems (see, e.g., Ivanov 1973, Chap. 5 and 6; Frisch 1988, Chap. 8) most probably have no matrix counterparts. And what about asymptotic solutions? As we shall see in Paper II, the methods of the scalar asymptotic theory enable one to develop its matrix generalization, but it is highly non-trivial.

4. Monochromatic scattering is the particular case of CFR scattering corresponding to the rectangular profile. Dealing with resonance scattering, we are interested in the Doppler profile. How sensitive are the polarizing properties of scattering atmospheres to the shape of the absorption profile? In particular,

how seriously does frequency redistribution affect the polarization rate of the emergent radiation in the Doppler core of the line? Strangely enough, this natural question has never been discussed. This is one of the subjects of our Paper II.

5. In scalar line transfer problems, there are two well-known approximations, the so-called first and second order escape probability approximations. Are there matrix analogs of these approximations? This is an intriguing question, and at least partial answer to it we hope to present in a forthcoming paper of the present series.

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