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AN EXPEDIENT METHOD FOR CALCULATING *H*-MATRICES

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ABSTRACT

A rapidly converging method for computing **H**-matrices appropriate to several studies of the scattering of polarized light is discussed.

We consider the equation of transfer relevant to a mixture of Rayleigh- and isotropic-scattering laws (Bond and Siewert 1971):

$$\mu \frac{\partial}{\partial \tau} \boldsymbol{I}(\tau, \mu) + \boldsymbol{I}(\tau, \mu) = \tfrac{1}{2}\omega \boldsymbol{Q}(\mu) \int_{-1}^{1} \boldsymbol{Q}^T(\mu')\boldsymbol{I}(\tau, \mu')d\mu' , \tag{1}$$

where $\boldsymbol{Q}^T(\mu)$ denotes the transpose of $\boldsymbol{Q}(\mu)$ and

$$\boldsymbol{Q}(\mu) = \tfrac{3}{2} \frac{(c+2)^{1/2}}{c+2} \begin{vmatrix} c\mu^2 + \frac{2}{3}(1-c) & (2c)^{1/2}(1-\mu^2) \\ \frac{1}{3}(c+2) & 0 \end{vmatrix} . \tag{2}$$

Here $\boldsymbol{I}(\tau, \mu)$, with elements $I_l(\tau, \mu)$ and $I_r(\tau, \mu)$, is the intensity two-vector, τ is the optical variable, and μ is the direction cosine (as measured from the positive τ-axis) of the propagating radiation. Further, $\omega \in [0, 1]$ is the single-scattering albedo, and $c \in [0, 1]$ is a measure of the Rayleigh component of the scattering law (Chandrasekhar 1950).

As discussed previously (Pahor 1968; Schnatz and Siewert 1971), the 2×2 **H**-matrix required for half-space applications is sufficiently specified by the nonlinear equation

$$\boldsymbol{H}(\mu)\left[\boldsymbol{I} - \mu \int_0^1 \boldsymbol{H}^T(\mu')\boldsymbol{\Psi}(\mu') \frac{d\mu'}{\mu' + \mu}\right] = \boldsymbol{I} \tag{3a}$$

and the linear constraint

$$\left[\boldsymbol{I} + \eta_0 \int_0^1 \boldsymbol{H}^T(\mu')\boldsymbol{\Psi}(\mu') \frac{d\mu'}{\mu' - \eta_0}\right]\boldsymbol{M}(\eta_0) = \boldsymbol{0} . \tag{3b}$$

Here η_0 is the positive zero, in the complex plane cut from -1 to 1 along the real line, of the dispersion function

$$\Lambda(z) = \det \boldsymbol{\Lambda}(z) = \det \left[\boldsymbol{I} + z \int_{-1}^{1} \boldsymbol{\Psi}(\mu) \frac{d\mu}{\mu - z}\right] , \tag{4}$$

where the characteristic function is

$$\boldsymbol{\Psi}(\mu) = \tfrac{1}{2}\omega \boldsymbol{Q}^T(\mu)\boldsymbol{Q}(\mu) . \tag{5}$$

In addition, $\boldsymbol{M}(\eta_0)$ is the *normalized* vector such that

$$\boldsymbol{M}^T(\eta_0)\boldsymbol{M}(\eta_0) = 1 \quad \text{and} \quad \boldsymbol{\Lambda}(\pm\eta_0)\boldsymbol{M}(\eta_0) = \boldsymbol{0} . \tag{6}$$

More explicitly, we note (Bond and Siewert 1971)

$$\boldsymbol{M}(\eta_0) = [\Lambda_{22}^2(\eta_0) + \Lambda_{12}^2(\eta_0)]^{-1/2} \begin{vmatrix} \Lambda_{22}(\eta_0) \\ -\Lambda_{12}(\eta_0) \end{vmatrix} , \tag{7}$$

where

$$\Lambda_{22}(\eta_0) = 1 - \frac{9\omega c}{2(c+2)}\left[(1-\eta_0^2)^2\eta_0 \tanh^{-1}\frac{1}{\eta_0} - \eta_0^2(\eta_0^2 - \tfrac{5}{3})\right] \quad (8a)$$

and

$$\Lambda_{12}(\eta_0) = -\frac{9\omega(2c)^{1/2}}{4(c+2)}\left\{[\tfrac{1}{3}(c+2) - c(1-\eta_0^2)](1-\eta_0^2)\eta_0 \tanh^{-1}\frac{1}{\eta_0} + [\tfrac{1}{3}(2-c) - c(1-\eta_0^2)]\eta_0^2\right\}. \quad (8b)$$

To solve equations (3) accurately by a straightforward iterative procedure has proved, for some choices of the parameters ω and c, to be a very slowly converging process (Schnatz and Siewert 1971; Bond and Siewert 1971). In fact, for conservative cases, from one to two hundred iterations to achieve significant accuracy is common.

In this Note, we wish to present explicitly an alternative calculational procedure, due to Pahor (1968), and to report that this alternative computational method is vastly superior to solving equations (3) directly.

Since equation (3a) alone does not uniquely specify the $\boldsymbol{H}$-matrix, the principal idea is to incorporate in the calculation the linear constraint, equation (3b). To this end, we write (Pahor 1968)

$$\boldsymbol{H}(z) = \boldsymbol{U}\boldsymbol{D}(z)\boldsymbol{A}(z)\boldsymbol{U}^T, \quad (9)$$

where $\boldsymbol{U}$ and $\boldsymbol{D}(z)$ are given by

$$\boldsymbol{U} = \begin{vmatrix} M_1(\eta_0) & -M_2(\eta_0) \\ M_2(\eta_0) & M_1(\eta_0) \end{vmatrix} \quad \text{and} \quad \boldsymbol{D}(z) = \begin{vmatrix} \dfrac{\eta_0(1+z)}{\eta_0 + z} & 0 \\ 0 & 1 \end{vmatrix}, \quad (10)$$

and $\boldsymbol{A}(z)$ is the 2×2 matrix to be determined. We note that $\boldsymbol{U}$ is a unitary matrix. If we substitute equation (9) into equation (3a), pre-multiply the resulting equation by $\boldsymbol{D}^{-1}(\mu)\boldsymbol{U}^T$, and then post-multiply by $\boldsymbol{U}\boldsymbol{D}(\mu)$, we find

$$\boldsymbol{A}(\mu)\left[\boldsymbol{D}(\mu) - \mu\int_0^1 \boldsymbol{A}^T(\mu')\boldsymbol{K}(\mu')\boldsymbol{D}^{-1}(-\mu')\boldsymbol{D}(\mu)\frac{d\mu'}{\mu'+\mu}\right] = \boldsymbol{I}, \quad (11)$$

where

$$\boldsymbol{K}(\mu') = \boldsymbol{D}(\mu')\boldsymbol{U}^T\boldsymbol{\Psi}(\mu')\boldsymbol{U}\boldsymbol{D}(-\mu'). \quad (12)$$

If we use the algebraic relation

$$\boldsymbol{D}(\mu) = \boldsymbol{D}(-\mu') - \frac{\eta_0(1-\eta_0)(\mu+\mu')}{(\eta_0-\mu')(\eta_0+\mu)}\begin{vmatrix} 1 & 0 \\ 0 & 0 \end{vmatrix} \quad (13)$$

with equations (9) and (12), equation (11) can be written as

$$\boldsymbol{A}(\mu)\left[\boldsymbol{D}(\mu) + \eta_0\mu\frac{1-\eta_0}{\eta_0+\mu}\boldsymbol{U}^T\int_0^1 \boldsymbol{H}^T(\mu')\boldsymbol{\Psi}(\mu')\frac{d\mu'}{\eta_0-\mu'}\boldsymbol{M}(\eta_0)\begin{vmatrix} 1 \\ 0 \end{vmatrix}^T - \mu\int_0^1 \boldsymbol{A}^T(\mu')\boldsymbol{K}(\mu')\frac{d\mu'}{\mu'+\mu}\right] = \boldsymbol{I}. \quad (14)$$

The linear constraint expressed by equation (3b) can now be used to reduce equation (14) to the computational form

$$\boldsymbol{A}(\mu)\left[\boldsymbol{I} - \mu\int_0^1 \boldsymbol{A}^T(\mu')\boldsymbol{K}(\mu')\frac{d\mu'}{\mu'+\mu}\right] = \boldsymbol{I}. \quad (15)$$

We note that if $\boldsymbol{A}(\mu)$ is a solution of equation (15), then the $\boldsymbol{H}$-matrix calculated from

$$\boldsymbol{H}(\mu) = \boldsymbol{U}\boldsymbol{D}(\mu)\boldsymbol{A}(\mu)\boldsymbol{U}^T\,, \qquad \mu \in [0, 1]\,, \tag{16}$$

will inherently satisfy the constraint, equation (3b).

To form the required matrices $\boldsymbol{D}(z)$ and $\boldsymbol{U}$, in general, we first must calculate the positive zero η_0 of the dispersion function which, when equation (4) is expanded, can be written as

$$\Lambda(z) = \frac{c}{8}\Lambda_1(z)\Lambda_2(z) + [1 - c + \tfrac{3}{2}c(1 - \omega)z^2]\Lambda_0(z)\,, \tag{17}$$

where

$$\Lambda_\alpha(z) = (-1)^\alpha + 3(1 - z^2)\Lambda_0(z) - (-1)^\alpha 3(1 - \omega)z^2\,, \qquad \alpha = 1 \text{ and } 2\,, \tag{18}$$

with

$$\Lambda_0(z) = 1 + \tfrac{1}{2}\omega z\int_{-1}^{1}\frac{d\mu}{\mu - z}\,. \tag{19}$$

For conservative cases $\omega \to 1$, and thus $\eta_0 \to \infty$; we note the required special forms

$$\boldsymbol{D}(z) = \begin{vmatrix} 1 + z & 0 \\ 0 & 1 \end{vmatrix} \quad \text{and} \quad \boldsymbol{U} = (c + 2)^{-1/2}\begin{vmatrix} \sqrt{2} & -\sqrt{c} \\ \sqrt{c} & \sqrt{2} \end{vmatrix}\,, \qquad \omega = 1\,. \tag{20}$$

To calculate $\boldsymbol{H}(\mu)$ from equation (16), we have solved equation (15) iteratively for various choices of $\omega \in [0, 1]$ and $c \in [0, 1]$; we found the rate of convergence to be vastly superior to that reported previously (Schnatz and Siewert 1971; Bond and Siewert 1971). For example, the most slowly converging case, $\omega = 1$ and $c = 1$, converged to fourteen significant figures in eighteen iterations for an 81-point improved Gaussian-quadrature (Kronrod 1965) representation of the integration process.

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