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On eigenvalue calculations for radiative transfer models that include polarization effects

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I. Introduction

In a recent paper concerning the scattering of polarized light [1] Siewert and Pinheiro investigated the equation of transfer

$$\mu \frac{\partial}{\partial \tau} \boldsymbol{I}(\tau, \mu) + \boldsymbol{I}(\tau, \mu) = \frac{\omega}{2} \sum_{l=0}^{L} \boldsymbol{\Pi}_l(\mu) \boldsymbol{B}_l \int_{-1}^{1} \boldsymbol{\Pi}_l(\mu') \boldsymbol{I}(\tau, \mu')\, d\mu' \tag{1}$$

that defines the azimuthally symmetric component

$$\boldsymbol{I}(\tau, \mu) = \frac{1}{2\pi} \int_0^{2\pi} \boldsymbol{I}(\tau, \mu, \varphi)\, d\varphi \tag{2}$$

of the complete solution. Here the density vector $\boldsymbol{I}(\tau, \mu, \varphi)$ has the four Stokes parameters I, Q, U and V as components [2, 3, 4], $\omega \in (0, 1]$ is the albedo for single scattering and

$$\boldsymbol{\Pi}_l(\mu) = \mathrm{diag}\,\{P_l(\mu), R_l(\mu), R_l(\mu), P_l(\mu)\}, \tag{3}$$

where $P_l(\mu)$ denotes the Legendre polynomial of order l, $R_0(\mu) = R_1(\mu) = 0$ and, for $l \geq 2$,

$$R_l(\mu) = \left[\frac{(l-2)!}{(l+2)!}\right]^{1/2} (1 - \mu^2) \frac{d^2}{d\mu^2} P_l(\mu). \tag{4}$$

In addition, the matrices

$$\boldsymbol{B}_l = \begin{vmatrix} \beta_l & \gamma_l & 0 & 0 \\ \gamma_l & \alpha_l & 0 & 0 \\ 0 & 0 & \zeta_l & -\varepsilon_l \\ 0 & 0 & \varepsilon_l & \delta_l \end{vmatrix} \tag{5}$$

are defined in terms of the basic constants $\{\alpha_l, \beta_l, \gamma_l, \delta_l, \varepsilon_l, \zeta_l\}$ that have been used [5] to represent a scattering matrix of the form considered by Hovenier [6], *viz.*

$$\boldsymbol{F}(\xi) = \begin{vmatrix} a_1(\xi) & b_1(\xi) & 0 & 0 \\ b_1(\xi) & a_2(\xi) & 0 & 0 \\ 0 & 0 & a_3(\xi) & b_2(\xi) \\ 0 & 0 & -b_2(\xi) & a_4(\xi) \end{vmatrix}. \tag{6}$$

We note that $\beta_0 = 1$ and that $\alpha_0 = \alpha_1 = \gamma_0 = \gamma_1 = \varepsilon_0 = \varepsilon_1 = \zeta_0 = \zeta_1 = 0$.

Although $\boldsymbol{I}(\tau, \mu)$ is a four-vector, it is apparent from Eqs. (1), (3) and (5) that it is sufficient to investigate two two-vector problems. We therefore write

$$\mu \frac{\partial}{\partial \tau} \boldsymbol{\Psi}(\tau, \mu) + \boldsymbol{\Psi}(\tau, \mu) = \frac{\omega}{2} \sum_{l=0}^{L} \boldsymbol{P}_l(\mu) \boldsymbol{C}_l \int_{-1}^{1} \boldsymbol{P}_l(\mu') \boldsymbol{\Psi}(\tau, \mu')\, d\mu', \tag{7}$$

where

$$\boldsymbol{P}_l(\mu) = \mathrm{diag}\,\{P_l(\mu), R_l(\mu)\}, \tag{8}$$

and consider two cases:

$$A\colon\ \boldsymbol{\Psi}(\tau, \mu) = \begin{vmatrix} I(\tau, \mu) \\ Q(\tau, \mu) \end{vmatrix} \quad \text{with} \quad \boldsymbol{C}_l = \begin{vmatrix} \beta_l & \gamma_l \\ \gamma_l & \alpha_l \end{vmatrix} \tag{9a, b}$$

and

$$B\colon\ \boldsymbol{\Psi}(\tau, \mu) = \begin{vmatrix} V(\tau, \mu) \\ U(\tau, \mu) \end{vmatrix} \quad \text{with} \quad \boldsymbol{C}_l = \begin{vmatrix} \delta_l & \varepsilon_l \\ -\varepsilon_l & \zeta_l \end{vmatrix}. \tag{9c, d}$$

In developing elementary solutions of Eq. (7), Siewert and Pinheiro [1] found that the required eigenvalues were the zeros of det $\boldsymbol{\Lambda}(z)$, $z \notin [-1, 1]$, where the dispersion matrix $\boldsymbol{\Lambda}(z)$ was expressed as

$$\boldsymbol{\Lambda}(z) = \boldsymbol{I} + \frac{\omega}{2} z \int_{-1}^{1} \boldsymbol{K}(\mu) \sum_{l=0}^{L} \boldsymbol{P}_l(\mu) \boldsymbol{C}_l \boldsymbol{G}_l(z) \frac{d\mu}{\mu - z} \tag{10}$$

with

$$\boldsymbol{K}(\mu) = \mathrm{diag}\,\{1, R_2(\mu)\}. \tag{11}$$

In addition, the 2×2 polynomial matrices $\boldsymbol{G}_l(z)$ are defined as

$$\boldsymbol{G}_0(z) = \mathrm{diag}\,\{1, 0\}, \quad \boldsymbol{G}_1(z) = \mathrm{diag}\,\{k_0 z, 0\}, \tag{12a, b}$$

$$\boldsymbol{G}_2(z) = \mathrm{diag}\,\{\tfrac{1}{2}(k_0 k_1 z^2 - 1), 1\} \tag{12c}$$

and, for $l \geq 2$,

$$\boldsymbol{G}_{l+1}(z) = \boldsymbol{J}_{l+1}^{-1} [z \boldsymbol{h}_l \boldsymbol{G}_l(z) - \boldsymbol{J}_l \boldsymbol{G}_{l-1}(z)]. \tag{13}$$

Here

$$k_l = 2l + 1 - \omega C_l^{11}, \tag{14}$$

$$\boldsymbol{J}_l = \operatorname{diag}\{l, (1-\delta_{0,l})(1-\delta_{1,l})(l^2-4)^{1/2}\} \tag{15}$$

and

$$\boldsymbol{h}_l = (2l+1)\boldsymbol{I} - \omega \boldsymbol{C}_l. \tag{16}$$

We now proceed to develop some additional representations of $\Lambda(z)$ and to deduce, for $z \notin [-1, 1]$, a way to compute the zeros of det $\Lambda(z)$ that provides an alternative method to that discussed previously [1].

II. The dispersion matrix

We now follow a procedure used by İnönü [7] and Garcia and Siewert [8] in studies of the scalar form of the equation of transfer and let

$$\boldsymbol{Q}_l(z) = \frac{1}{2}\int_{-1}^{1} \boldsymbol{K}(\mu)\boldsymbol{P}_l(\mu)\frac{d\mu}{z-\mu} \tag{17}$$

so that we can write Eq. (10) as

$$\boldsymbol{\Lambda}(z) = \boldsymbol{I} - \omega z \sum_{l=0}^{L} \boldsymbol{Q}_l(z)\boldsymbol{C}_l\boldsymbol{G}_l(z). \tag{18}$$

As previously reported [1, 5] the matrices $\boldsymbol{P}_l(z)$ satisfy

$$(2l+1)z\boldsymbol{P}_l(z) = \boldsymbol{J}_{l+1}\boldsymbol{P}_{l+1}(z) + \boldsymbol{J}_l\boldsymbol{P}_{l-1}(z) \tag{19}$$

and

$$\int_{-1}^{1} \boldsymbol{P}_l(\mu)\boldsymbol{P}_{l'}(\mu)\,d\mu = \left(\frac{2}{2l+1}\right)\operatorname{diag}\{1, (1-\delta_{0,l})(1-\delta_{1,l})\}\,\delta_{l,l'}, \tag{20}$$

and thus we can readily deduce from Eq. (17) that

$$(2l+1)z\boldsymbol{Q}_l(z) = \operatorname{diag}\{\delta_{0,l}, \delta_{2,l}\} + \boldsymbol{J}_{l-1}\boldsymbol{Q}_{l-1}(z) + \boldsymbol{J}_l\boldsymbol{Q}_{l-1}(z). \tag{21}$$

If we now multiply Eq. (21) on the right by $\boldsymbol{G}_l(z)$, then multiply

$$\boldsymbol{h}_l z\boldsymbol{G}_l(z) = \boldsymbol{J}_{l-1}\boldsymbol{G}_{l-1}(z) + \boldsymbol{J}_l\boldsymbol{G}_{l-1}(z) \tag{22}$$

on the left by $\boldsymbol{Q}_l(z)$, subtract the resulting two equations one from the other and sum the result from $l = 0$ to $l = L$, we find we can use the ensuing expression to write Eq. (18) as

$$\boldsymbol{\Lambda}(z) = \boldsymbol{J}_{L+1}[\boldsymbol{Q}_L(z)\boldsymbol{G}_{L-1}(z) - \boldsymbol{Q}_{L+1}(z)\boldsymbol{G}_L(z)]. \tag{23}$$

In a similar way we can eliminate between Eqs. (19) and (21) to deduce that

$$\boldsymbol{K}(z) = \boldsymbol{J}_{L+1}[\boldsymbol{Q}_L(z)\boldsymbol{P}_{L+1}(z) - \boldsymbol{Q}_{L+1}(z)\boldsymbol{P}_L(z)], \tag{24}$$

and we can eliminate between Eqs. (19) and (22) to obtain

$$2z\boldsymbol{\Psi}(z) = \boldsymbol{K}(z)\boldsymbol{J}_{L+1}[\boldsymbol{P}_{L+1}(z)\boldsymbol{G}_L(z) - \boldsymbol{P}_L(z)\boldsymbol{G}_{L+1}(z)], \tag{25}$$

where

$$\boldsymbol{\Psi}(z) = \frac{\omega}{2}\boldsymbol{K}(z)\sum_{l=0}^{L}\boldsymbol{P}_l(z)\boldsymbol{C}_l\boldsymbol{G}_l(z). \tag{26}$$

Multiplying Eq. (23) by $\boldsymbol{P}_{L+1}(z)$ and using Eqs. (24) and (25), we find

$$\boldsymbol{P}_{L+1}(z)\boldsymbol{\Lambda}(z) = \boldsymbol{K}(z)\boldsymbol{G}_{L+1}(z) - 2z\boldsymbol{K}^{-1}(z)\boldsymbol{Q}_{L+1}(z)\boldsymbol{\Psi}(z), \tag{27}$$

and then considering that $z \notin [-1, 1]$, so that det $\boldsymbol{P}_{L+1}(z) \neq 0$, we can write

$$\boldsymbol{\Lambda}(z) = \boldsymbol{P}_{L+1}^{-1}(z)[\boldsymbol{K}(z)\boldsymbol{G}_{L+1}(z) - 2z\boldsymbol{K}^{-1}(z)\boldsymbol{Q}_{L+1}(z)\boldsymbol{\Psi}(z)]. \tag{28}$$

As $R_l(z)$ can [4] be expressed as

$$R_l(z) = \frac{1}{4}\left[\frac{(l+2)(l+1)}{l(l-1)}\right]^{1/2}(1-z^2)P_{l-2}^{(2,2)}(z), \tag{29}$$

where $P_l^{(\alpha,\beta)}(z)$ is used to denote a Jacobi polynomial [9] of degree l, we can, for $z \notin [-1, 1]$, use the asymptotic formulas for the Legendre polynomials and the Jacobi polynomials that are given [as Eqs. (8.21.1) and (8.21.9)] by Szegö [10] to conclude that

$$\lim_{L\to\infty}\boldsymbol{P}_{L+1}^{-1}(z)\boldsymbol{Q}_{L+1}(z) = \boldsymbol{0},\ z \notin [-1, 1]. \tag{30}$$

We therefore can readily deduce from Eq. (28) that

$$\boldsymbol{\Lambda}(z) = \lim_{L\to\infty}\boldsymbol{P}_{L+1}^{-1}(z)\boldsymbol{K}(z)\boldsymbol{G}_{L+1}(z),\ z \notin [-1, 1]. \tag{31}$$

It follows that the zeros of det $\boldsymbol{G}_{L+1}(z)$, $z \notin [-1, 1]$, will converge as $L \to \infty$ to the zeros of det $\boldsymbol{\Lambda}(z)$, $z \notin [-1, 1]$. We thus can, for $\nu_\beta, \xi_\beta \notin [-1, 1]$, approximate the requirement [1]

$$\boldsymbol{\Lambda}(\nu_\beta)\boldsymbol{M}(\nu_\beta) = \boldsymbol{0} \tag{32}$$

by

$$\boldsymbol{G}_{N+1}(\xi_\beta)\boldsymbol{M}_{N+1}(\xi_\beta) = \boldsymbol{0} \tag{33}$$

for sufficiently large N and for ξ_β sufficiently close to ν_β. Here $\boldsymbol{M}(\nu_\beta)$ and $\boldsymbol{M}_{N+1}(\xi_\beta)$ are null vectors of $\boldsymbol{\Lambda}(\nu_\beta)$ and $\boldsymbol{G}_{N+1}(\xi_\beta)$ respectively. Finally we can use Eqs. (19), (22) and (31) to show that

$$\Lambda(\infty) = \lim_{|z|\to\infty}\det\boldsymbol{\Lambda}(z) = \prod_{l=0}^{L}\det\left(\frac{1}{2l+1}\right)\boldsymbol{h}_l. \tag{34}$$

III. The eigenvalues

We note that an Nth order generalized spherical harmonics solution of Eq. (7) requires as eigenvalues *all* of the zeros of det $\boldsymbol{G}_{N+1}(z)$. We therefore proceed to formulate a convenient computational technique that allows us to find all of the zeros of det $\boldsymbol{G}_{N+1}(z)$; in order to avoid a zero at the origin, we consider N to be odd. The method, which is a generalization of the one that has proved accurate and easy to use for the scalar case [11, 12], is based on the fact that the 2×2 polynomial matrices $\boldsymbol{G}_l(z)$ for $l \geq 0$ are defined, after the first three are given, by Eq. (13). If we multiply Eq. (22) on the right by

$$\boldsymbol{M}_{N+1}(z) = \begin{vmatrix} G^{22}_{N+1}(z) + G^{12}_{N+1}(z) \\ -G^{21}_{N+1}(z) - G^{11}_{N+1}(z) \end{vmatrix} \tag{35}$$

and define

$$\boldsymbol{T}_l(z) = \boldsymbol{G}_l(z)\,\boldsymbol{M}_{N+1}(z), \tag{36}$$

then we obtain the system of equations

$$\boldsymbol{U}_1\,\boldsymbol{T}_1(z) = z\,\boldsymbol{T}_0(z) \tag{37a}$$

$$\boldsymbol{L}_l\,\boldsymbol{T}_{l-1}(z) + \boldsymbol{U}_{l+1}\,\boldsymbol{T}_{l+1}(z) = z\,\boldsymbol{T}_l(z), \quad l = 1, 2, \ldots, N-1, \tag{37b}$$

$$\boldsymbol{L}_N\,\boldsymbol{T}_{N-1}(z) = z\,\boldsymbol{T}_N(z) \tag{37c}$$

where for $l = 1, 2, \ldots, N$

$$\boldsymbol{U}_l = \boldsymbol{h}^{-1}_{l-1}\,\boldsymbol{J}_l \tag{38}$$

and

$$\boldsymbol{L}_l = \boldsymbol{h}_l^{-1}\,\boldsymbol{J}_l. \tag{39}$$

Letting $\boldsymbol{T}(\xi)$ denote the vector with elements $\boldsymbol{T}_0(\xi), \boldsymbol{T}_1(\xi), \ldots, \boldsymbol{T}_N(\xi)$, we write Eq. (37) as

$$\boldsymbol{W}\,\boldsymbol{T}(\xi) = \xi\,\boldsymbol{T}(\xi) \tag{40}$$

where the $(2N+2)\times(2N+2)$ matrix $\boldsymbol{W}$ is 2×2-block tridiagonal; *i.e.*

$$\boldsymbol{W} = \begin{vmatrix} \boldsymbol{0} & \boldsymbol{U}_1 & & \\ \boldsymbol{L}_1 & \ddots & \ddots & \\ & \ddots & \ddots & \boldsymbol{U}_N \\ & & \boldsymbol{L}_N & \boldsymbol{0} \end{vmatrix} \tag{41}$$

We note that the matrix $\boldsymbol{W}$ has two rows and two columns that are all zeros, and thus we conclude that the $2N$ zeros of det $\boldsymbol{G}_{N-1}(z)$ are the $2N$ non-zero eigenvalues of $\boldsymbol{W}$.

In order to be specific we consider the $I-Q$ problem and the $V-U$ problem separately.

A: *The $I-Q$ problem.* As there are available in the EISPACK package [13, 14] efficient and accurate FORTRAN subroutines for finding the eigenvalues of banded, real symmetric matrices, we proceed to reduce our eigenvalue problem to that form. First of all, however, some restrictions on the constants $\{\alpha_l, \beta_l, \gamma_l\}$ are relevant. We define

$$h_l = 2l+1-\omega\beta_l \quad \text{and} \quad \eta_l = 2l+1-\omega\alpha_l \tag{42a, b}$$

and make the assumptions that

$$h_l > 0 \quad \text{and} \quad h_l\eta_l - \omega^2\gamma_l^2 > 0 \tag{43a, b}$$

for all $l \geq 0$ if $\omega \neq 1$ and for all $l \geq 1$ if $\omega = 1$. Now since

$$\boldsymbol{h}_l = \begin{vmatrix} h_l & -\omega\gamma_l \\ -\omega\gamma_l & \eta_l \end{vmatrix} \tag{44}$$

is symmetric we define

$$\boldsymbol{H}_l = h_l^{-1/2} \begin{vmatrix} h_l & 0 \\ -\omega\gamma_l & \Delta_l \end{vmatrix}, \tag{45}$$

with

$$\Delta_l = (h_l\eta_l - \omega^2\gamma_l^2)^{1/2} \tag{46}$$

so that we can write

$$\boldsymbol{h}_l = \boldsymbol{H}_l\,\boldsymbol{H}_l^T. \tag{47}$$

Now defining

$$\boldsymbol{S}_l = \boldsymbol{H}^T_{l-1}, \quad l = 1, 2, 3, \ldots, N+1, \tag{48}$$

we find that the transformation

$$\boldsymbol{X} = \operatorname{diag}\{\boldsymbol{S}_1, \boldsymbol{S}_2, \ldots, \boldsymbol{S}_{N+1}\}\,\boldsymbol{W}\,\operatorname{diag}\{\boldsymbol{S}_1^{-1}, \boldsymbol{S}_2^{-1}, \ldots, \boldsymbol{S}_{N+1}^{-1}\} \tag{49}$$

yields the symmetric 2×2-block tridiagonal matrix

$$\boldsymbol{X} = \begin{vmatrix} \boldsymbol{0} & \boldsymbol{X}_1 & & \\ \boldsymbol{X}_1^T & \ddots & \ddots & \\ & \ddots & \ddots & \boldsymbol{X}_N \\ & & \boldsymbol{X}_N^T & \boldsymbol{0} \end{vmatrix} \tag{50}$$

where

$$\boldsymbol{X}_l = \boldsymbol{H}^{-1}_{l-1}\,\boldsymbol{J}_l\,\boldsymbol{H}_l^{-T} \tag{51}$$

for $l = 1, 2, 3, \ldots, N$.

To develop an alternative and computationally more efficient method for finding the eigenvalues of X, we first let $A_0(\xi), A_1(\xi), \ldots, A_N(\xi)$ denote the 2-vector components of $A(\xi)$, so that

$$X A(\xi) = \xi A(\xi). \tag{52}$$

Then we can eliminate the odd components of $A(\xi)$ in the system of equations represented by Eq. (52) to obtain an equivalent problem

$$\boldsymbol{Y}\boldsymbol{B}(\xi) = \xi^2 \boldsymbol{B}(\xi) \tag{53}$$

where the $(N+1)\times(N+1)$ symmetric $\boldsymbol{Y}$ matrix is given by

$$\boldsymbol{Y} = \begin{vmatrix} X_1 X_1^T & \boldsymbol{Y}_1 & & \\ \boldsymbol{Y}_1^T & \boldsymbol{D}_2 & \ddots & \\ & \ddots & \ddots & \boldsymbol{Y}_{J-1} \\ & & \boldsymbol{Y}_{J-1}^T & \boldsymbol{D}_J \end{vmatrix} \tag{54}$$

with $J = (N+1)/2$,

$$\boldsymbol{D}_\alpha = X_{2\alpha-2}^T X_{2\alpha-2} + X_{2\alpha-1} X_{2\alpha-1}^T, \tag{55}$$

for $\alpha = 2, \ldots J$, and

$$\boldsymbol{Y}_\alpha = X_{2\alpha-1} X_{2\alpha}, \tag{56}$$

for $\alpha = 1, 2, \ldots, J-1$. Noting that the matrix $\boldsymbol{Y}$ has one row and one column with all zeros and that for N odd the zeros of det $\boldsymbol{G}_{N+1}(z)$ occur in $\pm$ pairs, we find that the N squares of the $2N$ zeros of det $\boldsymbol{G}_{N+1}(z)$ are the N non-zero eigenvalues of $\boldsymbol{Y}$. Of course, we can obtain an equivalent eigenvalue problem in a similar way by eliminating the even components of $A(\xi)$.

Finally we note from Eq. (51) that X_1 is unbounded for the special case of $\omega = 1$, and thus a modification to the foregoing analysis is required for this case. We can readily deduce from Eq. (52) that two of the eigenvalues coalesce at infinity and that $A_0(\xi)$ and $A_1(\xi) \to 0$ as $\omega \to 1$. We therefore can find all of the $2(N-1)$ bounded zeros of det $\boldsymbol{G}_{N-1}(z)$ for the case $\omega = 1$ by deleting the first four rows and columns of X and finding the eigenvalues of

$$X_s = \begin{vmatrix} \boldsymbol{0} & X_3 & & \\ X_3^T & \ddots & \ddots & \\ & \ddots & \ddots & X_N \\ & & X_N^T & \boldsymbol{0} \end{vmatrix}. \tag{57}$$

Alternatively, the squares of the $2(N-1)$ bounded zeros are the $N-1$ eigenvalues of

$$\boldsymbol{Y}_s = \begin{vmatrix} X_3 X_3^T & \boldsymbol{Y}_2 & & \\ \boldsymbol{Y}_2^T & \boldsymbol{D}_3 & \ddots & \\ & \ddots & \ddots & \boldsymbol{Y}_{J-1} \\ & & \boldsymbol{Y}_{J-1}^T & \boldsymbol{D}_J \end{vmatrix}. \tag{58}$$

B: *The V–U problem.* Here

$$\boldsymbol{h}_l = \begin{vmatrix} m_l & -\omega\varepsilon_l \\ \omega\varepsilon_l & n_l \end{vmatrix} \tag{59}$$

and we assume that

$$m_l = 2l + 1 - \omega\delta_l > 0 \quad \text{and} \quad n_l = 2l + 1 - \omega\zeta_l > 0 \tag{60a, b}$$

for all l. We define

$$\boldsymbol{H}_l = m_l^{-1/2} \begin{vmatrix} m_l & 0 \\ -\omega\varepsilon_l & D_l \end{vmatrix}, \tag{61}$$

where

$$D_l = [m_l n_l + \omega^2 \varepsilon_l^2]^{1/2}, \tag{62}$$

so that we can write

$$\boldsymbol{h}_l = \boldsymbol{E}\boldsymbol{H}_l \boldsymbol{E}\boldsymbol{H}_l^T \tag{63}$$

where

$$\boldsymbol{E} = \text{diag}\,\{1, -1\}. \tag{64}$$

Now we let

$$\boldsymbol{S}_1 = \text{diag}\,\{(1-\omega\delta_0)^{1/2}, 1\} \tag{65a}$$

and

$$\boldsymbol{S}_l = \begin{vmatrix} 1 & 0 \\ 0 & i \end{vmatrix} \boldsymbol{H}_{l-1}^T, \quad l = 2, 3, \cdots, N+1, \tag{65b}$$

and find that

$$X = \text{diag}\,\{\boldsymbol{S}_1, \boldsymbol{S}_2, \cdots, \boldsymbol{S}_{N-1}\}\, \boldsymbol{W}\, \text{diag}\,\{\boldsymbol{S}_1^{-1}, \boldsymbol{S}_2^{-1}, \cdots, \boldsymbol{S}_{N+1}^{-1}\} \tag{66}$$

yields

$$X = \begin{vmatrix} \boldsymbol{0} & X_1 & & \\ X_1^T & \ddots & \ddots & \\ & \ddots & \ddots & X_N \\ & & X_N^T & \boldsymbol{0} \end{vmatrix} \tag{67}$$

where

$$X_1 = \operatorname{diag}\{[(1-\omega\delta_0)(3-\omega\delta_1)]^{-1/2}, 0\} \quad \text{and} \quad X_l = C^* H_{l-1}^{-1} E J_l H_l^{-T} C^*,$$

for $l = 2, 3, \cdots, N+1$. In addition (68 a, b)

$$C^* = \operatorname{diag}\{1, -i\}. \tag{69}$$

It is apparent that Eq. (67) defines a banded symmetric matrix which, for N odd, has $2N$ non-zero eigenvalues that are the desired zeros of det $G_{N+1}(z)$. It is also clear that the N non-zero eigenvalues of

$$Y = \begin{vmatrix} X_1 X_1^T & Y_1 & & & \\ Y_1^T & D_3 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & Y_{J-1} \\ & & & Y_{J-1}^T & D_J \end{vmatrix} \tag{70}$$

provide the N squares of the zeros of det $G_{N+1}(z)$. Here again

$$Y_\alpha = X_{2\alpha-1} X_{2\alpha} \tag{71}$$

for $\alpha = 1, 2, \cdots, J-1$ and

$$D_\alpha = X_{2\alpha-2}^T X_{2\alpha-2} + X_{2\alpha-1} X_{2\alpha-1}^T \tag{72}$$

for $\alpha = 2, 3, \cdots, J$.

We note that for the $I-Q$ problem the symmetric matrices X and Y are real, and so to find the eigenvalues we can use the EISPACK [13, 14] subroutines *BANDR* and *IMTQL1* which make use of the fact that X and Y are banded (7 bands). Although we have obtained symmetric banded matrices X and Y for the $V-U$ problem, we *cannot* use the subroutine *BANDR* to reduce either X or Y to tridiagonal form because they are not real (the 7 bands are alternately real and purely imaginary). As we do not at present have available a method for dealing efficiently with the X and Y matrices for the $V-U$ problem, we return our attention to the real non-symmetric banded matrix W as given by Eq. (41). If we carry out on W a "shuffle" two columns at a time and follow that by a similar row "shuffle", then we find the equivalent eigenvalue problem

$$\begin{vmatrix} 0 & A \\ B & 0 \end{vmatrix} E = \xi E \tag{73}$$

where

$$A = \begin{vmatrix} U_1 & & & \\ L_2 & U_3 & & \\ & L_4 & \ddots & \\ & & L_{N-1} & U_N \end{vmatrix} \tag{74}$$

and

$$B = \begin{vmatrix} L_1 & U_2 & & \\ & L_3 & U_4 & \\ & & \ddots & U_{N-1} \\ & & & L_N \end{vmatrix}. \tag{75}$$

It is clear from Eq. (73) that we can find the desired eigenvalues ξ by considering

$$\Upsilon E_T = \xi^2 E_T \tag{76 a}$$

or

$$\Xi E_B = \xi^2 E_B \tag{76 b}$$

where $\Upsilon = AB$ and $\Xi = BA$. To be explicit, we write, for example,

$$\Upsilon = \begin{vmatrix} U_1 L_1 & U_1 U_2 & & & \\ L_2 L_1 & U_3 L_3 + L_2 U_2 & U_3 U_4 & & \\ & L_4 L_3 & \ddots & \ddots & \\ & & \ddots & \ddots & U_{N-2} U_{N-1} \\ & & & L_{N-1} L_{N-2} & U_N L_N + L_{N-1} U_{N-1} \end{vmatrix} \tag{77}$$

where we continue to consider N to be odd.

IV. Numerical results

For our numerical examples of the foregoing development, we use the three basic scattering laws considered by Vestrucci and Siewert [15]. The first of these three problems (model I) was introduced by Kuščer and Ribarič [16] for the scattering of light, with wave number k, by small spherical particles of radius a. The basic constants $\{\alpha, \beta, \gamma, \delta, \varepsilon, \zeta\}$ for this model are given in terms of

$$\alpha = (ka)^2 (n^2+2)^2 [30(n^2+2) + 36(ka)^2(n^2-2)]^{-1} \tag{78 a}$$

and

$$\beta = 5(ka)^2 (n^2+2)^2 (2n^2+3)^{-1} [30(n^2+2) + 36(ka)^2(n^2-2)]^{-1} \tag{78 b}$$

in Table 1. Here n is the index of refraction of the particle with respect to the surrounding medium. In Table 2 we list, for the specific case of $n = 1.33$ and $ka = \frac{1}{2}$, what we believe to be converged (as $N \to 39$) results for the zeros of det $\Lambda(z)$ relevant to the $I-Q$ problems for the two cases $\omega = 0.99$ and $\omega = 1$. These zeros, as well as those for the $I-Q$ problems for models II and III, were obtained by using the *FORTRAN* subroutines *BANDR* and *IMTQL1* of the EISPACK program package [13, 14] to find all of the eigenvalues of both the X and Y matrices.

Table 1
The basic constants for model I.

l	α_l	β_l	γ_l	δ_l	ε_l	ζ_l
0	0	1	0	2α	0	0
1	0	$3(\alpha + \frac{3}{5}\beta)$	0	$\frac{3}{2}$	0	0
2	3	$\frac{1}{2}$	$-\frac{1}{2}(6)^{1/2}$	$\alpha + 3\beta$	0	$6(\alpha + \frac{1}{3}\beta)$
3	4β	$\frac{6}{5}\beta$	$-\frac{2}{5}(30)^{1/2}\beta$	0	0	0

Table 2
The zeros of det $\Lambda(z)$ for the I–Q problem.

Model	$\omega = 0.99$	$\omega = 1$
I	5.943273020500	∞
II	1.019535723105	1.025112345119
	8.052579861387	∞
III	1.030780435341	1.032732805841
	1.038869411971	1.040948232700
	1.139072646734	1.143424021509
	1.153451577057	1.157940124966
	1.392584925216	1.406188855190
	1.454513843050	1.473542228691
	10.153828385407	∞

Model II is for the Mie scattering of light, with wavelength $\lambda = 0.951\,\mu$m, by a gamma distribution [17] of spherical particles with an effective radius $r_{eff} = 0.2\,\mu$m, effective variance $v_{eff} = 0.07$ and index of refraction $n = 1.44$. For this problem we use the constants $\{\alpha, \beta, \gamma, \delta, \varepsilon, \zeta\}$ reported, with $L = 13$, by Vestrucci and Siewert [15]. Model III is similar to model II but for the case $\lambda = 0.782\,\mu$m, $r_{eff} = 1.05\,\mu$m, $v_{eff} = 0.07$ and $n = 1.43$. Again we use the constants $\{\alpha, \beta, \gamma, \delta, \varepsilon, \zeta\}$, with $L = 60$, given previously [15]. We note that the constants $\{\alpha, \beta, \gamma, \delta, \varepsilon, \zeta\}$ for all three of these test problems were deduced [16, 18, 19] for the case of $\omega = 1$; however, to avoid tabulating more of these constants, we use these same constants for the case $\omega = 0.99$.

We note that the results given in Table 2 were obtained for model II as $N \to 39$ and for model III as $N \to 99$; in all cases the results have been confirmed by using the method of ref. 1 to compute the zeros of det $\Lambda(z)$. In addition, since a generalized spherical harmonics solution of Eq. (1) requires all of the zeros of det $\boldsymbol{G}_{N+1}(\xi)$, we have used forward recursion to compute the $\boldsymbol{G}$ polynomials and thus to conclude, by investigating det $\boldsymbol{G}_{N+1}(\xi \pm \varepsilon)$, that the eigenvalues $\xi \in [0,1]$ of the $\boldsymbol{Y}$ matrix found for the considered I–Q problems were correct to at least twelve significant figures for the values of N used.

For the V–U problems we have used the driver subroutine ***RG*** in the EISPACK package [13] to find the desired zeros of det $\Lambda(z)$ by computing the eigenvalues of both $\boldsymbol{W}$ and $\boldsymbol{Y}$. It is clear, of course, that the $\boldsymbol{Y}$ matrix is $(N+1) \times (N+1)$, with one row and one column of zeros, and so $\boldsymbol{Y}$ has an advantage

Table 3
The zeros of det $\Lambda(z)$ for the V–U problem.

Model	$\omega = 0.99$	$\omega = 1$
I	1.190017413515	1.195085765596
II	1.896261279525	1.927064027809
III	1.028957515744 ± i4.81030348741 (−3)	1.030742388691 ± i4.97361854630 (−3)
	1.133801054671 ± i2.359049300598 (−3)	1.137760548820 ± i2.434360980922 (−3)
	1.364325970300 ± i1.068168843827 (−2)	1.376053759131 ± i1.198389958861 (−2)
	3.288868706929	3.428684684420

over the $\boldsymbol{W}$ matrix, which is $(2N+2) \times (2N+2)$, in that less computer storage is required for the calculation of the eigenvalues. We also found that we could use the subroutine ***RG*** even in very high order ($N = 499$) to find the eigenvalues of $\boldsymbol{Y}$. On the other hand, we were not able to use ***RG*** to find the eigenvalues of $\boldsymbol{W}$ for, say, $N \to 59$. We list in Table 3 what we believe to be converged results for the zeros of det $\Lambda(z)$ for the V–U problems corresponding to the three scattering laws considered. It is clear that for V–U problems we can have complex zeros of det $\Lambda(z)$, $z \notin [-1, 1]$. We also found complex zeros of det $\boldsymbol{G}_{N+1}(z)$ that had a real part contained in the interval (0,1) of the real axis. We also found, as we expected, that the imaginary parts of these complex zeros appeared to diminish as N was increased.

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Abstract

Several representations of the dispersion matrix $\Lambda(z)$ basic to analytical solutions for a theory of radiative transfer that includes the effects of polarization are reported, and a method for computing the zeros of det $\Lambda(z)$ is discussed. Numerical results are given for several specific models.

Zusammenfassung

Verschiedene Darstellungen der Dispersionsmatrix $\Lambda(z)$, welche grundlegende Bedeutung für die analytischen Lösungen der Theorie der Strahlungsübertragung mit Polarisation hat, werden angegeben. Eine Methode zur Berechnung der Nullstellen von det $\Lambda(z)$ wird diskutiert. Es werden numerische Ergebnisse für verschiedene Modelle angegeben.

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Convergence of the inner-outer iteration scheme

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1. Introduction

The problem of determining the multiplication factor and the fundamental mode neutron distribution within the finite differenced approximation to the neutron diffusion equation is usually solved with the inner-outer iteration scheme. The inner iterations are carried out to obtain the neutron flux distribution from a given fission source distribution while in the outer iterations the fission source and the multiplication factor are improved. Hageman [1] has shown that the eigenvalue problem of multigroup diffusion theory is modified when finite number of inner iterations are performed. Though the conditions required for the convergence of inner-outer scheme have not been analysed by Hageman [1], he has shown that the converged solutions are the fundamental mode and eigen value. From numerical experimentation it has been observed that the inner-outer iteration scheme converges when a "sufficient number" of inner iterations are performed [1, 2, 3] and the convergence of the scheme depends on the number of inner iterations [1, 2]. However, the mathematical analysis of the scheme has been carried out only for few special cases [2]. It appears that the main difficulties in the analysis stem from the non-linear nature of the scheme (since the fundamental eigenvalue also is unknown) and the non-commutation of the inner and outer iteration matrices.

In this paper we attempt to derive a set of sufficient conditions which would guarantee convergence of the scheme. Accordingly, in Sec. 2 we start from the modified eigenvalue problem of Hageman [1] and reexpress it in a convenient basis. In Sec. 3 we derive a set of sufficient conditions and an expression for the asymptotic convergence rate of the scheme. Sec. 4 is devoted to the study of few special cases. Firstly we consider a problem when inner and outer iteration matrices commute and show that just one inner iteration is sufficient for obtaining convergence. We then proceed to show that an earlier result of Wachspress [2] is contained in our analysis. Next we generalise this result to a case not considered earlier. Finally, Sec. 5 gives our conclusions.