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On Incorporating Linear Constraints into H-Matrix Calculations

By C. E. Siewert,[1]) Service d'Etudes des Réacteurs et de Mathématiques Appliquées, Centre d'Etudes Nucléaires de Saclay, Gif-sur-Yvette, France, and E. E. Burniston, Mathematics Dept, North Carolina State University, Raleigh, N.C., USA

1. Introduction

Some years ago Kriese and Siewert [1] used an idea of Pahor [2], and Pahor and Larson [3], which can be seen to be closely related to the computational scheme suggested by Shure and Natelson [4], to incorporate the linear constraint into the calculation of the **H** matrix applicable to the scattering of polarized light. It was found [1] that for weakly absorbing media, $\omega \approx 1$, the developed equation for the **A** matrix converged by iteration much more quickly than the usual **H** equation, which as discussed by Lenoble [5] appeared, from a numerical point-of-view, not to converge at all. This same approach of developing an equation for a function simply related to the **H** matrix was also used in neutron-transport studies by Kriese et al. [6] whose **L** equation is very similar to the mentioned **A** equation. In a work devoted to the scalar version of the **L** equation [7], it was shown that the non-linear L equation had a unique solution that yielded the correct H function. The question of how to improve the calculation of the **H** matrix has recently been discussed by Mullikin [8].

In addition to the fact that the **L** equation has led to a more expedient method for computing **H** matrices, we note that Bowden and Zweifel [9] were able to use the L equation for one-speed theory to prove, from the functional analysis approach, the existence and uniqueness of the scalar H function, as defined by the non-linear H equation and one linear constraint, for multiplying media, $c > 1$. Thus, since to date only the singular integral equation approach [10] has been able to deal with factorizations of dispersion matrices for multiplying media, the utility of the **L** equation appears to be greater than one only of computational merit.

Here we wish to discuss the general case for **H** matrices when there may be more than one linear constraint and to show that the developed **L** equation has a unique solution that yields the desired **H** matrix. We consider first that the dispersion matrix can be written as

$$\mathbf{\Lambda}(z) = \mathbf{I} + z \int_{-1}^{1} \mathbf{\Psi}(x) \frac{dx}{x - z}, \tag{1}$$

where $\mathbf{\Psi}(x)$ is the characteristic matrix. We assume that $\mathbf{\Lambda}^T(z) = \mathbf{\Lambda}(-z)$ and that we know already that $\mathbf{\Lambda}(z)$ can be factored as

$$\mathbf{\Lambda}^T(z) = \mathbf{H}^{-T}(-z)\mathbf{H}^{-1}(z). \tag{2}$$

[1]) Permanent address: Nuclear Engineering Dept, North Carolina State University, Raleigh, N.C. 27607, USA.

Here $\mathbf{H}(\mu)$ satisfies the non-linear integral equation

$$\mathbf{H}^{-1}(\mu) = \mathbf{I} - \mu \int_0^1 \mathbf{H}^T(x)\mathbf{\Psi}(x)\frac{dx}{x+\mu}, \quad \mu \in [0, 1], \tag{3}$$

and the constraints

$$\left[\mathbf{I} + \nu_\alpha \int_0^1 \mathbf{H}^T(x)\mathbf{\Psi}(x)\frac{dx}{x-\nu_\alpha}\right]\mathbf{M}(\nu_\alpha) = \mathbf{0}, \quad \alpha = 1, 2, 3, \ldots, \kappa, \tag{4}$$

and $\mathbf{H}(z)$ is defined by

$$\mathbf{H}^{-1}(z) = \mathbf{I} - z \int_0^1 \mathbf{H}^T(x)\mathbf{\Psi}(x)\frac{dx}{x+z}, \quad z \notin (-1, 0). \tag{5}$$

Also, κ is the index, i.e., the number of $\pm$ pairs of zeros of $\Lambda(z) = \det \mathbf{\Lambda}(z)$ in the complex plane cut from -1 to 1 along the real axis. In addition, $\mathbf{M}(\nu_\alpha)$ is a *normalized* null vector of $\mathbf{\Lambda}(\nu_\alpha)$:

$$\mathbf{\Lambda}(\nu_\alpha)\mathbf{M}(\nu_\alpha) = \mathbf{0} \quad \text{and} \quad \mathbf{M}^T(\nu_\alpha)\mathbf{M}(\nu_\alpha) = 1. \tag{6}$$

2. Analysis

We first construct a matrix $\mathbf{U}_1$ that has $\mathbf{M}(\nu_1)$ as the first column and the remaining elements chosen such that

$$\mathbf{U}_1\mathbf{U}_1^T = \mathbf{I}. \tag{7}$$

Then we consider

$$\mathbf{\Lambda}_1(z) = \mathbf{D}_1(z)\mathbf{U}_1^T\mathbf{\Lambda}(z)\mathbf{U}_1\mathbf{D}_1(-z) \tag{8}$$

where $\mathbf{D}_1(z)$ is the unit matrix except for the 1–1 element which is

$$\left[\mathbf{D}_1(z)\right]_{11} = \frac{\nu_1(1+z)}{\nu_1 + z}. \tag{9}$$

It is clear that (i) $\mathbf{\Lambda}_1(z)$ is a matrix of sectionally analytic functions, as is $\mathbf{\Lambda}(z)$, (ii) $\mathbf{\Lambda}_1^T(z) = \mathbf{\Lambda}_1(-z)$, (iii) $\mathbf{\Lambda}_1(z)$ is bounded at infinity, (iv) $\mathbf{\Lambda}_1(0) = \mathbf{I}$ and (v) $\mathbf{\Lambda}_1(z)$ has associated with it the index $\kappa - 1$. Elementary considerations are sufficient to show the existence of $\mathbf{U}_1$. We can continue by writing

$$\mathbf{\Lambda}_2(z) = \mathbf{D}_2(z)\mathbf{U}_2^T\mathbf{\Lambda}_1(z)\mathbf{U}_2\mathbf{D}_2(-z) \tag{10}$$

where the first column of $\mathbf{U}_2$ is the normalized null vector of $\mathbf{\Lambda}_1(\nu_2)$,

$$\mathbf{U}_2\mathbf{U}_2^T = \mathbf{I}, \tag{11}$$

and $\mathbf{D}_2(z)$ is the unit matrix except for

$$\left[\mathbf{D}_2(z)\right]_{11} = \frac{\nu_2(1+z)}{\nu_2 + z}. \tag{12}$$

It is clear that $\mathbf{\Lambda}_2(z)$ has the same properties as $\mathbf{\Lambda}(z)$ except that the index associated with $\mathbf{\Lambda}_2(z)$ is $\kappa - 2$. Thus it follows that

$$\mathbf{\Lambda}_\kappa(z) = \mathbf{D}_\kappa(z)\mathbf{U}_\kappa^T\mathbf{D}_{\kappa-1}(z)\mathbf{U}_{\kappa-1}^T \cdots \mathbf{D}_1(z)\mathbf{U}_1^T\mathbf{\Lambda}(z)\mathbf{U}_1\mathbf{D}_1(-z) \cdots \mathbf{U}_{\kappa-1}\mathbf{D}_{\kappa-1}(-z)\mathbf{U}_\kappa\mathbf{D}_\kappa(-z) \tag{13}$$

has index zero; but otherwise $\mathbf{\Lambda}_\kappa(z)$ has the same properties as $\mathbf{\Lambda}(z)$.

We now define

$$\mathbf{L}^{-T}(-z) = \mathbf{D}_\kappa(-z)\mathbf{U}_\kappa^T\mathbf{D}_{\kappa-1}(-z)\mathbf{U}_{\kappa-1}^T\cdots\mathbf{D}_1(-z)\mathbf{U}_1^T\mathbf{H}^{-T}(-z)\mathbf{U}_1\cdots\mathbf{U}_{\kappa-1}\mathbf{U}_\kappa \tag{14}$$

so that we can write

$$\mathbf{\Lambda}_\kappa^T(z) = \mathbf{L}^{-T}(-z)\mathbf{L}^{-1}(z). \tag{15}$$

Since $\mathbf{L}^{-1}(z)$ is sectionally analytic in the complex plane cut from -1 to 0 along the real axis, is bounded at infinity, and is unity at $z = 0$, we can use Cauchy's formula to deduce

$$\mathbf{L}^{-1}(z) = \mathbf{I} - z\int_0^1 \mathbf{L}^T(x)\mathbf{K}(x)\frac{dx}{x+z}, \tag{16}$$

where

$$\mathbf{K}(x) = \mathbf{D}_\kappa(x)\mathbf{U}_\kappa^T\mathbf{D}_{\kappa-1}(x)\mathbf{U}_{\kappa-1}^T\cdots\mathbf{D}_1(x)\mathbf{U}_1^T\mathbf{\Psi}(x)\mathbf{U}_1\mathbf{D}_1(-x)\cdots \mathbf{U}_{\kappa-1}\mathbf{D}_{\kappa-1}(-x)\mathbf{U}_\kappa\mathbf{D}_\kappa(-x). \tag{17}$$

If in Eqn. (16) we consider $z \in [0, 1]$, we get the non-linear $\mathbf{L}$ equation

$$\mathbf{L}^{-1}(\mu) = \mathbf{I} - \mu\int_0^1 \mathbf{L}^T(x)\mathbf{K}(x)\frac{dx}{x+\mu}, \quad \mu\in[0, 1]. \tag{18}$$

We now wish to show that Eqn. (18) has a unique solution which when used in Eqn. (14) yields the desired $\mathbf{H}$ matrix. If we write Eqn. (18) as

$$\mathbf{L}^T(\mu)\left[\mathbf{I} - \mu\int_0^1 \mathbf{K}^T(x)\mathbf{L}(x)\frac{dx}{x+\mu}\right] = \mathbf{I} \tag{19}$$

and post multiply Eqn. (19) by

$$\mathbf{I} + \mu P\int_0^1 \mathbf{L}^T(x)\mathbf{K}(x)\frac{dx}{x-\mu}$$

then we can use some partial-fraction analysis to obtain the singular integral equation

$$\mathbf{L}^T(\mu)\mathbf{\lambda}_\kappa(\mu) = \mathbf{I} + \mu P\int_0^1 \mathbf{L}^T(\eta)\mathbf{K}(\eta)\frac{d\eta}{\eta-\mu}, \quad \mu\in(0, 1), \tag{20}$$

where

$$\mathbf{\lambda}_\kappa(\mu) = \mathbf{I} + \mu P\int_{-1}^1 \mathbf{K}(x)\frac{dx}{x-\mu}. \tag{21}$$

If we now show that Eqn. (20) has a unique solution, then so will Eqn. (18) have a unique solution.

We introduce

$$\mathbf{N}(z) = \frac{1}{2\pi i}\int_0^1 \mathbf{L}^T(x)\mathbf{K}(x)\frac{dx}{x-z} \tag{22}$$

and follow our previous work [10, 11] and that of Muskhelishvili [12] to find

$$\mathbf{I} + 2\pi i z\mathbf{N}(z) = [\mathbf{X}_{\kappa,asy}^{-T}(z) - \mathbf{X}_{\kappa,asy}^{-T}(0) + \mathbf{X}_\kappa^{-T}(0) + z\mathbf{F}(z)]\mathbf{X}_\kappa^T(z), \tag{23}$$

where $\mathbf{F}(z)$ is a matrix of polynomials (to be determined) and $\mathbf{X}_\kappa(z)$ is a canonical solution (of ordered normal form at infinity) of the Riemann–Hilbert problem defined by

$$\mathbf{X}_\kappa^+(t) = \mathbf{G}_\kappa(t)\mathbf{X}_\kappa^-(t), \quad t\in(0, 1). \tag{24}$$

Here

$$\mathbf{G}_\kappa(t) = [\mathbf{\Lambda}_\kappa^+(t)]^T[\mathbf{\Lambda}_\kappa^-(t)]^{-T}. \tag{25}$$

We note that

$$\lim_{|z|\to\infty} \mathbf{X}_\kappa(z) \begin{bmatrix} z^{\kappa_{\kappa,1}} & & & 0 \\ & z^{\kappa_{\kappa,2}} & & \\ & & \ddots & \\ 0 & & & z^{\kappa_{\kappa,n}} \end{bmatrix} = \mathbf{K}, \quad \det \mathbf{K} \neq 0, \tag{26}$$

where $\kappa_{\kappa,\alpha}$ are the partial indices corresponding to $\mathbf{G}_\kappa(t)$. Clearly

$$\sum_{\alpha=1}^{n} \kappa_{\kappa,\alpha} = 0. \tag{27}$$

Since $z\mathbf{N}(z)$ must be bounded as $|z| \to \infty$, it follows from Eqn. (23) that $\mathbf{F}(z) \equiv \mathbf{0}$ if $\kappa_{\kappa,\alpha} \geq 0$, $\alpha = 1, 2, 3, \ldots, n$; thus we would find

$$\mathbf{I} + 2\pi i z\mathbf{N}(z) = \mathbf{X}_\kappa^{-T}(0)\mathbf{X}_\kappa^T(z) \tag{28}$$

and a unique $\mathbf{L}(\mu)$:

$$\mathbf{L}(\mu) = \frac{1}{2\pi i\mu}\mathbf{K}^{-T}(\mu)[\mathbf{X}_\kappa^+(\mu) - \mathbf{X}_\kappa^-(\mu)]\mathbf{X}_\kappa^{-1}(0). \tag{29}$$

On the other hand, should any of the $\kappa_{\kappa,\alpha}$ be negative then $z\mathbf{N}(z)$ would be unbounded as $|z| \to \infty$, and thus there would be no solution to Eqn. (20). Thus a solution to Eqn. (18), if it exists, is unique. Since we have assumed a factorization of $\mathbf{\Lambda}(z)$ in Eqn. (2), we know that $\mathbf{H}^{-1}(\mu)$ exists and thus so does $\mathbf{L}^{-1}(\mu)$. Based on this assumption, we deduce that the solution to Eqn. (18) is unique and that by way of Eqn. (14) it must yield the desired $\mathbf{H}$ matrix.

It is clear that to relax the assumption of Eqn. (2) we should try to prove that all $\kappa_{\kappa,\alpha}$ are non negative. We hope to pursue this point in a later work.

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Abstract

A method of computing **H** matrices appropriate to (for example) studies of multigroup neutron-transport theory and rarefied-gas dynamics is proposed.

Zusammenfassung

Eine Methode zur Berechnung von **H**- Matrizen, die z.B. für Studien von Problemen der Mehrfachgruppen-Neutronen-Transport-Theorie und der Dynamik verdünnter Gase geeignet ist, wird vorgeschlagen.

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