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A METHOD FOR COMPUTING THE DISCRETE SPECTRUM BASIC TO MULTI-GROUP TRANSPORT THEORY

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Abstract—Elementary considerations are used to develop a computational method for establishing the discrete spectrum for a general multi-group model basic to radiation transport.

INTRODUCTION

We consider here the multi-group transport equation written as

$$\mu \frac{\partial}{\partial z} \boldsymbol{\Psi}(z, \mu) + \mathbf{S}\boldsymbol{\Psi}(z, \mu) = \sum_{l=0}^{L} P_l(\mu)\mathbf{T}_l \int_{-1}^{1} P_l(\mu')\boldsymbol{\Psi}(z, \mu')\, \mathrm{d}\mu' \tag{1}$$

where the Legendre polynomials are denoted by $P_l(\mu)$ and the transfer matrices $\mathbf{T}_l$ are such that particle transfer (by, say, scattering and/or fission) between and within all energy groups is allowed. In addition, the elements $\psi_1(z, \mu)$, $\psi_2(z, \mu), \ldots, \psi_M(z, \mu)$ of the M-vector $\boldsymbol{\Psi}(z, \mu)$ are the group angular fluxes, the elements $s_1, s_2, \ldots, s_M$ of the diagonal $\mathbf{S}$ matrix are the group total cross sections, z is the position variable measured in cm and μ is the direction cosine, with respect to the positive z axis, that defines the direction of motion.

In order to use dimensionless units we introduce an optical variable $x = zs_{\min}$, where $s_{\min}$ is the minimum of the set $\{s_i\}$, and rewrite equation (1) as

$$\mu \frac{\partial}{\partial x} \boldsymbol{\Psi}(x, \mu) + \boldsymbol{\Sigma}\boldsymbol{\Psi}(x, \mu) = \sum_{l=0}^{L} P_l(\mu)\mathbf{C}_l \int_{-1}^{1} P_l(\mu')\boldsymbol{\Psi}(x, \mu')\, \mathrm{d}\mu' \tag{2}$$

where the diagonal matrix $\boldsymbol{\Sigma}$ has entries $\sigma_i = s_i/s_{\min}$ and where the dimensionless transfer matrices are defined by $\mathbf{C}_l = \mathbf{T}_l/s_{\min}$.

THE DISPERSION FUNCTION

In order to find elementary solutions of equation (2) we start by substituting

$$\boldsymbol{\Psi}(\xi : x, \mu) = \exp(-x/\xi)\boldsymbol{\Phi}(\xi, \mu) \tag{3}$$

into equation (2) to obtain

$$(\xi\boldsymbol{\Sigma} - \mu\mathbf{I})\boldsymbol{\Phi}(\xi, \mu) = \xi \sum_{k=0}^{L} P_k(\mu)\mathbf{C}_k\mathbf{G}_k(\xi)\mathbf{M}(\xi) \tag{4}$$

where we have defined

$$\mathbf{G}_k(\xi)\mathbf{M}(\xi) = \int_{-1}^{1} P_k(\mu)\boldsymbol{\Phi}(\xi, \mu)\, \mathrm{d}\mu. \tag{5}$$

We can now multiply equation (4) by $P_l(\mu)$ and integrate over μ from -1 to 1 to find

$$[\xi \mathbf{h}_l \mathbf{G}_l(\xi) - (l+1)\mathbf{G}_{l+1}(\xi) - l\mathbf{G}_{l-1}(\xi)]\mathbf{M}(\xi) = \mathbf{0} \tag{6}$$

where we have defined

$$\mathbf{h}_l = (2l+1)\boldsymbol{\Sigma} - 2\mathbf{C}_l. \tag{7}$$

We now define

$$\mathbf{G}_0(\xi) = \mathbf{I} \tag{8}$$

so that

$$\int_{-1}^{1} \boldsymbol{\Phi}(\xi, \mu)\, d\mu = \mathbf{M}(\xi). \tag{9}$$

We thus consider the polynomial matrices $\mathbf{G}_l(\xi)$ to be defined for all ξ by equation (8) and the recursion formula

$$\xi \mathbf{h}_l \mathbf{G}_l(\xi) = (l+1)\mathbf{G}_{l+1}(\xi) + l\mathbf{G}_{l-1}(\xi) \tag{10}$$

for $l \geqslant 0$.

For the discrete spectrum $\xi \notin [-1, 1]$, we can solve equation (4) to obtain

$$\boldsymbol{\Phi}(\xi, \mu) = \xi(\xi\boldsymbol{\Sigma} - \mu\mathbf{I})^{-1}\mathbf{G}(\xi, \mu)\mathbf{M}(\xi) \tag{11}$$

where

$$\mathbf{G}(\xi, \mu) = \sum_{l=0}^{L} \mathbf{C}_l \mathbf{G}_l(\xi) P_l(\mu), \tag{12}$$

and we can integrate equation (11) to find

$$\boldsymbol{\Lambda}(\xi)\mathbf{M}(\xi) = \mathbf{0} \tag{13}$$

where

$$\boldsymbol{\Lambda}(\xi) = \mathbf{I} + \xi \int_{-1}^{1} (\mu\mathbf{I} - \xi\boldsymbol{\Sigma})^{-1}\mathbf{G}(\xi, \mu)\, d\mu. \tag{14}$$

We therefore take our dispersion function to be $\Lambda(\xi) = \det \boldsymbol{\Lambda}(\xi)$, so that the discrete spectrum here can be defined as those values of $\xi \notin [-1, 1]$ such that

$$\Lambda(\xi) = 0. \tag{15}$$

BASIC IDENTITIES

We now follow a procedure reported by İnönü[1] and Garcia and Siewert[2] for the one-group model and develop for the considered multi-group model a set of identities that provides the basis of our computational method for establishing the discrete spectrum.

We define, for $\xi \notin [-1, 1]$,

$$\mathbf{Q}_l(\xi) = \int_{-1}^{1} (\mu\mathbf{I} - \xi\boldsymbol{\Sigma})^{-1} P_l(\mu)\, d\mu \tag{16}$$

so that we can write the $\boldsymbol{\Lambda}$ matrix as

$$\boldsymbol{\Lambda}(\xi) = \mathbf{I} + \xi \sum_{l=0}^{L} \mathbf{Q}_l(\xi)\mathbf{C}_l\mathbf{G}_l(\xi). \tag{17}$$

Multiplying equation (16) by $(2l+1)\xi$ and using partial-fraction analysis and the recursion formula

$$(2l+1)\mu P_l(\mu) = (l+1)P_{l+1}(\mu) + lP_{l-1}(\mu), \tag{18}$$

we find that the $\mathbf{Q}_l(\xi)$ satisfy the recursion formula

$$(2l+1)\xi\boldsymbol{\Sigma}\mathbf{Q}_l(\xi) = (l+1)\mathbf{Q}_{l+1}(\xi) + l\mathbf{Q}_{l-1}(\xi) - 2\delta_{0,l}\mathbf{I}. \tag{19}$$

We can now multiply equation (10) on the left by $\mathbf{Q}_l(\xi)$, multiply equation (19) on the right by $\mathbf{G}_l(\xi)$, subtract one of the two resulting equations from the other and then sum the resulting equation from $l = 0$ to $l = L$ to find, after noting equation (17),

$$\Lambda(\xi) = \tfrac{1}{2}(L+1)[\mathbf{Q}_{L+1}(\xi)\mathbf{G}_L(\xi) - \mathbf{Q}_L(\xi)\mathbf{G}_{L+1}(\xi)]. \tag{20}$$

Introducing matrices $\boldsymbol{\Pi}_l(\xi) = \text{diag}\{P_l(\sigma_1\xi),\ P_l(\sigma_2\xi), \ldots, P_l(\sigma_M\xi)\}$ and noting equation (18), we now write

$$(2l+1)\xi\boldsymbol{\Sigma}\boldsymbol{\Pi}_l(\xi) = (l+1)\boldsymbol{\Pi}_{l+1}(\xi) + l\boldsymbol{\Pi}_{l-1}(\xi). \tag{21}$$

Now multiplying equation (19) by $\boldsymbol{\Pi}_l(\xi)$, multiplying equation (21) by $\mathbf{Q}_l(\xi)$, taking the difference and then summing over l, we find the identity

$$\mathbf{I} = \tfrac{1}{2}(L+1)[\mathbf{Q}_{L+1}(\xi)\boldsymbol{\Pi}_L(\xi) - \mathbf{Q}_L(\xi)\boldsymbol{\Pi}_{L+1}(\xi)]. \tag{22}$$

In a similar manner we can find from equations (10) and (21) that

$$\xi\sum_{l=0}^{L}\boldsymbol{\Pi}_l(\xi)\mathbf{C}_l\mathbf{G}_l(\xi) = \tfrac{1}{2}(L+1)[\boldsymbol{\Pi}_{L+1}(\xi)\mathbf{G}_L(\xi) - \boldsymbol{\Pi}_L(\xi)\mathbf{G}_{L+1}(\xi)]. \tag{23}$$

Finally we multiply equation (20) by $\boldsymbol{\Pi}_{L+1}(\xi)$ and use equations (22) and (23) to obtain

$$\boldsymbol{\Pi}_{L+1}(\xi)\Lambda(\xi) = \mathbf{G}_{L+1}(\xi) + \xi\mathbf{Q}_{L+1}(\xi)\sum_{l=0}^{L}\boldsymbol{\Pi}_l(\xi)\mathbf{C}_l\mathbf{G}_l(\xi). \tag{24}$$

If we consider that $\mathbf{C}_l = \mathbf{0}$ for $l > L$, we can write, for $\xi \notin [-1, 1]$,

$$\Lambda(\xi) = \boldsymbol{\Pi}_{N+1}^{-1}(\xi)\left[\mathbf{G}_{N+1}(\xi) + \xi\mathbf{Q}_{N+1}(\xi)\sum_{l=0}^{L}\boldsymbol{\Pi}_l(\xi)\mathbf{C}_l\mathbf{G}_l(\xi)\right] \tag{25}$$

for any $N \geqslant L$. In particular since Robin[3] has shown that the Legendre function of the second kind

$$Q_l(\xi) = \frac{1}{2}\int_{-1}^{1} P_l(\mu)\frac{d\mu}{\xi - \mu} \tag{26}$$

vanishes as $l \to \infty$ for all $\xi \notin [-1, 1]$ we conclude from equations (16) and (25) that

$$\Lambda(\xi) = \lim_{N\to\infty}\boldsymbol{\Pi}_{N+1}^{-1}(\xi)\mathbf{G}_{N+1}(\xi), \quad \xi \notin [-1, 1]. \tag{27}$$

It thus follows that the zeros of $\det\mathbf{G}_{N+1}(\xi)$ that lie outside the interval $[-1, 1]$ will approximate the desired discrete spectrum with better and better accuracy as N increases.

A COMPUTATIONAL METHOD

As we wish to approximate our exact problem

$$\Lambda(\xi)\mathbf{M}(\xi) = \mathbf{0} \tag{28}$$

by

$$\mathbf{G}_{N+1}(\xi)\mathbf{N}(\xi) = \mathbf{0}, \tag{29}$$

we now let

$$\mathbf{T}_l(\xi) = \mathbf{G}_l(\xi)\mathbf{N}(\xi), \tag{30}$$

for $l = 0, 1, 2, \ldots, N$, and multiply equation (10) by $\mathbf{N}(\xi)$ to obtain

$$l\mathbf{h}_l^{-1}\mathbf{T}_{l-1}(\xi) + (l+1)\mathbf{h}_l^{-1}\mathbf{T}_{l+1}(\xi) = \xi\mathbf{T}_l(\xi) \tag{31}$$

for $l = 0, 1, \ldots, N$. Equation (31) along with the termination condition $\mathbf{T}_{N+1}(\xi) = \mathbf{0}$ can be expressed as an eigenvalue problem for the $M(N+1)$ zeros of $\det \mathbf{G}_{N+1}(\xi)$. However, we prefer first to consider N to be odd and to eliminate the odd-order Ts in equation (31); we find, for $l = 0, 2, 4, \ldots, N-1$, that

$$\mathbf{X}_l\mathbf{T}_{l-2}(\xi) + \mathbf{Y}_l\mathbf{T}_l(\xi) + \mathbf{Z}_l\mathbf{T}_{l+2}(\xi) = \xi^2\mathbf{T}_l(\xi) \tag{32}$$

where

$$\mathbf{X}_l = l(l-1)\mathbf{h}_l^{-1}\mathbf{h}_{l-1}^{-1}, \tag{33a}$$

$$\mathbf{Y}_l = l^2\mathbf{h}_l^{-1}\mathbf{h}_{l-1}^{-1} + (l+1)^2\mathbf{h}_l^{-1}\mathbf{h}_{l+1}^{-1} \tag{33b}$$

and

$$\mathbf{Z}_l = (l+1)(l+2)\mathbf{h}_l^{-1}\mathbf{h}_{l+1}^{-1}. \tag{33c}$$

Equation (32) and the truncation condition $\mathbf{T}_{N+1}(\xi) = \mathbf{0}$ can now be expressed as the eigenvalue problem

$$\mathbf{A}\mathbf{X} = \xi^2\mathbf{X} \tag{34}$$

where

$$\mathbf{A} = \begin{bmatrix} \mathbf{Y}_0 & \mathbf{Z}_0 & & & & \\ \mathbf{X}_2 & \mathbf{Y}_2 & \mathbf{Z}_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & \mathbf{X}_{N-3} & \mathbf{Y}_{N-3} & \mathbf{Z}_{N-3} \\ & & & & \mathbf{X}_{N-1} & \mathbf{Y}_{N-1} \end{bmatrix} \tag{35}$$

is $M(N+1)/2$ square and the $\mathbf{X}$ vector has entries $\mathbf{T}_0(\xi), \mathbf{T}_2(\xi), \ldots, \mathbf{T}_{N-1}(\xi)$. It follows that the $J = M(N+1)/2$ eigenvalues of $\mathbf{A}$ provide the squares of the $J \pm$ pairs of zeros of $\det \mathbf{G}_{N+1}(\xi)$.

NUMERICAL RESULTS

Having generalized previous works,[4–7] on scalar problems, and works on a four-vector polarization problem in radiative transfer[8,9] to the case of multi-group transport theory, we now report some numerical results that indicate the accuracy with which the zeros of $\det \mathbf{G}_{N+1}(\xi)$, $\xi \notin [-1, 1]$, approximate the discrete spectrum defined by $\det \Lambda(\xi) = 0$, $\xi \notin [-1, 1]$.

Although the matrix $\mathbf{A}$ defined by equation (35) is banded (and sparse for $N \gg M$) we have not made use of this structure here. We have simply used the driver program RG in the EISPACK collection[10,11] to compute the eigenvalues.

For our first set of numerical examples we consider the four $L = 0$ data cases that were defined by Forster[12] and used by Kriese, Siewert and Yener[13] for two-group critical calculations in neutron transport theory. Thus we write

$$(\mathbf{T}_0)_{11} = \tfrac{1}{2}[\sigma_{11s} + (1-\chi)\bar{\nu}_1\sigma_{1f}] \tag{36a}$$

$$(\mathbf{T}_0)_{12} = \tfrac{1}{2}[\sigma_{12s} + (1-\chi)\bar{\nu}_2\sigma_{2f}] \tag{36b}$$

$$(\mathbf{T}_0)_{21} = \tfrac{1}{2}\chi\bar{\nu}_1\sigma_{1f} \tag{36c}$$

and

$$(\mathbf{T}_0)_{22} = \tfrac{1}{2}[\sigma_{22s} + \chi\bar{\nu}_2\sigma_{2f}] \tag{36d}$$

and use the data in Table 1 to define the $\mathbf{S}$ and $\mathbf{T}_0$ matrices basic to equation (1). In Table 2 we list the exact results[13] for the discrete eigenvalues for these four cases and the values of N we require here to duplicate, to the given degree of accuracy, these discrete eigenvalues.

To have a more challenging test case we considered the analytical 20-group model, with $L = 10$, that was used by Garcia and Siewert.[14] This 20-group model, defined in Ref. [14], was used for a

Table 1. Two-group macroscopic cross sections (in cm^{-1})

Case	s_1	σ_{11s}	$\bar{\nu}_1\sigma_{1f}$	σ_{12s}	s_2	σ_{22s}	$\bar{\nu}_2\sigma_{2f}$	χ
I	0.54628	0.4241	0.2425	0.0045552	0.33588	0.3198	0.0070425	1.0
II	2.52025	2.44383	0.12658	0.029227	0.65696	0.62568	0.002621	1.0
III	0.3456	0.26304	0.1728	0.072	0.216	0.07824	0.167184	0.575
IV	0.336	0.23616	0.2503392	0.0432	0.2208	0.0792	0.29016	0.575

Table 2. Discrete eigenvalues

Case	Eigenvalue	N
I	i 1.81477 (2)	5
II	i 3.54785	5
III	i 6.72584 (−1)	11
IV	i 4.80216 (−1)	15

radiation shielding study, and so there is no fission nor any up-scattering in the model. For this problem there is only one discrete eigenvalue $\xi \notin [-1, 1]$; for $N = 69$ we obtained a result that agreed with the published result to nine significant figures.

To conclude we note that the **A** matrix defined by equation (35) can, especially for many-group problems, become very large as N increases. It is clear that there can be cases where the size of **A** becomes unmanageable before N is sufficiently large so as to yield very accurate, say 10 figures, results for the desired eigenvalues. For these cases some alternative computational method, e.g. Newton's method applied to $\Lambda(\xi)$, may be required.

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