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The relationship between the normalization coefficient and dispersion function for the multigroup transport equation*

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An explicit formula for the discrete Case normalization coefficient is presented in terms of functions related to the dispersion function. These functions are easily determined and provide the normalization coefficient without need of prior evaluation of the eigenvectors.

The single-group (reduced) transport equation[1]

$$(z-\mu)\phi(\mu)=\frac{cz}{2}\int_{-1}^{1}d\mu'\,\phi(\mu') \tag{1}$$

is an eigenvalue equation for z: setting

$$\int_{-1}^{1}d\mu\,\phi(\mu)=1, \tag{2}$$

one obtains ($z\notin[-1,1]$)

$$\phi(\mu)=\frac{cz/2}{z-\mu} \tag{3}$$

with z determined by reimposing (2) upon (3):

$$1=\int_{-1}^{1}\phi(\mu)\,d\mu=\frac{cz}{2}\int_{-1}^{1}\frac{d\mu}{z-\mu}\equiv M(z).$$

That is, the eigenvalues z are the zeroes of the function $\Omega(z)$, where

$$\Omega(z)=1-\frac{cz}{2}\int\frac{d\mu}{z-\mu}=1-M(z). \tag{4}$$

Had ϕ been multicomponented (as for multigroup equations), the eigenvalues z would similarly have been the zeroes of a function $\Omega(z)$, which then is the determinant of the coefficients of the linear system analogous to (1):

$$\Omega(z)\equiv\det(\mathbf{I}-\mathbf{M}(z)). \tag{5}$$

That is, (4) is simply the one-dimensional case of (5). We shall write the explicit form of the matrix $\mathbf{M}(z)$ later.

A normalization factor N is defined for a solution to (1), according to

$$N\equiv\int_{-1}^{1}d\mu\,\mu\phi^2(\mu). \tag{6}$$

By utilizing the solution (3) [with z replaced by z_0, where $\Omega(z_0)=0$], it is easy to verify that the value of N satisfies the well-known formula

$$N=\tfrac{1}{2}cz_0{}^2\Omega'(z_0)=-\tfrac{1}{2}cz_0{}^2M'(z_0). \tag{7}$$

For multi-group equations for particular (and small, e.g., two) numbers of groups results similar to (7) have surfaced in the literature.[2] In this paper we attempt to determine just what the connection between N and Ω' is for a fairly general class of nonconstant, nonisotropic multigroup equations.

To be exact, we investigate the equation[3]

$$(\Sigma z-\mu\mathbf{I})\cdot\boldsymbol{\phi}(\mu)=z\sum_{m=1}^{\alpha}\mathbf{A}^m(\mu)\cdot\int_{-1}^{1}d\mu'\,\mathbf{B}^m(\mu')\circ\boldsymbol{\phi}(\mu') \tag{8}$$

for an α-fold degenerate nonconstant, nonisotropic scattering kernel, with Σ the diagonal matrix of cross-sections:

$$\Sigma=\begin{pmatrix}\sigma_1 & & & 0\\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_N\end{pmatrix}$$

for an N-group problem.

With $\mathbf{M}(z)$ the $N\alpha\times N\alpha$ matrix,

$$M^{(m)(n)}_{i\ \ \ j}(z)\equiv z\int_{-1}^{1}d\mu\,B^{(m)}_{ir}(\mu)(\Sigma z-\mu\mathbf{I})^{-1}_{rs}A^{(n)}_{sj}(\mu), \tag{9}$$

we shall establish that

$$N_i=-z_i{}^2\lambda_i'(z_i)=z_i{}^2\Omega'(z_i)\prod_{m\neq i}[1-\lambda_m(z_i)]^{-1} \tag{10}$$

where $\lambda_i(z)$ is ith eigenvalue of $\mathbf{M}$, and

$$\Omega=\det(\mathbf{I}-\mathbf{M})=\prod_{i=1}^{N\alpha}[1-\lambda_i(z)]$$

In analogy to the solution of (1), one solves (8) by isolating $\boldsymbol{\phi}$. Defining

$$\int_{-1}^{1}d\mu\,\mathbf{B}^{(m)}(\mu)\cdot\boldsymbol{\phi}(\mu)\equiv\boldsymbol{\beta}^{(m)} \tag{11}$$

upon multiplying by $(\Sigma z-\mu\mathbf{I})^{-1}$,

$$\boldsymbol{\phi}(\mu)=z(\Sigma z-\mu'\mathbf{I})^{-1}\cdot\sum_{m=1}^{\alpha}\mathbf{A}^{(m)}(\mu)\cdot\boldsymbol{\beta}^{(m)}.$$

Next, multiply by $\mathbf{B}^{(n)}(\mu)$ and integrate over μ:

$$\begin{aligned}\int_{-1}^{1}\mathbf{B}^{(n)}(\mu)\circ\boldsymbol{\phi}(\mu)\,d\mu&=\boldsymbol{\beta}^{(n)}\\ &=\sum_{m=1}^{\alpha}\left(\int_{-1}^{1}d\mu\,\mathbf{B}^{(n)}(\mu)\cdot z(\Sigma z-\mu'\mathbf{I})^{-1}\cdot\mathbf{A}^{(m)}(\mu)\right)\cdot\boldsymbol{\beta}^{(m)}\\ &\equiv\sum_{m=1}^{\alpha}\mathbf{M}^{(n)(m)}(z)\circ\boldsymbol{\beta}^{(m)}.\end{aligned}$$

That is, $\sum_m(\delta^{nm}\mathbf{I}-\mathbf{M}^{(n)(m)}(z))\boldsymbol{\beta}^{(m)}=0$, where $\mathbf{M}^{(n)(m)}$ is defined by (9). Clearly, this is a usual homogeneous system of equations in $N\alpha$ dimensions. Thus, apart from direct product subscripting, an α-fold degenerate kernel presents the identical mathematical problems as the onefold kernel $\mathbf{A}(\mu)\cdot\ \mathbf{B}(\mu')$. Accordingly, with no loss of generality, we consider the notationally simpler problem of the onefold degenerate kernel:

$$(\mathbf{I}-\mathbf{M}(z))\circ\boldsymbol{\beta}=0,\quad\boldsymbol{\phi}=z(\Sigma z-\mu\mathbf{I})^{-1}\circ\mathbf{A}\circ\boldsymbol{\beta}, \tag{12}$$

where

$$\mathbf{M}(z) = \int_{-1}^{1} d\mu\, \mathbf{B}(\mu) \cdot z(\Sigma z - \mu \mathbf{I})^{-1} \cdot \mathbf{A}(\mu), \tag{13}$$

$$\boldsymbol{\beta} \equiv \int_{-1}^{1} \mathbf{B}(\mu) \cdot \boldsymbol{\phi}(\mu)\, d\mu. \tag{14}$$

Next, define the adjoint solution $\boldsymbol{\phi}^*$:

$$\boldsymbol{\phi}^* \cdot (\Sigma z - \mu \mathbf{I}) = z\left(\int d\mu'\, \boldsymbol{\phi}^*(\mu') \cdot \mathbf{A}(\mu')\right) \cdot \mathbf{B}(\mu). \tag{15}$$

In an identical fashion to the above, with

$$\boldsymbol{\beta}^* \equiv \int_{-1}^{1} d\mu\, \boldsymbol{\phi}^*(\mu) \cdot \mathbf{A}(\mu) \tag{16}$$

one obtains

$$\boldsymbol{\beta}^* \cdot (\mathbf{I} - \mathbf{M}(z)) = 0 \quad \text{and}$$

and

$$\boldsymbol{\phi}^* = \boldsymbol{\beta}^* \cdot \mathbf{B} \cdot z(\Sigma z - \mu \mathbf{I})^{-1}. \tag{17}$$

($\boldsymbol{\beta}$ differs from $\boldsymbol{\beta}^*$ only when $\mathbf{M}$ is *nonsymmetric.*) The solubility of either (12) or (17) is exactly the eigenvalue condition $\Omega(z) = 0$, where

$$\Omega(z) \equiv \det(\mathbf{I} - \mathbf{M}(z)), \tag{18}$$

with $\boldsymbol{\beta}$ and $\boldsymbol{\beta}^*$, respectively, right and left eigenvectors of $\mathbf{M}$ corresponding to the eigenvalue $+1$; the condition on a z_0 is that $\mathbf{M}(z_0)$ should possess the eigenvalue $+1$.

Corresponding to the mth zero of $\Omega(z)$ [i.e., $\Omega(z_m) = 0$] is a $\boldsymbol{\beta}^{(m)}$ and $\boldsymbol{\beta}^{*(m)}$. As a natural normalization for that solution, we choose

$$\boldsymbol{\beta}^{*(m)} \cdot \boldsymbol{\beta}^{(m)} = 1 \tag{19}$$

and shortly comment on when this condition is tenable: At this point we cannot yet even comment on orthogonality of different modes. Normalization on the solution through (19), having been set, the normalization coefficient is determined:

$$N_m \equiv \int_{-1}^{1} d\mu\, \mu \boldsymbol{\phi}^*(\mu) \cdot \boldsymbol{\phi}(\mu)$$
$$= z_m{}^2 \int_{-1}^{1} d\mu\, \boldsymbol{\beta}^{*(m)} \cdot \mathbf{B}(\mu) \cdot \mu(\Sigma z - \mu \mathbf{I})^{-2} \cdot \mathbf{A}(\mu) \cdot \boldsymbol{\beta}^{(m)}$$
[by (12) and (17)]

and

$$N_m = -z_m{}^2 \boldsymbol{\beta}^{*(m)} \cdot \mathbf{M}'(z_m) \cdot \boldsymbol{\beta}^{(m)} \quad [\text{where } \mathbf{M}' \equiv (d/dz)\mathbf{M}]. \tag{20}$$

Equation (20) establishes some connection between N and $\mathbf{M}$, although it requires the evaluation of both $\boldsymbol{\beta}$ and $\boldsymbol{\beta}^*$ prior to calculating N. It is our goal to provide an evaluation of N independent of explicit $\boldsymbol{\beta}$ dependence. Unfortunately, Eqs. (12) and (17) are not valid for all z: Rather, they are a compatable system of equations only for certain specific values of z (i.e., the z_m). Accordingly, neither of (12) or (17) can be differentiated to be useful in (20). Thus, we are forced to pose a more flexible eigenvalue problem for $\mathbf{M}$. Clearly, for any z, we can evaluate the elements of $\mathbf{M}(z)$ and pose its eigenvalue problem. Equation (12) poses a more restricted problem, in that it seeks out those special values of z for which the eigenvalue is $+1$: For other values of z, $\mathbf{M}$ will possess eigenvalues different from 1 and z-dependent:

$$\mathbf{M}(z) \cdot \boldsymbol{\gamma}(z) = \lambda(z)\boldsymbol{\gamma}(z), \tag{21}$$

where

$$\lambda(z_m) = 1.$$

For a given z, there will, in general, be N different eigenvalues:

$$\lambda_m(z), \quad m = 1, \ldots, N$$

and, in general, at a z_m satisfying $\Omega(z_m) = 0$, only one λ will achieve the value $+1$. Accordingly, we label the z-dependent eigenvalues with the same index that labels the z's that satisfy $\Omega(z) = 0$:

$$\lambda_m(z_m) \equiv 1. \tag{22}$$

[Should $\Omega(z) = 0$ possess a degenerate root, evidently exactly that number of the λ's must simultaneously achieve the value $+1$ at that z-value.] For z_m, (21) becomes

$$\mathbf{M}(z_m) \cdot \boldsymbol{\gamma}_m(z_m) = \boldsymbol{\gamma}_m(z_m),$$

where $\boldsymbol{\gamma}^{(m)}(z)$ is the eigenvector associated with λ_m. That is,

$$\boldsymbol{\beta}^{(m)} = \boldsymbol{\gamma}_m(z_m). \tag{23}$$

Similarly,

$$\boldsymbol{\gamma}_m^*(z) \cdot \mathbf{M}(z) = \lambda_m(z)\boldsymbol{\gamma}_m^*(z) \tag{24}$$

and

$$\boldsymbol{\beta}^{*(m)} = \boldsymbol{\gamma}_m^*(z_m). \tag{25}$$

We are now in a position to examine orthonormality questions.

$$\mathbf{M}(z) \cdot \boldsymbol{\gamma}_m(z) = \lambda_m(z)\boldsymbol{\gamma}_m(z)$$
$$\Rightarrow \boldsymbol{\gamma}_n^*(z) \cdot \mathbf{M}(z) \cdot \boldsymbol{\gamma}_m(z) = \lambda_m(z)\boldsymbol{\gamma}_n^*(z) \cdot \boldsymbol{\gamma}_m(z)$$

and

$$\boldsymbol{\gamma}_n^*(z) \cdot \mathbf{M}(z) = \lambda_n(z)\boldsymbol{\gamma}_n^*(z)$$
$$\Rightarrow \boldsymbol{\gamma}_n^*(z) \cdot \mathbf{M}(z) \cdot \boldsymbol{\gamma}_m(z) = \lambda_n(z)\boldsymbol{\gamma}_n^*(z) \cdot \boldsymbol{\gamma}_m(z),$$

i.e.,

$$(\lambda_m(z) - \lambda_n(z))\boldsymbol{\gamma}_n^*(z) \cdot \boldsymbol{\gamma}_m(z) = 0 \tag{26}$$

so that

$$\boldsymbol{\gamma}_n^*(z) \cdot \boldsymbol{\gamma}_m(z) = 0 \quad \text{for } \lambda_m(z) \neq \lambda_n(z). \tag{27}$$

Should all the eigenvalues be distinct, then these $\boldsymbol{\gamma}_m$'s must span the N-dimensional space. Since, by (27), $\boldsymbol{\gamma}_n^*$ is orthogonal to $N-1$ linearly independent vectors, and is nonnull, it must have a projection upon the last, so that by appropriate normalization coefficients of the $\boldsymbol{\gamma}$'s, one can set

$$\boldsymbol{\gamma}_n^* \cdot \boldsymbol{\gamma}_m = \delta_{nm}. \tag{28}$$

Accordingly, by defining

$$G_{im} \equiv (\boldsymbol{\gamma}_m)_i, \quad (\boldsymbol{\gamma}_n^*)_i = G_{ni}^{-1}, \tag{29}$$

where (28) also guarantees G's invertibility. Clearly,

G accomplishes $\mathbf{M}$'s diagonalization

$$\gamma_n^* \cdot \mathbf{M} \cdot \gamma_m = \lambda_m \gamma_n^* \cdot \gamma_m$$
$$\Leftrightarrow \quad (\mathbf{G}^{-1} \cdot \mathbf{M} \cdot \mathbf{G})_{mn} = \lambda_m \delta_{mn} \equiv (\Lambda)_{mn}. \tag{30}$$

However, with degenerate eigenvalues and $\mathbf{M}$ nonsymmetric, diagonalization is not in general possible. Should it be possible, $\mathbf{M}$'s spectrum is termed complete. We assume completeness from this point onwards. This is important because it guarantees the validity of the normalization posited in (19): Set $m=n$ in (28) and evaluate at $z=z_m$:

$$1 = \gamma_m^*(z_m) \cdot \gamma_m(z_m) = \beta^{*(m)} \cdot \beta^{(m)}.$$

Also,

$$\begin{aligned}\Omega(z) &= \det(\mathbf{I} - \mathbf{M}(z)) = \det \mathbf{G}^{-1}(z)\mathbf{G}(z) \cdot \det(\mathbf{I} - \mathbf{M}(z)) \\ &= \det(\mathbf{G}^{-1}(z) \cdot (\mathbf{I} - \mathbf{M}(z)) \cdot \mathbf{G}(z)) \\ &= \det(\mathbf{I} - \Lambda(z)) \\ &= \prod_{m=1}^{N} [1 - \lambda_m(z)]. \end{aligned} \tag{31}$$

Since (21) holds for all z, we can differentiate it:

$$\mathbf{M}'(z) \cdot \gamma_m(z) + \mathbf{M}(z) \cdot \gamma_m'(z) = \lambda_m'(z)\gamma_m(z) + \lambda_m(z)\gamma_m'(z)$$

or

$$\mathbf{M}'(z) \cdot \gamma_m(z) = \lambda_m'(z)\gamma_m(z) + (\lambda_m(z)\mathbf{I} - \mathbf{M}(z)) \cdot \gamma_m'(z).$$

Projecting upon γ_m^*, paying attention to (24) and (28), we obtain

$$\begin{aligned}&\gamma_m^*(z) \cdot \mathbf{M}'(z) \cdot \gamma_m(z) \\ &= \lambda_m'(z)\gamma_m^*(z) \cdot \gamma_m(z) + \gamma_m^*(z) \cdot (\lambda_m(z)\mathbf{I} - \mathbf{M}(z)) \cdot \gamma_m'(z) \\ &= \lambda_m'(z).\end{aligned}$$

Finally, evaluating at $z=z_m$,

$$\begin{aligned}&\gamma_m^*(z_m) \cdot \mathbf{M}'(z_m) \cdot \gamma_m(z_m) \\ &= \beta^{*(m)} \cdot \mathbf{M}'(z_m) \cdot \beta^{(m)} = \lambda_m'(z_m)\end{aligned}$$

so that

$$N_m = z_m^2 \lambda_m'(z_m) \quad \text{where } \lambda_m(z_m) = 1. \tag{32}$$

Thus, knowledge of the $\lambda(z)$*'s suffices to determine at once the* z_m*'s and* N_m*'s.* To rewrite (32) in terms of Ω, differentiate (31):

$$\Omega'(z_m) = -\lambda_m'(z_m) \prod_{i \neq m} [1 - \lambda_i(z_m)]$$

or

$$\Omega'(z_m) = (N_m / z_m^2) \prod_{i \neq m} [1 - \lambda_i(z_m)]. \tag{33}$$

It is, at this point, perhaps useful to explicate these ideas by examining a two-group equation with constant, isotropic kernel,[4]

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & \sigma \end{pmatrix}, \quad \mathbf{A} \cdot \mathbf{B} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \equiv \mathbf{C},$$

$$(\Sigma z - \mu \mathbf{I}) \cdot \phi(\mu) = z\mathbf{C} \cdot \int_{-1}^{1} d\mu\, \phi(\mu'),$$

and

$$\phi^*(\mu)(\Sigma z - \mu \mathbf{I}) = z \int_{-1}^{1} \phi^*(\mu')\, d\mu' \cdot \mathbf{C}.$$

Defining

$$\begin{aligned}\beta &= \int d\mu'\, \phi(\mu'), \\ \beta^* &= \int d\mu'\, \phi^*(\mu') \cdot \mathbf{C},\end{aligned} \tag{34}$$

we have

$$\mathbf{M}(z) = z \int_{-1}^{1} d\mu\, (\Sigma z - \mu \mathbf{I})^{-1} \cdot \mathbf{C} \tag{35}$$

with β and β^* right and left eigenvectors. Writing out (35), we have

$$\begin{aligned}\mathbf{M}(z) &= \begin{pmatrix} z \int_{-1}^{1} d\mu/(z-\mu) & 0 \\ 0 & z \int_{-1}^{1} d\mu/(\sigma z - \mu) \end{pmatrix} \cdot \mathbf{C} \\ &\equiv \begin{pmatrix} f(z) & 0 \\ 0 & (1/\sigma) f(\sigma z) \end{pmatrix} \cdot \mathbf{C}. \end{aligned} \tag{36}$$

Calculating $\lambda(z)$:

$$\det\left(\lambda \mathbf{I} - \begin{pmatrix} f(z) & 0 \\ 0 & (1/\sigma) f(\sigma z) \end{pmatrix} \cdot \mathbf{C}\right) = 0, \tag{37}$$

which, after some algebra, reduces to

$$\lambda^2 - \lambda[C_{11} f(z) + (C_{22}/\sigma) f(\sigma z)] + (C/\sigma) f(z) f(\sigma z) = 0,$$
$$C \equiv \det \mathbf{C}. \tag{38}$$

Differentiating (38),

$$2\lambda\lambda' - \lambda'[C_{11} f(z) + (C_{22}/\sigma) f(\sigma z)] - \lambda[C_{11} f'(z) + C_{22} f'(\sigma z)] + (C/\sigma) f'(z) f(\sigma z) + C f(z) f'(\sigma z) = 0.$$

Solving for λ' and setting $\lambda = 1$, $z = z_0$,

$$\lambda' = -\frac{(C/\sigma) f'(z_0) f(\sigma z_0) + C f(z_0) f'(\sigma z_0) - [C_{11} f'(z_0) + C_{22} f'(\sigma z_0)]}{2 - C_{11} f(z_0) - (C_{22}/\sigma) f(\sigma z_0)}$$

so that

$$N_0 = -z_0^2 \lambda'(z_0) = C z_0^2 \frac{(1/\sigma) f'(z_0) f(\sigma z_0) + f(z_0) f'(\sigma z_0) - (1/C)[C_{11} f'(z_0) + C_{22} f'(\sigma z_0)]}{2 - C_{11} f(z_0) - (C_{22}/\sigma) f(\sigma z_0)}. \tag{39}$$

To evaluate z_0, one sets $\lambda = 1$ in (38), which of course, is simply $\Omega(z_0) = 0$ as can be seen by setting $\lambda = 1$ in (37). Since f is a perfectly definite function

$$f(z) = z \int_{-1}^{1} d\mu/(z-\mu) = z \ln|(1+z)/(1-z)| = 2z \tanh^{-1}(1/z),$$

once z_0 is evaluated, N_0 is obtained from (39) without further computation. It is to be recalled here that N_0 of (39) is the normalization factor for the solution normalized to $\beta^* \cdot \beta = 1$, or

$$\left(\int d\mu\, \phi^*(\mu)\right) \cdot \mathbf{C} \cdot \left(\int d\mu\, \phi(\mu)\right) = 1.$$

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[1]K.M. Case, Ann. Phys. (N.Y.) **9**, 1 (1960).
[2]A comprehensive review has been given by N.J. McCormick and I. Kuscer, Advan. Nucl. Sci. Tech. (N.Y.) **7**, 181 (1973). An extensive list of references is incorporated.
[3]Ref. 2, esp. Ref. 76 in Ref. 2.
[4]C.E. Siewert and P.S. Shieh, J. Nucl. Energy **21**, 385 (1967).