PHYSOR-2006, ANS Topical Meeting on Reactor Physics
Organized and hosted by the Canadian Nuclear Society. Vancouver, BC, Canada. 2006 September 10-14

On the Spectrum and Elementary Solutions of Level Symmetric Discrete Ordinates Equations in Nodal Reactor Computations

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Abstract

We report on recent improvements in the theory of spectral nodal methods for the numerical solution of multidimensional discrete ordinates multiplication eigenvalue problems with anisotropic scattering in rectangular geometry. We describe an efficient numerical scheme for generating the spectrum and the elementary solutions of basic transverse-integrated S_N equations for the special case of level symmetric quadratures. Generation of spectrum and elementary solutions is an important step in the (spectral) nodal strategy of estimating neutron multiplication factor and node-average power densities in nodal reactor computations. Numerical results are given to illustrate the scheme.

KEYWORDS: Nuclear reactors, one-speed, discrete ordinates, level symmetric quadratures, spectrum, elementary solutions

1. Introduction

As part of our effort to further develop the theory of spectral nodal methods for the numerical solution of multidimensional energy-independent discrete ordinates (S_N) neutron transport problems with anisotropic scattering, we have recently proposed [1] a numerical scheme for generating the spectrum and the elementary solutions of very basic transverse-integrated S_N equations [2–5] for general quadrature sets. These equations result from the application of the transverse integration technique to xyz-geometry S_N equations for multiplication eigenvalue problems [6,7]. Generation of the spectrum of these transverse-integrated equations is an important step in the (spectral) nodal strategy of estimating neutron multiplication factor and the node-average power density distribution in nodal reactor computations. More recently, we have noticed that our scheme can be made more efficient for the special case of level symmetric (LQ_N) quadrature sets [7,8]. In this article, we give the underlying theory, and we show how our scheme can be made more efficient for LQ_N sets.

This article is organized as follows. In Section 2, we set forth the governing equations, and we derive the transverse-integrated S_N equations to which our scheme does apply. In Section 3, we briefly describe our recently developed scheme for general quadrature sets. In Section 4, we infer basic and important properties of the spectrum and elementary solutions for LQ_N sets and, as a result, we define a more efficient strategy of generating spectrum and elementary solutions. In

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Section 5, we illustrate the strategy with numerical results for a sample problem, and in Section 6 we conclude this article with a discussion.

2. The Governing Equations and Transverse Integration

2.1 XYZ-Geometry Discrete Ordinates Equations

We begin by considering a homogeneous spatial node R_{ijk} of a nuclear reactor core model defined by $x_{i-1/2} \le x \le x_{i+1/2}$, $y_{j-1/2} \le y \le y_{j+1/2}$, $z_{k-1/2} \le z \le z_{k+1/2}$ on a system of three-dimensional Cartesian coordinates. We assume that R_{ijk} is isotropic and that the transport of neutrons through R_{ijk} is governed by the xyz-geometry S_N equations

$$\vec{\Omega}_m \bullet \vec{\nabla}\psi_m(x,y,z) + \sigma_t \psi_m(x,y,z) = \sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} \sigma_\ell \sum_{n=1}^{M} \omega_n P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) \psi_n(x,y,z), (x,y,z) \in R_{ijk}, m = 1:M. \quad (1)$$

Since our aim here is the generation of the spectrum and the elementary solutions, there is no point to consider interface/boundary conditions for equations (1).

Notation in equations (1) is quite usual [7]. The positive integer M is to denote the number of discrete directions/weights considered in the S_N equations (1). Each discrete direction m has its angular weight ω_m, and is represented by the (unit) vector $\vec{\Omega}_m \equiv (\xi_m, \eta_m, \zeta_m)$ defined on the surface of a unit sphere. Here, $\xi_m \equiv \sin\theta_m \cos\phi_m$, $\eta_m \equiv \sin\theta_m \sin\phi_m$, and $\zeta_m \equiv \cos\theta_m$, with θ_m and ϕ_m standing for the polar and azimuthal angles, respectively. The quantity $\psi_m(x,y,z)$ is the angular flux of neutrons travelling in direction m at (x,y,z); σ_t is the macroscopic total neutron cross section everywhere in R_{ijk}; $\sigma_\ell \equiv \sigma_{s,\ell} + \delta_{0\ell}\nu\sigma_f/k$, where $(2\ell+1)\sigma_{s,\ell}$ is the ℓth-order component of the Legendre expansion of the neutron scattering phase function everywhere in R_{ijk}, $\delta_{0\ell}$ is the Kronecker delta, ν is the average number of neutrons yielded in a neutron fission reaction everywhere in R_{ijk}, σ_f is the macroscopic fission neutron cross section everywhere in R_{ijk}, and k is the neutron multiplication factor; P_ℓ denotes the ℓth-degree Legendre polynomial; and $\vec{\Omega}_m \bullet \vec{\Omega}_n$ is the cosine of the scattering angle defined by the discrete directions m and n. The nonnegative integer L is to indicate that the Legendre expansion of the scattering phase function has been truncated after (L+1) terms.

2.2 Transverse-Integrated Equations

Transverse integration is to be understood as a linear operator technique for the derivation of systems of S_N equations whose unknowns are one-dimensional spatial moments of the angular flux $\psi_m(x,y,z)$. Here, it consists of applying the linear operator

$$\frac{(2r+1)(2s+1)}{V_\alpha W_\beta} \int_{v_{\alpha-1/2}}^{v_{\alpha+1/2}} \int_{w_{\beta-1/2}}^{w_{\beta+1/2}} dw\, dv\, P_r\left[\frac{2(v-v_\alpha)}{V_\alpha}\right] P_s\left[\frac{2(w-w_\beta)}{W_\beta}\right](\bullet) \quad (2)$$

to both sides of equations (1) to yield a system of M transverse-integrated S_N equations whose unknowns are one-dimensional spatial (Legendre) moments of order r and s of the angular flux. We note that the linear operator (2) is written in compact form. Given the spatial variable u and

the nonnegative integers r and s, it represents the analytic integration of the rs-Legendre-weighted S_N equations (1) over the rectangle $(v_{\alpha-1/2},v_{\alpha+1/2})$ x $(w_{\beta-1/2},w_{\beta+1/2})$ in the (transverse) vw plane at u, where $V_\alpha \equiv v_{\alpha+1/2} - v_{\alpha-1/2}$, $W_\beta \equiv w_{\beta+1/2} - w_{\beta-1/2}$, and the midpoints v_α and w_β are defined by $(v_{\alpha+1/2} + v_{\alpha-1/2})/2$ and $(w_{\beta+1/2} + w_{\beta-1/2})/2$, respectively. Therefore, given r and s, the linear operator (2) is a shorthand notation for three transverse integration operations on Eqs. (1), each of which being represented by a row of symbols in Table 1.

Table 1: Chart of symbols for transverse integration.

u	v	w	α	β	V_α	W_β
x	y	z	j	k	Y_j	Z_k
y	x	z	i	k	X_i	Z_k
z	x	y	i	j	X_i	Y_j

Let us illustrate with a sample operator for arbitrary r and s. For u = y, we have

$$\frac{(2r+1)(2s+1)}{X_i Z_k} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{z_{k-1/2}}^{z_{k+1/2}} dz\, dx\, P_r\left[\frac{2(x-x_i)}{X_i}\right] P_s\left[\frac{2(z-z_k)}{Z_k}\right](\bullet). \tag{3}$$

Application of operator (3) to equations (1) yields the M transverse-integrated S_N equations

$$\eta_m \frac{d}{dy}\psi_m^{rs}(y) + \sigma_t \psi_m^{rs}(y) = \sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi}\sigma_\ell \sum_{n=1}^{M} \omega_n P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n)\psi_n^{rs}(y) -$$
$$\xi_m \left\{\frac{(2r+1)}{X_i}\left[\psi_m^s(x_{i+1/2},y) + (-1)^{r+1}\psi_m^s(x_{i-1/2},y)\right] - \psi_m^{r's}(y)\right\} -$$
$$\zeta_m \left\{\frac{(2s+1)}{Z_k}\left[\psi_m^r(y,z_{k+1/2}) + (-1)^{s+1}\psi_m^r(y,z_{k-1/2})\right] - \psi_m^{rs'}(y)\right\}, \quad m = 1:M, \tag{4}$$

where

$$\psi_m^{rs}(y) \equiv \frac{(2r+1)(2s+1)}{X_i Z_k} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{z_{k-1/2}}^{z_{k+1/2}} dz\, dx\, P_r\left[\frac{2(x-x_i)}{X_i}\right] P_s\left[\frac{2(z-z_k)}{Z_k}\right] \psi_m(x,y,z), \tag{5}$$

is the Legendre spatial moment of $\psi_m(x,y,z)$ of order r in x and order s in z, and the remaining moments are suitably approximated by either exponential or polynomial functions [5,6,10].

The transverse-integrated equations (4) (and their x and z counterparts) are the starting point for the derivation of the (spectral) auxiliary equations that make up the discretized equations of the spectral nodal method for multidimensional multiplication eigenvalue problems [3–5]. Their unknowns are the Legendre moments (5) for all m from 1 to M. Therefore, the transverse-integrated equations (4) (and their x and z counterparts) can be seen as a system of M coupled ordinary differential equations of the first order in M unknown functions – the Legendre moments (5). Solution to equations (4) can be expressed in terms of the solution to the homogeneous part of equations (4) and of particular solutions tailored by the approximating

functions used for the "transverse leakage" terms [5,6] on their right hand sides. In the coming section, we consider the homogeneous version

$$\eta_m \frac{d}{dy}\psi_m^{rs}(y) + \sigma_t \psi_m^{rs}(y) = \sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} \sigma_\ell \sum_{n=1}^{M} \omega_n P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) \psi_n^{rs}(y),\ m = 1:M, \tag{6}$$

of equations (4), and we describe a numerical scheme for generating their spectrum and corresponding elementary solutions in order that we may be able to write the homogeneous solution of equations (4) as a linear combination of these elementary solutions. A discussion on the approximating functions for the transverse leakage terms and on particular solutions to equations (4) for low r and s can be found elsewhere [2,6,10]. We note that the form of the homogeneous equations (6) does not depend on r and s. Therefore, we may simply write

$$\eta_m \frac{d}{dy}\psi_m(y) + \sigma_t \psi_m(y) = \sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} \sigma_\ell \sum_{n=1}^{M} \omega_n P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) \psi_n(y),\ m = 1:M. \tag{7}$$

3. A Scheme for Generating the Spectrum and Elementary Solutions

In this section, we briefly describe our recently developed scheme [1] for the generation of the spectrum and elementary solutions of the S_N equations (7) (as well as for their x and z counterparts). An elementary solution is an ordered set of exponential functions of the form

$$\psi_{m,r}(y) = a_m^y(\nu_r^y) \exp(\sigma_t y / \nu_r^y),\ m = 1:M,\ y_{j-1/2} \le y \le y_{j+1/2}, \tag{8}$$

where ν_r^y belongs to the spectrum of the S_N equations (7); $a_m^y(\nu_r^y)$, m = 1 : M, are the angular components of the corresponding elementary solution. Now, if we substitute (8) into (7), and we first-order operate on the left hand sides of the resulting equations, we get

$$\eta_m \frac{\sigma_t}{\nu_r} a_m^y(\nu_r^y) \exp(\sigma_t y / \nu_r^y) + \sigma_t a_m^y(\nu_r^y) \exp(\sigma_t y / \nu_r^y) =$$
$$\sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} \sigma_\ell \sum_{n=1}^{M} \omega_n P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) a_n^y(\nu_r^y) \exp(\sigma_t y / \nu_r^y),\ m = 1:M. \tag{9}$$

Since $\exp(\sigma_t y / \nu_r^y) \neq 0$ for all y and assuming that R_{ijk} is a material region ($\sigma_t \neq 0$), we can divide equations (9) by $\sigma_t \exp(\sigma_t y / \nu_r^y)$ and write

$$\frac{\eta_m}{\nu_r} a_m^y(\nu_r^y) + a_m^y(\nu_r^y) = \sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} c_\ell \sum_{n=1}^{M} \omega_n P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) a_n^y(\nu_r^y),\ m = 1:M, \tag{10}$$

where $c_\ell \equiv \sigma_\ell / \sigma_t$. After suitable reformulation [1], we arrive at the algebraic eigenvalue problem

$$\sum_{n=1}^{M} \frac{1}{\eta_m} \left\{ -\delta_{mn} + \omega_n \left[\sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} c_\ell P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) \right] \right\} a_n^y(\nu_r^y) = \frac{1}{\nu_r^y} a_m^y(\nu_r^y),\ m = 1:M. \tag{11}$$

In matrix notation, we may write

$$\underline{\underline{A}}^{y}\,\vec{a}(\nu_r^y)=\frac{1}{\nu_r^y}\vec{a}(\nu_r^y). \tag{12}$$

The M-dimensional square matrix $\underline{\underline{A}}^{y}$ with (known) entries

$$A_{mn}^{y}\equiv\frac{1}{\eta_m}\left\{-\delta_{mn}+\omega_n\left[\sum_{\ell=0}^{L}\frac{(2\ell+1)}{4\pi}c_\ell P_\ell(\vec{\Omega}_m\bullet\vec{\Omega}_n)\right]\right\};m,n=1:M, \tag{13}$$

is a matrix whose eigenvalues $(\nu_r^y)^{-1}$, r = 1 : M, are corresponding reciprocals of the elements of the spectrum $\{\nu_r^y\}$ of the S_N equations (7), and whose corresponding eigenvectors

$$\vec{a}(\nu_r^y)\equiv[a_1^y(\nu_r^y),a_2^y(\nu_r^y),a_3^y(\nu_r^y),\ldots,a_M^y(\nu_r^y)]^T,\ r=1:M, \tag{14}$$

are ordered sets of angular components of the corresponding elementary solutions. Solution to the algebraic eigenvalue problem (12) can be achieved by means of modern computer algebra packages such as MAPLE [11], or with conventional matrix eigensystem packages such as EISPACK [12]. Once the algebraic eigenvalue problem (12) is solved, the elementary solutions (8) become available. We note that the scheme here is readily applied for *arbitrary order of anisotropic scattering* and for an *arbitrary set of directions and weights* in the S_N equations (1). This is in contrast to a scheme developed by de Barros and Larsen for anisotropic scattering up to the first order and symmetric quadrature sets [2].

Similar results stand for the other Cartesian directions, i.e.

$$\xi_m\frac{d}{dx}\psi_m(x)+\sigma_t\psi_m(x)=\sum_{\ell=0}^{L}\frac{(2\ell+1)}{4\pi}\sigma_\ell\sum_{n=1}^{M}\omega_n P_\ell(\vec{\Omega}_m\bullet\vec{\Omega}_n)\psi_n(x),\ m=1:M, \tag{15}$$

and

$$\zeta_m\frac{d}{dz}\psi_m(z)+\sigma_t\psi_m(z)=\sum_{\ell=0}^{L}\frac{(2\ell+1)}{4\pi}\sigma_\ell\sum_{n=1}^{M}\omega_n P_\ell(\vec{\Omega}_m\bullet\vec{\Omega}_n)\psi_n(z),\ m=1:M, \tag{16}$$

respectively. Spectra and elementary solutions for these yz- and xy-integrated equations can be likewise determined. The x and z counterparts of entries (13) are given by

$$A_{mn}^{x}\equiv\frac{1}{\xi_m}\left\{-\delta_{mn}+\omega_n\left[\sum_{\ell=0}^{L}\frac{(2\ell+1)}{4\pi}c_\ell P_\ell(\vec{\Omega}_m\bullet\vec{\Omega}_n)\right]\right\};m,n=1:M, \tag{17}$$

and

$$A_{mn}^{z}\equiv\frac{1}{\zeta_m}\left\{-\delta_{mn}+\omega_n\left[\sum_{\ell=0}^{L}\frac{(2\ell+1)}{4\pi}c_\ell P_\ell(\vec{\Omega}_m\bullet\vec{\Omega}_n)\right]\right\};m,n=1:M, \tag{18}$$

respectively. Note that the entries (13), (17) and (18) have a common term in curly brackets, and that the difference from one another is determined by the row multipliers $(1/\eta_m)$, $(1/\xi_m)$ and $(1/\zeta_m)$. So, we can generate the M-dimensional square matrix, say $\underline{\underline{A}}$, with entries

$$A_{mn} \equiv -\delta_{mn} + \omega_n \left[\sum_{\ell=0}^{L} \frac{(2\ell+1)}{4\pi} c_\ell P_\ell(\vec{\Omega}_m \bullet \vec{\Omega}_n) \right]; m, n = 1 : M, \tag{19}$$

and use the appropriate row multipliers in order to pass the corresponding matrix on to the eigenproblem solver. This unifying approach enhances the algorithm for computing the spectra (eigenvalues) and elementary solutions (eigenvectors) of equations (7), (15) and (16) for general quadratures.

4. The Special Case of LQ_N Sets

The scheme described in Section 3 can be made more efficient for the widely used LQ_N sets [7,8]. Aside the welcome property of mirror symmetry across the $\xi = 0$, $\eta = 0$, and $\zeta = 0$ planes, the LQ_N sets are invariant with respect to 90° rotations about the directional cosine axes ξ, η, and ζ. An important consequence of this 90° rotational invariance is that, given a completely arbitrary order $\vec{\Omega}_1, \vec{\Omega}_2, \ldots, \vec{\Omega}_M$ to the M = N(N+2) discrete directions of an LQ_N set, there exists a permutation $\vec{\Omega}_{p_1}, \vec{\Omega}_{p_2}, \ldots, \vec{\Omega}_{p_M}$ defined by a 90° rotation, which preserves angular weights, i.e., $\omega_m = \omega_{p_m}$, m = 1 : M, scattering cosines, i.e., $\vec{\Omega}_m \bullet \vec{\Omega}_n = \vec{\Omega}_{p_m} \bullet \vec{\Omega}_{p_n}$; m, n =1: M, and corresponding sets of directional cosines, i.e., $\alpha_m = \kappa_{p_m}$, m = 1 : M; $\alpha, \kappa \in \{\xi, \eta, \zeta\}$; $\alpha \neq \kappa$, with α and κ set by the 90° rotation. For example, there exists a permutation defined by a 90° rotation about the ζ axis, namely, a rotation from the positive ξ axis towards the positive η axis, such that $\omega_m = \omega_{p_m}$, $\vec{\Omega}_m \bullet \vec{\Omega}_n = \vec{\Omega}_{p_m} \bullet \vec{\Omega}_{p_n}$, and $\xi_m = \eta_{p_m}$; m, n = 1 : M. Similar results follow from permutations defined by 90° rotations about the ξ and η axes. Considering the entries (13) and (17) and the results of the preceding example, we can state the following: there exists a permutation $\vec{\Omega}_{p_1}, \ldots, \vec{\Omega}_{p_M}$ defined by a 90° rotation about the ζ axis such that

$$\underline{\underline{A}}^y \Big|_p = \underline{\underline{A}}^x, \tag{20}$$

where the quantity on the left hand side of equation (20) is matrix $\underline{\underline{A}}^y$ constructed from the permutation $\vec{\Omega}_{p_1}, \ldots, \vec{\Omega}_{p_M}$, and $\underline{\underline{A}}^x$ is the matrix with entries (17) constructed from our arbitrarily ordered set $\vec{\Omega}_1, \ldots, \vec{\Omega}_M$. From elementary matrix algebra [13], we have

$$\underline{\underline{A}}^y \Big|_p = E_K \ldots E_2 E_1 \underline{\underline{A}}^y E_1 E_2 \ldots E_K, \text{ K finite} \tag{21}$$

where E_t, t = 1 : K, are elementary matrices for row/column interchanging, K is an M-dependent positive integer, and $\underline{\underline{A}}^y$ is constructed from $\vec{\Omega}_1, \ldots, \vec{\Omega}_M$.

We are now in position to justify the importance of the 90° rotational invariance of LQ_N sets for spectrum generation. For this task, we turn to the algebraic eigenvalue problem (12). Suppose that this problem is solved and so, $(\nu_r^y)^{-1}$ and $\underline{a}(\nu_r^y)$, r = 1 : M, are available quantities. We left multiply both sides of (12) by $E_K \ldots E_2 E_1$ to get the matrix identity

$$E_K ... E_2 E_1 \underline{\underline{A}}^y \vec{a}(\nu_r^y) = \frac{1}{\nu_r^y} E_K ... E_2 E_1 \vec{a}(\nu_r^y), \tag{22}$$

which is valid for all r from 1 to M. Since E_t, t = 1 : K, are invertible [13], we may write

$$E_K ... E_2 E_1 \underline{\underline{A}}^y E_1 E_2 ... E_K E_K^{-1} ... E_2^{-1} E_1^{-1} \vec{a}(\nu_r^y) = \frac{1}{\nu_r^y} E_K ... E_2 E_1 \vec{a}(\nu_r^y), r = 1 : M. \tag{23}$$

Since $E_t^{-1} = E_t$ for all t [13], we must have

$$E_K ... E_2 E_1 \underline{\underline{A}}^y E_1 E_2 ... E_K E_K ... E_2 E_1 \vec{a}(\nu_r^y) = \frac{1}{\nu_r^y} E_K ... E_2 E_1 \vec{a}(\nu_r^y), r = 1 : M. \tag{24}$$

We define the M-dimensional column matrices

$$\vec{b}(\nu_r^y) \equiv E_K ... E_2 E_1 \vec{a}(\nu_r^y) = [a_{p_1}^y(\nu_r^y), a_{p_2}^y(\nu_r^y), a_{p_3}^y(\nu_r^y), \ldots, a_{p_M}^y(\nu_r^y)]^T, r = 1 : M, \tag{25}$$

and we substitute (25) into (24) to get

$$E_K ... E_2 E_1 \underline{\underline{A}}^y E_1 E_2 ... E_K \vec{b}(\nu_r^y) = \frac{1}{\nu_r^y} \vec{b}(\nu_r^y), r = 1 : M. \tag{26}$$

We substitute results (20) and (21) into equation (26) to finally get

$$\underline{\underline{A}}^x \vec{b}(\nu_r^y) = \frac{1}{\nu_r^y} \vec{b}(\nu_r^y), r = 1 : M. \tag{27}$$

Since $\vec{a}(\nu_r^y) \neq \vec{0}_M$, the null M-dimensional column matrix, $\vec{b}(\nu_r^y) \neq \vec{0}_M$, cf. definition (25), and $\vec{b}(\nu_r^y)$ is thus an eigenvector of $\underline{\underline{A}}^x$ associated with the eigenvalue $(\nu_r^y)^{-1}$, r = 1 : M. Therefore, all eigenvalues of $\underline{\underline{A}}^y$ are eigenvalues of $\underline{\underline{A}}^x$, with corresponding eigenvectors $\vec{b}(\nu_r^y)$ given by (25). Since $\underline{\underline{A}}^x$ is an M-dimensional square matrix, there can be no eigenvalues of $\underline{\underline{A}}^x$ other than $(\nu_r^y)^{-1}$, r = 1 : M, and so, *all* eigenvalues and eigenvectors of $\underline{\underline{A}}^x$ are determined.

Similar results hold for the M-dimensional square matrix $\underline{\underline{A}}^z$, whose entries are given by expression (18). There exists a permutation $\vec{\Omega}_{q_1}, \ldots, \vec{\Omega}_{q_M}$ defined by a 90° rotation about the ξ axis (a rotation from the positive ζ axis towards the positive η axis) such that

$$\underline{\underline{A}}^y \Big|_q = \underline{\underline{A}}^z, \tag{28}$$

where the quantity on the left hand side of equation (28) is matrix $\underline{\underline{A}}^y$ constructed from the permutation $\vec{\Omega}_{q_1}, \ldots, \vec{\Omega}_{q_M}$, and $\underline{\underline{A}}^z$ is constructed from $\vec{\Omega}_1, \ldots, \vec{\Omega}_M$. Similarly, we have

$$\underline{\underline{A}}^{y}\Big|_{q} = F_K \ldots F_2 F_1 \underline{\underline{A}}^{y} F_1 F_2 \ldots F_K , \tag{29}$$

where F_t, t = 1 : K, are elementary matrices for row/column interchanging. Following similar steps from (22) through (27), we obtain

$$\underline{\underline{A}}^{z}\, \vec{c}(\nu_r^y) = \frac{1}{\nu_r^y}\, \vec{c}(\nu_r^y), r = 1 : M, \tag{30}$$

where $(\nu_r^y)^{-1}$, r = 1 : M, are eigenvalues of $\underline{\underline{A}}^{z}$,

$$\vec{c}(\nu_r^y) \equiv F_K \ldots F_2 F_1 \vec{a}(\nu_r^y) = [a_{q_1}^y(\nu_r^y), a_{q_2}^y(\nu_r^y), a_{q_3}^y(\nu_r^y), \ldots, a_{q_M}^y(\nu_r^y)]^T, r = 1 : M, \tag{31}$$

are corresponding eigenvectors and, from the above arguments, *all* eigenvalues and eigenvectors of $\underline{\underline{A}}^{z}$ are determined.

From the above results, it is apparent that the scheme outlined in Section 3 can be used more efficiently for spectrum generation for the special case of LQ_N sets. Given an arbitrary order $\vec{\Omega}_1, \ldots, \vec{\Omega}_M$ to the discrete directions of an LQ_N set, we construct matrix $\underline{\underline{A}}^{y}$, and we generate its eigenvalues $(\nu_r^y)^{-1}$ and corresponding eigenvectors $\vec{a}(\nu_r^y)$, r = 1 : M, using either conventional or advanced numerical linear algebra packages [11,12]. Then, from the permutations $p_1, \ldots, p_M$ (defined by a 90° rotation about the ζ axis from the positive ξ axis towards the positive η axis) and $q_1, \ldots, q_M$ (defined by a 90° rotation about the ξ axis from the positive ζ axis towards the positive η axis), the eigenvectors $\vec{b}(\nu_r^y)$, r = 1 : M, of matrix $\underline{\underline{A}}^{x}$, cf. definition (25), and $\vec{c}(\nu_r^y)$, r = 1 : M, of matrix $\underline{\underline{A}}^{z}$, cf. definition (31), can be readily obtained, without further matrix eigenvalue/eigenvector computations.

5. Numerical Results

We have used our previously developed FORTRAN routines [1,14] to construct matrix $\underline{\underline{A}}^{y}$, and the driver routine RG of EISPACK [12] to generate its eigenvalues $(\nu_r^y)^{-1}$, r = 1 : M, and corresponding eigenvectors $\vec{a}(\nu_r^y)$, r = 1 : M. We have written an additional routine to make the row interchange operations on the eigenvectors $\vec{a}(\nu_r^y)$ for an efficient generation of the eigenvectors $\vec{b}(\nu_r^y)$ and $\vec{c}(\nu_r^y)$, r = 1 : M, of matrices $\underline{\underline{A}}^{x}$ and $\underline{\underline{A}}^{z}$, respectively.

We illustrate the efficient use, as described in the last paragraph of Section 4, of the scheme outlined in Section 3 with numerical results for an LQ_4 (M = 24) problem. We set L = 6 in equations (1), and we assume that node R_{ijk} has $c_0 = 0.9733$, $c_1 = 0.1755$, $c_2 = 0.1449$, $c_3 = 0.1613$, $c_4 = 0.0569$, $c_5 = -0.0098$, and $c_6 = 0.0046$ [1]. We have used the LQ_4 directions and weights (normalized to 4π) tabulated in Chapter 4 of the book of Lewis and Miller Jr. [7]. The discrete directions have been ordered quite arbitrarily, and the permutations $p_1, \ldots, p_{24}$ and $q_1, \ldots, q_{24}$ evaluated from the 90°-rotation prescriptions of Section 4.

In Table 2, we show the twenty-four elements ν_r^y of the spectrum (reciprocals of the eigenvalues) of the transverse-integrated S_N equations (7) (matrix $\underline{\underline{A}}^{y}$). The angular components of the corresponding elementary solutions (eigenvectors $\vec{a}(\nu_r^y)$, r = 1 : 24) are bulky

to be properly tabulated here. For this reason, they can be made available electronically upon request to the author. The angular components of the elementary solutions of the S_N equations (15) and (16) have been checked against (and matched) corresponding results generated independently with the scheme outlined in Section 3. We should note that $\nu_r^y \neq \eta_m$ for all m and r. This is in contrast with an assumption made in the scheme described in the work of de Barros and Larsen [2] – the directional cosines belong to the spectrum – and so, extension to anisotropic scattering of arbitrary order of the scheme developed by de Barros and Larsen, as it stands, may not be feasible.

Table 2: Spectrum of the transverse-integrated S_N equations (7).

r	ν_r^y	r	ν_r^y	r	ν_r^y
1	–0.3666205	9	–0.4070590	17	–0.9369657
2	+0.3666205	10	+0.4070590	18	+0.9369657
3	–0.3937389	11	–0.4131845	19	–1.0079720
4	+0.3937389	12	+0.4131845	20	+1.0079720
5	–0.3937389	13	–0.4131845	21	–1.0079720
6	+0.3937389	14	+0.4131845	22	+1.0079720
7	–0.4010709	15	–0.6177368	23	–3.9651961
8	+0.4010709	16	+0.6177368	24	+3.9651961

6. Concluding Remarks

We have described an efficient scheme for the generation of the spectrum and elementary solutions of transverse-integrated S_N equations for LQ_N sets. We began by inferring basic and important properties of the systems of transverse-integrated S_N equations for LQ_N sets, namely: i) the systems of xy-, xz-, and yz-integrated S_N homogeneous equations have the same spectrum; and ii) the angular components for the other systems can be readily computed from those generated for a reference system (we have considered the xz-integrated S_N homogeneous equations as the reference system in our developments). As a result, we were able to prevent unnecessary (and expensive for high N) matrix eigenvalue/eigenvector computations. We note that the scheme here can be readily applied to those challenging problems where the Legendre order of anisotropic scattering is high. This positive feature does not seem to be shared by the scheme reported by de Barros and Larsen in Ref. [2].

We intend to extend the scheme developed here to energy-dependent problems using multigroup theory [15]. The starting point is a numerical scheme for multigroup problems with azimuthal symmetry developed by the author [16]. An energy-dependent extension is important to take into account the energy change in scattering events [17] and, particularly in nuclear reactor applications, to account for the difference between the energies of neutrons newly born from fission and of those causing fission in thermal nuclear reactors.

Acknowledgements

The author wishes to thank A. C. M. Alvim and H. Alves Filho for their helpful comments concerning this work.

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