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On the spectrum of discrete–ordinates neutron transport problems

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ABSTRACT

Over the last six decades, the discrete spectrum of the neutron transport operator has been widely studied. Significant theoretical results can be found in the literature regarding the one–speed linear transport equation with anisotropic scattering. In this study, the discrete–ordinates (S_N) transport problem with anisotropic scattering has been considered and the discrete spectrum results in multiplying media have been corroborated. The numerical results obtained for the dominant S_N eigenvalues agreed with the ones for the analytic problem reported in the literature up to a triplet scattering order. A compact methodology to perform the spectral analysis to multigroup S_N problems with high anisotropy order in the scattering and fission reactions is also presented in this paper.

Keywords: **transport equation, discrete ordinates, spectral analysis, discrete eigenvalues, anisotropic scattering**

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1. INTRODUCTION

Case (1960) presented a general procedure with the intent to analytically solve the Boltzmann Transport Equation (BTE) by the expansion of its solution into a complete set of eigenfunctions [1]. This is, undoubtedly, one of the most remarkable studies in the field of neutral particle transport theory [2]. Even though eigenfunctions might present a lack of utility in the solution to practical nuclear engineering problems, this method has been applied among different fields in physics seeking a comprehensive mathematical understanding [2, 3]. Case found an analytic solution to the steady–state, homogeneous BTE in slab geometry considering one–speed particles and isotropic scattering. Over the past 60 years, the method has been applied to more complex problems that may consider energy dependence, multiplying media, anisotropic scattering, heterogeneity, and/or multiple dimensions [2, 4].

Case proved that the solutions are given by two discrete modes corresponding to a $\pm$ pair of eigenvalues that lie outside interval $(-1;\ +1)$, in addition to a complimentary continuous eigenvalue spectrum over the interval $[-1;\ +1]$ [1]. This pair of discrete dominant eigenvalues are conventionally referred to as c–eigenvalues [5] since they depend on the material cross section by

$$c = \frac{\Sigma_S\ +\ \nu\,\Sigma_f}{\Sigma_T} \quad .$$

In regard to obtaining a discrete eigenvalue spectrum, besides the monoenergetic problem with isotropic scattering [1], the main results have been applied to problems considering linearly anisotropic scattering [6], and more recently, arbitrary–order anisotropic scattering [4, 7, 8]. In Section 2 of this paper, the methodology described by Sahni and Tureci [4] is summarized and the main results for all the mentioned cases are presented.

To the best of this author's knowledge, no published work has extended these results to include multigroup these results to multigroup transport problems in the discrete–ordinates (S_N) formulation considering arbitrary order of anisotropy on the scattering and fission reactions. The procedures described here present a general solution to the problem cited before, including the possibility of obtaining eigenvalues over the complex plane. The spectral analysis for the S_N BTE that supports the discrete eigenvalues of the Case's spectrum has also been performed.

2. MATERIALS AND METHODS

According to the notation used by Sahni and Tureci [4], the steady–state BTE for one–speed neutrons in a slab–geometry homogeneous media can be written as

$$\mu \frac{\partial}{\partial x}\psi(x,\,\mu) + \Sigma_T\,\psi(x,\,\mu) \;=\; \frac{c\,\Sigma_T}{2}\sum_{l=0}^{L} b_l\,P_l(\mu)\int_{-1}^{1} d\mu'\;P_l(\mu')\,\psi(x,\,\mu') \qquad . \tag{1}$$

In Equation (1), the conventional terms apply: Σ_T is the total macroscopic cross–section, c is the mean number of secondary neutrons per collision, b_l depend on the scattering function with b_0 = 1, and $P_l(\mu)$ are the Legendre polynomials of degree l. The quantities x and $\mu \in [-1;\,+1]$ are the spatial coordinate and the direction variable, respectively, and $\psi(x,\,\mu)$ is the neutron flux.

To solve Equation (1), the method of separation of variables is applied by the substitution

$$\psi(x,\,\mu) = \phi_\xi(\mu)\,e^{\frac{-\Sigma_T\,x}{\xi}} \qquad , \tag{2}$$

that yields

$$\frac{1}{\mu}\,\phi_\xi(\mu)\; - \frac{c}{2\mu}\sum_{l=0}^{L} b_l\,P_l(\mu)\;\int_{-1}^{1} d\mu'\;P_l(\mu')\,\phi_\xi(\mu') \;=\; \frac{1}{\xi}\,\phi_\xi(\mu) \qquad . \tag{3}$$

At this point, the recursion relations for Legendre polynomials are applied along with some algebraic manipulations to obtain the transcendental equation

$$\frac{c\,\xi}{2}\sum_{l=0}^{L} b_l\;\int_{-1}^{1} d\mu'\;P_l(\mu')\,\phi_\xi(\mu')\int_{-1}^{1} d\mu\,\frac{P_l(\mu)}{\xi-\mu}\;-\;1\;=\;0\quad,\quad \xi \notin [-1;1] \qquad , \tag{4}$$

whose roots are the discrete values of ξ and appear in $\pm$ pairs. Moreover, if ξ is a complex number, then its complex conjugate $\bar{\xi}$ is also a root.

From the material properties of the media (i.e., values of c and b_l), one can deduct the type of the roots of Equation (4). Table 1 summarizes results for different anisotropy orders: isotropic scattering $(L = 0)$ [1], linearly anisotropic scattering $(L = 1)$ [6], and quadratic $(L = 2)$ and triplet $(L = 3)$ anisotropic scattering [4].

Table 1: Discrete eigenvalues under different conditions.

	Conditions	Discrete eigenvalues		
$L = 0$	$c > 1$	one pair of real roots $\pm \xi_0$		
	$c < 1$	one pair of imaginary roots $\pm \xi_0$		
$L = 1$	$c > 1$	one pair of real roots $\pm \xi_0$		
	$c < 1, b_1 < 0$	one pair of imaginary roots $\pm \xi_0$		
	$b_1 > 0, 1 < c < 1 + 1/b_1$	one pair of imaginary roots $\pm \xi_0$		
	$b_1 > 0, c > 1 + 1/b_1$	one quartet or two pairs of roots	$b_1 c < 3$	one real and one imaginary
			$b_1 c > 3$	both imaginary or both real
$L = 2$	$c > 1$	one pair of real roots $\pm \xi_0$		
	$c < 1, b_2 < 0$	one pair of imaginary roots $\pm \xi_0$		
	$b_2 > 0, 1 < c < 2/3\,(1 + 1/b_2)$	one pair of imaginary roots $\pm \xi_0$		
	$b_2 > 0, c > 2/3\,(1 + 1/b_2)$	one quartet or two pairs of roots	$b_2 c < 5$	one real and one imaginary
			$b_2 c > 5$	both imaginary or both real
$L = 3$	$c > 1$	one pair of real roots $\pm \xi_0$		
	$c < 1, b_3 < 0$	one pair of imaginary roots $\pm \xi_0$		
	$b_3 > 0, 1 < c < 6/11\,(1 + 1/b_3)$	one pair of imaginary roots $\pm \xi_0$		
	$b_3 > 0, c > 6/11\,(1 + 1/b_3)$	one quartet or two pairs of roots	$b_3 c < 7$	one real and one imaginary
			$b_3 c > 7$	both imaginary or both real

Source: Data from the work by Sahni and Tureci [4].

2.1. Spectral analysis of the S_N transport equations

The time–independent multigroup S_N BTE with $L-$'th order of anisotropy on both the scattering and fission terms within a region Υ of a multiplying slab [9, 10] is considered with appropriate boundary conditions

$$\mu_m \frac{d}{dx}\psi_{mg}(x) + \Sigma_{T\,g}\,\psi_{mg}(x) = \sum_{l=0}^{L}\frac{2l+1}{2}P_l(\mu_m)\sum_{g'=1}^{G}\Sigma_{Sg'\to g}^{(l)}\sum_{n=1}^{N}P_l(\mu_n)\,\omega_n\,\psi_{ng'}(x)$$
$$+\frac{\chi_g}{k_{eff}}\sum_{l=0}^{L}\frac{2l+1}{2}P_l(\mu_m)\sum_{g'=1}^{G}\nu_{g'}\,\Sigma_{f\,g'}^{(l)}\sum_{n=1}^{N}P_l(\mu_n)\,\omega_n\,\psi_{ng'}(x)\quad , \tag{5}$$
$$x\in\Upsilon\ ,\quad m=1{:}N\ ,\quad g=1{:}G\ .$$

The angular quadrature of order N is defined by the discrete directions (μ_m) and their associated weights (ω_m). The quantity $\psi_{mg}(x)$ is the angular flux of particles with energy within the group g traveling in direction μ_m; χ_g represents the spectrum of neutrons appearing in group g due to fission; $\Sigma_{Sg'\to g}^{(l)}$ and $\Sigma_{f\,g'}^{(l)}$ are the Legendre moments of the macroscopic differential scattering and fission cross section, respectively; $\nu_{g'}$ is the average number of neutrons in group g' released in each fission reaction; and k_{eff} is the multiplication factor.

Equation (5) can be rewritten aiming an analogous form to Equation (1) for the monoenergetic analytic problem as

$$\mu_m \frac{d}{dx}\psi_{mg}(x) + \Sigma_{T\,g}\,\psi_{mg}(x) = \sum_{g'=1}^{G}\frac{c_{g'\to g}\,\Sigma_{T\,g'}}{2}\sum_{l=0}^{L}b_{g'\to g}^{(l)}\,P_l(\mu_m)\sum_{n=1}^{N}P_l\,(\mu_n)\,\omega_n\,\psi_{ng'}(x)\quad ,$$
$$x\in\Upsilon\ ,\quad m=1{:}N\ ,\quad g=1{:}G\ , \tag{6}$$

with the definitions:

$$c_{g'\to g} = \frac{\Sigma_{Sg'\to g}^{(0)} + \dfrac{\chi_g\,\nu_{g'}\,\Sigma_{f\,g'}^{(0)}}{k_{eff}}}{\Sigma_{T\,g'}} \quad \text{and} \quad b_{g'\to g}^{(l)} = \begin{cases} 1 & , \quad l=0 \text{ and } g'=g \\ 0 & , \quad c_{g'\to g}=0 \\ \dfrac{(2l+1)\left(\Sigma_{Sg'\to g}^{(l)} + \dfrac{\chi_g\,\nu_{g'}\,\Sigma_{f\,g'}^{(l)}}{k_{eff}}\right)}{\Sigma_{Sg'\to g}^{(0)} + \dfrac{\chi_g\,\nu_{g'}\,\Sigma_{f\,g'}^{(0)}}{k_{eff}}} & , \quad \text{otherwise} \end{cases}\ . \tag{7}$$

To solve the homogeneous equation, Equation (6), it is considered the function

$$\psi_{mg}(x) = a_{mg}(\xi)\ e^{-\frac{x}{\xi}} \quad . \tag{8}$$

It is noteworthy that Equation (8) is analogous to the ansatz in Equation (2). Now, this expression is substituted into Equation (6) to obtain, after some operations, an eigenvalue problem of order NG

$$\sum_{g'=1}^{G}\sum_{n=1}^{N}\left\{\delta_{m,n}\,\delta_{g,g'}\,\frac{\Sigma_{T\,g}}{\mu_m} - \frac{c_{g'\to g}\,\Sigma_{T\,g'}\,\omega_n}{2\mu_m}\sum_{l=0}^{L} b_{g'\to g}^{(l)}\,P_l(\mu_m)\,P_l(\mu_n)\right\}a_{ng'}(\xi) = \frac{1}{\xi}\,a_{mg}(\xi) \quad . \tag{9}$$

By solving this eigenvalue problem, a set of NG linearly independent eigenfunctions defined in Equation (8) for $x \in \Upsilon$ is obtained.

3. RESULTS AND DISCUSSION

For high quadrature orders, the dominant eigenvalues obtained from the S_N problem should agree with the discrete eigenvalues from the one–speed analytic problem. Sahni and Tureci [4] reported the discrete eigenvalues calculated considering several combinations of values of c and b_l for three test cases: (a) linearly anisotropic scattering ($b_0, b_1 \neq 0$, otherwise $b_l = 0$), (b) isotropic+pure quadratic scattering ($b_0\,, b_2 \neq 0$, otherwise $b_l = 0$), and (c) isotropic+pure triplet scattering ($b_0, b_3 \neq 0$, otherwise $b_l = 0$).

The eigenvalue problem from the S_N BTE, Equation (9), was solved for all the examples reported by Sahni and Tureci [4]. It was started at low orders of the Gauss–Legendre quadrature that were increased up to obtain S_N results in agreement with the discrete Case's spectrum within a range of less than 100 pcm. The *RMatrixEVD* subroutine from the ALGLIB library [11] was used, in order to find the eigenvalues (real and imaginary parts) and eigenvectors of a general matrix.

Tables 2 to 4 show the results obtained from solving the S_N eigenvalue problem published by Sahni and Tureci [4]. In all cases, the moduli of the dominant eigenvalues and the relative deviations in pcm with respect to the reference values are presented. One can observe that for a quadrature order $N = 64$, the relative deviation is less than 80 pcm in all cases.

Table 2: The discrete eigenvalues for linearly anisotropic scattering $(L = 1)^{a}$.

$c \setminus b_1$	-0.9	0.6		0.9	
0.8	1.269769136 (0.03)[b]	1.5319699636 (0.04)		1.6087164379 (0.04)	
1.5	0.5811518597i (0.02)	0.8120788574i (0.005)		0.9078974421i (0.02)	
3.0	0.2039774078i (0.01)	0.3248994249i (0.01)	1.0002732641 (8.22)	0.4254805876i (0.04)	1.2809237676 (0.11)
4.0	0.1439582693i (0.003)	0.2399911569i (0.02)	1.1327124051 (0.04)	0.4026092026i (0.27)	0.5566781230i (0.41)

[a] Only the magnitude of real or purely imaginary eigenvalue pair is tabulated.
[b] relative deviation (pcm) with respect to the discrete analytic eigenvalue [4].

Table 3: The discrete eigenvalues for linearly anisotropic scattering $(L = 2)^{a}$.

$c \setminus b_2$	-1.0	0.5		1.5	
0.8	1.3902078564 (0.03)[b]	1.4187852618 (0.04)		1.4486484525 (0.04)	
1.5	0.712095766i (0.02)	0.67386471i (0.01)		0.6317760051i (0.004)	1.0309375337 (0.004)
3.0	0.2785204395i (0.005)	0.2364960112i (0.0001)	1.0057660256 (0.01)	0.2045765429i (0.003)	2.3007655785 (0.19)
4.0	0.2041791731i (0.003)	0.1664595861i (0.003)	1.0410302996 (0.001)	0.1415999511i (0.01)	1: 6038876543i (0.15)

[a] Only the magnitude of real or purely imaginary eigenvalue pair is tabulated.
[b] relative deviation (pcm) with respect to the discrete analytic eigenvalue [4].

Table 4: The discrete eigenvalues for linearly anisotropic scattering $(L = 3)^a$.

$\boldsymbol{c} \setminus \boldsymbol{b_3}$	-1.0	0.5		1.0	
0.8	1.4053567858 $(0.03)^b$	14090532489 (0.03)		1.4107235544 (0.03)	
1.5	$0.6841100404i$ (0.01)	$0.6920605429i$ (0.01)		$0.6953423810i$ (0.01)	1.0029060860 (0.125)
3.0	$0.2399919939i$ (0.002)	$0.585796957i$ (0.004)	1.0068223847 (0.01)	$0.2663092301i$ (0.01)	1.0936625073 (0.001)
10.0	$0.0595745983i$ (80.2)	$00713391099i$ (26.0)	1.4377274882 (0.03)	$0.0778750654i$ (13.0)	$19751716742i$ (0.03)

[a] Only the magnitude of real or purely imaginary eigenvalue pair is tabulated.
[b] relative deviation (pcm) with respect to the discrete analytic eigenvalue [4].

3.1. Solution to the S_N BTE

As a result of the previous analysis, in this subsection, a methodology to obtain the analytic solution to the slab–geometry multigroup S_N BTE in multiplying media [12–14] is proposed. It is remarked that the presented procedures can also be used to derive the homogeneous component of the general solution in fixed–source problems [15–20]. Equation (5) can be represented in matrix form as

$$\frac{d}{dx}\mathbf{\Psi} = \mathbf{M}\,\mathbf{\Psi} \quad , \tag{10}$$

where $\mathbf{M}$ is the NG–order square matrix with entries

$$M_{mg,ng'} = \frac{1}{\mu_m}\left\{-\delta_{m,n}\,\delta_{g,g'}\,\Sigma_{T\,g} + \sum_{l=0}^{L}\frac{2l+1}{2}\,P_l(\mu_m)\,P_l(\mu_n)\,\omega_n\left[\Sigma_{Sg'\to g}^{(l)} + \frac{\chi_g}{k_{eff}}\nu_{g'}\,\Sigma_{f\,g'}^{(l)}\right]\right\}$$

$$m = 1{:}N\ ,\ \ g = 1{:}G\ ,\ \ n = 1{:}N\ ,\ \ g' = 1{:}G\ , \tag{11}$$

and $\mathbf{\Psi}$ is a column matrix whose entries are $\psi_{mg}(x)$. The solution to the homogeneous system of ordinary differential equations in Equation (10) can be written as

$$\boldsymbol{\Psi}^{\mathrm{H}}(x) = \sum_{k=1}^{NG} \alpha_k \; v_k \, e^{\xi_k x} \qquad , \tag{12}$$

where v_k are the eigenvectors associated to the eigenvalues ξ_k of matrix M. Depending on the material parameters, the NG eigenvalues ξ_k can appear in $\pm$ real pairs, imaginary or complex conjugate. Since the input of matrix M are real numbers, the real eigenvalues will be associated to real eigenvectors, and the complex conjugate eigenvalues will be associated to complex conjugate eigenvectors.

As it is the case, when $\xi = p + qi$ and $\bar{\xi} = p - qi$ are a pair of eigenvalues, the eigenvectors associated to ξ and $\bar{\xi}$ are $\mathbf{v} = \mathbf{a} + \mathbf{b}i$ and $\bar{\mathbf{v}} = \mathbf{a} - \mathbf{b}i$, respectively [21]. After some operations, two real–valued solutions are obtained

$$\boldsymbol{\Psi}_{\mathbf{1}}(x) = (a \, \cos qx - b \, \sin qx) \, e^{p\,x} \quad \text{and} \quad \boldsymbol{\Psi}_{\mathbf{2}} = (b \, \cos qx + a \, \sin qx) \, e^{p\,x} \quad . \tag{13}$$

Therefore, if K_R real eigenvalues and K_C complex conjugate pairs are found, i.e., $K_R + 2K_C = NG$, a set of NG linearly independent eigenfunctions is obtained, and the solution to Equation (5) within region Υ is

$$\begin{aligned} \boldsymbol{\Psi}^{\mathrm{H}}(x) = {} & \sum_{k=1}^{K_R} \alpha_k \, \mathbf{v}_k \, e^{\xi_k x} \\ & + \sum_{j=1}^{K_C} \left\{ \beta_j \left(\mathbf{a}_j \cos q_j x - \mathbf{b}_j \sin q_j x \right) + \beta'_j \left(\mathbf{b}_j \, \cos q_j x + \mathbf{a}_j \, \sin q_j x \right) \right\} \, e^{p_j x} \end{aligned} \tag{14}$$

where α_i, β_j and β'_j are arbitrary constants to be determined. Equation (14) can be represented in matrix form as

$$\boldsymbol{\Psi}(x) = [\mathbf{M_R} \, \mathbf{I}_{e\cos}(x) + \mathbf{N_R} \, \mathbf{I}_{e\sin}(x)] \, \boldsymbol{\alpha} \qquad , \tag{15}$$

with the definition of matrices

$$\mathbf{M_R} = \begin{bmatrix} \mathrm{v}_{1,1} & \cdots & \mathrm{v}_{1,K_R} & \mathrm{a}_{1,1} & \mathrm{b}_{1,1} & \cdots & \mathrm{a}_{1,K_C} & \mathrm{b}_{1,K_C} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathrm{v}_{NG,1} & \cdots & \mathrm{v}_{NG,K_R} & \mathrm{a}_{NG,1} & \mathrm{b}_{NG,1} & \cdots & \mathrm{a}_{NG,K_C} & \mathrm{b}_{NG,K_C} \end{bmatrix} \qquad ,$$

$$\mathbf{N_R} = \begin{bmatrix} 0 & \cdots & 0 & -\mathrm{b}_{1,1} & \mathrm{a}_{1,1} & \cdots & -\mathrm{b}_{1,K_C} & \mathrm{a}_{1,K_C} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & -\mathrm{b}_{NG,1} & \mathrm{b}_{NG,1} & \cdots & -\mathrm{b}_{NG,K_C} & \mathrm{a}_{NG,K_C} \end{bmatrix} ,$$

$$\mathbf{I}_{e\cos}(x) = diag\left\{e^{\xi_1 x}, \cdots, e^{\xi_{K_R} x}, e^{p_1 x}\cos q_1 x\,, e^{p_1 x}\cos q_1 x\,, \cdots, e^{p_{K_C} x}\cos q_{K_C} x\,,\ e^{p_{K_C} x}\cos q_{K_C} x\right\} ,$$

$$\mathbf{I}_{esin}(x) = diag\left\{0, \cdots, 0\,,\ e^{p_1 x} sin\, q_1 x\,, e^{p_1 x} sin\, q_1 x\,, \cdots\,,\ e^{p_{K_C} x} sin\, q_{K_C} x\,,\ e^{p_{K_C} x} sin\, q_{K_C} x\right\}$$

and

$$\boldsymbol{\alpha} = \left[\alpha_1\,,\ \cdots,\ \alpha_{K_R}\,,\ \beta_1\,,\ \beta_1^{'}\,,\ \cdots\,,\ \beta_{K_C}\,,\ \beta_{K_C}^{'}\right]^T .$$

The terminology presented here for the spectral analysis can be used in the development and implementation of spectral nodal methods to obtain accurate and efficient numerical solutions to the S_N BTE in slab–geometry. It is noteworthy that the notation used here is general and compact, nevertheless, it can be modified, and one should perform the construction of the matrices and the order of the operations aiming at computational efficiency.

4. CONCLUSION

In this paper, the spectral analysis of the S_N BTE with anisotropic scattering has been performed and the results with the discrete Case's eigenvalues from the analytic transport problem have been compared. As one could anticipate, for a quadrature order high enough, the dominant S_N eigenvalues agree with the discrete spectrum. A simplification for the procedures to obtain the analytic solution of the S_N BTE considering high–order anisotropic events in the scattering and fission sources was also presented. This simplification has been presented in a compact form and includes the possibility of obtaining complex eigenvalues from the spectral analysis. The present methodology shall be applied not only to slab–geometry problems but also to multidimensional spectral nodal methods that use transverse integration procedures.

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