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Spherical Harmonics and Energy Polynomial Solution of the Boltzmann Equation for Neutrons*-I

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The approximate solution of the source-free energy-dependent Boltzmann transport equation for neutrons in plane geometry and isotropic scattering case was given by Leonard and Ferziger using a truncated development in a series of energy-polynomials for the energy dependent neutron flux and solving exactly for the angular dependence. The presence in the general solution of eigenfunctions belonging to a continuous spectrum gives rise to difficult analytical problems in the application of their method even to simple problems To avoid such difficulties, the angular dependence is treated in this paper by a spherical harmonics method and a general solution of the energy-dependent transport equation in plane geometry and isotropic scattering is obtained, in spite of the appearance of matrices as argurnent of the angular polynomials.

Uma solução aproximada da equação de transporte de Boltzmann para neutrons, sem fonte, poli-energética, em geometria plana e espalhamento isotrópico, foi obtida por Leonard e Ferziger. Estes autores, utilizando um desenvolvimento truncado em uma série de polinômios na energia para descrever a dependência energética do fluxo de neutrons, obtiveram uma solução exata para a dependência angular. A presença, na solução geral, de auto-funções pertencentes a um espectro contínuo de autovalores, dá origem a problemas analíticos dificeis mesmo quando se consideram casos simples. Para evitar tais dificuldades, a dependência angular do fluxo de neutrons é tratada neste trabalho pelo método de esféricas harmônicas. A solução geral da equação de transporte em geometria plana e espalhamento isotrópico é obtida, apesar do aparecimento de matrizes como argumentos dos polinômios angulares considerados.

Introduction

The source-free energy-dependent Boltzmann equation for neutrons in plane geometry has bem the subject of a considerable number of papers since 1962. The origin of this sudden interest in this problem can be traced back to the fundamental work of Case' who developed the now called "singular eigenfunctions method". Case's work dealt with the energy-independent case and the extension to the energy-dependent case was basically due to the Zelazny and Kusze11[2], Bednarz and Mika[3] and Leonard and

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Ferziger[4,5]. Whereas the work of Zelazny and Kuszell was based in the multi-group method, Leonard and Ferziger used the polynomial method to treat the energy dependence of the neutron flux.

The method of Leonard and Ferziger gives an approximate solution of the source-free energy dependent Boltzmann equation in plane geometry: it is approximate as far as the energy dependence of the solution is concerned, but it is exact in the angular variable, and can be applied to infinite or finite medium problems.

The use of an extension of Case's method by Leonard and Ferziger led to the appearance, in the general solution, of eigenfunctions belonging to a discrete as well as a continuous spectrum of eigenvalues: and the presence of eigenfunctions belonging to a continuous spectrum of eigenvalues gave rise to difficult analytical problems in the application even to simple practical problems. As a matter of fact, the angular dependence is obtained exactly but only formally. When one wants to apply their general solution to real problems on finite media, the exactness of the angular dependence is ultimately lost, since the Fredholm equations that result must be solved approximately.

Such difficulties motivated the work to be presented in this paper. in which the angular dependence of the neutron flux is treated approximately by the wellknown spherical harmonics method and a general solution of the Boltzmann equation in plane geometry can be obtained in a form that closely resembles the solution of the energy – independent case.

The plan of this paper is asfollows: in Part 1, the energy-dependent transport equation is reduced to a system of coupled matrix equations that is quite similar to the system of algebraic equations wellknown in the spherical harmonics method of solution of the energy-independent transport equation, In Part 2, the equation that determines the eigenvalues is obtained, as well as the corresponding eigenfunctions. The general solution of the Boltzmann equation in an arbitrary order of approximation in the energy and angle variables, for the case of isotropic scattering and plane geometry, is also explicitly given. In Part 3, some conclusions are presented as well as the plan to extend this method to other geometries.

1. The Transgort Equation in the Energy-Angle Polynomial Method

For the case of plane symmetry, the source-free energy dependent Boltzmann equation for a non-multiplying homogeneous and isotropic medium, can be written as follows:

$$\mu \frac{\partial}{\partial x} \phi(x, E, \mu) + \sum_t(E)\, \phi(x, E, \mu)$$

$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} \int_0^{\infty} dE' \sum_s^l (E' \to E)\, P_l(\mu) \int_{-1}^{+1} d\mu'\, P_l(\mu')\, \phi(x, E', \mu'), \qquad (1)$$

where $\Sigma_s^l(E' \to E)$ is the l- moment of the scattering kernel for neutron scattering from energy E' to E; μ is the cosine of the angle between the direction of travel of the neutron and the x-axis. All distances are measured in terms of the maximum free path $(1/\Sigma_t(\min))$: all cross sections appearing in (1) are dimensionless. If the further assumption is made that the scattering is isotropic, then

$$\sum_s^l (E' \to E) = \sum_s^l \cdot \delta_{l0}\,,$$

and Eq. (1) reduces to equation (2.1) of the paper of Leonard and Ferziger[5]. This simplification will be made later on in this paper.

Following the method of energy-polynomial approximation of Leonard and Ferziger (Ref. 4, hereafter referred to as F & L), $\phi(x, E, \mu)$ is developed in a series of a complete set of orthonormal functions of the energy, $g_j(E)$:

$$\phi(x, E, \mu) = \sum_{j=0}^{\infty} q_j(x, \mu)\, g_j(E), \qquad (2)$$

$$\int_0^{\infty} dE\, g_j(E)\, g_k(E) = \delta_{jk}\,. \qquad (3)$$

An approximate solution of the exact equation (1) in the case of isotropic scattering kernel, was given by F & L by a truncation procedure: they retained, in the development (2) only the first (L + 1) terms:

$$\phi(x, E, \mu) = \sum_{j=0}^{L} q_j(x, \mu)\, g_j(E). \qquad (4)$$

Such a truncation procedure can be expected to give good results as long as $\Sigma_t(E)$ is a smooth function of the energy; one can hardly expect this method to give good results in the resonance region of those media containing heavy elements, specially uranium and thorium. In the thermal region, $\Sigma_t(E)$ varies smoothly and (4) can be expected to give good results with a reasonable low value for L and a suitable choice of the $g_j(E)$.

Considering then only the thermal region, the moments of the scattering kernel satisfy the detailed balance condition[7], that is:

$$M(E) \sum_s^l (E \to E') = M(E') \sum_s^l (E' \to E), \qquad (5)$$

where

$$M(E) = Ee^{-E} \tag{6}$$

is the Maxwellian distribution and the energy E is measured in units of kT.

It is usual, in this case, to symmetrize the scattering kernel. This is done defining $\psi(x, E, \mu)$ by

$$\phi(x, E, \mu) = \sqrt{M(E)}\,\psi(x, E, \mu). \tag{7}$$

Using (7), Eq. *(1)* can be written as

$$\mu \frac{\partial}{\partial x}\psi(x, E, \mu) + \sum_t(E)\,\psi(x, E, \mu)$$

$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} \int_0^{\infty} dE' \cdot \sum_{ss}^{l}(E' \to E)\, P_l(\mu) \int_{-1}^{+1} d\mu'\, P_l(\mu')\,\psi(x, E', \mu'), \tag{8}$$

where $\Sigma_{ss}^{l}(E' \to E)$, defined by

$$\sum_{ss}^{l}(E' \to E) = \left[M(E')\right]^{1/2} \sum_{s}^{l}(E' \to E), \tag{9}$$

is symmetric due to Eq. (5).
To simplify, let us put

$$\psi(x, E, \mu) = \sum_{j=0}^{L} f_j(x, \mu)\, g_j(E). \tag{10}$$

Eq. (4) is then substituted by

$$\phi(x, E, \mu) = \sqrt{M(E)} \sum_{j=0}^{L} f_j(x, \mu)\, g_j(E), \tag{11}$$

and, by a suitable choice of the functions $g_j(E)$, the truncated development *(11)* can be made to represent the deviation from the Maxwellian distribution of the actual neutron spectrum. This, again, reinforces our argument that in the thermal region – where, in the absence of absorption, the neutron spectrum in an infinite medium deviates little from a Maxwellian one -- low values of L will be sufficient to account for deviations due to absorption or leakage in finite media.

Substituting *(10)* in (8) and using (3), one obtains immediately

$$\sum_{j=0}^{L} \left\{ \mu \frac{\partial}{\partial x} f_j(x,\mu) \cdot \delta_{jk} + V_{kj}\, f_j(x,\mu) \right\} =$$

$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int_{-1}^{+1} d\mu'\, P_l(\mu') \sum_{j=0}^{L} \alpha_{kj}^{l}\, f_j(x,\mu'), \qquad (12)$$

where

$$V_{kj} = \int_0^{\infty} dE\, g_k(E)\, \Sigma_t(E)\, g_j(E), \qquad (13)$$

$$\alpha_{kj}^{l} = \int_0^{\infty} dE \int_0^{\infty} dE'\, g_k(E)\, \Sigma_{ss}^{l}(E' \to E)\, g_j(E'). \qquad (14)$$

This is a system of finite coupled integro-differential equations in which the expiicit dependence of the energy was eliminated.

If $\Sigma_t(E)$ is energy-independent (constant cross-section approximation, in the sense used by Davison[7] or Ferziger and Leonard[6]), V_{kj} is a diagonal matrix and (12) can be reduced to the case considered by Ferziger and Leonard[6], that is, to a set of uncoupled energy-independente problems.

Defining now the matrices

$[V]$ = symmetric square matrix of order (L + 1), with elements V_{kj}.
$[a']$ = symmetric square matrix of order (L + 1), with elements α_{kj}^{l},
$|f(x,\mu)\rangle$ = column matrix (vector) of order (L + 1), with elements $f_j(x, p)$,

the system (12) can be written, in matrix notation, as

$$\mu \frac{\partial}{\partial x} |f(x,\mu)\rangle + [V]\, |f(x,\mu)\rangle$$

$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int_{-1}^{+1} d\mu'\, P_l(\mu')\, [\alpha^l]\, |f(x,\mu')\rangle. \qquad (15)$$

It is important to notice that the matrices $[V]$ and $[a']$ will couple *all* components of the vector $|f(x,\mu)\rangle$. If a partial decoupling could be obtained, the solution of (15) would be very much simplified.

Such decoupling, in case of isotropic scattering, was done by F & L[4], allowing these outhors to obtain exact solutions in the variable μ, in any finite order of approximation L of the energy polynomial approximation.

Considering (15) a partial decoupling will be obtained using the same method used by F & L.

Since [V] is real and symmetric, there exists an orthogonal matrix [O] such that the similarity transformation

$$[\mathcal{O}]^{-1}[V][\mathcal{O}] = [\beta] \tag{16}$$

gives a diagonal matrix $[\beta]$. This similarity transformation gives also

$$[\mathcal{O}]^{-1}[\alpha^l][\mathcal{O}] = [\gamma^l], \tag{17}$$

$$[\mathcal{O}]^{-1}|f(x,\mu)\rangle = |h(x,\mu)\rangle, \tag{18}$$

where $[\gamma^l]$ is again symmetric but not diagonal.

Using Eqs. (16), (17) and (18), one gets from Eq. (15):

$$\mu\frac{\partial}{\partial x}|h(x,\mu)\rangle + [\beta]|h(x,\mu)\rangle = \sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu)\int_{-1}^{+1}d\mu'\,P_l(\mu')[\gamma^l]|h(x,\mu')\rangle \tag{19}$$

The translational invariance of this system suggests to look for solutions of the form:

$$|h(x,\mu)\rangle = \exp(-x/\nu).|h(\nu,\mu)\rangle. \tag{20}$$

With the ***Ansatz*** (20). Eq. (19) gives

$$\left(-\frac{\mu}{\nu}[I] + [\beta]\right)|h(\nu,\mu)\rangle = \sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu)\int_{-1}^{+1}d\mu'\,P_l(\mu')[\gamma^l]|h(\nu,\mu')\rangle, \tag{21}$$

where [I] denotes the identity matrix.

Up to this point, but for the generality of the considering a fully anisotropic kernel, the treatment is the same as the one developed by F & L[4].

The solution of Eq. (21), even with two terms in the second member – linearly anisotropic scattering kernel – was not considered by F & L and it seems that it will be very hard to be obtained.

Now there will be an essential departure from the F & L method: instead

of trying to solve exactly Eq. (21), the spherical harmonics method will be used to solve for the angular dependence of $|h(\nu, p))$.

Putting

$$|h(\nu, \mu)\rangle = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(\mu) \,|\, B_n(\nu)\rangle, \tag{22}$$

one gets, from Eq. (21),

$$-\sum_{n=0}^{\infty} \frac{2n+1}{2} \frac{1}{\nu} \mu P_n(\mu) \,|\, B_n(\nu)\rangle + \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(\mu) [\beta] \,|\, B_n(\nu)\rangle$$
$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) [\gamma^l] \sum_{n=0}^{\infty} \frac{2n+1}{2} \int_{-1}^{+1} d\mu' \, P_l(\mu') \, P_n(\mu) \,|\, B_n(\nu)\rangle. \tag{23}$$

Since

$$(2n+1) \mu P_n(\mu) = (n+1) P_{n+1}(\mu) + n P_{n-1}(\mu), \tag{24}$$

one gets from Eq. (23), upon multiplication by $P_m(\mu)$, integration in $d\mu$ and use of

$$\int_{-1}^{+1} d\mu \, P_m(\mu) \, P_n(\mu) = \frac{2}{2m+1} \delta_{mn}, \tag{25}$$

the following system of matrix equations:

$$(m+1) \,|\, B_{m+1}(\nu)\rangle + m \,|\, B_{m-1}(\nu)\rangle - (2m+1) \nu [\beta] \,|\, B_m(\nu)\rangle$$
$$= -(2m+1) \nu [\gamma^m] \,|\, B_m(\nu)\rangle, \qquad m = 0, 1, 2, \ldots . \tag{26}$$

It is important to notice that now the matrices $[\beta]$ and $[\gamma^m]$ couple only the various components of each single vector like $|B_m(\nu)\rangle$: the coupling of components of different vectors is completely absent. And furthermore, such coupling between components of a single vector is due only to the presence of the non-diagonal matrices $[\gamma^m]$, since $[\beta]$ being a diagonal matrix does not bring any coupling.

The number of coupling matrices $[\gamma^m]$ is equal to the number of moments of the scattering kernel that one wants to consider. For example, if the isotropic scattering kernel is considered, as did F & L[4], only the matrix $[\gamma^0]$ differs from zero, and *(26)* reduces to:

$$(m+1) \,|\, B_{m+1}(\nu)\rangle + m \,|\, B_{m-1}(\nu)\rangle - (2m+1) \nu [\beta] \,|\, B_m(\nu)\rangle$$
$$= -\nu [\gamma^0] \,|\, B_0(\nu)\rangle \, \delta_{m0}, \qquad m = 0, 1, 2, \ldots . \tag{27}$$

So, the isotropic kernel couples only the components of the vector $|B_0(v)\rangle$. Considering a linearly anisotropic kernel, there will be two matrices $[\gamma^0]$ and $[\gamma^1]$ differing from zero; and whereas $[\gamma^0]$ will introduce coupling between the components of $|B_0(v)\rangle$, $[\gamma^1]$ will do the same between the components of $|B_1(v)\rangle$.

The diagonalization of the $[V]$ matrix of Eq. (15) was really important; without such a diagonalization, there would be in the left member of *(27)* a coupling between the components of all vectors and no only of the vector $|B_0(v)\rangle$ in the isotropic case.

Finally, since $[\beta]$ is diagonal, the system *(27)* has a structure that closely parallels the one of the system that occurs in the energy-independent or constant cross-section case and that has been extensively studied and applied[8,9,10].

The coupling introduced between the coniponents of $|B_0(v)\rangle$ in equation *(27)* can be dealt with without difficulty, as will be seen in Sec. *2.*

2. Eigenvalues and Eigenfunctions in the Energy-Angle Pohynomial Approximation: Isotropic Case

Considering Eq. *(26)* and keeping only a finite number of $(N+1)$ terms in the expansion (22), one obtains the following system of matrix equations:

$$(m+1)\,|B_{m+1}(v)\rangle + m\,|B_{m-1}(v)\rangle - (2m+1)\,v\,[\beta]\,|B_m(v)\rangle = -(2m+1)\,v\,[\gamma^m]\,|B_m(v)\rangle, \qquad m = 0, 1, \ldots, N-1, \tag{28}$$

$$N\,|B_{N-1}(v)\rangle - (2N+1)\,v\,[\beta]\,|B_N(v)\rangle = -(2N+1)\,v\,[\gamma^N]\,|B_N(v)\rangle. \tag{29}$$

If one considers, for the sake of simplicity, the isotropic case. only $[\gamma^0]$ will be different from zero and Eqs. (28) and *(29)* reduce to

$$(m+1)\,|B_{m+1}(v)\rangle + m\,|B_{m-1}(v)\rangle - (2m+1)\,v\,[\beta]\,|B_m(v)\rangle = -v\,[\gamma^0]\,|B_0(v)\rangle\,\delta_{m,0}, \qquad m = 0, 1, 2, \ldots, N-1, \tag{30}$$

$$N\,|B_{N-1}(v)\rangle - (2N+1)\,v\,[\beta]\,|B_N(v)\rangle = 0. \tag{31}$$

The solution of (28), *(29)* for the linearly anisotropic case could be obtained without difficulty using a general method developed by Travelli[11].

Up to now, v was an arbitrary parameter: now it will be determined by imposing the condition that the homogeneous system (30), (31) has non-trivial solutions.

Following a method developed by Kofink[12] for the energy-independent case, the following system of (N + 1) equations and $(N + 2)$ unknowns is considered:

$$(m+1)\,|\,B_{m+1}(v)\rangle + m\,|\,B_{m-1}(v)\rangle - (2m+1)\,v\,[\beta]\,|\,B_m(v)\rangle = -v\,[\gamma^0]\,|\,B_0(v)\rangle\,\delta_{m0}\,, \qquad m = 0, 1, \ldots, N-1, \tag{32}$$

$$(N+1)\,|\,B_{N+1}(v)\rangle + N\,|\,B_{N-1}(v)\rangle - (2N+1)\,v\,[\beta]\,|\,B_N(v)\rangle = 0. \tag{33}$$

$$|\,B_{N+1}(v)\rangle = 0, \tag{34}$$

the system (32)-(33) reduces to (30)-(31).

Kofink's method consists in obtaining a solution of the system (32), (33) without any restriction on v; then, Eq. (34) will determine the values of v that allow the existence of non-trivial solutions of the original system (30), (31).

It is easily shown that

$$|\,B_n(v)\rangle = \{P_n([v\beta]) - W_{n-1}([v\beta])\cdot[v\gamma^0]\}\,|\,B_0(v)\rangle \tag{35}$$

is a solution of the system (32), (33), with no restriction on v; and $|\,B_0(v)\rangle$ is an arbitrary vector, different from zero.

In Eq. (35), $W_{n-1}(x)$ is the non-singular part of the Legendre functions of second kind[13].

It is worthwhile to notice that the diagonal character of the matrix $[\beta]$ plays again an important part. Indeed, $[v\beta]$ being a diagonal matrix, there is no difficulty at all due to its presence as argument of polynomials like P_n or W_{n-1}.

Eqs. (34) and (35) give the characteristic determinantal equation

$$\|\,P_{N+1}([v\beta]) - W_N([v\beta])\cdot[v\gamma^0]\,\| = 0 \tag{36}$$

that determines the (L + 1)$(N + 1)$ eigenvalues v.

If N is odd, all roots of (36) will be different from zero; and furthermore. the $(L + 1)(N + 1)$ roots occurs in pairs, that is, to each positive root $(+ |\nu_s|)$ there corresponds a negative one $(- |\nu_s|)$, with $s = 1, 2, \ldots \frac{1}{2}(N + 1)(L + 1)$.

From now on the approximation in which there are $(L + 1)$ terms in the energy polynomial expansion and $(N + 1)$ terms in the Legendre (angular) expansion will be called a $P_N L_L$ approximation; and N will always be considered to be odd, as is usual in the energy-independent case.

The characteristic equation (36) is in a form which is convenient for studying the behaviour of the eigenvalues $\pm \nu$, when $N \to \infty$. This is due to the fact that the determinantal equation (36) is always of order $(L + 1)$: when N increases, only the order of P_{N+1} and W_N will increase.

The vector eigenfunctions $|B_n(\nu)\rangle$ $(n = 0, 1 \ldots N)$ are now compietely determined by (35), with the only restriction that ν is no more an arbitrary parameter but must be a member of the set $\pm \nu_s (s = 1, 2, \ldots \frac{1}{2}(N + 1)(L + 1))$.

Finally, the general solution of the linear Boltzmann equation in the $P_N L_L$ approximation (N odd) will be given, in the isotropic case and plane geometry, by

$$\phi(x, E, \mu) = \sqrt{M(E)} \left\{ \sum_{s=1}^{\frac{1}{2}(N+1)(L+1)} \sum_{j=0}^{L} \sum_{n=0}^{N} \left[C_s^{(+)} A_j^n(+\nu_s) \exp(-x/\nu_s) + C_s^{(-)} A_j^{(n)}(-\nu_s) \exp(x/\nu_s) \right] \frac{2n+1}{2} P_n(\mu)\, g_j(E), \right. \tag{37}$$

where the $A_j^n(\nu)$ denote the components of a vector $|A_n(\nu)\rangle$ which are given by

$$|A_n(\nu)\rangle = [\mathcal{O}]\, |B_n(\nu)\rangle \tag{38}$$

or

$$|A_n(\nu)\rangle = [\mathcal{O}]\, [H_n]\, |B_0(\nu)\rangle, \tag{39}$$

with

$$[H_n] = P_n([\nu\beta]) - W_{n-1}([\nu\beta]) \cdot [\nu\gamma^0]. \tag{40}$$

The $C_s^{(+)}$ and $C_s^{(-)}$ are $(L + 1)(N + 1)$ arbitrary coefficients to be determined by boundary conditions appropriate to a particular physical problem.

The analysis of the behaviour of the eigenvalues and eigenfunctions given by (36) and (35) when $N \to \infty$, as well as numerical comparison with some results given by F & L, will be presented in another paper.

3. Concluding Remarks

The general solution (37) has been applied to the solution of the energy-dependent Milne problem in a medium that scatters and absorbs neutrons[14]. The study of the same problem but considering the influence of a linearly anisotropic scattering kernel was also carried out[15], and both works will be shortly submitted to publication.

As could be anticipated looking at the simple and compact nature of (37), it can be applied in a way that permits complete and detailed studies to be made, using even small computers and without too long computing times.

The extension of this method to spherical and cylindrical geometries is being studied.

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