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Eigenvalue Theorems for the Discrete Form of the Multigroup Diffusion- and Transport Equations

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Abstract

The existence of a positive, greatest, single and unique eigenvalue is proved for the discrete form of the multigroup diffusion equations and for the discrete multigroup Boltzmann equations; the convergence of outer iterations may be concluded. The following assumptions are made:

1) A neutron introduced at any point in the reactor may diffuse to all locations of the assembly (i.e. the diffusion regions for all energy groups are the same).
2) Only downscattering is permitted
3) The fission transfer matrix is multiplicative.

Then a necessary and sufficient condition is derived for the existence of a greatest single eigenvalue (k-effective) and the corresponding non-negative eigenvector (neutron flux).

Sätze über Eigenwerte der diskreten Form der Multigruppen Diffusions- und Transport-Gleichung

Zusammenfassung

Für die diskreten Multigruppengleichungen der Diffusions- und Transporttheorie wird die Existenz eines größten, reellen, positiven und einfachen Eigenwertes mit einem zugehörigen nichtnegativen Flußvektor sowie die Konvergenz der äußeren Iterationen bewiesen. Dabei werden folgende Annahmen gemacht:

1) Der zu berechnende Reaktor besteht aus nur einem Diffusionsgebiet
2) Es gibt keine Aufwärtsstreuung
3) Die Spaltquerschnitte sind multiplikativ (d.h. $\chi_g \cdot \nu\sigma^{\kappa}{}_f$).

Contents

Introduction

When the diffusion- or transport-equation is substituted by consistent difference equations, the steady state neutron reactor problem leads to a matrix eigenvalue problem

$$A\ x = \frac{1}{\lambda} \cdot F\ x$$

It is of interest to know under what conditions the greatest eigenvalue λ (k-effective) is real, positive and single.

In 1958, G.Birkhoff and R.S.Varga (/1/) proved an existence theorem for the diffusion theory problem. They assumed the physical problem to be transitive (a neutron of any energy has non-zero progeny at all energies and locations), which implies A^{-1} to be irreducible.

In 1968, R.Fröhlich (/4/) replaced the conditions of transitivity by some weak conditions of connectedness which he showed to be sufficient and necessary for the existence of unique positive normalized eigenvector and a corresponding single positive greatest eigenvalue. The diffusion theory problem he considered was permitted to include arbitrary up- and downscattering and a non-multiplicative fission transfer matrix.

In this paper it is shown that, if the fission matrix is multiplicative (i.e. with elements $\chi_g \cdot (\nu\sigma_f)^k$) and only downscattering is permitted, if furthermore the diffusion regions are identical with the reactor assembly for each group, the greatest eigenvalue λ is positive and single, provided that not all eigenvalues are zero. Contrary to /4/ the corresponding neutron flux is not strictly positive (i.e. it can have certain zero components). The existence of non-zero eigenvalues depends on a graph theory condition

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which can be described as follows: Associate each energy group g with a geometrical point P_g and connect P_i with P_j by a directed line $\overrightarrow{P_iP_j}$ if neutrons located anywhere in the region may change their energy by fission or scattering from energy group i to energy group j. If and only if there is at least one closed path, a greatest single eigenvalue exists with a corresponding eigenvalue $x \geqq o$.

In section I this is shown for the diffusion problem. Section II is concerned with the transport theory problem. Finally, in Section IV the Diamond Difference Scheme (/2/) for the numerical solution of the transport problem is treated as an example.

I. The Diffusion Equation

1. The Multigroup Diffusion Equations

Section I is concerned with the diffusion equations, a system of second order elliptic partial differential equations:

$$(1) \qquad -D_g \Delta\Phi^g + \sigma_t^g \Phi^g - \sum_{k \leqq g} \sigma_{k\to g} \Phi^k = \frac{1}{\lambda} \sum_{k=1}^{G} \chi_g \cdot \nu \cdot \sigma_f^k \cdot \Phi^k$$

with boundary conditions

$$(2) \qquad \frac{\partial \Phi^g}{\partial n} + \alpha^g \Phi^g = 0$$

where n is the outward directed normal. We suppose all the coefficients to be non-negative. Our aim is to find the greatest eigenvalue λ and its associated solution Φ. λ is a measure of the reactivity of a reactor whose materials are specified by the non-negative coefficients of Eq.(1).

2. Matrix Equations

The numerical solution of (1), (2) may be performed by substituting Eqs.(1) and (2) by consistent difference equations defining approximations $\tilde{\Phi}_i^g$ for discrete lattice points (/5/). If u_g is a vector containing all the discrete values $\tilde{\Phi}_i^g$ for each group index g, from (1), (2), we obtain the matrix equations

$$(3) \qquad (T_g - S_{gg})\ u_g = \frac{1}{\lambda}\ \chi_g \sum_{k=1}^{G} F_k u_k + \sum_{k<g} S_{gk} u_k$$

$$(g = 1,\ 2,\ \ldots,\ G)$$

where

$$(4) \qquad S_{gk} = \begin{pmatrix} \sigma^1_{k\to g} & & & O \\ & \sigma^2_{k\to g} & & \\ & & \ddots & \\ O & & & \sigma^I_{k\to g} \end{pmatrix}$$

$$(5) \qquad F_k = \begin{pmatrix} (\nu\sigma_f)^k_1 & & & O \\ & (\nu\sigma_f)^k_2 & & \\ & & \ddots & \\ O & & & (\nu\sigma_f)^k_I \end{pmatrix}$$

our assumptions yield:

$$(6) \qquad S_{gk} \geqq 0; \quad F_k \geqq 0; \quad \chi_k \geqq 0$$

We further assume that

(7) $$(T_g - S_{gg})^{-1} > 0 \qquad (g=1,2, \dots G)$$

The physical meaning of (7) is that if any neutron with the energy of group index g enters the region, it may diffuse or be scattered to all locations of the space. If $T_g^{-1} > 0$ (i.e. neutrons may diffuse to all locations) and the greatest eigenvalue of $T_g^{-1} S_{gg}$ is less than 1 (mostly satisfied if $\sigma_{g \to g} < \sigma_t$), then

$$(T_g - S_{gg})^{-1} = \sum_{j=0}^{\infty} (T_g^{-1} S_{gg})^j \cdot T_g^{-1}$$

and (7) is valid.

The matrix equation (3) may be written more compactly if we define the vector

$$v = (u_1, u_2, \dots, u_G)'$$

and the matrices

(8) $$A = \begin{pmatrix} (T_1 - S_{11}) & & & 0 \\ -S_{21} & (T_2 - S_{22}) & & \\ -S_{31} & -S_{32} & (T_3 - S_{33}) & \\ \dots & \dots & \dots & \dots \\ -S_{G1} & -S_{G2} & \dots & (T_G - S_{GG}) \end{pmatrix}$$

(9) $$B = \begin{pmatrix} \chi_1 I & & & 0 \\ & \chi_2 I & & \\ & & \ddots & \\ 0 & & & \chi_G I \end{pmatrix}$$

$$F=\begin{pmatrix} F_1 & F_2 & \cdots & F_G \\ F_1 & F_2 & \cdots & F_G \\ \cdots & \cdots & \cdots & \cdots \\ F_1 & F_2 & \cdots & F_G \end{pmatrix}$$

Then, from (3) we have

(10) $$A\ v = \frac{1}{\lambda}\ BFv$$

It is easy to show that

(11) $$A^{-1}=\begin{pmatrix} A_{11} & & & \\ A_{21} & A_{22} & & 0 \\ A_{31} & A_{32} & A_{33} & \\ \cdots & \cdots & \cdots & \cdots \\ A_{G1} & A_{G2} & \cdots & A_{GG} \end{pmatrix}$$

with

(12) $$A_{ii} = (T_i - S_{ii})^{-1} > 0$$

and

(13) $$A_{i+k,i} = \sum_{i=q_1<q_2<\ldots q_n=i+k} A_{q_nq_n} S_{q_nq_{n-1}} A_{q_{n-1}q_{n-1}} S_{q_{n-1}q_{n-2}} A_{q_{n-2}q_{n-2}} \cdots A_{q_2q_2} S_{q_2q_1} A_{q_1q_1}$$

and, consequently, $A_{i+k,i} \geqq 0$

<u>Lemma 1.1:</u> 1) Let $\tau_{gk} = \sup_i \sigma^i_{k\to g}$ and r>s. Then, $A_{rs}>o$ if and only if there exist some integers $S=q_1<q_2<q_3<\ldots<q_n=r$ such that

(15) $$\tau_{q_n q_{n-1}} \cdot \tau_{q_{n-1} q_{n-2}} \cdots \tau_{q_2 q_1} > o$$

2) $A_{rs}>o$ or $A_{rs}\equiv o$

<u>Proof:</u> If each S_{qp} in any term of the sum (13) has at least one diagonal element $\sigma_{p\to g}>o$, we have $A_{qq}S_{qp}A_{pp}>o$ with regard to (12) and, consequently, $A_{i+k,i}>o$. Thus, if (15) is satisfied for some integers q_i, $A_{rs}>o$. On the other hand, if $A_{rs}>o$, there must be some matrices

$$S_{rq_n} \neq o; \quad S_{q_n q_{n-1}} \neq o; \; \ldots, \; S_{q_2 s} \neq o,$$

which implies (15).

Obviously, $A_{rs}\equiv o$ if and only if all possible products (15) are zero (i.e. there exists no "matrix chain" $S_{rq_n}\neq o$; $S_{q_n q_{n-1}}\neq o; \ldots, S_{q_2 s}\neq o$).

The geometrical interpretation of Lemma 1.1 by the graph theory is useful. Consider G points $P_1, P_2, \ldots P_G$ in the plane. If $\tau_{gk}>o$, the points P_k and P_g may be connected by a directed path from P_k to P_g. We shall say that there is a path from P_i to P_j if there exist some integers $i=q_1<q_2<\ldots<q_n=j$ such that each directed path $P_{q_i}\to P_{q_{i+1}}$ exists. For example, in Figure 1

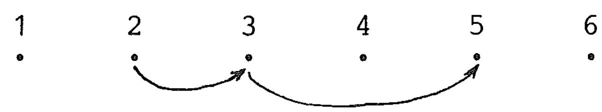

fig. 1

a path from P_2 to P_5 exists.

Lemma 1.1 implies then: $A_{rs}>o$ if and only if there exists a path from P_s to P_r.

The physical meaning of Lemma 1.1 is: $A_{rs}>o$ if and only if each neutron being located anywhere in the reactor and having the energy of energy-group s, may be transported by diffusion and scattering to any point of the reactor having the energy of energy-group r afterwards.

We obtain from Eq.(10):Using (11),

(16) $$M \cdot v = \lambda \cdot v$$

with

(17) $$M=\begin{pmatrix} E_1 \cdot F_1 & E_1 \cdot F_2 & \cdots & E_1 \cdot F_G \\ E_2 \cdot F_1 & E_2 \cdot F_2 & \cdots & E_2 \cdot F_G \\ \cdots & \cdots & \cdots & \cdots \\ E_G \cdot F_1 & E_G \cdot F_2 & \cdots & E_G \cdot F_G \end{pmatrix}$$

and

(18) $$E_j = \chi_1 A_{j1} + \chi_2 A_{j2} + \dots + \chi_j A_{jj}$$

From Lemma 1.1 we have

(19) $$E_j > o \quad \text{or} \quad E_j \equiv o$$

(20) $E_j>o$ if and only if (a) or (b) is true:

(a) $\chi_j>o$

(b) In a graph (see Fig.1) there exists at least one path from a point P_i with $i<j$ and $\chi_i>o$ to P_j.

3. Mathematical Theorems

Matrix M from (16) may be transformed to some "normal forms" which are given by (21):

(21a) $$M_1 = \begin{pmatrix} A & o \\ B & o \end{pmatrix}$$

(21b) $$M_2 = \begin{pmatrix} A & B \\ o & o \end{pmatrix}$$

(21c) $$M_3 = \begin{pmatrix} M_2 & o \\ C & o \end{pmatrix} = \left(\begin{array}{cc|c} A & B & \\ o & o & 0 \\ \hline \multicolumn{2}{c|}{C} & o \end{array}\right)$$

where A is quadratic and $A \geqq o$, $B \geqq o$, $C \geqq o$. A is an irreducible matrix and satisfies the assumptions of

<u>THEØREM 1.1</u> Let $A \geqq o$, irreducible and $Ax = \lambda x$; $x \geqq o$; $x \neq o$. Then $\lambda = \rho(A)$ is a single eigenvalue and $x > o$.

Here $\rho(A)$ means the spectral radius of A $(= |\lambda_{max}|)$. $x > o$ means that each coordinate of x is greater than zero. This theorem was proved by Perron and Frobenius (/3/,/8/).

<u>THEØREM 1.2</u> If M_j $(j=1,2,3)$ are defined by (21) and if $A \geqq o$; $B \geqq o$; $C \geqq o$, the following statements are true:

(1) If $M_j x_j = \lambda_j x_j$; $x_j \neq o$; then $\lambda = o$ or λ is an eigenvalue of A.

(2) $\rho(M_1) = \rho(M_2) = \rho(M_3) = \rho(A)$

(3) If A is irreducible; $M_j x_j = \lambda_j x_j$; $x_j \geq o$; $x_j \neq o$; $\lambda_j \neq o$, $\lambda_j = \rho(A)$ is a single eigenvalue.

The proof is simple. If, for example, $M_1 x_1 = \lambda_1 x_1$ and $x_1 \neq o$; then $Ax_1^1 = \lambda_1 x_1^1$; $Bx_1^1 = \lambda_1 x_1^2$ and (1) is valid. The same is true for M_2, M_3. (3) follows from (1), (2) and theorem 1.1.

Some properties of a matrix structured like (17) are specified in

THEØREM 1.3: Let E_j, F_j ($j=1,2,\ldots G$) be nxn-matrices with

a) $E_j > o$ or $E_j \equiv o$

b) $F_j \geq o$

c) $M = (E_i F_k)$ (see (17))

Then there exists a permutation matrix P such that PMP^T adopts one of the following "normal forms":

(1) $PMP^T = M_j$ ($j=1,2,3$) with A irreducible (see (21))

(2) $PMP^T = o$

(3) $PMP^T > o$

(4) $PMP^T = \begin{pmatrix} A & O \\ B & O \end{pmatrix}$ with $A = (nxn)$ and $A = o$.

(P^T=transposed matrix)

Proof: If $M \equiv o$ or $M > o$, (2) and (3) will be accepted. Let Let $M \not\equiv o$ and $M \not> o$. Then M contains an entry $m_{ij} = o$. Thus, $E_m \cdot F_n = (\sum_j e_{ij} f_{jk})$ contain o and $\sum_j e_{ij} f_{jk} = o$ for at least one i,k. From a) it follows that either $e_{ij} > o$ and thus $f_{jk} = o$ for all values of j, or $e_{ij} = o$ for all values of j.

Consequently if $m_{ij}=o$, $m_{ij}=o$ for all values of j or $m_{ij}=o$ for all values of i. Thus, if M has an entry o, then the column or the row defined by the entry is zero.

<u>Case 1:</u> M has no zero-columns. Then a permutation matrix P may be chosen such that all the zero-rows are transported to the bottom of the matrix and $PMP^T=M_2$ with $A>o$ (irreducible)

<u>Case 2:</u> M has no zero-rows. Then P may be chosen such that all the zero-columns are transported to the right side and $PMP^T=M_1$ with $A>o$ (irreducible)

<u>Case 3:</u> M has zero-rows and zero-columns. First a permutation matrix P_c may be chosen such that

$$P_c M P_c^T = M_1 \qquad \text{(see (21a))}$$

If $A\equiv o$, we have (4) of theorem 3.
If $A\not\equiv o$, we chose P_r such that $P_r A P_r^T = \begin{pmatrix} A_{11} & D \\ O & O \end{pmatrix}$ with $A_{11}>o$. (This is possible because A has only zero-rows).
For

$$\tilde{P}_r = \begin{pmatrix} P_r & O \\ O & I \end{pmatrix} \text{ it follows}$$

$$\tilde{P}_r P_c M P_c^T \tilde{P}_r^T = M_3 \text{ with } A_{11}>o \text{ (irreducible).}$$

<u>THEØREM 1.4</u> Let E_j, F_j satisfy the assumptions of theorem 1.3, in addition, let
$Mx=\lambda x$; $x\geq o$; $x\not\equiv o$
Then
(1) $\lambda=o$ or $\lambda=\rho(M)>o$
(2) $\rho(M)>o$ is a single eigenvalue
(3) $\lambda>o$ if and only if there exists a j such that $E_j>o$ and $F_j\not\equiv o$.

Proof: From theorem 1.3 it follows that $\lambda = o$ if the "normal forms" (2) or (4) are adopted; otherwise $\lambda = \rho(M) > o$ is a single eigenvalue (see theorem 1.2). It remains to prove (3). Let $\lambda = \rho(M) > o$ and for all values of $j: E_j \equiv o$ or $F_j \equiv o$. Then for each j M has a zero-column and a zero-row, respectively. Then, $\det(\lambda I - M) = \pm\lambda^n$ and $\rho(M) = o$ are in contradiction to the assumption. If, conversely $E_j > o$, $F_j \neq o$ for at least one j, then $E_j \cdot F_j$ has a positive diagonal entry, and so M has at least one positive diagonal entry. Consequently, M may be transformed to the "normal forms" (1), (3) of theorem 1.3 only which have none-zero positive eigenvalues. From theorem 1.2, (3) it follows that $\rho(M) = \lambda$ is a single eigenvalue.

4. Existence Theorems

The numerical formulation of (1), (2) was given by (see(3))

$$(T_g - S_{gg}) ug = \frac{1}{\lambda}\chi_g \sum_{k=1}^{G} F_k u_k + \sum_{k<g} S_{gk} u_k$$

where S_{gk}, F_k are defined by (4), (5) and

$$S_{gk} \geqq o; \quad F_k \geqq o.$$

We further assumed:

$$T_g^{-1} > o; \quad \rho(T_g^{-1} S_{gg}) < 1$$

or

$$(T_g - S_{gg})^{-1} > o.$$

On these assumtions we immediately obtain from theorem 1.4

THEØREM 1.5: If $u_g \geq o$ and $u_h \neq o$ for at least one h, if further $\lambda \neq o$, then

(1) λ is real

(2) $\lambda > o$

(3) λ is the greatest eigenvalue

(4) λ is a single eigenvalue.

The question whether $\lambda > o$ exists can easily be answered by the graph-theory. In (20) it was stated that $E_j > o$ if and only if either $\chi_j > o$ or if a path exists from a point P_i with $i < j$, $\chi_i > o$ to P_j. We now extend the concept of our graph by drawing an additional directed path from P_r to P_s if $\chi_s \cdot (\nu\sigma_f)^r > o$ for at least one special point. (i.e. if $\chi_s > o$ and $F_r \neq o$). If $\chi_k (\nu\sigma_f)^k > o$, we combine P_k with itself as shown in Figure 2:

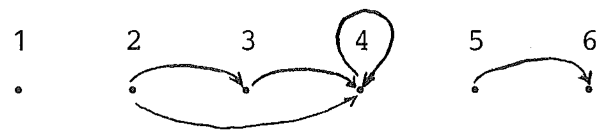

Figure 2.

If G(M) is the graph of M in the meaning of Fig.2, we say that G(M) contains a closed path, if for at least one point P_j a path combining P_j with itself exists.

From (20) we get the equivalence of the two statemants:

(1) There exists a j such that $E_j > o$ and $F_j \neq o$

(2) G(M) contains at least one closed path.

From this and from theorem 1.4 it follows immediately:

THEØREM 1.6: On the assumptions made in theorem 1.5 the greatest single eigenvalue $\lambda > o$ exists if and only if the graph G(M) contains at least one closed path.
If no closed path exists, all eigenvalues of M are zero.

The physical meaning is clear: Neutron having changed their energy due to fission must be able "to return" by scattering. If no path exists, no neutron circulation occurs and the multiplication factor is zero. If neutron circulation exists, the greatest eigenvalue is real, positive and single.

II. The Transport Theory Problem

1. The Multigroup Transport Equations

Section II is concerned with the linear Boltzmann equation

(1) $$\Omega\cdot\nabla\Phi^g + \sigma_t^g\Phi^g - \sum_{k\leq g} \sigma_{k\to g}\psi^k = \frac{1}{\lambda}\sum_{k=1}^{G}\chi_g(\nu\sigma_f)^k\psi^k$$

with $\Phi^g = \Phi^g(r,\Omega)$

(2) $$\psi^g = \oint \Phi^g(r,\Omega)\ \overline{d\Omega}$$

r is a space vector and Ω is a direction vector with $||\Omega||=1$. Φ^g is the neutron flux dependent on space, angle and the energy-group-index g. The integral (2) is extended over the unit sphere. Φ and λ (= k-effective) exist if some boundary conditions are defined. They usually are given in one of the following forms:

(3a) Vacuum: $\Phi^g(r,\Omega)=o$ for $\Omega\cdot n<o$ if n is an outward directed normal vector on the boundary.

(3b) Reflexion: $\Phi^g(\tilde{r},\Omega_1)=\Phi^g(\tilde{r},\Omega_2)$ if Ω_2 is the direction of neutrons having been reflected at the boundary.

(3c) Periodicity: $\Phi^g(\tilde{r},\Omega)=\Phi^g(\tilde{r}+a,\Omega)$, if $\tilde{r}$ and $\tilde{r}+a$ are boundary points and $a=(l_x,0,0)'$ and $a=(0,l_y,0)'$ and $a=(0,0,l_z)$, respectively, (d=diameter of the reactor).

2. Matrix Equations

For the numerical solution of the eigenvalue problem (1),(3) by the difference method we substitute the solution $\Phi^g(r,\Omega)$ by a set of function values $\Phi^g_{i,m} \approx \Phi^g(r_i,\Omega_m)$ $(i=1,2,\dots,I;\ m=1,2,\dots,M)$. The discrete directions Ω_m may be chosen such that

$$(4) \qquad \oint \Phi^g(r,\Omega)\overline{d\Omega} \approx \sum_{m=1}^{M} w_m \, \Phi^g_{i,m}$$

with suitable associated weights $w_m \geq 0$. We assume $\sum w_m = 4\pi$ (see /5/,/7/). Substituting (4) into (1) and replacing the left side of (1) by consistent difference equations (/2/,/5/), we obtain, observing (3):

$$(5) \qquad (T_g - S_{gg})u_g = \frac{1}{\lambda}\chi_g \sum_{k=1}^{G} F_k u_k + \sum_{k<g} S_{gk} u_k$$

where u_g is a vector with

$$u_g = (\Phi^g_{1,1};\ \Phi^g_{1,2},\dots,\Phi^g_{1,M},\Phi^g_{2,1},\dots,\Phi^g_{1,M},\dots\Phi^g_{I,M})$$

and S_{gk}, F_k are block matrices

$$(6) \qquad S_{gk} = \begin{pmatrix} W_s^1 & & & 0 \\ & W_s^2 & & \\ & & \ddots & \\ 0 & & & W_s^I \end{pmatrix}$$

$$(7) \qquad F_k = \begin{pmatrix} W_f^1 & & & 0 \\ & W_f^2 & & \\ & & \ddots & \\ 0 & & & W_f^I \end{pmatrix}$$

with

$$(8) \qquad W_s^i = \begin{pmatrix} \sigma_{k\to g}^i \cdot W_1 & \sigma_{k\to g}^i \cdot W_2 & \cdots & \sigma_{k\to g}^i \cdot W_M \\ \sigma_{k\to g}^i \cdot W_1 & \sigma_{k\to g}^i \cdot W_2 & \cdots & \sigma_{k\to g}^i \cdot W_M \\ \cdots & \cdots & \cdots & \cdots \\ \sigma_{k\to g}^i \cdot W_1 & \sigma_{k\to g}^i \cdot W_2 & \cdots & \sigma_{k\to g}^i \cdot W_M \end{pmatrix}$$

$$(9) \qquad W_f^i = \begin{pmatrix} (\nu\sigma_f)^i W_1 & (\nu\sigma_f)^i W_2 & \cdots & (\nu\sigma_f)^i W_M \\ (\nu\sigma_f)^i W_1 & (\nu\sigma_f)^i W_2 & \cdots & (\nu\sigma_f)^i W_M \\ \cdots & \cdots & \cdots & \cdots \\ (\nu\sigma_f)^i W_1 & (\nu\sigma_f)^i W_2 & \cdots & (\nu\sigma_f)^i W_M \end{pmatrix}$$

T_g is a $(I \cdot M) \times (I \cdot M)$-matrix (difference operator). We make the following assumption:

$$(10) \qquad S_{gk} \geqq 0$$

$$(11) \qquad F_k \geqq 0$$

$$(12) \qquad \chi_k \geqq 0$$

$$(13) \qquad (T_g - S_{gg})^{-1} > 0$$

(10), (11), (12) imply the positivity of the cross-sections. (13) guarantees that a neutron of energy g may travel everywhere by diffusion or by scattering. As we have assumed an isotopic scattering, this assumption is physically convenient.

Matrix Equation (5) may be written more compactly if we define the vector

$$V=\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_G \end{pmatrix}$$

and the matrices:

$$A=\begin{pmatrix} (T_1-S_{11}) & & & 0 \\ -S_{21} & (T_2-S_{22}) & & \\ -S_{31} & -S_{32} & (T_3-S_{33}) & \\ \cdots & \cdots & \cdots & \cdots \\ -S_{G1} & \cdots & \cdots & (T_G-S_{GG}) \end{pmatrix}$$

$$B=\begin{pmatrix} \chi_1 I & & & \\ & \chi_2 I & & 0 \\ & & \ddots & \\ 0 & & & \chi_G I \end{pmatrix}$$

$$F=\begin{pmatrix} F_1 & F_2 & \cdots & F_G \\ F_1 & F_2 & \cdots & F_G \\ \cdots & \cdots & \cdots & \cdots \\ F_1 & F_2 & \cdots & F_G \end{pmatrix}$$

Then, from (5) we obtain

(14) $$A\ v = \frac{1}{\lambda}\ B\ F\ v$$

As in chapter I, it is easily shown that

(15) $$A^{-1} = \begin{pmatrix} A_{11} & & & & \\ A_{21} & A_{22} & & & O \\ A_{31} & A_{32} & A_{33} & & \\ \cdots & \cdots & \cdots & \cdots & \\ A_{G1} & A_{G2} & \cdots & \cdots & A_{GG} \end{pmatrix}$$

with

(16) $$A_{ii} = (T_i - S_{ii})^{-1} > o$$

and

(17) $$A_{i+k,i} = \sum_{i=q_1<q_2<\ldots<q_n=i+k} A_{q_nq_n} S_{q_nq_{n-1}} A_{q_{n-1}q_{n-1}} S_{q_{n-1}q_{n-2}} A_{q_{n-2}q_{n-2}} \cdots\cdots A_{q_2q_2} S_{q_2q_1} A_{q_1q_1}$$

and consequently, $A_{i+k,i} \geq o$.

(6) implies that $S_{gk} \neq o$ if and only if $\sigma^{i}_{k\to g} > o$ for at least one i. Consequently, the considerations of the proof of Lemma 1.1 (chapt.I) can be applied to the matrices accuring in (17). This leads to

Lemma 2.1: 1) Let $\tau_{gk}=\sup_i \sigma^i_{k\to g}$ and $r>s$. Then, $A_{rs}>o$ if and only if some integers $s=q_1<g_2<\cdots<q_n=r$ exist such that $\tau_{q_nq_{n-1}}\tau_{q_{n-1}q_{n-2}}\cdots\tau_{q_2q_1}>o$

2) $A_{rs}>o$ or $A_{rs}\equiv o$

As in chapter I we state: $A_{rs}>o$ if and only if the graph G(M) (see I,4) contains a directed path from P_s to P_r.

From (14) we obtain using (15):

(18) $$M\ v = \lambda\ v$$

where

(19) $$M=\begin{pmatrix} E_1F_1 & E_1F_2 & \cdots & E_1F_G \\ E_2F_1 & E_2F_2 & \cdots & E_2F_G \\ \cdots & \cdots & \cdots & \cdots \\ E_GF_1 & E_GF_2 & \cdots & E_GF_G \end{pmatrix}$$

and

(20) $$E_j = \chi_1A_{j1}+\chi_2A_{j2}+ \cdots +\chi_jA_{jj}$$

From Lemma 2.1 we have

(21) $E_j>o$ or $E_j\equiv o$

(22) $E_j>o$ if and only if (a) or (b) applies:

(a) $\chi_j>o$

(b) In a graph G(M) there exists at least one path from a point P_i with $i<j$ and $\chi_i>o$ to P_j (Definition of G(M): chapt. I,4).

3. Existence Theorems

As in I,4 we obtain from theorem 1.4 assuming (10),(11), (12),(13):

THEØREM 2.1: If $u_g \geqq o$ and $u_h \neq o$ for at least one h, if further $\lambda \neq o$, then
(1) λ is real
(2) $\lambda > o$
(3) λ is the greatest eigenvalue
(4) λ is a single eigenvalue

The question whether $\lambda > o$ exists may be answered by the graph theory. Having G points (one for each group), we draw a directed line from P_k to P_g if

(a) $\sigma^i_{k \to g} > o$ for one i at least or

(b) $\chi_g (\nu \cdot \sigma_f)^i_k > o$ for one i at least.

Then, in analogy with I,4 we obtain:

THEØREM 2.2: On the assumption made in theorem 2.1 the greatest single eigenvalue $\lambda > o$ exists if and only if the graph G(M) contains one closed path at least.
If no closed path exists, all the eigenvalues of M are zero.

The existence of $\lambda > o$ is not dependent on the choice of the discrete directions Ω_m or the weights W_m. This is due to the fact that the source was assumed to be isotropical.

III. Outer and Inner Iterations

The computation of the greatest eigenvalue may be performed by the following well-known procedure (/5/,/10/):

If $v^o > o$ and $v^{n+1} = \frac{Mv^n}{||Mv^n||}$ (outer iterations) ($M \geqq o$)

then $||v^i|| = 1$, $v^i \geqq o$ and, consequently there exist integers q_i such that

$$v^{q_i} \longrightarrow v \qquad (i \longrightarrow \infty)$$

with

$$v = \frac{Mv}{||Mv||}$$

From the assumptions of M we may conclude, using theorem 1.5 (theorem 2.1, respectively) that the normalized vector v is a unique fix point so that

$$v^n \longrightarrow v \quad \text{and} \quad ||Mv^n|| \longrightarrow \lambda \qquad (n \to \infty)$$

The inversion of the matrix M may be accomplished by the following iterations

$$T_g u_g^{p+1} = S_{gg} u_g^p + r_g$$

with

$$r_g = \frac{1}{\lambda} \chi_g \sum_{k=1}^{G} F_k u_k^n + \sum_{k<g} S_{gk} u_k^{n+1}$$

where n is the iteration index of the outer iterations. We assumed

$$(T_g - S_{gg})^{-1} > o$$

If the difference equations provide non-negative fluxes, then

$$T_g^{-1} \geqq o$$

and $R=T_g-S_{gg}$ is a regular splitting. This implies (/9/, page 89):

(23) $$\rho(T_g^{-1} \cdot S_{gg})<1$$

Consequently, the inner iterations converge.

Summarizing we can state:

<u>THEØREM 3.1:</u> Let $T_g u_g = \frac{1}{\lambda}\chi_g \sum_{k=1}^{G} F_k u_k + \sum_{k \lesseqqgtr g} S_{gk} u_k$ with

$F_k \geqq o$; $S_{gk} \geqq o$; $\chi_g \geqq o$; $T_g^{-1} \geqq o$; $(T_g-S_{gg})^{-1}>o$

for all k,g.

Let further the graph G contain at least one closed path. Then the outer and inner iterations converge.

Omission of the assumption $T_g^{-1} \geqq o$ implies convergence of outer iterations only.

IV. Example: The Diamond Difference Scheme

The Diamond Difference Scheme provides numerical solutions for the Boltzmann equation. A description is found in /2/ and /5/. For one-dimensional fluxes $\Phi(x,\mu)$ the difference equations are written as

$$(1) \qquad \mu_m \frac{\phi^g_{i+1,m} - \phi^g_{i,m}}{\Delta x} + \sigma^g_t \; \phi^g_{i+\frac{1}{2},m} = S_g$$

$$(2) \qquad \phi^g_{i+\frac{1}{2},m} = 0.5 \cdot (\Phi^g_{i+1,m} + \phi^g_{i,m})$$

where

$$(3) \qquad S_g = \frac{1}{\lambda} \chi_g \sum_{\substack{k=1 \\ m \leq M}}^{G} W_m (\nu\sigma_f)^k \; \phi^k_{i+\frac{1}{2},m} + \sum_{\substack{k=g \\ m \leq M}} \sigma_{k\to g} \; \phi^k_{i+\frac{1}{2},m} \cdot W_m$$

with non-negative cross-sections.

Substituting ϕ_{i+1} in (1) by (2) gives omitting the index g)

$$(4) \qquad \phi_{i+\frac{1}{2},m} = (2\mu_m \phi_{i,m} + \Delta x \cdot S_g) / (2\mu_m + \Delta x \cdot \sigma_t)$$

and from (2):

$$(5) \qquad \phi_{i+1,m} = 2 \; \phi_{i+\frac{1}{2},m} - \phi_{i,m}$$

$$= \frac{(2\mu_m - \Delta x \cdot \sigma_t) \; \Phi_{i,m} + 2 \cdot \Delta x \cdot S_g}{2\mu_m + \Delta x \cdot \sigma_t}$$

If $\mu_m > o$, $\phi_{1,m}$ is an inward directed boundary flux and therefore defined by boundary conditions. Formula (5) enables us to compute $\phi_{2,m} \cdot \Phi_{3,m}$ ... successively. If $\phi_{1,m} \geqq o$, $S_g \geqq o$, $2\mu_m - \Delta x \cdot \sigma_t \geqq o$, then

$\Phi_{i,m} \geq o$ for all values of i. In the case of $\mu_m < o$ we use a formula which can be evaluated as (5):

$$(6) \qquad \Phi_{i,m} = \frac{(2|\mu_m| - \Delta x \cdot \sigma_t)\ \Phi_{i+1,m} + 2 \cdot \Delta x \cdot S_g}{2|\mu_m| + \Delta x \cdot S_g}$$

Then, starting with the inward directed boundary flux $\Phi_{I,m} \geq o$, we get $\Phi_{I-1,m}$, $\phi_{I-2,m}$ ... $\Phi_{1,m}$ successively, each being non-negative if $S_g = o$ and $2|\mu_m| - \Delta x \cdot \sigma_t \geq o$. This implies that under vacuum boundary conditions a non-negative source leads to non-negative fluxes if

$$(7) \qquad \Delta x \leq 2|\mu_m|\ \lambda_f$$

with $\lambda_f = 1/\sigma_t$ (mean free path). In the formalism of chapter II we obtain:

$$(8) \qquad T_g^{-1} \geq o$$

Furthermore, it can be proved that

$$(9) \qquad (T_g - S_{gg})^{-1} > o$$

if (7) is satisfied and $\sigma_{g\to g} < \sigma_t$ (/6/). Thus, from theorem 3.1 we may conclude the convergence of outer and inner iterations if the graph theory condition is satisfied). Applying theorem 2.1 and theorem 2.2 we can summarize.

<u>THEØREM 4.1:</u> Let the difference equations (1),(2),(3) be given to solve the transport-problem defined in II. Let all the cross sections and χ_g be non-negative and

$$\Delta x \leq 2|\mu_m|\ \lambda_f^g \qquad (\lambda_f^g = 1/\sigma_t^g)$$

$$\sigma_{g\to g} < \sigma_t^g$$

for $g=1,2,\ldots G$; $m=1,2,\ldots M$. Let further the graph defined in I contain one closed path at least. Then we have:

(1) There exists a greatest single eigenvalue $\lambda > o$ with non-negative fluxes

(2) If $u_g \geq o$ $(g=1,2,\ldots G)$ are eigenvector-fluxes, then the associated eigenvalue is the greatest one

(3) The outer iterations converge

(4) The inner iterations converge.

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