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The Multigroup Diffusion Equations of Reactor Physics

G. J. Habetler

M. A. Martino

July 28, 1958

Operated for the
United States Atomic
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UC-34, Physics and Mathematics
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THE MULTIGROUP DIFFUSION EQUATIONS OF REACTOR PHYSICS

G. J. Habetler, M. A. Martino

July 28, 1958

H. E. Stevens

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KNOLLS ATOMIC POWER LABORATORY
Schenectady, New York
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ABSTRACT

The partial differential equations of the multigroup diffusion model of reactor physics are shown to have solutions both in the time-independent and time-dependent problems, and the usually assumed behavior of these solutions is shown to be mathematically valid. The method of spectral representation is developed for the multigroup diffusion operator.

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THE MULTIGROUP DIFFUSION EQUATIONS OF REACTOR PHYSICS

G. J. Habetler, M. A. Martino

INTRODUCTION

This report is concerned with some fundamental mathematics concerning the partial differential equations for the multigroup diffusion model of reactor theory. The existence and uniqueness of a positive eigenfunction (the fundamental mode) and adjoint eigenfunction (importance function) are established for both the time-independent and time-dependent problems. The corresponding eigenvalue is shown to have minimum modulus in the time-independent case and maximum real part in the time-dependent case. These results are applied to an analysis of certain iterative techniques for the solution of the principal eigenfunction and eigenvalue and also to an asymptotic analysis of the reactor process. Perturbation theory and an analysis of variational methods will be developed in another paper.

Considering the widespread usage of the multigroup diffusion model, both as a theoretical reference frame[†] and as a basis for reactor calculations, it is somewhat surprising that the common concepts of criticality and perturbation theory have had no previous mathematical justification for this model. In the absence of this justification a type of pseudo-mathematical theory has evolved in a rather classical way; that is, statements concerning certain non-self-adjoint differential operators (such as the existence of biorthogonal expansions) have been postulated to reflect inductive reasonings from various self-adjoint counterparts and also from practical experience. These postulates, although not always rigorously true, have remained acceptable because they have not given rise to any practical difficulties. Useful as this approach has been, it is clearly desirable to put this theory on a more firm mathematical foundation.

Recently a corresponding theory was developed by G. Birkhoff and R. S. Varga^{††} for discrete space approximations to the multigroup model, which provided a rigorous theory for the finite-difference reactor equations used in many calculational schemes. For the exploration of

[†]A. M. Weinberg, "Current Status of Nuclear Reactor Theory," Am. J. Phys. 20 (1952), pp. 401-412.

^{††}G. Birkhoff and R. S. Varga, "Reactor Criticality and Non-Negative Matrices," WAPD-166, August, 1957.

certain variational and integral transform methods and for a better general understanding of the multigroup concept, it is desirable to extend these results to the continuous space model. It is possible that this extension can be obtained from certain convergence arguments applied to discrete space approximations; however, we have found that the continuous space theory can be obtained directly, and the latter approach is used here. It is interesting to note the parallel ideas involved here and in the earlier work of Birkhoff and Varga. Whereas the work of Birkhoff and Varga in WAPD-166 is mainly derived from generalizations of the Perron-Frobenius fixed-point property of positive matrices (which leave the hyperoctant of "positive" vectors invariant), the work herein is derived from Jentzsch's theorem on integral operators with positive kernel and the Krein-Rutman generalization to completely continuous operators leaving invariant a (positive) cone in a Banach space. Essentially, then, this work is a natural extension of the work in WAPD-166.

In the next section the partial differential equations of the multigroup diffusion model are introduced and the associated operators are defined. Following that, in the section titled Mathematical Preliminaries, the main mathematical theory of this work is developed for later use; this section can be ignored by those readers who are interested only in the applications, which are found in the remaining sections.

THE DIFFERENTIAL EQUATIONS

The reactor R is assumed to occupy a connected region of finite extent in space; we will also use the symbol R for the region occupied by the reactor. It will be convenient to assume that R is an open set; this is not a restrictive condition, for if it is not open we may replace R by its interior set. Further, R is assumed to be the composite of a finite number of material subregions. More precisely, we assume that there are a finite number of convex, open, simply connected, disjoint regions $R_1, R_2, \dots, R_m$, such that $\bar{R} = \bigcup_{i=1}^m \bar{R}_i$ (the bar denotes topological closure in the Euclidean metric). If the number of energy groups is n , there are given $2n^2 + n$ real-valued functions (the diffusion equation coefficients) $d_j(r), a_{jk}(r), f_{jk}(r)$ ($1 \leq j, k \leq n, r \in R$); the a_{jk} and f_{jk} [d_j] have continuous and bounded first [second] order partial derivatives in each R_i ($1 \leq i \leq m; 1 \leq j, k \leq n$). Certain arithmetic restrictions will be placed on these coefficients later. For now, we content ourselves with pointing out that these coefficients are generally discontinuous across the boundaries (material interfaces) of the subregions R_i .

Suppose $\Phi = (\phi_1(r), \phi_2(r), \dots, \phi_n(r))$ where

- a. Each $\phi_j(r)$ has bounded and continuous second-order derivatives inside the subregions R_i .
- b. $\phi_j(r)$ and the normal component of $d_j(r) \cdot \text{grad } \phi_j(r)$ are continuous across the material interfaces.[†]
- c. $\phi_j(r)$ satisfies the boundary condition $\phi_j(r) + \alpha_j(r) \frac{\partial \phi_j}{\partial n} = 0$ (outgoing normal) along the boundary of R for a given piecewise continuous function $\alpha_j(r) \geq 0$, $1 \leq j \leq n$.

(1)

A function $\Phi = (\phi_1, \phi_2, \dots, \phi_n)$ satisfying Conditions (1a), (1b), and (1c) above will be said to belong to the class C , denoted $\Phi \in C$.

For any $\Phi \in C$, define the differential operators

$$\mathcal{D}_j \Phi = \text{div } (d_j(r) \text{ grad } \phi_j(r)) \quad 1 \leq j \leq n \quad (2)$$

and let $\mathcal{D}$ be the diagonal matrix of differential operators given by

$$\mathcal{D} = (\mathcal{D}_{jk}) = \begin{pmatrix} \mathcal{D}_1 & & 0 \\ & \mathcal{D}_2 & \\ 0 & & \ddots \\ & & & \mathcal{D}_n \end{pmatrix}, \quad (3)$$

where δ_{jk} is the Kronecker delta. Also, define two matrices of scalar functions by

$$A = (a_{jk}(r)) ; F = (f_{jk}(r)) \quad (4)$$

With certain restrictions on A and F , to be specified below, the differential equations of reactor kinetics for the multigroup diffusion model become^{††}

$$\frac{\partial \Phi(r, t)}{\partial t} = (\mathcal{D} + A + \nu F) \Phi(r, t) + S(r, t) \quad (5)$$

[†]That is, continuous at every point which is common to the topological closure of exactly two subregions and at which the normal direction to the common boundary is defined. This is the self-adjoint "current" condition for the material interfaces.

^{††}Equation (5) does not include the effect of delayed neutrons, which is not considered in this paper.

Here $\Phi(r,t) = (\phi_1(r,t), \phi_2(r,t), \dots, \phi_n(r,t))$ represents the neutron flux in the n energy levels at point $r \in R$, time t ;
 $\mathcal{S}(r,t) = (\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_n)$ is the extraneous (nonfission) flux source production rate at point r , time t ; the parameter ν represents the expected number of fission neutrons per fission; d_j , a_{jk} ($j \neq k$), a_{jj} , f_{jk} are, respectively, the diffusion coefficients, energy change (slowing down or up-scattering according to $j > k$ or $j < k$) cross sections, negative removal cross sections, and fission cross sections, all multiplied by the average group velocity for group j . It follows that

$$\begin{aligned} d_j(r) &\geq 0 \\ a_{jk}(r) &\geq 0 & j \neq k \\ a_{jj}(r) &\leq 0 \\ f_{jk}(r) &\geq 0 & 1 \leq j, k \leq n \end{aligned} \tag{6}$$

Two standard problems are connected with Equation (5). The first is an eigenvalue problem: namely, the determination of the smallest value of ν for which a steady-state solution is possible without the aid of an extraneous source. In this, the so-called "time-independent" problem, Equation (5) reduces to

$$-(\mathcal{D} + A) \Phi(r) = \nu F \Phi(r); \tag{7}$$

the second variable of Φ is dropped since Φ is presumed to be steady.

The second problem, the so-called "time-dependent" problem, is that of obtaining the solution to the differential Equation (5) for a given value of ν and $\mathcal{S}(r,t)$, such that the solution satisfies an initial condition, say, at $t = 0$. The existence and uniqueness of this solution must be established for the given initial flux distribution $\Phi(r,0)$. Of particular importance in the study of the time-dependent problem is the determination of the asymptotic behavior of the solution $\Phi(r,t)$ of Equation (5) for large values of t . The time-independent and time-dependent problems will be discussed in the later sections of this report.

Returning to the conditions in (6), it is seen that we have not yet ruled out certain trivial models which do not represent working reactors, for example, the case $F \equiv 0$. In order to obtain a more complete theory for nontrivial models, we need to postulate conditions which ensure that fissions will occur and that neutrons migrate in position and energy. Specifically, we will assume that there is a positive number δ such that

$$d_j(r) \geq \delta > 0 \tag{8}$$

$j = 1, 2, \dots, n;$

also, we postulate a transitivity condition as follows. Define sets $R_{jk} \subset R$ so that R_{jk} consists of those points $r \in R$ for which either $a_{jk}(r) > 0$ or $f_{jk}(r) > 0$ (or both). We say that the model described in Equation (5) or (7) is transitive if, given any two positive integers $j \leq n$, $k \leq n$, there exists a finite sequence of numbers $j = \alpha_0, \alpha_1, \dots, \alpha_{q-1}, \alpha_q = k$ such that the Lebesgue measure of $R_{\alpha_i, \alpha_{i+1}}$ is positive for $i = 0, 1, \dots, q-1$. A transitive model, then, has the property that the expected[†] progeny of a neutron of energy group j is not zero in energy group k for all $j, k \leq n$. A simple and common example of a transitive process occurs when $f_{1,n}, a_{n,n-1}, a_{n-1,n-2}, \dots, a_{2,1}$ all take on positive values on a set of positive measure (which set may be different for each of the n functions); all models considered below will be assumed to be transitive. Also, we will specifically require that $f_{1,n}(r) \neq 0$.

MATHEMATICAL PRELIMINARIES

The Operator $\mathcal{D}$

Applying Green's theorem to each of the ordinary diffusion operators $\mathcal{D}_j$ of Equation (2), we obtain for $\Phi, \Psi \in C$ (again letting lower case letters represent the components of Φ and Ψ),

$$\begin{aligned} \int_R \psi_j(r) \cdot \mathcal{D}_j \phi_j(r) \, dV_r - \int_R \phi_j(r) \cdot \mathcal{D}_j \psi_j(r) \, dV_r \\ = \sum_{i=1}^m \lim_{\epsilon \rightarrow 0} \oint_{B_{i,\epsilon}} d_j(r) \left(\psi_j(r) \frac{\partial \phi_j}{\partial n} - \phi_j(r) \frac{\partial \psi_j}{\partial n} \right) d\sigma \end{aligned} \quad (9)$$

where $B_{i,\epsilon}$ is the ϵ -contraction of the boundary B_i of subregion R_i ; that is, $B_{i,\epsilon}$ is the locus of all points at distance ϵ from B_i along the inward drawn normals. On account of the continuity Conditions (1a) and (1b), the limit boundary integrals in the right member of Equation (9) cancel in pairs over the segments of the B_i which are common boundaries for two subregions. The remaining boundary integrals taken over the boundary of R are also zero since ϕ_j and ψ_j both satisfy Condition (1c). Thus, the right member of Equation (9) is zero; so each $\mathcal{D}_j$ - and, therefore, also $\mathcal{D}$ - is self-adjoint.

[†]Statistical expectation.

It is well known that each $\mathcal{D}_j$ has a Green's function $G_j(r,s)$; these kernels may be constructed by passing to the limit from the corresponding Green's functions for the discrete approximations, which are in turn constructable by random walk methods.[†] For reference, we list the following cogent properties of $G_j(r,s)$:

- a. $\int_R G_j(r,s) \mathcal{D}_j \phi_j(s) dV_s = \phi_j(r)$ for any ϕ_j satisfying Conditions (1a) and (1c).
 - b. $G_j(r,s)$ is continuous for all $r,s \in \bar{R}$, provided $r \neq s$.
 - c. $G_j(r,s)$ has continuous first-order partial derivatives provided $r \neq s$ and r and s are each interior to some subregion.
 - d. For a fixed s_0 interior to some R_i , $G_j(r,s_0)$ satisfies the boundary Conditions (1b) and (1c).
 - e. There exists a number M such that
- $$|G_j(r,s)| \leq \frac{M}{|r-s|} \quad \text{and} \quad \left| \frac{\partial G_j}{\partial x} \right| + \left| \frac{\partial G_j}{\partial y} \right| + \left| \frac{\partial G_j}{\partial z} \right| \leq \frac{M}{|r-s|^2},$$
- where $|r-s|$ is the Euclidean distance between r and s and differentiation is with respect to either of the two arguments of G_j .
- f. $G_j(r,s) = G_j(s,r) < 0$ for all $r,s \in R$, $r \neq s$.

(10)

Property (10a) shows that the diagonal matrix of integral operators

$$\mathcal{D}^{-1} = \begin{pmatrix} \int G_1 & & 0 \\ & \int G_2 & \\ 0 & & \ddots \\ & & & \int G_n \end{pmatrix} \quad (11)$$

is inverse to $\mathcal{D}$ in the sense that $\mathcal{D}^{-1}\mathcal{D}\phi = \phi$ for all $\phi \in C$.

[†]See, for example, J. D. Tamarkin and W. Feller, Partial Differential Equations, Chaps. 5 through 7 (Brown University Press, 1941).

The class C has a natural imbedding in the Hilbert space $\mathcal{H}$ of complex vector functions[†] $\Phi = (\phi_1, \phi_2, \dots, \phi_n)$ for which

$$\|\Phi\| = \sum_{i=1}^n \int_R |\phi_i(r)|^2 dV_r \quad (12)$$

is finite. Condition (10e) and Schwarz's inequality show that $\|\mathcal{D}^{-1}\Phi\| \leq K \|\Phi\|$ for some number K independent of Φ . Hence, $\mathcal{D}^{-1}$ is a continuous (bounded) operator defined on all of $\mathcal{H}$. The range of $\mathcal{D}^{-1}$ (the set of all images $\mathcal{D}^{-1}\Phi$), which we denote by $\mathcal{M}$, is, therefore, a closed subspace of $\mathcal{H}$ and $\mathcal{M} \subset C$. The operator $\mathcal{D}$ can be extended to $\mathcal{M}$ by the obvious definition. $\mathcal{D}(\mathcal{D}^{-1}\Phi) = \Phi$; we assume $\mathcal{D}$ is so extended.

Since R is finite, Condition (10e)^{††} guarantees

$$\iint_{R \times R} |G_j(r,s)|^2 dV_r dV_s < +\infty, \quad (13)$$

so that $\mathcal{D}^{-1}$ is a completely continuous operator on $\mathcal{H}$;‡ that is, $\mathcal{D}^{-1}$ maps every bounded subset of $\mathcal{H}$ into a compact set. Since $\mathcal{D}^{-1}$ is also self-adjoint, it has a complete sequence of orthonormal eigenfunctions,

$$\mathcal{D}^{-1}\Omega_j = \frac{1}{\omega_j} \Omega_j \quad j = 1, 2, \dots \quad (14)$$

We may write the eigenvalues here as $\frac{1}{\omega_j}$, since $\mathcal{D}(\mathcal{D}^{-1}\Omega_j) = \Omega_j$ implies that the eigenvalues of $\mathcal{D}^{-1}$ are nonzero. Furthermore, the numbers ω_j have no finite point of accumulation.^{‡‡} Also Equation (14) shows that $\Omega_j \in \mathcal{M}$ and

$$\mathcal{D}\Omega_j = \omega_j \Omega_j \quad j = 1, 2, \dots \quad (15)$$

[†]Strictly speaking, the elements of $\mathcal{H}$ are classes of functions Φ such that Φ and Φ_1 belong to the same class if their values agree almost everywhere. We shall loosely identify the elements of $\mathcal{H}$ with their representative functions.

^{††}Condition (10e) is stated for the three-dimensional model. The corresponding inequalities, $G_j(r,s) \leq M_1 - M_2 \log |r-s|$ in two dimensions and $|G_j(r,s)| \leq M$ in one dimension, show that (13) is valid in all three cases.

[‡]See F. Riesz and B. Sz.-Nagy, Functional Analysis (Frederick Ungar Publishing Co., 1955), pp. 242-244.

^{‡‡}Ibid., pp. 177-190.

THEOREM 1. $\mathcal{D}$ has a complete sequence of orthonormal eigenfunctions, given by Equation (15), such that $\omega_j < 0$, $j = 1, 2, \dots$.

Proof: From the above the theorem will follow if it is shown that the eigenvalues of each $\mathcal{D}_k$ ($1 \leq k \leq n$) are negative. Assume $\mathcal{D}_k \phi = \lambda \phi$ for some $k \leq n$. Since $\mathcal{D}_k$ is self-adjoint, $\phi(r)$ can be assumed to be real-valued. Green's formula gives

$$\begin{aligned} \lambda \int_R \phi^2(r) dV_r &= \int_R \phi(r) \mathcal{D}_k \phi(r) dV_r \\ &= - \int_R d_k(r) \|\text{grad } \phi\|^2 dV_r + \int_{\text{Bdry } R} d_k \phi \frac{\partial \phi}{\partial n} d\sigma. \end{aligned} \quad (16)$$

Conditions (1c) and (6) imply that the last member of Equation (16) is nonpositive, vanishing only if ϕ is a constant. In the latter case the boundary Condition (1c) implies $\phi(r) \equiv 0$, so that ϕ is not an eigenfunction. This concludes the proof.

The Subspace $\mathcal{M}$

In preparation for the determination of the analytic behavior of the solutions of Equations (5) and (7), we now discuss the local properties of the members of $\mathcal{M}$.

THEOREM 2. The elements of $\mathcal{M}$ are continuous functions on $\bar{R}$.

Proof: Extend the definition of the Green's function $G_j(r, s)$ so that $G_j(r, s) = 0$ if either r or s is exterior to $\bar{R}$. Let $S_h(r)$ denote the solid sphere with its center at r and radius $h > 0$. From Condition (10c) we have

$$\int_{S_h(r)} |G_j(r, s)|^2 dV_s \leq M^2 \int_{S_h(0)} \frac{dV_s}{|s|^2} = 4\pi h M^2;$$

hence, $\int_{S_h(r)} |G_j(r, s)|^2 dV_s$ converges to zero as h approaches zero uniformly in r , $j = 1, 2, \dots, n$.

Now suppose $\Psi \in \mathcal{M}$, say $\Psi = \mathcal{G}^{-1}\phi$. Schwarz's inequality gives

$$\begin{aligned} |\Psi_j(r) - \Psi_j(r_0)|^2 &\leq \left[\int_R |G_j(r, s) - G_j(r_0, s)| \cdot |\phi_j(s)| dV_s \right]^2 \\ &\leq \int_R |\phi_j^2(s)| dV_s \left[\int_{S_h(r_0)} |G_j(r, s) - G_j(r_0, s)|^2 dV_s \right. \\ &\quad \left. + \int_{CS_h(r_0)} |G_j(r, s) - G_j(r_0, s)|^2 dV_s \right], \end{aligned} \quad (17)$$

where CS denotes the complement of set S. With reference to the last member of (17), the first integral inside the brackets has been shown above to converge to zero with h ; the second integral inside the same brackets can be made arbitrarily small for a fixed h by taking $|r - r_0|$ small enough, since $G_j(r, s)$ is uniformly continuous over the set $S_{h/2}(r_0) \times CS_h(r_0)$. Hence, $\lim_{r \rightarrow r_0} \psi_j(r) = \psi_j(r_0)$ for each $j = 1, 2, \dots, n$, q.e.d.

THEOREM 3. Suppose $\Psi = \mathcal{O}^{-1}\Phi$, where $\Phi(r)$ is bounded and continuous in each subregion R_i , $1 \leq i \leq m$; then $\Psi(r)$ has continuous first-order partial derivatives in each R_i and satisfies the boundary Conditions (1b) and (1c). If, in addition, $\Phi(r)$ has continuous first-order partial derivatives in each R_i , then $\Psi(r)$ also satisfies Condition (1a).

Proof: Given $\epsilon > 0$, let $\Sigma_\epsilon = \left\{ r \mid \text{dist} \left(r, \bigcup_{i=1}^m B_i \right) < \epsilon \right\}$; Σ_ϵ is the set of all points less distant than ϵ from at least one of the boundaries B_i of the subregions R_i . The Green's functions $G_j(r, s)$ have uniformly continuous partial derivatives with respect to r at a fixed point $r_0 \in R_i$ for all s in $U_\epsilon = C(S_\epsilon(r_0) \cup \Sigma_\epsilon)$. Furthermore, Condition (10e) implies

$$\text{that}^\dagger \int_{U_\epsilon} \frac{\partial G_j(r, s)}{\partial x} \phi_j(s) dV_s \text{ converges to } \int_R \frac{\partial G_j(r, s)}{\partial x} \phi_j(s) dV_s$$

uniformly with respect to r in a neighborhood of r_0 . Thus, the conditions for differentiation of the Cauchy-Riemann integral are fulfilled^{††} and

$$\frac{\partial \psi_j}{\partial x}(r) = \int_R \frac{\partial G_j(r, s)}{\partial x} \phi_j(s) dV_s.$$

To see that this is continuous, let $|\phi_j(s)| \leq M_1$. Then Condition (10e) implies

$$\int_{S_\epsilon(r_0)} \left| \frac{\partial G_j(r, s)}{\partial x} \phi_j(s) \right| dV_s \leq 4\pi\epsilon M \cdot M_1,$$

$$\text{so that } \frac{\partial \psi_j(r)}{\partial x} = \lim_{\epsilon \rightarrow 0} \int_{CS_\epsilon(r_0)} \frac{\partial G_j(r, s)}{\partial x} \phi_j(s) dV_s \text{ uniformly in a}$$

neighborhood of r_0 ; but, as before, the latter integral is - for all sufficiently small ϵ - continuous at r_0 , and so $\frac{\partial \psi_j}{\partial x}$ (being a uniform limit

[†]Derivatives $\frac{\partial G_j(r, s)}{\partial x}$, $\frac{\partial G_j(r, s)}{\partial y}$, and $\frac{\partial G_j(r, s)}{\partial z}$ are with respect to the coordinate components of r .

^{††}E. C. Titchmarsh, The Theory of Functions (Oxford University Press, 1950), p. 59.

of continuous functions) is continuous at r_0 . Continuity of $\frac{\partial \psi_j}{\partial y}$ and $\frac{\partial \psi_j}{\partial z}$ follows similarly, as do the boundary Conditions (1b) and (1c).

The last statement in Theorem 3 is a slight extension of a standard result, which may be found in Methoden der Mathematischen Physik.[†] The extension here does not assume that $\Psi(r)$ is continuous on the boundaries B_i . The alteration of the proof is obvious - one simply applies the standard proof to each R_i separately. This concludes the proof of Theorem 3.

COROLLARY. The eigenfunctions of $\mathcal{D}$ belong to C .

Proof: Suppose $\mathcal{D}\Omega = \omega\Omega$, so $\Omega = \omega\mathcal{D}^{-1}\Omega$. Since $\mathcal{D}^{-1}\Omega$ belongs to $\mathcal{M}$, Theorem 2 shows that Ω is continuous (and therefore bounded) on the closed set $\bar{R}$; hence, the first part of Theorem 3 applies to Ω . Thus, Ω has continuous first-order partial derivatives in each R_i , and Theorem 3 shows that Ω satisfies Conditions (1a), (1b), and (1c), q.e.d.

Existence Theorem for Positive Integral Operators

The later developments will depend principally on the following theorem, which is an extension of a result given by M. G. Krein and M. A. Rutman.^{††} The Krein-Rutman result is, in turn, a generalization of a classical existence theorem for integral operators with positive kernels discovered by R. Jentzsch.[‡]

In Theorem 4 we will consider matrices whose elements are integral operators; these matrices operate on the elements $\Phi \in \mathcal{H}$. Letting $(T\Phi)_i$ denote the i^{th} component of the transform of Φ by T , $1 \leq i \leq n$, we consider T of the form

$$(T\Phi)_i = \int_R \sum_{j=1}^n K_{ij}(r,s) \phi_j(s) dV_s$$

where $\Phi(s) = (\phi_1(s), \phi_2(s), \dots, \phi_n(s))$, and the K_{ij} are prescribed

[†]R. Courant and D. Hilbert, Methoden der Mathematischen Physik (J. Springer, 1927), Vol. I, pp. 365-367.

^{††}M. G. Krein and M. A. Rutman, "Linear Operators Leaving Invariant a Cone in Banach Space," Uspekhi Matem. Nauk (N.S.) 3, Sec. 6, pp. 3-95.

[‡]R. Jentzsch, "Über Integralgleichungen mit Positivem Kern," J. Reine Angew. Math. 141 (1912), pp. 235-244.

kernels satisfying $K_{ij}(r,s) \geq 0$ and $\sum_{i,j} \iint_{R \times R} |K_{ij}(r,s)|^2 dV_r dV_s < +\infty$.

We will employ the usual notation for iterated kernels:

$$(T^p \Phi)_i = \int_R \sum_{j=1}^n K_{ij}^{(p)}(r,s) \phi_j(s) dV_s$$

where $K_{ij}^{(1)} = K_{ij}$ and $K_{ij}^{(p)}(r,s) = \sum_{k=1}^n \int_R K_{ik}(r,t) K_{kj}^{(p-1)}(t,s) dV_t$

for any integer $p > 1$. Finally, we introduce n measurable subsets of R , denoted $M_1, M_2, \dots, M_n$, and denote the Lebesgue measure of M_i by σ_i ;

the only assumption we make on the M_i is that $\sum_{i=1}^n \sigma_i > 0$.

THEOREM 4. Suppose the integral operator T is defined on $\mathcal{H}$, as above, such that for some positive integer p , $K_{ij}^{(p)}$ is continuous and $K_{ij}^{(p)}(r,s) > 0$ for almost all[†] $r \in M_i$, $s \in R$, and $K_{ij}^{(p)}(r,s) = 0$ for $r \notin M_i$. Then T has a positive real eigenvalue, λ_0 , which is simple and greater than the absolute value of any other eigenvalue of T . The eigenfunctions belonging to λ_0 are all proportional to the principal eigenfunction of T , which is uniquely determined by the normalizing conditions: $\Phi^0(r) = (\phi_1^0(r), \phi_2^0(r), \dots, \phi_n^0(r))$, $\phi_j^0(r) > 0$ for $r \in M_j$, $\phi_j^0(r) = 0$ for $r \notin M_j$, $1 \leq j \leq n$; and $\|\Phi\|^2 = \sum_{j=1}^n \int_{M_j} [\phi_j^{(0)}(r)]^2 dV_r = 1$.

The adjoint operator, given by $(T^* \Psi)_i = \sum_{j=1}^n \int_R K_{ji}(s,r) \psi_j(s) dV_s$,

also possesses a unique principal eigenfunction $\Psi^0(r)$ satisfying $\psi_j^0(r) > 0$ for all $r \in R$, $1 \leq j \leq n$, and $(\Phi^0, \Psi^0) = 1$. Finally, if $X(r) = (x_1(r), x_2(r), \dots, x_n(r))$ is a member of $\mathcal{H}$ with $x_j(r) \geq 0$,

[†]That is, all points in M_i except possibly for an exceptional subset of Lebesgue measure zero.

$1 \leq j \leq n$, and satisfying $\|X\|^2 = \sum_{i=1}^n \int_R x_i^2(r) dV_r > 0$, then

$\lim_{m \rightarrow \infty} \frac{T^m X}{\|T^m X\|} = \Phi^0$ in the norm topology on $\mathcal{H}$.

Proof: Letting $\|T\| = \underset{\substack{\Phi \in \mathcal{H} \\ \Phi \neq 0}}{\text{l.u.b.}} \frac{\|T\Phi\|}{\|\Phi\|}$, then the so-called "spectral radius" of T , which is the maximum of the magnitudes of the eigenvalues of T , is given by[†]

$$|\lambda|_{\max} = \lim_{m \rightarrow \infty} \|T^m\|^{1/m} \leq \|T\|; \quad (18)$$

the limit always exists. By hypothesis, $\sigma_i > 0$ for at least one value of i ; we may suppose $\sigma_1 > 0$, and we can select a closed set $N_1 \subset M_1$ such that the measure of N_1 is $\sigma_0 > 0$. Since

$$\omega(r) = \sum_{j=1}^n \int_R K_{1j}^{(p)}(r,s) K_{1j}^{(p)}(s,r) dV_s$$

is continuous and positive on the closed set N_1 , it follows that g.l.b. $\omega(r) = \omega_0 > 0$. Now taking $\hat{\Phi} = (1, 1, \dots, 1)$ throughout R , $r \in N_1$ we have

$$\|T^p \hat{\Phi}\|^2 = \sum_{i,j} \iint_{R \times R} [K_{ij}^{(p)}(r,s) K_{ij}^{(p)}(s,r)] dV_r dV_s \geq \sigma_0 \omega_0$$

and

$$\|T^{kp} \hat{\Phi}\|^2 \geq \sigma_0^k \omega_0^k. \quad (19)$$

From Equations (18) and (19) we find, $|\lambda|_{\max} \geq \frac{(\sigma_0 \omega_0)^{1/2p}}{(nV)^{1/2}}$, where V is the volume of R , so that T must have at least one nonzero eigenvalue.

It follows^{††} from Theorem 6.1 of Krein and Rutman[‡] that T possesses a positive eigenvalue, λ_0 , which is not less than the absolute value of any other eigenvalue of T , and to λ_0 there corresponds at least one eigenfunction Φ^0 for T and Ψ^0 for T^* such that the components of Φ^0 and Ψ^0

[†]See Riesz, op. cit., p. 425.

^{††}Note T leaves invariant the cone of those $\Phi \in \mathcal{H}$ whose components $\phi_j(r)$ are nonnegative almost everywhere in R .

[‡]Krein and Rutman, op. cit.

are nonnegative throughout R , and $\|\Phi^0\| = (\Phi^0, \Psi^0) = 1$. Also, since

$$\phi_i^0(r) = \frac{1}{\lambda_0^p} \int_R \sum_{j=1}^n K_{ij}^{(p)}(r,s) \phi_j^0(s) dV_s, \text{ the hypotheses for } K_{ij}^{(p)}$$

imply that $\phi_i^0(r) > 0$ if $r \in M_i$ and $\phi_i^0(r) = 0$ otherwise. The same argument applied to the adjoint shows that each component of Ψ^0 is positive everywhere in R .

We now show that λ_0 is strictly greater than the modulus of all other eigenvalues of T . Suppose, then, that λ_1 is another eigenvalue of T with $|\lambda_1| = \lambda_0$, and let $T\Phi^1 = \lambda_1\Phi^1$, $\|\Phi^1\| = 1$. Thus, we have

$$\phi_i^1(r) = \frac{1}{\lambda_1^p} \int_R \sum_{j=1}^n K_{ij}^{(p)}(r,s) \phi_j^1(s) dV_s \quad 1 \leq i \leq n.$$

Taking absolute values,

$$|\phi_i^1(r)| \leq \frac{1}{\lambda_0^p} \int_R \sum_{j=1}^n K_{ij}^{(p)}(r,s) |\phi_j^1(s)| dV_s;$$

multiplying by $\psi_i^0(r)$, summing on i , and integrating gives

$$(\lambda_0^p |\Phi^1|, \Psi^0) \leq (T^p |\Phi^1|, \Psi^0) = (|\Phi^1|, T^{*p} \Psi^0) = (\lambda_0^p |\Phi^1|, \Psi^0), \quad (20)$$

$$\begin{aligned} \text{where } |\Phi^1(r)| &= |(\phi_1^1(r), \phi_2^1(r), \dots, \phi_n^1(r))| \\ &= (|\phi_1^1(r)|, |\phi_2^1(r)|, \dots, |\phi_n^1(r)|). \end{aligned}$$

The equality of the first and last members of (20) requires that the first relation be an equality; and since the components of Ψ^0 are everywhere positive, we must have

$$T^p |\Phi^1| = \lambda_0^p |\Phi^1| \quad (21)$$

and, as before, $|\phi_i^1(r)| > 0$ for $r \in M_i$, $1 \leq i \leq n$.

$$\begin{aligned} \text{Let } \theta_j(r) &= 2\pi \arg \phi_j^1(r) & r \in M_j \\ &= 0 & r \notin M_j \end{aligned}$$

so we can write

$$\Phi^0(r) = \left(e^{i\theta_1(r)} \phi_1(r), e^{i\theta_2(r)} \phi_2(r), \dots, e^{i\theta_n(r)} \phi_n(r) \right). \quad (22)$$

Rewriting Equation (19), we obtain

$$\begin{aligned} \sum_{k=1}^n \int_R K_{jk}^{(p)}(r,s) |\phi_k^1(s)| dV_s &= \lambda_0 \phi_j^0(r) = \lambda_0 e^{i\theta_j(r)} \phi_j^1(r) \\ &= \frac{\lambda_0}{\lambda_1} e^{i\theta_j(r)} \sum_{k=1}^n \int_R K_{jk}^{(p)}(r,s) \phi_k^1(s) dV_s, \quad 1 \leq j \leq n. \end{aligned} \quad (23)$$

However, if $r \in M_j$ so that $\phi_j^0(r) > 0$, the first member of Equation (21) will be strictly greater than the absolute value of the last member of Equation (21) unless the argument of $\phi_k^1(s)$ is constant, independent of k and s , wherever $s \in M_k$. Thus, the relationship in (20) implies $\theta_j(r) = \alpha$, $r \in M_j$, for some real α . Therefore, $e^{-i\alpha}\phi^1$ has nonnegative components, and so (20) and the definition of ϕ^0 give $T\phi^1 = \lambda_0\phi^1$. But, by definition, $T\phi^1 = \lambda_1\phi^1$, and we conclude $\lambda_0 = \lambda_1$.

Next, to show that λ_0 is a simple eigenvalue of T , note that the contrary implies the existence[†] of a solution $\hat{\phi}$ of

$$T\hat{\phi} = \lambda_0\hat{\phi} \quad (24)$$

which is orthogonal to ψ^0 . But we have just shown that any solution of Equation (24) has a constant argument, so that $\hat{\phi} = \beta\tilde{\phi}$, where $\tilde{\phi}$ has nonnegative components for some complex number β . Since the components of ψ^0 are everywhere positive, $(\tilde{\phi}, \psi^0)$ cannot vanish unless $\tilde{\phi} \equiv 0$; so, λ_0 is simple. Incidentally, the observation in this paragraph shows that ψ^0 may be normalized by the condition $(\tilde{\phi}^0, \psi^0) = 1$.

The final statement of the theorem, concerning the convergence of $\frac{T^m X}{\|T^m X\|}$ to ϕ^0 , is given by Krein and Rutman.^{††} This concludes the proof of Theorem 4.

We will need to know something about the way in which λ_0 , ϕ^0 , and ψ^0 depend upon the kernel $K(r,s) = (K_{ij}(r,s))$. For this purpose we have the following perturbation theorem.

[†]B. Friedman, Principles and Techniques of Applied Mathematics (John Wiley & Sons, 1956), p. 131.

^{††}Krein and Rutman, op. cit., pp. 72, 73.

THEOREM 5. If the kernel K of Theorem 4 depends on a parameter α , denoted $K = K(r, s; \alpha)$, in such a way that $K(r, s; \alpha)$ satisfies the hypotheses of Theorem 4 for each α in a neighborhood of α_0 and such that

$$\lim_{\alpha \rightarrow \alpha_0} \sum_{i,j=1}^n \iint_{R \times R} |K_{ij}(r, s; \alpha) - K_{ij}(r, s; \alpha_0)|^2 dV_r dV_s = 0,$$

then the eigenvalue λ_α given by Theorem 4 for the kernel $K(r, s; \alpha)$ will be continuous at $\alpha = \alpha_0$; also the corresponding eigenfunction $\Phi_\alpha^0(r)$ and adjoint eigenfunction $\Psi_\alpha^0(r)$ will be continuous in the mean at α_0 :

$$\lim_{\alpha \rightarrow \alpha_0} \int_R \sum_{i=1}^n \left\{ \left| \phi_{\alpha,i}^0(r) - \phi_{\alpha_0,i}^0(r) \right|^2 + \left| \psi_{\alpha,i}^0(r) - \psi_{\alpha_0,i}^0(r) \right|^2 \right\} dV_r = 0.$$

Moreover, the convergence of $\Phi_\alpha^0(r)$ and $\Psi_\alpha^0(r)$ will be uniform in r if the kernel $K(r, s; \alpha)$ is continuous in its variables jointly.

The proof of Theorem 5 for continuous scalar kernels is given[†] by H. F. Bueckner,^{††} who makes use of a result of Tricomi concerning continuity properties of Fredholm determinants. The general case is a consequence of a theorem of F. Wolf.[‡]

A Spectral Theorem

In preparation for the spectral theory which follows we want to recall the usual definition of generalized eigenvector.^{‡‡} An ordered set of vectors $x_0, x_1, \dots, x_k$ belonging to a complex vector space for which

$$Tx_0 = \lambda x_0$$

$$Tx_j = \lambda x_j + x_{j-1} \quad j = 1, 2, \dots, k$$

is termed a set of generalized eigenvectors for the linear transformation T corresponding to the eigenvalue λ . Inspection of the Jordan canonical form of a finite square matrix M of complex numbers will show that the set

[†]It is essential to note that the eigenvalue λ_{α_0} is simple.

^{††}H. F. Bueckner, Die Praktische Behandlung von Integral Gleichungen (J. Springer, 1952), Secs. 6, 24, 27.

[‡]See Theorem 4.15 of F. Wolf, "Analytic Perturbation of Operators in Banach Spaces," Math. Annalen 124 (1952), pp. 317-333.

^{‡‡}See Friedman, op. cit., pp. 67-70.

of generalized eigenvectors of M forms a complete set in their vector space. This is not generally true, however, for linear operators on spaces of infinite dimension.

Let T be a linear operator defined on a linear submanifold $\mathcal{J}$ (not necessarily topologically closed) of a Banach space $\mathcal{B}$. T is said to be a "closed" operator provided that for all sequences of elements $x_1, x_2, \dots$ of $\mathcal{J}$ for which $\{x_j\}$ converges, say to x , and $\{Tx_j\}$ converges, say to y , then $x \in \mathcal{J}$ and $Tx = y$.

The following theorem, which is due to M. A. Naimark,[†] shows that a closed operator T for which $R_\mu = (\mu I - T)^{-1}$ (the resolvent of T) is suitably well-behaved has a complete set of generalized eigenfunctions.^{††}

THEOREM 6. Let T be a closed linear operator defined on a linear manifold dense in the Hilbert space $\mathcal{H}$ whose resolvent, $R_\mu = (\mu I - T)^{-1}$, is completely continuous for some $\mu = \mu_0$. Suppose that there exists a sequence of circumferences in the complex plane $C_1, C_2, \dots$ with a common center at the origin of coordinates such that

- There are no eigenvalues of T on any C_k .
- The radius r_k of C_k increases without limit as k approaches infinity.
- For all $x \in \mathcal{H}$, $\lim_{m \rightarrow \infty} \sup_{\mu \in C_n} \|R_\mu f\| = 0$.

Then the generalized eigenvectors of T span $\mathcal{H}$, and every $x \in \mathcal{H}$ has a conditionally[‡] convergent expansion in these generalized eigenvectors.

Proof: If λ is an eigenvalue of T , then $\frac{1}{\mu_0 - \lambda}$ is an eigenvalue of R_{μ_0} . Since R_{μ_0} is completely continuous, it follows that T has, at most, a countable number of eigenvalues and these eigenvalues have no

[†]M. A. Naimark, "On Some Criteria of Completeness of the System of Eigen and Associated Vectors of a Linear Operator in Hilbert Space," Doklady Akad. Nauk S.S.S.R. (N.S.) 98 (1954), pp. 727-730.

^{††}Theorem 6 has a direct extension to the case where $\mathcal{H}$ is a Banach space and $\|R_\mu f\|$ has polynomial growth (of degree l independent of f) on the $\{C_k\}$ at ∞ , and the domain of T^{l+2} is dense in $\mathcal{H}$. [See M. A. Martino, "An Extension of a Spectral Theorem of M. A. Naimark," Notices Am. Math. Soc. 5, No. 3 (1958).]

[‡]The precise meaning is given in the proof.

finite point of accumulation; also, T has a pure point spectrum.[†] We may enumerate the eigenvalues of T , say $\lambda_1, \lambda_2, \dots$, such that $\lambda_1, \lambda_2, \dots, \lambda_{k_q}$ are those which are interior to C_q . Then, if μ_0 is interior to C_q , we have^{††}

$$\frac{1}{2\pi i} \oint_{C_q} \frac{R_\mu f}{\mu - \mu_0} d\mu = \left[R_{\mu_0} - \sum_{j=1}^{k_q} P_j(\mu_0) \right] f \quad (25)$$

where $P_j(\mu_0)$ is a projection onto the finite dimensional space spanned by the generalized eigenvectors corresponding to λ_j . On the other hand,

$$\left\| \frac{1}{2\pi i} \oint_{C_q} \frac{R_\mu f}{\mu - \mu_0} d\mu \right\| \leq \text{l.u.b.}_{\mu \in C_q} \|R_\mu f\| \frac{1}{2\pi} \cdot \frac{2\pi r_n}{r_n - |\mu_0|}; \quad (26)$$

hence, by hypothesis (c) the first member of Equation (25) converges (in norm) to zero as q approaches infinity. Thus,

$$R_{\mu_0} f = \lim_{n \rightarrow \infty} \sum_{j=1}^{k_n} P_j(\mu_0) f, \quad (27)$$

so that the generalized eigenvectors of T span the range of R_{μ_0} . Since $R_{\mu_0}(\mu_0 - T)f = f$, the range R_{μ_0} includes the domain of definition of $\mu_0 - T$, which by assumption is dense in $\mathcal{H}$. We conclude that the generalized eigenvectors of T span $\mathcal{H}$.

Equation (27) does not necessarily imply that $\sum_{j=1}^{\infty} P_j(\mu_0) f$ converges,

for the Inequality (26) provides a proof of convergence of Equation (27) only if the projections P_j corresponding to eigenvalues in each of the annular regions $A_k = C_k - C_{k-1}$ are grouped together. Thus, if we set

$$Q_k = \sum_{j=k_{q-1}+1}^{k_q} P_j(\mu_0) \text{ (with } k_0 = 0), \text{ we have } R_{\mu_0} f = \sum_{k=1}^{\infty} Q_k f; \text{ the latter}$$

[†]See M. A. Martino, "Concerning the Multigroup Diffusion Operator," KAPL-1867, September 20, 1957, pp. 18-19.

^{††}See A. E. Taylor, "Spectral Theory of Closed Distributive Operators," Acta Math. 84 (1950), pp. 189-224.

series is absolutely convergent in norm. The Q_k are projections onto the finite dimensional subspaces spanned by the generalized eigenvectors belonging to eigenvalues in A_k , $k = 1, 2, \dots$.

THE TIME-INDEPENDENT PROBLEM

The time-independent problem has been defined by the eigenvalue equation

$$-(\mathcal{D} + A) \Phi(r) = \nu F \Phi(r). \quad (7)$$

From Equation (4) $A = (a_{jk}(r))$; it is convenient to separate A into two triangular matrices, $A = L + U$, as follows:

$$\begin{aligned} L_{jk} &= a_{jk} & j &\geq k \\ &= 0 & j &< k \\ U_{jk} &= 0 & j &\geq k \\ &= a_{jk} & j &< k. \end{aligned} \quad (28)$$

The Time-Independent Problem without Up-Scattering

If there is no up-scattering, then U , defined in Equation (28), is identically zero, so that Equation (7) becomes

$$-(\mathcal{D} + L) \Phi(r) = \nu F \Phi(r). \quad (29)$$

Now the one-group diffusion-absorption operators which comprise the diagonal of the left member of Equation (29), namely $-(\mathcal{D}_j + a_{jj})$, are self-adjoint with respect to the components of $\Phi \in C$, and these operators possess

Green's functions $G_j(r, s) > 0$, so that $-(\mathcal{D}_j + a_{jj})^{-1} = \int_R dV_s G_j(r, s)$;

A direct calculation verifies that $(\mathcal{D} + L)$ has the inverse given by

$$\left. \begin{aligned} \text{a. } (\mathcal{D} + L)_{jj}^{-1} &= - \int_R dV_s G_j(r, s) & (1 \leq j \leq n) \\ \text{b. } (\mathcal{D} + L)_{jk}^{-1} &= 0 & (j < k) \\ \text{c. } (\mathcal{D} + L)_{jk}^{-1} &= - \sum_{m=k+1}^j (\mathcal{D} + L)_{jm}^{-1} L_{mk} (\mathcal{D} + L)_{kk}^{-1} & (j > k) \end{aligned} \right\} \quad (30)$$

The definition (30c) is given inductively for increasing values of $j - k$. It follows from Equations (6), (8), and (30) and the transitivity postulate (p. 15) that we may write:

$$-(\mathcal{D} + L)^{-1} = \left(\int_R dV_s H_{jk}(r, s) \right), \quad (31)$$

$$\text{where } H_{jk}(r, s) \equiv 0 \quad (j < k) \\ > 0 \quad (j \geq k).$$

Since $\mathcal{D} + L$ is invertible, any eigenvalue ν of Equation (29) must be nonzero. If we write $\lambda = 1/\nu$, Equation (29) becomes

$$-(\mathcal{D} + L)^{-1} F \Phi = \lambda \Phi. \quad (32)$$

Consider the range of F ; i.e., the set $\mathcal{H}_I$ of all images $\Phi_1 = F\Phi$. On $\mathcal{H}_I$ Equation (32) becomes

$$-F(\mathcal{D} + L)^{-1} \Phi_1 = \lambda \Phi_1. \quad (33)$$

Let

$$N_j = \left\{ r \in R \mid f_{jk}(r) = 0 \quad 1 \leq k \leq n \right\},$$

and let M_j be the complement of N_j in R . From Equation (31) we see that we may write

$$-F(\mathcal{D} + L)^{-1} = \left(\int_R dV_s \sum_m f_{jm}(r) H_{mk}(r, s) \right).$$

From Equation (8), Equation (31), and the transitivity postulate following Equation (8) it may be verified that

$$\int_R dV_t \sum_{p, m, n} f_{jp}(r) H_{pm}(r, t) f_{mn}(t) H_{nk}(t, s) > 0 \quad (34)$$

for all $r \in M_j$ and $s \in R$. Thus, for $p = 2$, $-F(\mathcal{D} + L)^{-1}$ satisfies the conditions of Theorem 4 and we obtain Theorem 7.

THEOREM 7. The time-independent eigenvalue problem with no up-scattering, Equation (33), has a positive dominant eigenvalue λ_0 (i.e., $\lambda_0 > |\lambda_k|$ for all $\lambda_k \neq \lambda_0$) which is simple, corresponding to an eigenfunction $\Phi^0 = (\phi_1^0, \phi_2^0, \dots, \phi_n^0)$ with $\phi_j^0(r) > 0$ for $r \in M_j$ and $\phi_j^0(r) = 0$ for $r \in N_j$, $1 \leq j \leq n$; the adjoint eigenfunction corresponding to λ_0 has all its components positive throughout R .

The Time-Independent Problem with Up-Scattering

For the time-independent problem with up-scattering, Equation (7) may be rewritten as

$$-(\mathcal{D} + L + U) \Phi(r) = \nu F \Phi(r), \quad (35)$$

where L and U are as before [Equation (28)], and U is not identically zero. We assume ν to be nonzero and rewrite Equation (35) as

$$-(\mathcal{D} + L)^{-1} (F + \lambda U) \Phi = \lambda \Phi, \quad (36)$$

where $\lambda = 1/\nu$. Consider the range of $F + U$; i.e., the set $\hat{\mathcal{A}}$ of all images $\hat{\Phi} = (F + U)\Phi$. On $\hat{\mathcal{A}}$, Equation (36) becomes[†]

$$-(F + \lambda U)(\mathcal{D} + L)^{-1} \hat{\Phi} = \lambda \hat{\Phi}. \quad (37)$$

In what follows we will derive an extension of Theorem 7 to Equation (37). To do this, we make one further assumption concerning the diffusion equation coefficients besides those listed under Differential Equations (pp. 12 to 15). We assume that for all r and k

$$-\sum_j a_{jk}(r) \geq c \sum_j f_{jk}(r) \quad (38)$$

for some $c > 0$.^{††}

Let

$$Q_j = \left\{ r \in R \mid f_{jk}(r) + U_{jk}(r) = 0 \quad 1 \leq k \leq n \right\}$$

[†]Note that the range of $F + \lambda U$ is independent of $\lambda > 0$.

^{††}This postulate reflects the physical requirement that each fission be derived from a neutron capture. By allowing $c < 1$, this theory applies to the case where the average number of fission neutrons per fission is group-dependent.

and let P_j be the complement of Q_j in R . We shall call $\Phi = (\phi_1, \phi_2, \dots, \phi_n)$ "positive in the range of $F + U$ " if $\phi_j(r) > 0$ for $r \in P_j$ and $\phi_j(r) = 0$ for $r \in Q_j, 1 \leq j \leq n$.

Consider the eigenvalue problem

$$-(F + \alpha U)(\mathcal{D} + L)^{-1}\Phi_\alpha = \mu_\alpha \Phi_\alpha \quad (39)$$

where α is a real, positive parameter. For a given $\alpha \geq 0$, Theorem 4 assures us that Equation (39) has a dominant eigenvalue μ_α^0 which is positive and simple, corresponding to a positive eigenfunction in the range of $F + U$. Concerning this dominant eigenvalue μ_α^0 , we have the following lemmas.

LEMMA 1. For $U \neq 0$ and $\alpha > 0$, μ_α^0 is a monotonic increasing continuous function of α .

Proof: Since $-(F + \alpha U)(\mathcal{D} + L)^{-1}$ with $\alpha > 0$ satisfies the condition of theorem 5, μ_α^0 is a continuous function of α for $\alpha > 0$. To show the monotony, consider the eigenfunction Φ_α^0 corresponding to the dominant eigenvalue μ_α^0 of Equation (39) and the adjoint eigenfunction $\Psi_{\alpha+\delta\alpha}^0$ corresponding to the dominant eigenvalue $\mu_{\alpha+\delta\alpha}^0$ of Equation (39) with $\alpha+\delta\alpha$ replacing α :

$$-(F + \alpha U)(\mathcal{D} + L)^{-1}\Phi_\alpha^0 = \mu_\alpha^0 \Phi_\alpha^0$$

and

$$-(\mathcal{D} + L^*)^{-1} [F^* + (\alpha + \delta\alpha) U^*] \Psi_{\alpha+\delta\alpha}^0 = \mu_{\alpha+\delta\alpha}^0 \Psi_{\alpha+\delta\alpha}^0.$$

Taking the inner product of the first of these equations with $\Psi_{\alpha+\delta\alpha}^0$ and the second with Φ_α^0 and subtracting, we obtain

$$-\delta\alpha \left(U(\mathcal{D} + L)^{-1} \Phi_\alpha^0, \Psi_{\alpha+\delta\alpha}^0 \right) = (\mu_{\alpha+\delta\alpha}^0 - \mu_\alpha^0) \left(\Phi_{\alpha+\delta\alpha}^0, \Psi_\alpha^0 \right).$$

Since Φ_α^0 is positive in the range of $F + U$ and $\Psi_{\alpha+\delta\alpha}^0$ is positive everywhere in R , $\left(\Phi_\alpha^0, \Psi_{\alpha+\delta\alpha}^0 \right) > 0$. Since $-(\mathcal{D} + L)^{-1} \Phi_\alpha^0$ has all positive components and $U \neq 0$, $-\left(U(\mathcal{D} + L)^{-1} \Phi_\alpha^0, \Psi_{\alpha+\delta\alpha}^0 \right) > 0$. Thus, we have the result that for $\delta\alpha > 0$, $\mu_{\alpha+\delta\alpha}^0 > \mu_\alpha^0$; i.e., μ_α^0 is monotonically increasing.

LEMMA 2. There exists a positive number A such that for $\alpha > A$, $\mu_\alpha^0 < \alpha$.

Proof: We rewrite Equation (39) for the dominant eigenvalue and corresponding eigenfunction as

$$-\left(\frac{F}{\alpha} + U\right)(\mathcal{D} + L)^{-1} \Phi_{\alpha}^0 = \frac{\mu_{\alpha}^0}{\alpha} \Phi_{\alpha}^0. \quad (40)$$

Let $\bar{\Phi}_{\alpha} = -(\mathcal{D} + L)^{-1} \Phi_{\alpha}^0$. From the definition of $(\mathcal{D} + L)^{-1}$ in Equation (30) we see that $\bar{\Phi}_{\alpha}$ belongs to the class C and all its components are positive everywhere in R.[†] Equation (40) for $\bar{\Phi}_{\alpha}$ becomes

$$-\frac{\mu_{\alpha}^0}{\alpha} (\mathcal{D} + L) \bar{\Phi}_{\alpha} = \left(\frac{F}{\alpha} + U\right) \bar{\Phi}_{\alpha}.$$

With the notation previously introduced, this equation is equivalent to the group equations

$$\frac{\mu_{\alpha}^0}{\alpha} \left(-d_j \nabla^2 \phi_{\alpha,j} - \sum_{k \leq j} a_{jk} \phi_{\alpha,k} \right) = \frac{1}{\alpha} \sum_k f_{jk} \phi_{\alpha,k} + \sum_{k > j} a_{jk} \phi_{\alpha,k} \quad (1 \leq j \leq n),$$

where $\bar{\Phi}_{\alpha} = (\phi_{\alpha,1}, \phi_{\alpha,2}, \dots, \phi_{\alpha,n})$.

Summing the group equations over j, we obtain

$$\begin{aligned} \frac{\mu_{\alpha}^0}{\alpha} \left(- \sum_j d_j \nabla^2 \phi_{\alpha,j} + \sum_j \sigma_j \phi_{\alpha,j} \right) + \left(\frac{\mu_{\alpha}^0}{\alpha} - 1 \right) \sum_j \sum_{k < j} a_{jk} \phi_{\alpha,k} \\ = \frac{1}{\alpha} \sum_{j,k} f_{jk} \phi_{\alpha,k}, \end{aligned}$$

where $\sigma_j = - \sum_k a_{kj}$. Integrating over R, we obtain

$$\begin{aligned} \frac{\mu_{\alpha}^0}{\alpha} \left(- \sum_j \int_{\Gamma} d_j \frac{\partial \phi_{\alpha,j}}{\partial n} dS + \sum_j \int_R \sigma_j \phi_{\alpha,j} dV \right) \\ + \left(\frac{\mu_{\alpha}^0}{\alpha} - 1 \right) \sum_j \sum_{k < j} \int_R a_{jk} \phi_{\alpha,k} dV = \frac{1}{\alpha} \sum_{j,k} \int_R f_{jk} \phi_{\alpha,k} dV. \quad (41) \end{aligned}$$

[†]Note that the transitivity assumption on $F + U$ ensures that P_1 has positive measure and $\phi_{\alpha,1}^0(r) > 0$ for $r \in P_1$.

Since $\bar{\Phi}_\alpha$ belongs to the class C,

$$- \sum_j \int_{\Gamma} d_j \frac{\partial \phi_{\alpha,j}}{\partial n} dS > 0;$$

the other integrals in Equation (41) are obviously positive. From Equation (38) we obtain

$$\sum_j \int_R \sigma_j \phi_{\alpha,j} dV \geq c \sum_{j,k} \int_R f_{jk} \phi_{\alpha,k} dV.$$

Therefore, Equation (41) shows that if $\alpha > \frac{1}{c}$, then $\frac{\mu_\alpha^0}{\alpha} < 1$, q.e.d.

If we use these lemmas, Theorem 7 can be extended to include models with up-scattering.

THEOREM 8. The time-independent eigenvalue problem in arbitrary dimension

$$-(F + \lambda U)(\mathcal{D} + L)^{-1} \Phi = \lambda \Phi \quad (42)$$

has a positive dominant eigenvalue λ_0 (i.e., $\lambda_0 > |\lambda_k|$ for all $\lambda_k \neq \lambda_0$) which is simple, corresponding to an eigenfunction which is positive in the range of $F + U$ and to an adjoint eigenfunction whose components are positive throughout R.

Proof: For the eigenvalue problem (39) as α approaches zero, μ_α^0 approaches the dominant eigenvalue of Equation (42) with $U \equiv 0$. Thus, for α sufficiently small, $\mu_\alpha^0 > \alpha$. From Lemma 2 we see that for α sufficiently large $\mu_\alpha^0 < \alpha$. Since by Lemma 1 μ_α^0 is a monotonic increasing, continuous function of α , there exists one and only one value of α , call it λ_0 , such that $\mu_{\lambda_0}^0 = \lambda_0$. Thus, λ_0 is an eigenvalue of Equation (42). From the definition of μ_α^0 , the corresponding eigenfunction is positive in the range of $F + U$, and the adjoint eigenfunction is positive everywhere in R. Moreover, the eigenvalue λ_0 is simple, as can be seen by applying Theorem 7 to Equation (39) with $\alpha = \lambda_0$.

Consider any other eigenvalue $\lambda_1 \neq \lambda_0$ of Equation (42):

$$-(F + \lambda_1 U)(\mathcal{D} + L)^{-1} \Phi^1 = \lambda_1 \Phi^1.$$

Since $-(\mathcal{D} + L)^{-1}$ is a positive integral operator with the form given in Equation (31),

$$-(\mathcal{D} + L)^{-1} = \left(\int_R dV_s H_{jk}(r, s) \right)$$

$$\text{where } H_{jk}(r, s) \equiv 0 \quad (j < k) \\ > 0 \quad (j \geq k),$$

it follows that

$$|\lambda_1| |\Phi^1| \leq -(F + |\lambda_1| U)(\mathcal{D} + L)^{-1} |\Phi^1|, \quad (43)$$

where we define $|\Phi^1| = (|\phi_1^1|, |\phi_2^1|, \dots, |\phi_n^1|)$. Since $-(F + |\lambda_1| U)(\mathcal{D} + L)^{-1}$ satisfies the conditions of Theorem 4, we have for its dominant eigenvalue and corresponding adjoint eigenfunction

$$\mu_{|\lambda_1|}^0 \Psi_{|\lambda_1|}^0 = -(\mathcal{D} + L^*)^{-1} (F^* + |\lambda_1| U^*) \Psi_{|\lambda_1|}^0. \quad (44)$$

Taking the inner product of Expression (43) with $\Psi_{|\lambda_1|}^0$ and of Equation (44) with $|\Phi^1|$, we obtain

$$\left(|\lambda_1| - \mu_{|\lambda_1|}^0 \right) \left(|\Phi^1|, \Psi_{|\lambda_1|}^0 \right) \leq 0.$$

Since $\Psi_{|\lambda_1|}^0$ is positive everywhere in R and $|\Phi^1|$ is positive on the range of $F + U$, we have $|\lambda_1| \leq \mu_{|\lambda_1|}^0$. From an inspection of the behavior of μ_{α}^0/α , we see that this implies that $\lambda_0 \geq |\lambda_1|$.

It remains to be shown that $\lambda_0 = |\lambda_1|$ implies $\lambda_1 = \lambda_0$. Let

$$A_1 = -(F + \lambda_1 U)(\mathcal{D} + L)^{-1} \quad i = 0, 1; \lambda_0 > 0; |\lambda_1| = \lambda_0;$$

and assume

$$A_1 \Phi^i = \lambda_1 \Phi^i \quad \Phi^i = (\phi_1^i, \phi_2^i, \dots, \phi_n^i); \phi_j^i(r) > 0 \text{ for } r \in P_j$$

$$A_1^* \Psi^i = \bar{\lambda}_1 \Psi^i \quad \Psi^i = (\psi_1^i, \psi_2^i, \dots, \psi_n^i); \psi_j^i(r) > 0 \text{ for } r \in R.$$

Defining as before $|\Phi| = (|\phi_1|, |\phi_2|, \dots, |\phi_n|)$ and " $\Phi \geq \Psi$ " to mean $\phi_j \geq \psi_j$, $j = 1, 2, \dots, n$, we have

$$\lambda_0 |\Phi^1| \leq A_0 |\Phi^1|, \quad (45)$$

so that

$$(\lambda_0 |\Phi^1|, \Psi^0) \leq (A_0 |\Phi^1|, \Psi^0) = (|\Phi^1|, A_0^* \Psi^0) = (\lambda_0 |\Phi^1|, \Psi^0). \quad (46)$$

Thus, the inequality sign in Expression (46) is ruled out, and since Ψ^0 is positive for $r \in R$, the inequality sign in Expression (45) is also impossible; i.e., $\lambda_0 |\Phi^1| = A_0 |\Phi^1|$. Because of the uniqueness of the normalized eigenfunction corresponding to λ_0 , $|\Phi^1| = \Phi^0$. Hence, we may write

$$\Phi^0(r) = |\Phi^1(r)| = \left(e^{i\theta_1(r)} \phi_1^1(r), e^{i\theta_2(r)} \phi_2^1(r), \dots, e^{i\theta_n(r)} \phi_n^1(r) \right).$$

If we introduce the notation

$$A_i = \left(\int_R dV_s \quad {}^i K_{jk}(r,s) \right),$$

we have

$$\begin{aligned} \sum_{k=1}^n \int_R {}^0 K_{jk}(r,s) |\phi_k^1(s)| dV_s &= \lambda_0 \phi_j^0(r) = \lambda_0 e^{i\theta_j(r)} \phi_j^1(r) \\ &= \frac{\lambda_0}{\lambda_1} e^{i\theta_j(r)} \sum_{k=1}^n \int_R {}^1 K_{jk}(r,s) \phi_k^1(s) dV_s \\ &\quad 1 \leq j \leq n. \end{aligned} \quad (47)$$

Now choose the index j and a point $r \in R$ such that $\phi_j^0(r) > 0$. Expanding Equation (47), we have

$$\begin{aligned} 0 < \lambda_0 \phi_j^0(r) &= \sum_{k,\ell=1}^n f_{jk}(r) \int_R H_{k\ell}(r,s) |\phi_\ell^1(s)| dV_s \\ &\quad + \frac{1}{\lambda_0} \sum_{k,\ell=1}^n U_{jk}(r) \int_R H_{k\ell}(r,s) |\phi_\ell^1(s)| dV_s \\ &= \frac{\lambda_0}{\lambda_1} e^{i\theta_j(r)} \left[\sum_{k,\ell=1}^n f_{jk}(r) \int_R H_{k\ell}(r,s) \phi_\ell^1(s) dV_s \right. \\ &\quad \left. + \frac{1}{\lambda_1} \sum_{k,\ell=1}^n U_{jk}(r) \int_R H_{k\ell}(r,s) \phi_\ell^1(s) dV_s \right], \end{aligned} \quad (48)$$

where $H_{jk}(r,s)$ is the Green's matrix for $-(\mathcal{D} + L)^{-1}$.

Each term of the penultimate member of Equation (48) is nonnegative, and at least one of these terms is positive; also, each term of that member is clearly the absolute value of its correspondent in the final member of Equation (48). Now the sum of two nonzero complex numbers has a smaller magnitude than the sum of their respective absolute values, unless the two numbers have the same argument. So in order for Equation (48) to hold, all terms in the last member must have the same argument; likewise, in the integrations it is necessary that whenever $\phi_\ell^1(s) \neq 0$, the argument of $\phi_\ell^1(s)$ be constant, independent of s and ℓ .

Hence, for some complex number α , $|\alpha| = 1$, the components of $\alpha \phi^1(s)$ are real and nonnegative for all s , and necessarily then $\alpha \phi^1 = \phi^0$. Thus, ϕ^0 satisfies

$$A_0 \phi^0 = \lambda_0 \phi^0 \quad (49)$$

$$A_1 \phi^0 = \lambda_1 \phi^0$$

Subtracting the second of Equations (49) from the first, we get

$$\frac{\lambda_1 - \lambda_0}{\lambda_0 \lambda_1} \left[-U(\mathcal{D} + L)^{-1} \phi^0 \right] = (\lambda_0 - \lambda_1) \phi^0 \quad (50)$$

Since ϕ^0 and $-U(\mathcal{D} + L)^{-1} \phi^0$ have nonnegative real components, Equation (50) together with $|\lambda_1| = \lambda_0$ implies that $\lambda_1 = \pm \lambda_0$. If $\lambda_1 = -\lambda_0$, we may add Equations (49) to get $-F(\mathcal{D} + L)^{-1} \phi^0 = 0$. But this is impossible, since the n^{th} component of $-(\mathcal{D} + L)^{-1} \phi^0$ is everywhere positive, and by hypothesis $f_{1n}(r) > 0$ on a set of positive measure. We conclude $\lambda_1 = \lambda_0$, q.e.d.

Iterative Solution of the Time-Independent Problem

On the basis of what has been established, it can be shown that the dominant eigenvalue and corresponding eigenfunction of the time-independent problem can be found by means of an iterative procedure.

For the time-independent problem with no up-scattering, let

$$T = -F(\mathcal{D} + L)^{-1}$$

The eigenvalue problem becomes

$$T\phi = \lambda\phi$$

The iterative process

$$\begin{aligned} y^{(n+1)} &= T x^{(n)} \\ \lambda^{(n+1)} &= \|y^{(n+1)}\| \\ x^{(n+1)} &= \frac{1}{\lambda^{(n+1)}} y^{(n+1)} \end{aligned} \quad (51)$$

for an initial guess $x^{(0)}$ (which we assume to be normalized and ≥ 0 everywhere in R) will then yield the desired results.

$$\lim_{n \rightarrow \infty} x^{(n)} = \phi^0$$

$$\lim_{n \rightarrow \infty} \lambda^{(n)} = \lambda_0$$

This follows from the fact that T satisfies the conditions of Theorem 4.

Of course, the rate of convergence of the iterative process (51) is determined by $|\lambda_1|/\lambda_0$, where λ_1 is the modulus of the eigenvalue (s) with the next largest modulus to λ_0 . For, if we define the operator T_1 by

$$T_1 x = T x - \lambda_0(x, \psi^0) \phi^0,$$

where ψ^0 is the adjoint eigenfunction corresponding to λ_0 , we see that the eigenvalues of T_1 all lie in the circle $|\lambda| \leq |\lambda_1|$; i.e.

$$\lim_{n \rightarrow \infty} \sqrt[n]{\|T_1^n\|} = |\lambda_1|.$$

Since $(T_1 x^{(0)}, \psi^0) = 0$, we have

$$T^n x^{(0)} = T_1^n x^{(0)} + \lambda_0^n (x^{(0)}, \psi^0) \phi^0. \quad (52)$$

From (51) we see that

$$x^{(n)} = \frac{T^n x^{(0)}}{\prod_{k=1}^n \lambda^{(k)}} = \frac{T_1^n x^{(0)}}{\|T^n x^{(0)}\|},$$

and, thus, Equation (52) yields

$$x^{(n)} - \phi^0 = \frac{T_1^n x^{(0)}}{\|T_1^n x^{(0)}\|} + \left[\frac{\lambda_0^n (x^{(0)}, \psi^0)}{\|T^n x^{(0)}\|} - 1 \right] \phi^0. \quad (53)$$

Dividing Equation (52) by λ_0^n , we obtain

$$\frac{T_1^n x(o)}{\lambda_0^n} = \frac{T_1^n x(o)}{\lambda_0^n} + (x(o), \psi^o) \phi^o.$$

Thus, we have

$$\left\| \frac{T_1^n x(o)}{\lambda_0^n} - (x(o), \psi^o) \phi^o \right\| = \frac{1}{\lambda_0^n} \|T_1^n x(o)\|.$$

If we assume that the eigenvalues with modulus $|\lambda_1|$ are simple,[†] we see that asymptotically

$$\left\| \frac{T_1^n x(o)}{\lambda_0^n} - (x(o), \psi^o) \phi^o \right\| \sim a \left(\frac{|\lambda_1|}{\lambda_0} \right)^n. \quad (54)$$

From Equation (53) and from (54) we obtain

$$\|x(n) - \phi^o\| \sim b \left(\frac{|\lambda_1|}{\lambda_0} \right)^n. \quad (55)$$

For the time-independent problem with up-scattering, let

$$T_\lambda = -(F + \lambda U)(Q + L)^{-1}.$$

The eigenvalue problem becomes

$$T_\lambda \phi = \lambda \phi.$$

The iterative scheme

$$\begin{aligned} y_p^{(n+1)} &= T_{\alpha_p} x_p^{(n)} \\ \beta_p^{(n+1)} &= \|y_p^{(n+1)}\| \\ x_p^{(n+1)} &= \frac{1}{\beta_p^{(n+1)}} y_p^{(n+1)} \\ \alpha_{p+1} &= \lim_{n \rightarrow \infty} \beta_p^{(n)} \\ x_{p+1}^{(o)} &= \lim_{n \rightarrow \infty} x_p^{(n)} \end{aligned} \quad (56)$$

[†]If the eigenvalues are not simple, then the right hand side of (54) becomes $a \frac{n!}{(n-p)!} \left(\frac{|\lambda_1|}{\lambda_0} \right)^{n-p}$, where p is the length of the largest generalized eigenfunction chain corresponding to an eigenvalue with modulus $|\lambda_1|$.

then converges to the desired result

$$\begin{aligned}\lim_{p \rightarrow \infty} \alpha_p &= \lambda_0 \\ \lim_{p \rightarrow \infty} x_p^{(0)} &= \Phi^0.\end{aligned}\tag{57}$$

This follows from the fact that α_{p+1} is the dominant eigenvalue of $T\alpha_p$. For if we write

$$\alpha_p \psi_{p-1}^0 = T_{\alpha_{p-1}}^* \psi_{p-1}^0 = -(\mathcal{D} + L^*)^{-1} (F^* + \alpha_{p-1} U^*) \psi_{p-1}^0$$

$$\alpha_{p+1} \Phi_p^0 = T_{\alpha_p} \Phi_p^0 = -(F + \alpha_p U)(\mathcal{D} + L)^{-1} \Phi_p^0,$$

we obtain, by taking the inner product of the first equation with Φ_p^0 and the second with ψ_{p-1}^0 and subtracting,

$$(\alpha_{p+1} - \alpha_p) = (\alpha_p - \alpha_{p-1}) \frac{[-U(\mathcal{D} + L)^{-1} \Phi_p^0, \psi_{p-1}^0]}{(\Phi_p^0, \psi_{p-1}^0)}.$$

Since the term in brackets is positive, we see that if $\alpha_1 \geq \alpha_0$, then $\alpha_p \geq \alpha_{p-1}$ for all $p \geq 1$. But from what we have seen in proving Theorem 8 if we have $\alpha_1 \geq \alpha_0$, then $\alpha_0 \leq \lambda_0$. But then since $\alpha_p \geq \alpha_{p-1}$, we have $\alpha_p \leq \lambda_0$ for all $p \geq 0$. Hence, we have a monotonic increasing [decreasing] sequence converging from above [below] to λ_0 .

The limits in (56) do not have to be taken to ensure convergence to λ_0 and Φ^0 . An iterative scheme

$$\begin{aligned}y_p^{(n+1)} &= T_{\alpha_p} x_p^{(n)} \\ \beta_p^{(n+1)} &= \|y_p^{(n+1)}\| \\ x_p^{(n+1)} &= \frac{1}{\beta_p^{(n+1)}} y_p^{(n+1)} \\ \alpha_{p+1} &= \beta_p^{(N_p)} \\ x_{p+1}^{(0)} &= x_p^{(N_p)}\end{aligned}\tag{58}$$

will converge $\alpha_p \rightarrow \lambda_0$, $x_p^{(0)} \rightarrow \Phi^0$ if suitable restrictions are placed on the N_p . Convergence of (58) is ensured if N_p is such that

$$\left| \beta_p^{(N_p)} - \mu_{\alpha_p}^0 \right| < \left| \mu_{\alpha_p}^0 - \alpha_p \right|, \quad (59)$$

where $\mu_{\alpha_p}^0$ is the dominant eigenvalue of T_{α_p} . Since $\mu_{\alpha_p}^0$ is always between α_p and λ_0 , (59) will ensure

$$\left| \beta_p^{(N_p)} - \lambda_0 \right| < \left| \alpha_p - \lambda_0 \right|.$$

Although the iteration schemes examined above converge, other iterative processes may converge more rapidly. For the discrete space approximation to the time-independent problem with no up-scattering, for example, considerable effort has gone into accelerating the iterative process analogous to (51).[†] Similar techniques can be applied in the continuous case.

THE TIME-DEPENDENT PROBLEM

The time-dependent problem concerns the kinetics equation (5) for a given value of $v = v_0$. Set $B = A + v_0 F$, and the kinetics equation becomes

$$\frac{\partial \Phi}{\partial t} = (D + B) \Phi(r, t) + S(r, t). \quad (60)$$

The principal problem is that of determining the solution of Equation (60) for $t > 0$, given the initial flux $\Phi(r, 0)$; it is usually assumed that $\Phi(r, 0) \in C$.

The Analytic Case

Let us first restrict the problem to a simple, special case for which the solution to Equation (60) is evident; this will give an insight into a general method of solution. In this, which we call the "analytic case," we assume that the boundary Condition (1c) on R is simply $\Phi(r) = 0$. Also, denoting the boundary by Γ , we require that the spatial derivatives of all orders for $\Phi(r, 0)$ and $S(r, t)$ tend to zero as r approaches Γ uniformly in t . Further, in the interior of R these derivatives and those of the coefficients (6) are assumed to be continuous and to have polynomial growth as the order of the derivative increases. Finally, $\frac{\partial S}{\partial t}(r, t)$ is required to

[†]See, for example, G. Bilodeau and L. Hageman, "A Survey of Numerical Methods in the Solution of Diffusion Problems," WAPD-TM-64, July, 1957.

be continuous. It follows that these functions are all analytic in r and that there are no material interfaces in R . The above conditions are satisfied, for example, if $d_j(r)$, $a_{jk}(r)$, and $f_{jk}(r)$ are polynomials in r and if

$$\Phi(r,0) = P(r) e^{-\frac{1}{\rho(r)}}$$

$$\mathcal{J}(r,t) = Q(r,t) e^{-\frac{1}{\rho(r)}},$$

where P and Q are polynomials and $\rho(r)$ is the distance of r from Γ ,
 $\rho(r) = \text{g.l.b.}_{s \in \Gamma} |r - s|$.

Under the above assumptions for the analytic case it is clear that $(\mathcal{D} + B)^k \Phi(r,0)$ and $(\mathcal{D} + B)^k \mathcal{J}(r,t)$ belong to the class C for each $k, t \geq 0$, and these functions are majorized by $M \cdot (2k)^\alpha$ for some M and α uniformly in t . It follows that

$$\begin{aligned} \Phi(r,t) &= e^{t(\mathcal{D}+B)} \left[\Phi(r,0) + \int_0^t e^{-\tau(\mathcal{D}+B)} \mathcal{J}(r,\tau) d\tau \right] \\ &= \sum_{j,k=0}^{\infty} \frac{t^j}{j!} (\mathcal{D} + B)^j \left[\Phi(r,0) + \int_0^t \frac{(-\tau)^k}{k!} (\mathcal{D} + B)^k \mathcal{J}(r,\tau) d\tau \right]. \end{aligned} \quad (61)$$

To verify that $\Phi(r,t)$ satisfies Equation (60), note that the series in the last member of (61) and its derived series are uniformly and absolutely convergent, so that term-by-term differentiation is justified.

The solution (61) was easily obtained for the analytic case because $(\mathcal{D} + B)^k$ is defined on $\Phi(r,0)$ and $\mathcal{J}(r,t)$ for all k , and the resulting functions do not grow rapidly enough with k to prevent the desired convergence of (61). In general, since the coefficients $d_j(r)$ are discontinuous across internal interfaces, the function $\mathcal{D} \Phi(r,0)$ does not belong to $\mathcal{M}$, so that $\mathcal{D}^2 \Phi(r,0)$ is not even defined! Still, it is sometimes possible to represent $\Phi(r,0)$ and $\mathcal{J}(r,t)$ as the sum of functions for which the above technique applies. For example, if $\mathcal{D} + B$ has a complete set of eigenfunctions, $\{\Phi_i\}_{i=1}^{\infty}$, and if there are corresponding expansions

$$\Phi(r,0) = \sum \alpha_i \Phi_i(r)$$

$$\mathcal{J}(r,t) = \sum \beta_i(t) \Phi_i(r)$$

with sufficient convergence properties, we find that the direct analog of Equation (61), namely,

$$\Phi(r, t) = \sum_{i=1}^{\infty} e^{\lambda_i t} \left[\alpha_i + \int_0^t e^{-\lambda_i \tau} \beta_i(\tau) d\tau \right] \Phi_i(r), \quad (62)$$

is a solution of Equation (60), where $(\mathcal{D} + B)\Phi_i = \lambda_i \Phi_i$. The form of the solution (62) is particularly desirable, since it exhibits the asymptotic behavior of Φ for large t . We will study in detail two cases for which Equation (62) is valid.

The Homogeneous Model

If the coefficients $d_j(r)$, $a_{ij}(r)$, and $f_{ij}(r)$ are independent of r and if $\alpha_j(r) = \alpha(r)$ in the boundary condition (1c) is independent of j , we have the so-called homogeneous bare core problem, for which a spectral theory, alluded to above, is particularly simple. Defining $Q = \mathcal{D} + B$, we have in this case

$$Q = (Q_{ij}),$$

$$\text{where } Q_{ij} = \delta_{ij} d_j \nabla^2 + a_{ij} + v_0 f_{ij};$$

δ_{ij} is the Kronecker delta: $\delta_{ij} = 1$ or 0 according to whether $i = j$ or $i \neq j$, respectively.

Let $\ell_0(r)$, $\ell_1(r)$, $\dots$ be a complete orthonormal set of eigenfunctions for the Laplacian operator with the boundary conditions

$\ell_k(r) + \alpha(r) \frac{\partial \ell_k}{\partial n} = 0$ on Γ . The existence of this set follows from Theorem 1; thus,

$$\nabla^2 \ell_k(r) = \mu_k \ell_k(r), \quad r \in R.$$

For each integer $k \geq 0$ define $\mathcal{M}_k$ to be the n -dimensional subspace of $\mathcal{H}$ consisting of all functions Φ of the form $\Phi = (a_1 \ell_k, a_2 \ell_k, \dots, a_n \ell_k)$, where the a_j are arbitrary complex numbers. Each $\mathcal{M}_k$ is invariant under the transformation Q , so that the restriction of Q to $\mathcal{M}_k$ can be represented by an $n \times n$ matrix Q_k relative to a given basis in $\mathcal{M}_k$. Let $\xi_j^{(k)} = (\xi_{j,1} \ell_k, \xi_{j,2} \ell_k, \dots, \xi_{j,n} \ell_k)$, $1 \leq j \leq n$, be a basis for $\mathcal{M}_k$ which reduces Q_k to its Jordan canonical form; then, $\xi_1^{(k)}, \xi_2^{(k)}, \dots, \xi_n^{(k)}$ form a complete set of generalized eigenvectors in $\mathcal{M}_k$. Since the collection of subspaces $\mathcal{M}_0, \mathcal{M}_1, \dots$ spans $\mathcal{H}$, the generalized

eigenfunctions $\xi_j^{(k)}$, $1 \leq j \leq n$, $k = 0, 1, \dots$, also span $\mathcal{H}$.

Let $\eta_j^{(k)} = (\eta_{j,1}^{(k)}, \eta_{j,2}^{(k)}, \dots, \eta_{j,n}^{(k)})$, $1 \leq j \leq n$, be a corresponding complete set of eigenvectors for the transpose matrix Q_k^T . If the $\eta_j^{(k)}$ are properly ordered with respect to the $\xi_j^{(k)}$, every vector $x \in \mathcal{M}_k$ will have a biorthogonal expansion[†] given by $x = \sum_{j=1}^n (x, \eta_j^{(k)}) \xi_j^{(k)}$.^{††} Finally, since the eigenfunctions $\{\xi_j^{(k)}\}_{k=0}^\infty$ are complete and orthonormal, every function $\Phi \in \mathcal{H}$ can be represented by the sum of its orthogonal projections on the subspaces $\{\mathcal{M}_k\}$; that is,

$$\Phi = \sum_{k=0}^{\infty} \sum_{j=1}^n (\Phi, \eta_j^{(k)}) \xi_j^{(k)}. \quad (63)$$

Equation (63) represents a conditional convergence in the mean. That is,

letting $P_k \Phi = \sum_{j=1}^n (\Phi, \eta_j^{(k)}) \xi_j^{(k)}$ be the projection of Φ onto $\mathcal{M}_k$, the norm

$\left\| \Phi - \sum_{k=0}^N P_k \Phi \right\|$ converges to zero as $N \rightarrow \infty$. Although the convergence of the series

$\sum_{k=0}^{\infty} P_k \Phi$ is absolute - unaffected by a permutation of the terms - it does

not necessarily follow that the double series (63) is absolutely convergent, since the individual terms of (63) are not generally orthogonal.

The following theorem summarizes the principal results for the homogeneous model. The theorem is set in a rather general language to allow for the later generalization to another model.

THEOREM 9. For the homogeneous model, Q has a complete sequence of generalized eigenfunctions

$$\Phi_0 = \Phi_{0,0}$$

$$\Phi_{1,0}, \Phi_{1,1}, \dots, \Phi_{1,k_1}$$

$$\vdots \quad \vdots \quad \vdots$$

$$\vdots \quad \vdots \quad \vdots$$

$$\vdots \quad \vdots \quad \vdots$$

$$\Phi_{i,0}, \Phi_{i,1}, \dots, \Phi_{i,k_i} \quad k_i < n; i = 1, 2, \dots$$

[†]See Friedman, *op. cit.*, pp. 131-133.

^{††} (x, y) denotes the inner product of vectors x and y .

corresponding to eigenvalues $\lambda_0, \lambda_1, \dots$; that is,

$$Q\Phi_{i,0} = \lambda_i \Phi_{i,0}$$

$$Q\Phi_{i,j} = \lambda_i \Phi_{i,j} + \Phi_{i,j-1}, \quad 1 \leq j \leq k_i, \quad i = 0, 1, \dots$$

There exists a principal eigenvalue, λ_0 , which is real, simple, and algebraically larger than the real part of all other eigenvalues:

$$\lambda_0 > \sup_{j \geq 1} \operatorname{Re}(\lambda_j).$$

The adjoint equations

$$Q^*\Psi_{i,0} = \bar{\lambda}_i \Psi_{i,0}$$

$$Q^*\Psi_{i,j} = \bar{\lambda}_i \Psi_{i,j} + \Psi_{i,j-1}, \quad 1 \leq j \leq k_i; \quad i = 0, 1, \dots$$

have solutions. Φ_0 and $\Psi_0 = \Psi_{0,0}$ can be assumed to take on only positive values throughout R , and all the $\Phi_{i,j}$ and $\Psi_{i,j}$ belong to the class C defined by Conditions (1). Every $\Phi \in \mathcal{H}$ has a biorthogonal expansion

$$\Phi = \sum_{i=0}^{\infty} \left[\sum_{j=0}^{k_i} (\Phi, \Psi_{i,k_i-j}) \Phi_{i,j} \right]. \quad (64)$$

The series (64) is absolutely convergent in norm with respect to the index i , provided the bracketed terms are kept intact. Given an initial condition, $\Phi(r,0) = \sum_{i,j} a_{ij} \Phi_{ij}(r) \in C$, the unique solution of the kinetics equation with no extraneous source

$$\frac{\partial \Phi}{\partial t} = Q\Phi(r,t) \quad (65)$$

is given by

$$\Phi(r,t) = e^{tQ} \Phi(r,0) = \sum_{i=0}^{\infty} \sum_{j=0}^{k_i} a_{ij} e^{\lambda_i t} \sum_{q=0}^j \frac{\Phi_{i,j-q}(r) t^q}{q!}. \quad (66)$$

Provided $\Phi(r,0) \geq 0$ and $\Phi(r,0) \neq 0$, then $a_{0,0} > 0$ and the solution (66) is asymptotic with $a_{0,0} e^{\lambda_0 t} \Phi_0(r)$ for large t . Likewise given an ex-

traneous source, $\mathcal{J}(r,t) = \sum_{i,j} b_{ij}(t) \Phi_{i,j}(r)$, belonging to C for each t

and having integrable coefficients $b_{ij}(t)$, the solution to the inhomogeneous kinetics equation

$$\frac{\partial \Phi}{\partial t} = Q\Phi(r, t) + \mathcal{L}(r, t) \quad (60)$$

is given by

$$\begin{aligned} \Phi(r, t) &= e^{tQ} \left[\Phi(r, 0) + \int_0^t e^{-\tau Q} \mathcal{L}(r, \tau) d\tau \right] \\ &= \sum_{i=0}^{\infty} \sum_{j=0}^{k_i} \sum_{q=0}^j e^{\lambda_i t} \left[a_{ij} t^q + \int_0^t e^{-\lambda_i \tau} (t - \tau)^q b_{ij}(\tau) d\tau \right] \frac{\Phi_{i, j-q}}{q!}. \end{aligned} \quad (67)$$

Proof: The existence of the generalized eigenfunctions $\Phi_{i,j}$ and their adjoints $\Psi_{i,j}$, as well as the validity of the biorthogonal expansion (64), has already been shown. We shall now prove the statement concerning the principal eigenvalue λ_0 . To this end we first note that the Laplacian operator ∇^2 with the given boundary condition has, by (10), an inverse ∇^{-2} for which $-\nabla^{-2}$ satisfies the hypotheses of Theorem 4 for $p = 1$; so, ∇^2 possesses a unique (algebraically) largest eigenvalue μ_0 which is simple and corresponds to a unique normalized eigenfunction, say $\ell_0(r)$, which is positive throughout R .

We return now to the matrix representations M_k of Q restricted to $\mathcal{M}_k$, $k = 0, 1, \dots$, and assume that each M_k is taken relative to the natural basis of $\mathcal{M}_k$: namely, $z_j = (\delta_{1,j}, \delta_{2,j}, \dots, \delta_{n,j})\ell_k$, $1 \leq j \leq n$; then,

$$M_k = \mu_k D + A + v_0 F, \quad (68)$$

where D is the diagonal matrix of (constant) diffusion coefficients $d_1, d_2, \dots, d_n$, and A, v_0 , and F are as before. It is evident from Equation (68) that all the nondiagonal entries in M_k are nonnegative. On account of the transitivity condition postulated for $B = A + v_0 F$ (see p. 15) the matrices M_k are "essentially positive" in the sense of G. Birkhoff and R. S. Varga. It follows[†] that each matrix M_k possesses an eigenvector $v_k = (v_{k,1}, v_{k,2}, \dots, v_{k,n})\ell_k$, with $v_{k,j} > 0$, $1 \leq j \leq n$, and

$\sum_{j=1}^n v_{k,j}^2 = 1$, corresponding to a real, simple eigenvalue ρ_k larger than the

[†]See Theorem 1 of Birkhoff and Varga, op. cit.

real part of all other eigenvalues of M_k . Now if $\rho_0 > \rho_k$ for all $k > 0$, then clearly $\lambda_0 = \rho_0$ and $\Phi_0 = v_0 = (v_{0,1}, v_{0,2}, \dots, v_{0,n})$ satisfy the statement of the theorem. To show the dominance of $\rho_0 = \lambda_0$, let $w_k = (w_{k,1}, w_{k,2}, \dots, w_{k,n})$ be the positive eigenvector for the adjoint equation $M_k^* w_k = \rho_k w_k$; then,

$$\begin{aligned} \rho_0 (v_0, w_k) &= (M_0 v_0, w_k) = (v_0, M_0^* w_k) \\ &= (v_0, M_k^* w_k) + (\mu_0 - \mu_k) (v_k, Dw_k) \\ &= \rho_k (v_0, w_k) + (\mu_0 - \mu_k) (v_0, Dw_k). \end{aligned}$$

Since v_0 and w_k have positive components, the inner products (v_0, w_k) and (v_0, Dw_k) are positive; hence,

$$\rho_0 - \rho_k = \frac{(\mu_0 - \mu_k) (v_0, Dw_k)}{(v_0, w_k)} > 0 \quad k \geq 1$$

as claimed. The fundamental adjoint vector Ψ_0 is likewise obtained as $\Psi_0 = w_0$.

Proceeding with the proof of Theorem 9, we next show the validity of the solutions (66) and (67) for the kinetics equation without and with an extraneous source, respectively. So suppose $\Phi(r, 0) = \sum_{i=0}^{\infty} \sum_{j=1}^{k_i} a_{ij} \phi_{ij}(r) \in C$ and define

$$\Phi_N(r, t) = \sum_{i=0}^N \sum_{j=1}^{k_i} a_{ij} e^{\lambda_i t} \sum_{q=0}^j \frac{\phi_{i,j-q}(r)}{q!} t^q. \quad (69)$$

Differentiating Equation (69) termwise, we have

$$\begin{aligned} \frac{\partial \Phi_N}{\partial t} &= \lambda_i \Phi_N(r, t) + \sum_{i=0}^N \sum_{j=0}^{k_i} \sum_{q=0}^j e^{\lambda_i t} a_{i,j} \frac{\phi_{i,j-q-1}(r)}{q!} t^q \\ &\quad - Q \Phi_N(r, t). \end{aligned} \quad (70)$$

So, Equation (66) is the solution of Equation (65) provided the initial function $\Phi(r, 0)$ has a finite expansion in generalized eigenfunctions. To show that this result is true for the general $\Phi(r, 0) \in C$ is to show that Equation (70)

is maintained in the limit as $N \rightarrow \infty$. Now the eigenvalues μ_k of ∇^2 satisfy inequalities,[†]

$$\mu_k \leq -\alpha \sqrt{k}, \quad (71)$$

for some $\alpha > 0$ independent of k . Suppose that λ_k is an eigenvalue of M_k corresponding to an eigenvector $v = (v_1, v_2, \dots, v_n) \in \mathcal{H}_k$. Referring to Equation (68), we obtain

$$\lambda_k v_i = \mu_k d_i v_i + [(A + v_0 F)v]_i \quad 1 \leq i \leq n. \quad (72)$$

Suppose $|v_{i_0}| = \max_{1 \leq i \leq n} |v_i|$; so, Equation (72) gives

$$\begin{aligned} \lambda_k &\leq \mu_k \min_{1 \leq j \leq n} d_j + \left| \frac{[Bv]_{i_0}}{v_{i_0}} \right| \\ &\leq -\alpha \sqrt{k} \min_{1 \leq j \leq n} d_j + \sqrt{n} \|B\|. \end{aligned} \quad (73)$$

Since $k_i < n$, $i = 1, 2, \dots$, (73) shows for sufficiently large i that the terms of Equation (69) and its derived series (70) are majorized by the terms of a series

$$(A + Bt^n) \sum_{i=0}^{\infty} e^{-\gamma \sqrt{i} t}$$

for some positive numbers A , B , and γ and for all $t > 0$ uniformly in r . Hence, Equations (69) and (70) converge absolutely and uniformly in every closed interval $[a, b]$, where $0 < a < b < \infty$. So solution (66) may be differentiated termwise for all $t > 0$; hence, (66) does satisfy the homogeneous differential equation (65) for all $t > 0$. Again applying the above argument to $\Phi_N(r, t)$ as $N \rightarrow \infty$, we obtain

$$\lim_{t \rightarrow 0} \Phi(r, t) = \Phi(r, 0) = \sum_{i,j} a_{ij} \Phi_{ij}(r). \quad (74)$$

Since Theorem 3 implies that each $\Phi_{ij} \in C$, it follows in a similar fashion that $\Phi(r, t) \in C$ for all $t > 0$.

The solution (67) for the inhomogeneous equation (60) is obtained in an entirely analogous manner. In order to conclude the proof, it is necessary only to show that the solution (66) for the homogeneous equation

[†]See Courant and Hilbert, op. cit., Vol I, Sec. VI.4.

is asymptotic with $a_{0,0} e^{\lambda_0 t} \Phi_0(r)$ for large t if $\Phi(r,0) \geq 0$ and $\Phi(r,0) \neq 0$. Since Ψ_0 is positive throughout R , we have $a_{0,0} = (\Phi(r,0), \Psi_0(r)) > 0$. Therefore, since $\lambda_0 > \operatorname{Re}(\lambda_i)$ for $i > 0$, $\Phi(r,t)$, as given in (66), satisfies $\Phi(r,t) = a_{0,0} e^{\lambda_0 t} \Phi_0(r) + O(e^{(\lambda_1 - \lambda_0)t})$, which is the desired result.

The General One-Dimensional Model

We return now to the general multigroup diffusion operator $Q = D + A + \nu_0 F$. The supremum norm of an operator U on $\mathcal{H}$ will be denoted by $\|U\| = \sup_{\Phi \neq 0} \frac{\|U\Phi\|}{\|\Phi\|}$. An operator with finite norm is termed "bounded." Note that $B = A + \nu_0 F$ is a bounded operator on $\mathcal{H}$. As before, let the eigenvalues of $\mathcal{D}$ be $\{\omega_j\}_{j=1}^\infty$, and denote the resolvent of Q by $R_\alpha = (\alpha I - Q)^{-1}$. R_α is bounded provided α is not an eigenvalue of Q .

LEMMA 1. For any complex number α , let $\delta(\alpha) = \min_{j \geq 1} |\alpha - \omega_j|$.

If $\delta(\alpha) \geq 2\|B\|$, then $\|R_\alpha\| \leq \frac{2}{\delta(\alpha)}$.

Proof: Let $\Phi \in \mathcal{H}$, and suppose $\Phi = \sum a_i \Omega_i$ is its expansion in the eigenfunctions of $\mathcal{D}$. Then $(\alpha I - \mathcal{D})^{-1} \Phi = \sum \frac{a_i}{\alpha - \omega_i} \Omega_i$; so,

$$\|(\alpha I - \mathcal{D})^{-1} \Phi\|^2 = \sum \frac{|a_i|^2}{|\alpha - \omega_i|^2} \leq \frac{1}{\delta^2(\alpha)} \sum |a_i|^2 = \frac{\|\Phi\|^2}{\delta^2(\alpha)};$$

hence, $\|(\alpha I - \mathcal{D})^{-1}\| \leq \frac{1}{\delta(\alpha)}$. Therefore,

$$\|B(\alpha I - \mathcal{D})^{-1}\| \leq \|B\| \cdot \|(\alpha I - \mathcal{D})^{-1}\| \leq \frac{\|B\|}{\delta(\alpha)} \leq \frac{1}{2}.$$

The Neumann expansion,

$$U(\alpha) = [I - B(\alpha I - \mathcal{D})^{-1}]^{-1} = \sum_{k=0}^{\infty} [B(\alpha I - \mathcal{D})^{-1}]^k,$$

is, therefore, valid, and

$$\|U(\alpha)\| \leq \sum_{k=0}^{\infty} \|B(\alpha I - \mathcal{D})^{-1}\|^k \leq \sum_{k=0}^{\infty} 2^{-k} = 2.$$

Hence, we have

$$\|R_\alpha\| = \|(\alpha I - \mathcal{D})^{-1} U(\alpha)\| \leq \frac{2}{\delta(\alpha)}, \quad \text{q.e.d.}$$

LEMMA 2. There exists an increasing sequence of positive numbers $r_1, r_2, \dots$ with $\lim_{k \rightarrow \infty} r_k = +\infty$, such that g.l.b. $|r_k + \omega_j| \geq k + 2 \|B\|$, $j \geq 1$

$k = 1, 2, \dots$. That is, there exist gaps of arbitrarily large width between consecutive (negative) eigenvalues of $\mathcal{D}$.

Proof: The proof depends on the assumption of a single dimension, for which the region R consists of an open interval (a, b) on the real line. Referring to the notation of Equation (8), we see by comparison of the corresponding Green's functions that the eigenvalues of $\mathcal{D}$, respectively, dominate (in magnitude) those of

$$\delta \cdot \begin{pmatrix} \nabla^2 & & \\ & \nabla^2 & 0 \\ & 0 & \ddots \\ & & & \nabla^2 \end{pmatrix} \quad (n \times n),$$

which are given by $\left\{ -\frac{j^2 \pi^2}{(b-a)^2} \delta \right\}_{j=1}^{\infty}$ with multiplicity n . So $-\omega_k \geq \frac{k^2 \pi^2 \delta}{n^2 (b-a)^2}$,

$k = 1, 2, \dots$. Thus, for any positive number p , the number of eigenvalues ω_j for which $-\omega_j \leq p$ is not more than $\frac{(b-a)}{\pi} \sqrt{\frac{p}{\delta}} n$. Hence, in the interval $[0, -p]$ there must be a subinterval of length $\frac{\pi \sqrt{p \delta}}{(b-a)n}$ which contains none of the eigenvalues ω_j . The existence of the sequence $r_1, r_2, \dots$ is now evident.

Now by defining the sequence of circumferences in the complex plane $\{C_k\}$ to be concentric with the origin and having the radii $\{r_k\}$, respectively, as given in Lemma 2, it follows that g.l.b. $|\mu - \omega_j| \geq k + 2 \|B\|$, $j \geq 1, \mu \in C_k$

$k = 1, 2, \dots$. Therefore, by Lemma 1, we have

$$\text{l.u.b.}_{\mu \in C_k} \|R_\mu\| \leq \frac{2}{k} \quad k = 1, 2, \dots$$

DEFINITION: The projection operator onto the one-space spanned by Ω_k will be denoted by Π_k ; thus, $\Pi_k \Phi = (\Phi, \Phi_k) \Phi_k$, $k = 1, 2, \dots$

Theorem 10. For the one-dimensional model, the generalized eigenvectors of Q span $\mathcal{H}$ and every $\Phi \in \mathcal{H}$ has a biorthogonal expansion in these generalized eigenfunctions.

Proof: The circles $\{C_k\}$ defined above satisfy conditions a through c of Theorem 6; so, Theorem 10 will follow from Theorem 6 upon a demonstration that Q is closed and that R_μ is completely continuous for at least one value of μ .

To see that Q is closed, let $\phi_1, \phi_2, \dots$ be a sequence of members of $\mathcal{M}$ and $\Psi \in \mathcal{H}$, such that $\lim_{k \rightarrow \infty} \|\phi_k - \phi\| = \lim_{k \rightarrow \infty} \|Q\phi_k - \Psi\| = 0$; we need to show that $\Psi \in \mathcal{M}$ and $Q\phi = \Psi$. Now $Q = \mathcal{D} + B$, where B is bounded; hence, $B\phi_k$ converges in norm to $B\phi$. So,

$$\begin{aligned} \|\mathcal{D}\phi_k - (\Psi - B\phi)\| &= \|(Q\phi_k - \Psi) - B(\phi_k - \phi)\| \\ &\leq \|Q\phi_k - \Psi\| + \|B\phi_k - B\phi\| \rightarrow 0 \quad \text{as } k \rightarrow \infty. \end{aligned}$$

Since $\mathcal{D}^{-1}$ is bounded, we have

$$\|\phi_k - \mathcal{D}^{-1}(\Psi - B\phi)\| = \|\mathcal{D}^{-1}(\mathcal{D}\phi_k - \Psi + B\phi)\| \leq \|\mathcal{D}^{-1}\| \cdot \|\mathcal{D}\phi_k - (\Psi - B\phi)\| \rightarrow 0.$$

So,

$$\|\phi - \mathcal{D}^{-1}(\Psi - B\phi)\| \leq \|\phi - \phi_k\| + \|\phi_k - \mathcal{D}^{-1}(\Psi - B\phi)\| \rightarrow 0,$$

and we conclude $\phi = \mathcal{D}^{-1}(\Psi - B\phi)$. So ϕ is in the range of $\mathcal{D}^{-1}$; that is, in $\mathcal{M}$. Finally $Q\phi = \mathcal{D}[\mathcal{D}^{-1}(\Psi - B\phi)] + B\phi = \Psi$, as claimed.

To complete the proof of theorem 10 it is necessary only to show that R_μ is completely continuous for a suitable choice of μ ; namely,

$$\mu = \mu_0 = 1 + \|B\|. \quad \text{We have } \mathcal{D} = \sum_{j=1}^{\infty} \omega_j \Pi_j \text{ and } (\mathcal{D} - \mu_0 I)^{-1} = \sum_{j=1}^{\infty} \frac{1}{\omega_j - \mu_0} \Pi_j.$$

Since all $\omega_j < 0$, we have $\|(\mathcal{D} - \mu_0 I)^{-1}\| < \frac{1}{1 + \|B\|}$; so, $\|B(\mathcal{D} - \mu_0 I)^{-1}\| < 1$.

Therefore, $U_{\mu_0} = [I + B(\mathcal{D} - \mu_0 I)^{-1}]^{-1}$ is a bounded operator, and since $(\mathcal{D} - \mu_0 I)^{-1}$ is completely continuous, so is $R_{\mu_0} = (\mathcal{D} - \mu_0 I)^{-1} U_{\mu_0}$, q.e.d.

Following the notation of theorem 6 and the subsequent text, we let $A_k = C_k - C_{k-1}$, with $C_0 = 0$, and consider the spectral decomposition of Q given by the Cauchy integrals

$$\frac{1}{2\pi i} \oint_{\text{Bdry } A_k} \frac{R_\mu \phi}{\mu - \mu_0} d\mu,$$

where the contour integral is taken over the inside and outside boundaries of the annuli A_k in the usual sense.

THEOREM 11. The results of theorem 9 are valid for the general one-dimensional model. An absolutely convergent series for the solution of the homogeneous equation (65) is given by

$$\Phi(r, t) = \frac{1}{2\pi i} \sum_{k=1}^{\infty} \oint_{\text{Bdry } A_k} e^{\alpha t} R_{\alpha} \Phi(r, 0) d\alpha, \quad (76)$$

and this solution is asymptotic with the fundamental mode as t approaches infinity; also the solution of the corresponding inhomogeneous equation (60) is

$$\Phi(r, t) = \frac{1}{2\pi i} \sum_{k=1}^{\infty} \oint_{\text{Bdry } A_k} e^{\alpha t} R_{\alpha} \left\{ \Phi(r, 0) + \int_0^t e^{-\alpha \tau} f(r, \tau) d\tau \right\} d\alpha. \quad (77)$$

Proof: The solutions (76) and (77) follow from the spectral mapping theorem.[†] The dominance of the principal eigenvalue of Q can be obtained by expanding Equation (76) in generalized eigenfunctions, as provided in theorem 10. Then Equation (76) takes the form

$$\Phi(r, t) = \int_R K(r, s; t) \Phi(s, 0) ds. \quad (78)$$

If $\Phi(s, 0) \geq 0$ and $\Phi(s, 0) \not\equiv 0$, Equation (65) gives $\frac{\partial \Phi}{\partial t} = Q\Phi(r, t)$ for all $t \geq 0$. It follows that $\Phi(r, t) \geq \hat{\Phi}(r, t)$, where $\hat{\Phi}$ denotes the solution of the diffusion-absorption equation,

$$\frac{\partial \hat{\Phi}}{\partial t} = (\mathcal{D} - aI)\hat{\Phi},$$

with $a = \max_{\substack{1 \leq i \leq n \\ r \in R}} |a_{ii}(r)|$. Thus, $\Phi(r, t) > 0$ for all $t > 0$, $r \in R$. Since

the kernel of Equation (78) is continuous, it must be positive for all $t > 0$. Hence, we may apply Theorem 4 (with $p = 1$) to Equation (78), and Theorem 11 follows by noting that the eigenvalues of Q and those of the integral operator defined by Equation (78) are related by $\lambda_i \mapsto e^{t\lambda_i}$, respectively.

The General Two- and Three-Dimensional Models

If R has more than one dimension, the eigenvalues of $\mathcal{D}$, and, therefore, also those of Q , do not become sparse at $-\infty$; so, Theorem 6 does not apply, and the spectral representations given in theorems 10 and 11 do not obtain. However, the existence of the fundamental mode and its adjoint may be demonstrated as a result of Theorem 4.

[†]Taylor, op. cit.

THEOREM 12. For the general reactor model not exceeding three dimensions there exists for Q a simple, real eigenvalue λ_0 which is not less than the real part of any other eigenvalue of Q , $\lambda_0 \geq \operatorname{Re}(\lambda_k)$, $k = 1, 2, \dots$. The corresponding eigenfunction and adjoint eigenfunction, Φ_0 and Ψ_0 , respectively, are strictly positive on R and are the only eigenfunctions for Q and Q^* , respectively, which are everywhere nonnegative. Φ_0 and Ψ_0 satisfy the analytic conditions (1); that is, they belong to the class C .

Before proving Theorem 12, let us compare it with the stronger results of Theorem 9 for the homogeneous model of three dimensions or less and with Theorem 11 for the general model of one dimension. Theorem 12 does not provide solutions of the kinetics equations,[†] nor does it imply the asymptotic convergence of $\Phi(r, t)$ to the fundamental projection of $\Phi(r, 0)$. Also it establishes the existence of only the single eigenvalue λ_0 (perhaps none other exists in certain pathological cases). And finally the inequality $\lambda_0 \geq \operatorname{Re}(\lambda_k)$ is weaker than before.

Proof: We recall from the proof of Theorem 10 that the resolvent $R_\alpha = (\alpha I - \mathcal{D} - B)^{-1}$ is completely continuous and $\|R_\alpha\| \leq \frac{2}{\alpha}$, provided that α is real and $\alpha \geq 2\|B\| + 1$. R_α also satisfies an important positivity property. For if $B = (B_{ij})$ is the aforementioned matrix representation of B and

$$\gamma = - \min_{1 \leq j \leq n} \text{g.l.b.}_{r \in R} B_{jj}(r),$$

then the elements of the matrix $B_1 = B + \gamma I$ are everywhere nonnegative. Setting $\alpha_1 = \alpha + \gamma$, we have the Neumann expansion,

$$R_\alpha = [(\alpha + \gamma)I - \mathcal{D} - (B + \gamma I)]^{-1} = (\alpha_1 I - \mathcal{D})^{-1} \sum_{k=0}^{\infty} [B_1(\alpha_1 I - \mathcal{D})^{-1}]^k, \quad (79)$$

which is valid if $\|B_1(\alpha_1 I - \mathcal{D})^{-1}\| < 1$. Since $\|B_1\| \leq \gamma + \|B\|$ and $\|(\alpha_1 I - \mathcal{D})^{-1}\| \leq \frac{1}{\alpha_1}$, we have $\|B_1(\alpha_1 I - \mathcal{D})^{-1}\| \leq \frac{\gamma + \|B\|}{\gamma + \alpha}$, so that Equation (79) holds for all $\alpha > \|B\|$. Furthermore, $(\alpha_1 I - \mathcal{D})^{-1}$ is the

[†]The solution of the kinetics equation has recently been shown by K. Jörgens by means of the Hille-Yosida theorem in the theory of semi-groups. See "An Asymptotic Expansion in the Theory of Neutron Transport," Commun. Pure Appl. Math. 11 (1958), pp. 219-242.

integral operator given by the Green's kernel for the diffusion-absorption operator $\mathcal{Q} = \alpha_1 I$. This kernel is positive; so Equation (79) shows that R_α is an integral operator with positive kernel for which Theorem 4 applies. Let $\mu_0(\alpha)$ be the fundamental eigenvalue of R_α as given by Theorem 4, so that $\mu_0(\alpha) > |\mu_k(\alpha)|$ for all other eigenvalues $\mu_k(\alpha)$ of R_α . Then $\lambda_0 = \alpha - \frac{1}{\mu_0(\alpha)}$ is a real, simple eigenvalue of $\mathcal{Q}$. If there were another eigenvalue of $\mathcal{Q}$, say λ_1 , for which $\text{Re}(\lambda_1) > \lambda_0$, then for a sufficiently large positive number $\hat{\alpha}$ we would have $|\hat{\alpha} - \lambda_1| \leq (\hat{\alpha} - \lambda_0)$; so,

$$|\mu_1(\hat{\alpha})| = \frac{1}{|\hat{\alpha} - \lambda_1|} \geq \frac{1}{\hat{\alpha} - \lambda_0} = \mu_0,$$

which contradicts Theorem 4 for $R_{\hat{\alpha}}$. Hence, $\lambda_0 \geq \text{Re}(\lambda_k)$, as claimed. The admissibility of the eigenfunctions Φ_0 and Ψ_0 into class $\mathcal{C}$ follows, as before, from Theorem 3 (and this is where the requirement of three dimensions or less is used).

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