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MULTI - GROUP DIFFUSION METHODS

by

K. F. Hansen

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U.S. Atomic Energy Commission

April, 1962

Department of Nuclear Engineering
Massachusetts Institute of Technology
Cambridge, Massachusetts

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
DEPARTMENT OF NUCLEAR ENGINEERING
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PREFACE

The notes on Multigroup Diffusion Methods by Professor Hansen were developed in connection with the theoretical work of the M. I. T. Heavy Water Lattice Project. They have been found so enlightening and useful, both in the project and for teaching purposes at M. I. T., that it has seemed worthwhile to issue them in a form that will offer them a greater audience. We hope that, in this form, they will prove to be as useful to many others as they have been at M. I. T.

I. Kaplan
T. J. Thompson

ABSTRACT

The purpose of this report is to provide an introduction to the multi-group diffusion methods of reactor analysis. The report is divided into two sections: the first concerning the derivation of the multi-group equations from the age-diffusion equation; while the second portion pertains to numerical methods of solving the equations.

No new techniques of analysis are contained in the report. The mathematics has been kept simple in order that the approximations at each step are clearly apparent. The adjoint function is introduced and the reasons for considering the adjoint are repeatedly stressed.

The selection of numerical methods considered in the second section is by no means exhaustive. Simple illustrations of various iterative methods are included. Relations between the rates of convergence of various methods may be found in the references, along with proofs of various results quoted in the report.

TABLE OF CONTENTS

LIST OF FIGURES

PART I. GENERAL THEORY

The multigroup equations arise as approximations to the well-known age-diffusion theory. It should be noted that all of the approximations used in obtaining age-diffusion theory are contained in the multigroup equations to be derived subsequently. There is an expanding effort to improve the methods by using the Bolzmann transport equations as the basic slowing down equations. For the purpose of the report, we shall only consider the simplified age-diffusion equations.

1.1 AGE-DIFFUSION APPROXIMATIONS

For stationary, i.e., time independent problems, the general forms of the age-diffusion equations are:

$$\frac{\partial q}{\partial u}(\underline{r}, u) = \underline{\nabla} \cdot [D(\underline{r}, u)\, \underline{\nabla}\phi(\underline{r}, u)] - \Sigma_a(\underline{r}, u)\, \phi(\underline{r}, u) + S(\underline{r}, u), \qquad (1.1.1)$$

and

$$q(\underline{r}, u_{th}) = -\underline{\nabla} \cdot [D_{th}(\underline{r})\, \underline{\nabla}\phi_{th}(\underline{r})] + \Sigma_a^{th}(\underline{r})\, \phi_{th}(\underline{r}) - S_{th}(\underline{r}), \qquad (1.1.2)$$

where the usual definitions apply. We denote the thermal group flux and constants with the sub/super scripts th. The model of the slowing-down-diffusion process is the following. Neutrons are born with lethargies greater than zero but less than thermal lethargy. The slowing down equation, (1.1.1), applies between $u = 0$ and $u = u_{th}$. Below u_{th} we take the slowing down density, q, as zero and include all neutrons of lethargy greater than u_{th} as thermal neutrons. Thus, u_{th} represents the cut-off lethargy of the slowing down process. We take $u = 0$ at an energy such that no neutrons are born by any process above the reference energy; consequently, $q(\underline{r}, 0) = 0$.

The coupling condition between the flux and slowing down density

depends upon the properties of the medium under discussion. For an infinite nonabsorbing medium, we have

$$q(\underline{r}, u) = \xi \Sigma_s(\underline{r}, u)\ \phi(\underline{r}, u) \qquad (1.1.3)$$

where ξ is the logarithmic energy decrement and may be a function of position and lethargy. If weak absorption occurs during the slowing down, a more appropriate expression for $q(\underline{r}, u)$ would be

$$q(\underline{r}, u) = [\xi \Sigma_s(\underline{r}, u) + \gamma \Sigma_a(\underline{r}, u)]\ \phi(\underline{r}, u)\,. \qquad (1.1.4)$$

Furthermore, for finite media, additional terms dependent upon the geometry enter the coupling condition. For simplicity, we shall use Equation (1.1.3) as the coupling condition. The results to be derived can always be amended to account for other coupling conditions.

The source function $S(\underline{r}, u)$ consists of fission sources plus independent, extraneous sources. The fission source, $S_f(\underline{r}, u)$, is

$$S_f(\underline{r}, u) = \nu\chi(u)\left[\int_{-\infty}^{\infty} \Sigma_f(\underline{r}, u')\ \phi(\underline{r}, u')\ du' + \Sigma_f^{th}\phi_{th}(\underline{r})\right]. \qquad (1.1.5)$$

The integral over the nonthermal fissions is extended from $-\infty$ to $+\infty$ for later convenience. The function $\phi(\underline{r}, u)$ is zero for $u < 0$ or $u > u_{th}$. The thermal flux, $\phi_{th}(\underline{r})$, is assumed to be of a delta function nature. That is, $\phi_{th}(\underline{r})$ is zero except at $u = u_{th}$. Note that

$$\phi_{th}(\underline{r}) \neq \phi(\underline{r}, u_{th})\,. \qquad (1.1.6)$$

We take $\phi(\underline{r}, u_{th})$ as the slowing down flux at u_{th} as the limit u_{th} is approached from smaller u. Schematically, the flux is shown in Figure 1.1. The function $\phi(\underline{r}, u)$ is zero from $u = -\infty$ up to and including $u = 0$. Above $u = 0$, $\phi(\underline{r}, u)$ approaches a limiting value at $u = u_{th}$ from the left, i.e., lower u. $\phi(\underline{r}, u)$ drops to zero on the right-hand side of $u = u_{th}$, i.e., for $u > u_{th}$.

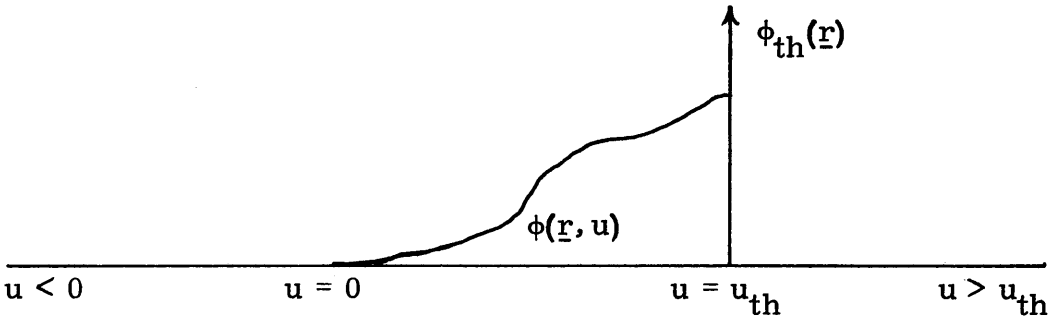

Figure 1. 1. Schematic representation of the slowing down and thermal fluxes.

Thus, $\phi(\underline{r}, u)$ has a step at $u = u_{th}$.

The function $\phi_{th}(\underline{r})$ is non-zero only at $u = u_{th}$. This impulse, or delta function, is superimposed upon $\phi(\underline{r}, u_{th})$. The thermal flux may also be written

$$\phi_{th}(\underline{r}) = \int_{-\infty}^{\infty} \phi_{th}(\underline{r}, u') \, \delta(u'-u_{th}) \, du' . \qquad (1. 1. 7)$$

The coefficient $\chi(u)$ is the fission spectrum, assumed independent of the energy of the neutron causing the fission. $\chi(u)$ is normalized such that

$$\int_{-\infty}^{\infty} \chi(u) \, du = 1 . \qquad (1. 1. 8)$$

Furthermore, we have assumed $\chi(u) = 0$, $u \leq 0$, and $\chi(u) = 0$, $u \geq u_{th}$, so that no neutrons are born with lethargies less than zero or greater than thermal cut-off. This implies that the thermal source function, $S_{th}(\underline{r})$, consists of extraneous sources only. We also assume ν, the neutrons per fission, independent of energy.

By use of the coupling condition (1. 1. 3), we may express the basic equations entirely in terms of the flux. We have, for Equation (1. 1. 1),

$$\frac{\partial}{\partial u}\left[\xi\Sigma_s\phi(\underline{r},u) - \underline{\nabla}\cdot[D\underline{\nabla}\phi(\underline{r},u)] + \Sigma_a\phi(\underline{r},u)\right.$$

$$\left. - \nu\chi(u)\left[\int_{-\infty}^{\infty}\Sigma_f\phi(\underline{r},u')\,du' + \Sigma_f^{th}\phi_{th}(\underline{r})\right]\right] = S_e(\underline{r},u) \tag{1.1.9}$$

where $S_e(\underline{r},u)$ is the extraneous source. For simplicity, we drop the arguments of the coefficients. Equation (1.1.2) becomes

$$-\xi\Sigma_s\phi(\underline{r},u_{th}) - \underline{\nabla}\cdot[D_{th}\underline{\nabla}\phi_{th}(\underline{r})] + \Sigma_a^{th}\phi_{th}(\underline{r}) = S_{th}(\underline{r})\,. \tag{1.1.10}$$

The first term on the left-hand side of Equation (1.1.10) may be written

$$-\xi\Sigma_s\phi(\underline{r},u_{th}) = -\int_{-\infty}^{\infty}\xi\Sigma_s(r,u')\,\phi(r,u')\,\delta(u'-u_{th})\,du'\,. \tag{1.1.11}$$

Equations (1.1.10) and (1.1.11) may be written in a compact form as

$$[A+\nu B]\,\underline{\Psi} = \underline{S}, \tag{1.1.12}$$

where we have the following definitions:

$$\underline{\Psi} = \begin{bmatrix}\phi(\underline{r},u)\\ \phi_{th}(\underline{r})\end{bmatrix} \quad ; \quad \underline{S} = \begin{bmatrix}S_e(\underline{r},u)\\ S_{th}(\underline{r})\end{bmatrix} \quad ; \tag{1.1.13a, b}$$

$$A = \begin{bmatrix}\frac{\partial}{\partial u}(\xi\Sigma_s\,\text{---}) - \underline{\nabla}\cdot[D\underline{\nabla}\,\text{---}] + \Sigma_a\,\text{---} & ; & 0\\ -\int_{-\infty}^{\infty}\xi\Sigma_s\,\text{---}\,\delta(u'-u_{th})\,du' & ; & -\underline{\nabla}\cdot[D_{th}\underline{\nabla}\,\text{---}] + \Sigma_a^{th}\,\text{---}\end{bmatrix} \tag{1.1.13c}$$

$$B = \begin{bmatrix}-\chi(u)\int_{-\infty}^{\infty}\Sigma_f\,\text{---}\,du' & ; & -\chi(u)\,\Sigma_f^{th}\,\text{---}\\ 0 & ; & 0\end{bmatrix} \tag{1.1.13d}$$

The underscore $\underset{\sim}{\ }$ indicates the appropriate argument is to be operated upon in the given position.

In a like manner, the reactor equations (1. 1. 1) and (1. 1. 2) may be written in terms of the slowing down density and thermal flux. We shall find the formulation in terms of the slowing down density convenient when we take up the multigroup equations.

The set of reactor equations (1. 1. 12) represents a coupled pair of integro-differential equations. The objective of the multigroup formulation is to reduce the two equations to a coupled set of simultaneous differential equations, which are, in general, easier to solve. Before outlining the reduction, we complete the formulation of the age-diffusion equation.

The boundary conditions applied to the age-diffusion equations are the usual conditions; namely, continuity of flux and current at interfaces between media, and vanishing of the flux at extrapolated boundaries. The continuity conditions are of the form

$$D(\underset{\sim}{r}_a, u)\ \underset{\sim}{\nabla}\phi(\underset{\sim}{r}_a, u) = D'(\underset{\sim}{r}_a, u)\ \underset{\sim}{\nabla}\phi'(\underset{\sim}{r}_a, u)\,, \qquad (1.\ 1.\ 14)$$

where prime denotes a different region, and $\underset{\sim}{r}_a$ is the radius vector at the interface. Flux continuity is then

$$\phi(\underset{\sim}{r}_a, u) = \phi'(\underset{\sim}{r}_a, u)\,. \qquad (1.\ 1.\ 15)$$

The diffusion approximation boundary condition at an exterior (vacuum) boundary is the vanishing of the inbound current. The approximation yields

$$d(u)\ \frac{d\phi(\underset{\sim}{r}_o, u)}{ds} + \phi(\underset{\sim}{r}_o, u) = 0\,, \qquad (1.\ 1.\ 16)$$

where $\underset{\sim}{r}_o$ is the radius vector to the bounding surface, s is arc length along the outbound normal, and d(u) is the extrapolation distance. In general, d is a function of u. For large reactors, it is not a bad approximation to assume d independent of lethargy. The boundary is then

$$\phi(\underset{\sim}{r}_o + d, u) = 0\,, \qquad \text{all } u\,. \qquad (1.\ 1.\ 17)$$

With the given boundary conditions, the equations (1. 1. 12) constitute an eigenvalue problem. For external sources equal zero, solutions for the equations exist only for certain values of the parameter ν. The usual study of the eigenvalue problem is to consider a given geometry and given nuclear properties; the allowed values of ν are then computed. One then compares the smallest computed ν with the known value of neutrons per fission, say ν_e. If the ratio $\nu/\nu_e < 1$, the assembly is then super-critical and one must change the size or constituency for criticality. Conversely, if $\nu/\nu_e > 1$, the assembly is sub-critical and appropriate corrections are necessary. The ratio ν/ν_e is a measure of the effective multiplication. That is,

$$\frac{\nu}{\nu_e} = \frac{1}{k_{eff}} . \qquad (1.1.18)$$

The remainder of this report is devoted to means of calculating the effective multiplication by appropriate simplification of the age-diffusion equation.

1.2 ADJOINT EQUATIONS

The equations adjoint to (1. 1. 12) and the solutions of these equations (the importance function) are useful in studying the effects of perturbations, and in computing eigenvalues. The reason for the utility stems from a principal of biorthogonality. We recall that two vectors are orthogonal if their dot product is zero; that is, if $\underline{x}$ and $\underline{y}$ are two non-zero vectors, they are orthogonal if

$$\underline{x} \cdot \underline{y} = 0 \qquad (1.2.1)$$

Two non-zero functions f, g, are orthogonal if

$$\int f(x)\, g(x)\, dx = 0 \qquad (1.2.2)$$

The integration is over the range of definition of the functions.

Physical problems are frequently solved by expansion of an arbitrary function in terms of the eigenfunctions of the given

operator.[1] The calculation of expansion coefficients is greatly facilitated if the eigenfunctions form a set of orthogonal functions. If the eigenfunctions are not orthogonal, the algebra is greatly simplified by introducing an auxiliary set of functions which are orthogonal to the original eigenfunctions. Such a relation between a function and an auxiliary function is called a biorthogonality relation.

The solutions of the adjoint equation, the adjoint functions, are biorthogonal to the solution of the original equation. In fact, the adjoint function is constructed in such a manner to guarantee the biorthogonality relation. We now define a functional relation that yields the adjoint operator and adjoint function and show that solution of the two operators are biorthogonal.

We first define the adjoint to a linear operator, say 0. If the operator 0 operates on a function ψ, then the functional relationship

$$\{\psi^*, 0\psi\} = \{\psi, 0^*\psi^*\} \tag{1.-2. 3}$$

defines the adjoint operator 0^* and the adjoint function ψ^*. The notation $\{\ \}$ denotes component multiplication in abstract vector notation. In continuous spaces the component multiplication is an integration.

We consider a simple eigenvalue problem, in one dimension, of the form.

$$0\psi_i = \lambda_i\psi_i . \tag{1. 2. 4}$$

To construct the adjoint, we multiply by ψ^* and integrate. We assume the variable of integration is x, and the region of interest is $a < x \leq b$. The functional relation is then,

$$\int_a^b \psi^* 0\psi_i \, dx = \lambda_i \int_a^b \psi^*\psi_i \, dx . \tag{1. 2. 5}$$

---

[1] We assume that the eigenfunctions are complete.

By Equation (1. 2. 3) we have

$$\int_a^b \psi_i 0^* \psi^* \, dx = \lambda_i \int_a^b \psi_i \psi^* \, dx . \qquad (1.2.6)$$

Thus, the adjoint equation is

$$0^* \psi^* = \lambda_i \psi^* . \qquad (1.2.7)$$

We denote solutions of this equation as ψ_i^*. Notice that the eigenvalue is the same for both 0 and 0*. To demonstrate the biorthogonality, consider the pair of equations

$$0\psi_i = \lambda_i \psi_i , \qquad (1.2.8)$$

$$0^* \psi_j = \lambda_j \psi_j^* . \qquad i \neq j \qquad (1.2.9)$$

We multiply the first equation by ψ_j^* and integrate, multiply the second by ψ_i and integrate, and subtract. We have

$$\int_a^b \left[\psi_j^* 0 \psi_i - \psi_i 0^* \psi_j \right] dx = (\lambda_i - \lambda_j) \int_a^b \psi_i \psi_j^* \, dx. \qquad (1.2.10)$$

By use of Equation (1. 2. 3) the left-hand side vanishes and since $\lambda_i \neq \lambda_j$, we have

$$\int_a^b \psi_i \psi_j^* \, dx = N^2 \delta ij \qquad (1.2.11)$$

where δij, the Kronecker delta

$$\begin{aligned} \delta ij &= 1 ; \quad i = j \\ &= 0 ; \quad i \neq j \end{aligned} \qquad (1.2.12)$$

and N^2 is a normalization constant.

For the method of constructing the adjoint operator and adjoint function as given by Equation (1. 2. 3), we see that solutions form a biorthogonal set of functions. We now consider the nature of the adjoint operator for the age-diffusion approximation. We define the quantity

$$\psi^* = \begin{bmatrix} \phi^*(\underline{r}, u) \\ \phi^*_{th}(\underline{r}) \end{bmatrix} \tag{1. 2. 13}$$

The functional relation (1. 2. 3), applied to Equation (1. 1. 12), can be written

$$\left\{ [\phi^*, \phi^*_{th}][A+\nu B] \begin{bmatrix} \phi \\ \phi_{th} \end{bmatrix} \right\} = \left\{ [\phi, \phi_{th}][A^*+\nu B^*] \begin{bmatrix} \phi^* \\ \phi^*_{th} \end{bmatrix} \right\}. \tag{1. 2. 14}$$

To simplify the derivation, we denote the matrix $[A+\nu B]$ as

$$[A+\nu B] = [C] = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix}, \tag{1. 2. 15}$$

and

$$[A^*+\nu B^*] = [C^*] = \begin{bmatrix} c^*_{11} & c^*_{12} \\ c^*_{21} & c^*_{22} \end{bmatrix}. \tag{1. 2. 16}$$

By the usual rules of matrix multiplication, we have

$$\int_{vol} \phi^* c_{11} \phi \, d(vol) = \int_{vol} \phi c^*_{11} \phi^* \, d(vol), \tag{1. 2. 17a}$$

$$\int_{vol} \phi^*_{th} c_{21} \phi \, d(vol) = \int_{vol} \phi c^*_{12} \phi^*_{th} \, d(vol), \tag{1. 2. 17b}$$

$$\int_{vol} \phi^* c_{12} \phi_{th} \, d(vol) = \int_{vol} \phi_{th} c^*_{21} \phi^* \, d(vol), \tag{1. 2. 17c}$$

$$\int_{vol} \phi^*_{th} c_{22} \phi_{th} \, d(vol) = \int_{vol} \phi_{th} c^*_{22} \phi^*_{th} \, d(vol). \tag{1. 2. 17d}$$

The volume integrations are to extend over the space occupied by the reactor and over the lethargy from $-\infty$ to $+\infty$. We illustrate the derivation of certain of the coefficients c^*_{ij}. The coefficient c_{11} is given by

$$c_{11} = \frac{\partial}{\partial u}(\xi\Sigma_s \text{---}) - \underline{\nabla}\cdot[D\underline{\nabla}\text{---}] + \Sigma_a \text{---} - \nu\chi(u)\int_{-\infty}^{\infty}\Sigma_f(u')\text{---}\,du'. \tag{1.2.18}$$

The first term of the functional $\int_{vol}\phi^* c_{11}\phi\, d(vol)$ is then

$$\int_{vol}\phi^*\frac{\partial}{\partial u}(\xi\Sigma_s\phi)\,d(vol) = \int_{\underline{r}}\int_{-\infty}^{\infty}\phi^*\frac{\partial}{\partial u}(\xi\Sigma_s\phi)\,du\,d\underline{r}. \tag{1.2.19}$$

If we integrate over lethargy by parts, we have

$$\int_{\underline{r}}\int_{-\infty}^{\infty}\phi^*\frac{\partial}{\partial u}(\xi\Sigma_s\phi)\,du\,d\underline{r} = \int_{\underline{r}}\phi^*\xi\Sigma_s\phi\Big|_{-\infty}^{\infty}d\underline{r} - \int_{\underline{r}}\int_{-\infty}^{\infty}\phi\xi\Sigma_s\frac{\partial}{\partial u}\phi^*\,du\,d\underline{r}. \tag{1.2.20}$$

Since $\phi = 0$ at $u = \pm\infty$, the first term of the right-hand side vanishes and we thus have for the first term of c_{11}^*, $-\xi\Sigma_s\frac{\partial}{\partial u}$. By application of Greens' theorem, we see the adjoint to $\underline{\nabla}\cdot[D\underline{\nabla}\text{---}] = \underline{\nabla}\cdot[D\underline{\nabla}\text{---}]$, i.e., the operator is self-adjoint. A similar result applies for the factor Σ_a. We now consider the final term of c_{11}. The last term of the functional is

$$\int_{vol}\phi^*\left[-\nu\chi(u)\int_{-\infty}^{\infty}\Sigma_f(u')\,du'\right]d(vol)$$

$$= \int_{\underline{r}}d\underline{r}\int_{-\infty}^{\infty}du\left[\phi^*\left\{-\nu\chi(u)\int_{-\infty}^{\infty}\Sigma_f(u')\,\phi(u')\,du'\right\}\right] \tag{1.2.21}$$

We interchange the integration over u' and u to obtain

$$= \int_{\underline{r}}d\underline{r}\int_{-\infty}^{\infty}du\,\phi(u)\left[-\nu\Sigma_f(u)\int_{-\infty}^{\infty}\chi(u')\,\phi^*(u')\,du'\right] \tag{1.2.22}$$

Collecting the results, we have

$$c_{11}^* = -\xi\Sigma_s\frac{\partial}{\partial u}(\text{---}) - \underline{\nabla}\cdot[D\underline{\nabla}\text{---}] + \Sigma_a\text{---} - \nu\Sigma_f(u)\int_{-\infty}^{\infty}\chi(u')\text{---}\,du'. \tag{1.2.23a}$$

By similar means we easily obtain

$$c_{21}^{*} = -\nu\Sigma_f^{th} \int_{-\infty}^{\infty} \chi(u') \sim du' , \tag{1.2.23b}$$

$$c_{12}^{*} = -\xi\Sigma_s^{th}\delta(u-u_{th}) \sim \tag{1.2.23c}$$

$$c_{22}^{*} = -\underline{\nabla}\cdot[D_{th}\underline{\nabla}\sim] + \Sigma_a^{th} \sim . \tag{1.2.23d}$$

Collecting the results in matrix form, the adjoint equations are of the form

$$[A^{*}+\nu B^{*}][\psi^{*}] , \tag{1.2.24}$$

with

$$A^{*} = \begin{bmatrix} -\xi\Sigma_s \frac{\partial}{\partial u} \sim - \underline{\nabla}\cdot[D\underline{\nabla}\sim] + \Sigma_a \sim \; ; \; -\Sigma_s^{th}\delta(u-u_{th}) \sim \\ 0 \; ; \; -\underline{\nabla}\cdot[D_{th}\underline{\nabla}\sim] + \Sigma_a^{th} \sim \end{bmatrix} \tag{1.2.25}$$

and

$$B^{*} = \begin{bmatrix} -\Sigma_f \int_{-\infty}^{\infty} \chi(u') \sim du' \; ; \; 0 \\ -\Sigma_f^{th} \int_{-\infty}^{\infty} \chi(u') \sim du' \; ; \; 0 \end{bmatrix} \tag{1.2.26}$$

The set of adjoint equations, in expanded form, is

$$-\xi\Sigma_s \frac{\partial}{\partial u}\phi^{*}(r,u) - \underline{\nabla}\cdot[D\underline{\nabla}\phi^{*}(r,u)] + \Sigma_a\phi^{*}(r,u)$$

$$= \nu\Sigma_f(u) \int_{-\infty}^{\infty} \chi(u')\,\phi^{*}(\underline{r},u')\,du' + \Sigma_s^{th}\phi_{th}^{*}(\underline{r})\,\delta(u-u_{th}) , \tag{1.2.27}$$

and

$$-\underline{\nabla}\cdot[D_{th}\underline{\nabla}\phi_{th}^{*}(\underline{r})] + \Sigma_a^{th}\phi_{th}^{*}(\underline{r}) = \nu\Sigma_f^{th} \int_{-\infty}^{\infty} \chi(u')\,\phi^{*}(\underline{r},u')\,du' . \tag{1.2.28}$$

Note that the source term for the thermal adjoint group consists of the fission spectrum sources weighted by the thermal fission cross section. There is no slowing down term into the thermal group. The sources for the slowing down equation consist of fission spectrum sources, weighted by the fission cross section, and a contribution from the thermal group at $u = u_{th}$. In effect, neutrons move up the lethargy scale from the thermal group into the slowing down group and then diffuse upward in lethargy. For this reason, the adjoint function is usually computed from $u = +\infty$ to $u = -\infty$. The function $\phi^*(\underline{r}, u)$ is zero for $u > u_{th}$, but does not necessarily vanish at $u = 0$.

The adjoint function must obey boundary conditions similar to the conditions on the original function. In the derivation of the adjoint to the operator $\underline{\nabla} \cdot [D\underline{\nabla}]$, Greens' theorem is used. In order to eliminate surface terms, it is necessary to assume $\phi^*(\underline{r}, u)$ vanishes at the extrapolated boundary. Continuity of flux and current lead to the same requirements on the adjoint and adjoint current at interfaces. The adjoint functions therefore have the same boundary conditions as the flux.

In later sections we shall indicate the utility of the importance function in solving the age-diffusion equations.

1.3 ELEMENTARY SOLUTIONS

In order to compare numerical approximations with exact expressions for the age-diffusion theory, we consider two elementary solutions of the equations. For a simple example, we treat a one-region, homogeneous, infinite reactor. In terms of the slowing down density, Equation (1. 1. 1) becomes

$$\frac{\partial q}{\partial u}(u) + \frac{\Sigma_a(u)}{\xi \Sigma_s(u)} q(u) = \nu\chi(u) \int_{-\infty}^{\infty} \frac{\Sigma_f(u')}{\xi \Sigma_s(u')} q(u')\, du' + \nu\chi(u)\, \Sigma_f^{th} \phi_{th} + S_e(u) \qquad (1.3.1)$$

For simplicity, we take $\Sigma_f(u') = 0$, so only thermal fission sources and extraneous sources are present. The basic equation becomes

$$\frac{\partial q(u)}{\partial u} + \frac{\Sigma_a(u)}{\xi\Sigma_s(u)} q(u) = \nu\chi(u)\,\Sigma_f^{th}\phi_{th} + S_e(u) \qquad (1.3.2)$$

The solution, with $q(0) = 0$, is

$$q(u) = \int_{-\infty}^{u} e^{-\int_{u'}^{u} \frac{\Sigma_a(u'')}{\xi\Sigma_s(u'')}\,du''} [\nu\Sigma_f^{th}\chi(u') + S_e(u')]\,du' . \qquad (1.3.3)$$

The thermal flux is given by

$$\phi_{th} = \frac{S_e^{th}}{\Sigma_a^{th}} + \frac{q(u_{th})}{\Sigma_a^{th}} . \qquad (1.3.4)$$

Inserting Equation (1.3.3) for $q(u_{th})$, we have

$$\phi_{th} = \frac{\frac{S_e^{th}}{\Sigma_a^{th}} + \frac{1}{\Sigma_a^{th}} \int_{-\infty}^{u_{th}} e^{-\int_{u'}^{u_{th}} \frac{\Sigma_a(u'')}{\xi\Sigma_s(u'')}\,du''} S_e(u')\,du'}{1 - \frac{\Sigma_f^{th}}{\nu\Sigma_a^{th}} \int_{-\infty}^{u_{th}} e^{-\int_{u'}^{u_{th}} \frac{\Sigma_a(u'')}{\xi\Sigma_s(u'')}\,du''} \chi(u')\,du'} \qquad (1.3.5)$$

In the absence of external sources, non-trival solutions exist if

$$\frac{1}{\nu} = \frac{\Sigma_f^{th}}{\Sigma_a^{th}} \int_{-\infty}^{u_{th}} e^{-\int_{u'}^{u_{th}} \frac{\Sigma_a(u'')}{\xi\Sigma_s(u'')}\,du''} \chi(u')\,du' . \qquad (1.3.6)$$

The integral is the fission spectrum weighted non-capture probability during slowing down. The exponential term is the resonance escape probability to thermal lethargy. The coefficient is the fraction of thermal neutrons that cause a fission. Equation (1.3.6) is merely

the four-factor formula for this simple example.

We now consider a finite homogeneous assembly with fissions occurring at all lethargies between 0 and u_{th}. The basic equations are then, for no external sources,

$$\frac{\partial q}{\partial u}(\underline{r}, u) + \frac{\Sigma_a}{\xi\Sigma_s} q(\underline{r}, u) = \frac{D}{\xi\Sigma_s} \nabla^2 q(\underline{r}, u) + \nu\chi(u) \int_{-\infty}^{\infty} \frac{\Sigma_f}{\xi\Sigma_s} q(r, u')\, du' + \nu\chi(u)\, \Sigma_f^{th}\, \phi_{th}(\underline{r}) \qquad (1.3.7)$$

and

$$-D_{th}\nabla^2\phi_{th}(\underline{r}) + \Sigma_a^{th}\phi_{th}(\underline{r}) = q(r, u_{th}) = \int_{-\infty}^{\infty} q(\underline{r}, u)\, \delta(u-u_{th})\, du . \qquad (1.3.8)$$

We shall assume the spatial dependence of the slowing-down density can be separated in spatial and lethargy dependent factors. We consider harmonics of the Helmholtz equation, $\nabla^2 q_n(\underline{r}, u) = B_n^2 q_n(\underline{r})$. For simplicity we drop the harmonic index on $q(\underline{r})$ and B^2. The same spatial harmonics for the thermal flux are used. We separate the spatial dependence and insert Equation (1.3.8) in (1.3.7), we have

$$\frac{\partial q}{\partial u}(u) + \left(\frac{\Sigma_a}{\xi\Sigma_s} + \frac{DB^2}{\Sigma_s}\right) q(u) = \nu\chi(u) \int_{-\infty}^{\infty} \left[\frac{\Sigma_f}{\xi\Sigma_s} + \frac{\Sigma_f^{th}}{D_{th}B^2 + \Sigma_a^{th}}\right] \delta(u'-u_{th})\, q(u')\, du' . \qquad (1.3.9)$$

Let

$$\frac{\Sigma_a}{\xi\Sigma_s} + \frac{DB^2}{\xi\Sigma_s} = \alpha(u) , \qquad (1.3.10)$$

and

$$\frac{\Sigma_f}{\xi\Sigma_s} + \frac{\Sigma_f^{th}}{D_{th}B^2 + \Sigma_a^{th}}\,\delta(u'-u_{th}) = \rho(u') \qquad (1.3.11)$$

The solution to (1.3.9) is then

$$q(u) = \nu \int_{-\infty}^{\infty} \rho(u')\,q(u') \int_{-\infty}^{u} \chi(\omega)\, e^{-\int_{\omega}^{u} a(u'')\,du''}\, d\omega\, du'. \qquad (1.3.12)$$

The result can be written

$$q(u) = \nu \int_{-\infty}^{\infty} K(u, u')\,q(u')\,du', \qquad (1.3.13)$$

with

$$K(u, u') = \left\{\frac{\Sigma_f(u')}{\xi\Sigma_s(u')} + \frac{\Sigma_f^{th}}{D_{th}B^2+\Sigma_a^{th}}\,\delta(u'-u_{th})\right\} \int_{-\infty}^{u} \chi(\omega)\, e^{-\int_{\omega}^{u}\left(\frac{\Sigma_a+DB^2}{\xi\Sigma_s}\right)du''}\, d\omega. \qquad (1.3.14)$$

The thermal flux is

$$\phi_{th} = \frac{\nu}{D_{th}B^2 + \Sigma_a^{th}} \int_{-\infty}^{\infty} K(u_{th}, u')\,q(u')\,du'. \qquad (1.3.15)$$

We define the function

$$Q = \nu \int_{-\infty}^{\infty} \rho(u')\,q(u')\,du', \qquad (1.3.16)$$

which is the fission source term, and is not a function of u.

The solutions are then, from (1.3.12) and (1.3.15),

$$q(u) = Q \int_{-\omega}^{u} \chi(\omega)\, e^{-\int_{\omega}^{u} a(u'')\,du''}\, d\omega, \qquad (1.3.17)$$

and

$$\phi_{th} = \frac{Q}{D_{th}B^2 + \Sigma_a^{th}} \int_{-\infty}^{\infty} \chi(\omega)\, e^{-\int_{\omega}^{u_{th}} a(u'')\, du''}\, d\omega. \quad (1.3.18)$$

Inserting the results (1.3.17) and (1.3.18) into the definition (1.3.16) yields

$$Q = \nu \int_{-\infty}^{\infty} \frac{\Sigma_f(u)}{\xi\Sigma_s(u)}\, Q \int_{-\infty}^{u} \chi(\omega)\, e^{-\int_{\omega}^{u} a(u'')\, du''}\, d\omega\, du +$$

$$+ \frac{\nu\Sigma_f^{th}}{D_{th}B^2 + \Sigma_a^{th}}\, Q \int_{-\infty}^{\infty} \chi(\omega)\, e^{-\int_{\omega}^{u_{th}} a(u'')\, du''}\, d\omega, \quad (1.3.19)$$

or equivalently,

$$\frac{1}{\nu} = \int_{-\infty}^{\infty} \left[\frac{\Sigma_f(u)}{\xi\Sigma_s(u)} \int_{-\infty}^{u} \chi(\omega)\, e^{-\int_{\omega}^{u} a(u'')\, du''}\, d\omega + \right.$$

$$\left. + \frac{\Sigma_f^{th}}{D_{th}B^2 + \Sigma_a^{th}}\, \chi(u)\, e^{-\int_{\omega}^{u_{th}} a(u'')\, du''} \right] du. \quad (1.3.20)$$

Equation (1.3.20) is the critical equation for this problem. The allowed values of ν can be determined from (1.3.20). Note that if $\Sigma_f(u) = 0$, then we have

$$1 = \frac{\nu\Sigma_f^{th} / \Sigma_a^{th}}{1 + L_{th}^2 B^2} \int_{-\infty}^{\infty} \chi(u)\, e^{-\int_{u}^{u_{th}} a(u'')\, du''}\, du. \quad (1.3.21)$$

This is the usual criticality condition where the integral represents the fission spectrum weighted non-resonance capture, non-escape probability.

To complete the discussion of the problem, we consider the set of adjoint equations. By the usual procedures we obtain the equations,

$$\frac{-\partial q^*(\underline{r}, u)}{\partial u} + \frac{\Sigma_a(u)}{\xi\Sigma_s(u)} q^*(\underline{r}, u) = \frac{D(u)}{\xi\Sigma_s(u)} \nabla^2 q^*(\underline{r}, u) + \frac{\nu\Sigma_f(u)}{\xi\Sigma_s(u)} \int_{-\infty}^{\infty} \chi(u') q^*(u')\, du' + \delta(u-u_{th})\, \phi^*_{th}(\underline{r}), \qquad (1.3.22)$$

and

$$-D_{th}\nabla^2\phi^*_{th}(\underline{r}) + \Sigma_a^{th}\phi^*_{th}(\underline{r}) = \nu\Sigma_f^{th} \int_{-\infty}^{\infty} \chi(u') q^*(\underline{r}, u')\, du'. \qquad (1.3.23)$$

Assuming the spatial dependence may be separated, the last equation yields

$$\phi^*_{th} = \frac{\nu\Sigma_f^{th}}{D_{th}B^2 + \Sigma_a^{th}} \int_{-\infty}^{\infty} \chi(u') q^*(u')\, du'. \qquad (1.3.24)$$

The adjoint slowing-down density is computed from $u = +\infty$ to u, for the reasons mentioned in the previous section. Using Equation (1.3.24) in (1.3.22), we have

$$\frac{-\partial q^*(u)}{\partial u} + \left\{\frac{\Sigma_a + DB^2}{\xi\Sigma_s}\right\} q^*(u) = \nu\left\{\frac{\Sigma_f(u)}{\xi\Sigma_s} + \frac{\Sigma_f^{th}\delta(u-u_{th})}{D_{th}B^2 + \Sigma_a^{th}}\right\} \int_{-\infty}^{\infty} \chi(u') q^*(u')\, du'. \qquad (1.3.25)$$

We again define

$$\alpha(u) = \frac{\Sigma_a(u) + D(u)B^2}{\xi\Sigma_s(u)} \qquad (1.3.26)$$

$$P(u) = \frac{\Sigma_f(u)}{\xi\Sigma_s} + \frac{\Sigma_f^{th}\delta(u-u_{th})}{D_{th}B^2 + \Sigma_a^{th}}. \qquad (1.3.27)$$

The solution to Equation (1.3.25) is then

$$q^*(u) = \nu \int_{-\infty}^{\infty} \chi(u')\, q^*(u') \int_{u}^{\infty} P(\omega)\, e^{-\int_u^{\omega} a(u'')\, du''} d\omega, \qquad (1.3.28)$$

or

$$q^*(u) = \nu \int_{-\infty}^{\infty} G(u, u')\, q^*(u')\, du', \qquad (1.3.29)$$

with

$$G(u, u') = \chi(u') \int_{\infty}^{u} \left\{ \frac{\Sigma_f(\omega)}{\xi\Sigma_s(\omega)} + \frac{\Sigma_f^{th}\delta(\omega-\omega_{th})}{D_{th}B^2+\Sigma_a^{th}} \right\} e^{-\int_u^{\omega} \left\{ \frac{\Sigma_a(u'')+DB^2}{\xi\Sigma_s(u'')} \right\} du''} d\omega. \qquad (1.3.30)$$

We define the function T as

$$T = \int_{-\infty}^{\infty} \chi(u)\, q^*(u)\, du. \qquad (1.3.31)$$

We multiply Equation (1.3.28) by $\chi(u)$ and integrate over all lethargy to obtain, after canceling the factor T,

$$\frac{1}{\nu} = \int_{-\infty}^{\infty} \chi(u) \int_{u}^{\infty} P(\omega)\, e^{-\int_u^{\omega} a(u'')\, du''} d\omega\, du. \qquad (1.3.32)$$

This represents the criticality condition of the adjoint solution. From the discussion in section 2, we know the eigenvalue, $1/\nu$, are the same for the original equation and for the adjoint.

For this particular problem we now prove the two criticality conditions are identical. We define the function $g(u-\omega)$ such that

$$g(u-\omega) = 1 \qquad u < \omega,$$
$$g(u-\omega) = 0 \qquad u > \omega. \tag{1.3.33}$$

Equation (1.3.32) can then be written

$$\frac{1}{\nu} = \int_{-\infty}^{\infty} \chi(u) \int_{-\infty}^{\infty} P(\omega)\, e^{-\int_{u}^{\omega} a(u'')\, du'''} g(u-\omega)\, d\omega\, du. \tag{1.3.34}$$

We now interchange the variables u and ω to obtain

$$\frac{1}{\nu} = \int_{-\infty}^{\infty} \chi(\omega) \int_{-\infty}^{\infty} P(u)\, e^{-\int_{\omega}^{u} a(u'')\, du''} g(\omega-u)\, d\omega\, du, \tag{1.3.35}$$

$$= \int_{-\infty}^{\infty} P(u) \int_{-\infty}^{u} \chi(\omega)\, e^{-\int_{\omega}^{u} a(u'')\, du''} d\omega\, du, \tag{1.3.36}$$

The last result follows since

$$g(\omega-u) = 1 \qquad \omega < u,$$
$$g(\omega-u) = 0 \qquad \omega > u. \tag{1.3.37}$$

From the definition of P(u) and a(u), the above result, Equation (1.3.36), is seen to be identical with Equation (1.3.20).

We now consider the use of the adjoint function in the calculation of eigenvalues.

1.4 METHOD OF SUCCESSIVE APPROXIMATIONS

In section 2 it was shown that a function and its adjoint form a biorthogonal set of functions. That is, if

$$\psi_n = \begin{bmatrix} q_n(\underline{r}, u) \\ \phi_{th}(\underline{r}) \end{bmatrix}, \tag{1.4.1}$$

and

$$\psi_m^* = \begin{bmatrix} q_m^*(\underline{r}, u) \\ \phi_{th}^*(\underline{r}) \end{bmatrix}, \tag{1.4.2}$$

then

$$\int_{vol} \psi_n \psi_m^* \, d(vol) = \delta_{nm}. \tag{1.4.3}$$

The basic reactor equations can be converted into an integral equation of the form

$$\frac{\psi(\underline{r}, u)}{\nu} = \int_{vol} K(\underline{r}, u; \underline{r}', u') \, \psi(\underline{r}', u') \, d(vol). \tag{1.4.4}$$

An example of such a formulation was given in the previous section.[1] In a similar manner, the adjoint function can be written in the form

$$\frac{\psi^*(\underline{r}, u)}{\nu} = \int_{vol} G(\underline{r}, u; \underline{r}', u') \, \psi^*(\underline{r}', u') \, d(vol). \tag{1.4.5}$$

The eigenvalue ν is the same for both Equations (1.4.4) and (1.4.5).

Equation (1.4.4) will be obeyed only for certain functions $\psi(\underline{r}, u)$. If we denote a trial solution of (1.4.4) as $\psi_o(\underline{r}, u)$, then we may generate a second approximation by using Equation (1.4.4). Thus, let

$$\psi_1(\underline{r}, u) = \int_{vol} K(\underline{r}, u; \underline{r}', u') \, \psi_o(\underline{r}', u) \, d(vol). \tag{1.4.6}$$

If $\psi_o(\underline{r}, u)$ is a solution of Equation (1.4.4), then we have

$$\frac{1}{\nu} = \frac{\psi_1(\underline{r}, u)}{\psi_o(\underline{r}, u)}. \tag{1.4.7}$$

On the other hand, if $\psi_1(\underline{r}, u)$ is not a solution, then Equation (1.4.7) is only an approximation. By recursion we then have

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[1] For more general problems, see Reference 2, Chapter 9.

$$\frac{1}{\nu} \approx \frac{\psi_p(\underline{r}, u)}{\psi_{p-1}(\underline{r}, u)} . \tag{1.4.8}$$

If the iteration converges, then Equation (1.4.8) provides a means of obtaining the eigenvalue ν. To prove the convergence, let us denote the integral operator of Equation (1.4.4) as 0. We denote the eigenfunctions as $\phi_i(\underline{r}, u)$ and the eigenvalues as ν_i. We assume the eigenfunctions are complete and hence

$$\psi_o(\underline{r}, u) = \sum_i a_i \phi_i(\underline{r}, u) \tag{1.4.9}$$

where the a_i are expansion coefficients. Using Equation (1.4.9) in Equation (1.4.6), we have

$$\psi_1(\underline{r}, u) = \sum_i a_i \left(\frac{1}{\nu_i}\right) \phi_i(\underline{r}, u) \tag{1.4.10}$$

and, in general

$$\psi_p(\underline{r}, u) = \sum_i a_i \left(\frac{1}{\nu_i}\right)^p \phi_i(\underline{r}, u) . \tag{1.4.11}$$

Let us assume $\nu_1 < \nu_2 < \ldots$. The dominant term in (1.4.11) is then the first term. After sufficient iterations, we have

$$\frac{1}{\nu_1} \approx \frac{\psi_p(\underline{r}, u)}{\psi_{p-1}(\underline{r}, u)} \approx \frac{a_1(1/\nu_1)^p \phi_i(\underline{r}, u)}{a_1(1/\nu_1)^{p-1} \phi_i(\underline{r}, u)} \tag{1.4.12}$$

The method is seen to converge to a limit value which is the reciprocal of the smallest eigenvalue of the operator. We are interested in the smallest eigenvalue since that is the first critical state of the reactor.

The expression (1.4.12) is rarely used as an approximation to the eigenvalue since the numerator and denominator are functions of $\underline{r}, u$. Usually the approximation is used in the form

$$\frac{1}{\nu} \approx \frac{\int_{\text{vol}} \psi_p(\underline{r}, u)\, d(\text{vol})}{\int_{\text{vol}} \psi_{p-1}(\underline{r}, u)\, d(\text{vol})} . \qquad (1.4.13)$$

A similar expression for the adjoint function may be derived;

$$\frac{1}{\nu} \approx \frac{\int_{\text{vol}} \psi^*_p(\underline{r}, u)\, d(\text{vol})}{\int_{\text{vol}} \psi^*_{p-1}(\underline{r}, u)\, d(\text{vol})} . \qquad (1.4.14)$$

The two approximations for the eigenvalue should yield the same result. Thus the adjoint may be used to provide a check calculation.

A more rapid convergence may be obtained by using the approximation

$$\frac{1}{\nu} = \frac{\int_{\text{vol}} \psi^*_{p-1}(\underline{r}, u)\, \psi_p(\underline{r}, u)\, d(\text{vol})}{\int_{\text{vol}} \psi^*_{p-1}(\underline{r}, u)\, \psi_{p-1}(\underline{r}, u)\, d(\text{vol})} . \qquad (1.4.15)$$

To show why the above approximation is more rapid, consider the expansions of $\psi_p(\underline{r}, u)$ and $\psi^*_{p-1}(\underline{r}, u)$,

$$\psi_p(\underline{r}, u) = \sum_i a_i \left(\frac{1}{\nu_i}\right)^p \phi_i(\underline{r}, u) , \qquad (1.4.16)$$

$$\psi^*_{p-1}(\underline{r}, u) = \sum_i b_i \left(\frac{1}{\nu_i}\right)^{p-1} \phi^*_i(\underline{r}, u) , \qquad (1.4.17)$$

where ϕ^*_i are the adjoint eigenfunctions. The expansion (1.4.15) is then

$$\frac{1}{\nu} = \frac{\sum_i a_i b_i \left(\frac{1}{\nu_i}\right)^{2p-1}}{\sum_i a_i b_i \left(\frac{1}{\nu_i}\right)^{2p-2}} = \frac{\left(\frac{1}{\nu_1}\right)^{2p-1}}{\left(\frac{1}{\nu_1}\right)^{2p-2}} \frac{\sum_i a_i b_i \left(\frac{\nu_1}{\nu_i}\right)^{2p-1}}{\sum_i a_i b_i \left(\frac{\nu_1}{\nu_i}\right)^{2p-2}} . \qquad (1.4.18)$$

This approximation converges to ν_1 as

$$\frac{1}{\nu} \simeq \frac{1}{\nu_1} + 0\left(\frac{\nu_1}{\nu_i}\right)^{2p}, \qquad (1.4.19)$$

where 0(x) means terms of the order of x. Thus, the approximation (1.4.15) approaches the limit with a square dependence upon the ratio $\frac{\nu_1}{\nu_i}$ (< 1). It is easily seen that (1.4.13) approaches the limit as the first power of $\frac{\nu_1}{\nu_i}$. The reason for the gain in rate of convergence is the biorthogonality of the function ϕ_i and ϕ_i^*. Thus, the adjoint is useful not only as a check but as a means of achieving the solution in fewer steps. Of course, computation of the adjoint is as involved as computing a new trial function, but we shall see that the multi-group adjoint equations are found as readily as the original equations.

In general, one cannot analytically use the method of successive substitutions. We now consider simplifying the equations to reduce the calculation to a more amenable form.

1.5 FORMATION OF THE MULTI-GROUP EQUATIONS

We shall consider two alternative methods of deriving the multi-group equations and indicate the differences and inherent approximations. The age-diffusion equations can be written

$$\frac{\partial q(\underline{r}, u)}{\partial u} = D(u)\nabla^2\phi(\underline{r}, u) - \Sigma_a(u)\,\phi(\underline{r}, u) + \mathcal{S}(\underline{r}, u), \qquad (1.5.1)$$

and

$$-D_{th}\nabla^2\phi_{th}(\underline{r}) + \Sigma_a^{th}\phi_{th}(\underline{r}) = q(\underline{r}, u_{th}) + S_e^{th}(\underline{r}). \qquad (1.5.2)$$

We have assumed the reactor is homogeneous within regions, and hence the coefficients are functions only of u within a region. The lethargy interval is from $0 \leq u \leq u_{th}$. We divide the interval into J sub-intervals and denote the points of division as u_j; $j = 0, 1, \ldots, J$, such that $u_o = 0$; $u_J = u_{th}$. The interval $u_j - u_{j-1}$ is denoted Δu_j.

If we integrate Equation (1.5.1) from u_{j-1} to u_j, we have

$$q(\underline{r}, u_j) - q(\underline{r}, u_{j-1}) = \int_{u_{j-1}}^{u_j} D(u) \nabla^2 \phi(\underline{r}, u)\, du - \int_{u_{j-1}}^{u_j} \Sigma_a(u)\, \phi(\underline{r}, u)\, du +$$

$$+ \int_{u_{j-1}}^{u_j} \mathcal{S}(\underline{r}, u)\, du . \qquad (1.5.3)$$

The source function consists of fission sources and extraneous sources. Thus we have

$$\mathcal{S}(\underline{r}, u) = \nu\chi(u)\left[\int_0^{u_{th}} \Sigma_f(u')\, \phi(\underline{r}, u')\, du' + \Sigma_f^{th}\phi_{th}(\underline{r})\right] + \mathcal{S}_e(\underline{r}, u), \qquad (1.5.4)$$

or,

$$\mathcal{S}(\underline{r}, u) = \nu\chi(u)\, Q(\underline{r}) + \mathcal{S}_e(\underline{r}, u), \qquad (1.5.5)$$

with

$$Q(\underline{r}) = \int_0^{u_{th}} \Sigma_f(u')\, \phi(\underline{r}, u')\, du' + \Sigma_f^{th}\phi_{th}(\underline{r}) . \qquad (1.5.6)$$

Since $\phi(\underline{r}, u) = 0$, $u < 0$ and $u > u_{th}$, we set the limits of integration as $0 - u_{th}$.

We assume the extraneous source is separable, of the form

$$\mathcal{S}_e(\underline{r}, u) = S_e(\underline{r})\, z(u) . \qquad (1.5.7)$$

We define the coefficients

$$\chi^j \Delta u_j = \int_{u_{j-1}}^{u_j} \chi(u)\, du, \qquad (1.5.8)$$

$$z^j \Delta u_j = \int_{u_{j-1}}^{u_j} z(u)\, du . \qquad (1.5.9)$$

The source is then

$$\int_{u_{j-1}}^{u_j} \mathcal{S}(\underline{r}, u)\, du = \nu Q(\underline{r})\, \chi^j \Delta u_j + S_e(\underline{r})\, z^j \Delta u_j . \qquad (1.5.10)$$

We now consider two different means of evaluating the diffusion and absorption terms. Consider the absorption first. We have

$$\int_{u_{j-1}}^{u_j} \Sigma_a(u)\, \phi(\underline{r}, u)\, du = \frac{\int_{u_{j-1}}^{u_j} \Sigma_a(u)\, \phi(\underline{r}, u)\, du}{\int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\, du} \int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\, du$$

$$= \overline{\Sigma_a^j}\, \overline{\phi^j}(\underline{r})\, \Delta u_j . \qquad (1.5.11)$$

where

$$\overline{\Sigma_a^j} = \frac{\int_{u_{j-1}}^{u_j} \Sigma_a(u)\, \phi(\underline{r}, u)\, du}{\int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\, du}, \qquad (1.5.12)$$

$$\overline{\phi^j}(\underline{r}) = \frac{\int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\, du}{\Delta u_j} . \qquad (1.5.13)$$

Similarly, the diffusion term can be written

$$\int_{u_{j-1}}^{u_j} D(u)\, \nabla^2 \phi(\underline{r}, u)\, du = \overline{D^j}\, \nabla^2\, \overline{\phi^j}(\underline{r})\, \Delta u_j , \qquad (1.5.14)$$

with

$$\overline{D^j} = \frac{\int_{u_{j-1}}^{u_j} D(u)\, \phi(\underline{r}, u)\, du}{\int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\, du} . \qquad (1.5.15)$$

In terms of the average values, the multi-group equations become

$$q(\underline{r}, u_j) - q(\underline{r}, u_{j-1}) = \left[\overline{D^j} \nabla^2 \overline{\phi^j}(\underline{r}) - \overline{\Sigma_a^j \phi^j} \right] \Delta u_j + \nu Q(\underline{r}) \chi^j \Delta u_j + \\ + S_e(\underline{r}) z^j \Delta u_j , \qquad (1.5.16)$$

$j = 1, 2, \ldots, J$. The thermal group can be included in the equations by denoting it with the superscript, J+1. We then have

$$-D^{J+1} \nabla^2 \phi^{J+1}(\underline{r}) - \Sigma_a^{J+1} \phi^{J+1}(\underline{r}) = q^J(\underline{r}) + S_e^{J+1}(\underline{r}) . \qquad (1.5.17)$$

We cannot proceed further in the analysis without having some relation between $q(\underline{r}, u_j)$, $(=q^j(\underline{r}))$, and $\overline{\phi^j}(\underline{r})$. A number of approximations are widely used, and we shall discuss these presently.

As a basis for deriving an alternative set of multi-group equations, we notice that the coefficients of Equations (1.5.16) are computed by averaging over the flux spectrum. If an original estimate of the flux spectrum is inaccurate, the coefficients must be corrected as a more accurate estimate is computed. This recomputation is laborious and time-consuming. In order to avoid such involved computations of coefficients, we look for an alternative formulation of the equations which may be easier to use.

We recall that the slowing-down density is, in general, a smoother function of the lethargy than the flux. If the basic equations are expressed in terms of the slowing-down density, then integrals over products of lethargy dependent coefficients and the slowing-down density may be approximated simply. To illustrate, we write the basic equation for slowing down as,

$$\frac{\partial q}{\partial u}(\underline{r}, u) = \frac{D(u)}{\xi \Sigma_s(u)} \nabla^2 q(\underline{r}, u) - \frac{\Sigma_a(u)}{\xi \Sigma_s(u)} q(\underline{r}, u) + \mathcal{S}(\underline{r}, u) . \qquad (1.5.18)$$

Integrating over the interval Δu_j yields

$$q^j(\underline{r}) - q^{j-1}(\underline{r}) = \int_{u_{j-1}}^{u_j} \frac{D(u)}{\xi\Sigma_s(u)} \nabla^2 q(\underline{r}, u)\, du - \int_{u_{j-1}}^{u_j} \frac{\Sigma_a(u)}{\xi\Sigma_s(u)} q(\underline{r}, u)\, du + \int_{u_{j-1}}^{u_j} \mathcal{S}(\underline{r}, u)\, du . \tag{1.5.19}$$

For the diffusion term, we have

$$\int_{u_{j-1}}^{u_j} \frac{D(u)}{\xi\Sigma_s(u)} \nabla^2 q(\underline{r}, u)\, du = \overline{\frac{D(u)}{\xi\Sigma_s(u)} \nabla^2 q(\underline{r}, u)}\, \Delta u_j . \tag{1.5.20}$$

If $q(\underline{r}, u)$ is indeed a slowly varying function of u and, if the interval Δu_j is small enough, then we use the approximation

$$\overline{\frac{D(u)}{\xi\Sigma_s(u)} \nabla^2 q(\underline{r}, u)} = \overline{\frac{D(u)}{\xi\Sigma_s(u)}}\, \nabla^2 \overline{q}(\underline{r}, u) . \tag{1.5.21}$$

Thus, we assume the average of the product is equal to the product of the averages. We compute the averages

$$\left(\overline{\frac{D(u)}{\xi\Sigma_s(u)}}\right)_j = \frac{1}{\Delta u_j} \frac{\int_{u_{j-1}}^{u_j} \frac{D(u)}{\xi\Sigma_s(u)}\, du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}} \int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)} = D^j a^j , \tag{1.5.22}$$

with

$$D^j = \frac{\int_{u_{j-1}}^{u_j} \frac{D(u)}{\xi\Sigma_s(u)}\, du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}} , \tag{1.5.23}$$

and

$$a^j = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)} . \tag{1.5.24}$$

Similarly, the absorption term is

$$\left(\overline{\frac{\Sigma_a(u)}{\xi\Sigma_s(u)}}\right)_j = \Sigma_a^j \alpha^j, \tag{1.5.25}$$

with

$$\Sigma_a^j = \frac{\int_{u_{j-1}}^{u_j} \frac{\Sigma_a(u)}{\xi\Sigma_s(u)}\,du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}}. \tag{1.5.26}$$

The set of multi-group equations are then

$$q^j(\underline{r}) - q^{j-1}(\underline{r}) = \alpha^j \Delta u_j \left[D^j \nabla^2 \bar{q}^j(\underline{r}) - \Sigma_a^j \bar{q}^j(\underline{r}) \right] + \int_{u_{j-1}}^{u_j} \mathcal{S}(\underline{r}, u)\,du, \tag{1.5.27}$$

$j = 1, 2, \ldots, J$. We denote

$$(\bar{q}(\underline{r}, u))_j = \bar{q}^j(\underline{r}). \tag{1.5.28}$$

To compare the two different methods, we compare $\overline{D^j}$ and D^j, and $\overline{\Sigma_a^j}$ and Σ_a^j. Note that $\overline{D^j}$ and $\overline{\Sigma_a^j}$ are rigorous, whereas D^j and Σ_a^j are approximations. From the definition of $\overline{D^j}$, (1.5.15), we have

$$\overline{D^j} = \frac{\int_{u_{j-1}}^{u_j} D(u)\,\nabla^2\phi(\underline{r}, u)\,du}{\int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\,du} = \frac{\int_{u_{j-1}}^{u_j} \frac{D(u)}{\xi\Sigma_s(u)}\,\nabla^2 q(r, u)\,du}{\int_{u_{j-1}}^{u_j} \frac{q(r, u)\,du}{\xi\Sigma_s(u)}}. \tag{1.5.29}$$

The average flux is

$$\bar{\phi}^j(\underline{r}) = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \phi(\underline{r}, u)\,du = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \frac{q(r, u)\,du}{\xi\Sigma_s(u)}. \tag{1.5.30}$$

Thus,

$$\overline{D^j}\nabla^2\,\overline{\phi^j}(\underline{r}) = \frac{1}{\Delta u_j}\,\frac{\displaystyle\int_{u_{j-1}}^{u_j}\frac{D(u)}{\xi\Sigma_s(u)}\,q(\underline{r},u)\,du}{\displaystyle\int_{u_{j-1}}^{u_j}\frac{q(r,u)\,du}{\xi\Sigma_s(u)}}\int_{u_{j-1}}^{u_j}\frac{q(r,u)\,du}{\xi\Sigma_s(u)}\,. \qquad (1.5.31)$$

If $q(\underline{r},u)$ is constant over the interval Δu_j, we have

$$\overline{D^j}\nabla^2\overline{\phi^j}(\underline{r}) = a^j D^j\nabla^2\overline{q^j}(\underline{r})\,. \qquad (1.5.32)$$

Thus, the two formulations are the same only if $q(\underline{r},u)$ is constant over Δu_j. If $q(\underline{r},u)$ varies only slightly, then the difference is small, and we may use the second formulation. Note the second formulation involves no weighting of coefficients with the spectrum and hence the coefficients are determined once and for all. A similar argument may be developed for the absorption terms.

In view of the simpler computation of coefficients, we shall use Equation (1.5.27) as the basic multi-group equations. It is to be realized that the error introduced at this step may be quite significant for some cases. The selection of the lethargy groups themselves is strongly influenced by the approximate form of the equations.

The next step in the derivation of the equations is to relate $q^j(\underline{r})$ and $\overline{q^j}(\underline{r})$. At this point, we must introduce further approximations into the formulation. In fact, the approximation used to relate $q^j(\underline{r})$ and $\overline{q^j}(\underline{r})$ must be made irrespective of how the coefficients are computed.

There are many different approximations used. Typical examples are as follows:

1) $\overline{q^j}(\underline{r}) = q^j(\underline{r}) \qquad u_{j-1} \leq u \leq u_j$
2) $\overline{q^j}(\underline{r}) = q^{j-1}(\underline{r})$
3) $\overline{q^j}(\underline{r}) = aq^j(\underline{r}) \qquad a$ constant
4) $\overline{q^j}(r) = [q^j(r)+q^{j-1}(r)]/2\,.$

Many other relations have been proposed. For our purposes, we shall derive the multi-group equations for two approximations, numbers 1 and 4, above.

For approximation 1, which assumes $q(\underline{r}, u)$ constant and equal to $q^j(\underline{r})$, the equation (1. 5. 27) becomes

$$q^j(\underline{r}) - q^{j-1}(\underline{r}) = a^j \Delta u_j \left[D^j \nabla^2 q^j(\underline{r}) - \Sigma_a^j q^j(\underline{r}) \right] + \int_{\Delta u_j} \mathcal{S}(\underline{r}, u)\, du . \quad (1.5.33)$$

The above equation can be rearranged in terms of the flux, if we take $q^j(\underline{r}) = (\xi \Sigma_s)^j \phi^j(\underline{r})$. We have,

$$D^j \nabla^2 \phi^j(\underline{r}) - \Sigma^j \phi^j(\underline{r}) = - \frac{(\xi \Sigma_s)^{j-1}}{(\xi \Sigma_s)^j} \frac{\phi^{j-1}(\underline{r})}{a^j \Delta u_j} - \frac{1}{(\xi \Sigma_s)^j a^j \Delta u_j} \int_{\Delta u_j} \mathcal{S}(\underline{r}, u)\, du , \quad (1.5.34)$$

with

$$\Sigma^j = \Sigma_a^j + \frac{1}{a^j \Delta u_j} .$$

The coefficient Σ^j represents a removal cross section and accounts for both absorption and scattering out of Δu_j. We write the equation as an inhomogeneous diffusion equation.

$$D^j \nabla^2 \phi^j(\underline{r}) - \Sigma^j \phi^j(\underline{r}) = -f^j . \quad (1.5.35)$$

and consider the function of f^j. The source integral is given in Equation (1. 5. 10) as

$$\int_{u_{j-1}}^{u_j} \mathcal{S}(\underline{r}, u)\, du = \nu Q(\underline{r})\, \chi^j \Delta u_j + S_e(\underline{r})\, z^j \Delta u_j , \quad (1.5.36)$$

with

$$Q(r) = \int_0^{u_{th}} \frac{\Sigma_f(u')}{\xi \Sigma_s(u')} q(\underline{r}, u')\, du' + \Sigma_f^{th} \phi_{th}(\underline{r}) . \quad (1.5.37)$$

If we assume $q(r, u)$ constant in each interval Δu_j, then we have

$$Q(\underline{r}) = \sum_{j=1}^{J} \beta^j \phi^j(\underline{r}) + \Sigma_f^{th} \phi_{th}(\underline{r}) , \tag{1.5.38}$$

with

$$\beta^j = (\xi\Sigma_s)^j \int_{u_{j-1}}^{u_j} \frac{\Sigma_f(u)}{\xi\Sigma_s(u)}\, du . \tag{1.5.39}$$

The function f^j is then

$$f^j = \frac{(\xi\Sigma_s)^{j-1}}{(\xi\Sigma_s)^j} \frac{\phi^{j-1}(\underline{r})}{a^j \Delta u_j} + \frac{\nu\chi^j}{(\xi\Sigma_s)^j a^j} \left\{ \sum_{j=1}^{J} \beta^j \phi^j(\underline{r}) + \Sigma_f^{th} \phi_{th}(\underline{r}) \right\}$$

$$+ \frac{z^j}{(\xi\Sigma_s)^j} \frac{1}{a^j} S_e(\underline{r}) . \tag{1.5.40}$$

The thermal group equation is merely

$$D^{J+1}\nabla^2\phi^{J+1}(\underline{r}) - \Sigma_a^{J+1}\phi^{J+1}(\underline{r}) = -(\xi\Sigma_s)^J \phi^J(\underline{r}) - S_e^{th}(\underline{r}) . \tag{1.5.41}$$

The entire collection of simultaneous equations can be written

$$D^j\nabla^2\phi^j(\underline{r}) - \Sigma^j\phi^j(\underline{r}) = -f^j, \qquad j=1, 2, \ldots, J+1 . \tag{1.5.42}$$

Note that all of the coefficients of Equations (1.5.42) can be computed irrespective of the value of $\phi^j(\underline{r})$. Before giving a physical interpretation to the terms in the equations, we develop a similar form for the linear approximation.

$$\overline{q^j}(\underline{r}) = [q^j(r) + q^{j-1}(r)]/2 . \tag{1.5.43}$$

The basic equation (1.5.27) becomes

$$(\xi\Sigma_s)^j\phi^j(\underline{r}) - (\xi\Sigma_s)^{j-1}\phi^{j-1}(\underline{r}) = a^j\Delta u_j \left[D^j \left\{ \frac{(\xi\Sigma_s)^j}{2} \nabla^2\phi^j(\underline{r}) + \frac{(\xi\Sigma_s)^{j-1}}{2} \nabla^2\phi^{j-1}(\underline{r}) \right\} - \right.$$

$$\left. - \Sigma_a^j \left\{ \frac{(\xi\Sigma_s)^j}{2} \phi^j(\underline{r}) + \frac{(\xi\Sigma_s)^{j-1}}{2} \phi^{j-1}(\underline{r}) \right\} \right] +$$

$$+ \int_{\Delta u_j} \mathcal{S}(\underline{r}, u)\, du . \tag{1.5.44}$$

We factor Equation (1. 5. 44) into the form

$$D^j \nabla^2 \phi^j(\underline{r}) - \Sigma^j \phi^j(\underline{r}) = -f^j , \tag{1. 5. 45}$$

where

$$\Sigma^j = \Sigma_a^j + \frac{2}{\alpha^j \Delta u_j} \tag{1. 5. 46}$$

and

$$f^j = \frac{(\xi\Sigma_s)^{j-1}}{(\xi\Sigma_s)^j}\left[D^j\nabla^2\phi^{j-1}(\underline{r}) - \left(\Sigma_a^j - \frac{2}{\alpha^j\Delta u_j}\right)\phi^{j-1}(\underline{r})\right] +$$

$$+ \frac{2}{(\xi\Sigma_s)^j\alpha^j\Delta u_j}\int_{\Delta u_j} \mathcal{S}(\underline{r}, u)\, du \tag{1. 5. 47}$$

We eliminate the ∇^2 term by using (1. 5. 45), that is

$$\nabla^2\phi^{j-1}(\underline{r}) = \frac{\Sigma^{j-1}}{D^{j-1}}\phi^{j-1}(\underline{r}) - \frac{f^{j-1}}{D^{j-1}} . \tag{1. 5. 48}$$

Hence, we have

$$f^j = \frac{(\xi\Sigma_s)^{j-1}}{(\xi\Sigma_s)^j}\left[\left\{\frac{D^j}{D^{j-1}}\Sigma^{j-1} + \frac{2}{\alpha^j\Delta u_j} - \Sigma_a^j\right\}\phi^{j-1}(\underline{r}) - \frac{D^j}{D^{j-1}} f^{j-1}\right] +$$

$$+ \frac{2}{(\xi\Sigma_s)^j\alpha^j\Delta u_j}\int_{\Delta u_j} \mathcal{S}(\underline{r}, u)\, du . \tag{1. 5. 49}$$

The source may again be written as a series of the form

$$\frac{2}{(\xi\Sigma_s)\alpha^j\Delta u_j}\int_{u_{j-1}}^{u_j} \mathcal{S}(r, u)\, du = \frac{2\nu\chi^j}{(\xi\Sigma_s)^j\alpha^j}\left\{\sum_{j=1}^{J}\gamma^j\phi^j(\underline{r}) + \Sigma_f^{th}\phi^{J+1}(\underline{r})\right\} +$$

$$+ \frac{2z^j}{(\xi\Sigma_s)^j\alpha^j} S_e(\underline{r}) , \tag{1. 5. 50}$$

where, for the linear approximation,

$$\gamma^j = (\xi\Sigma_s)^j \int_{u_{j-1}}^{u_j} \frac{\Sigma_f(u)}{\xi\Sigma_s(u)} \left\{ \frac{u-u_{j-1}}{\Delta u_j} \right\} du +$$

$$+ (\xi\Sigma_s)^{j+1} \int_{u_j}^{u_{j+1}} \frac{\Sigma_f(u)}{\xi\Sigma_s(u)} \left\{ \frac{u_{j+1}-u}{\Delta u_{j+1}} \right\} du . \qquad (1.5.51)$$

The various terms in Equations (1.5.45) and (1.5.48) are readily interpreted. The left-hand side consists of the leakage, absorption, and slowing-down terms. The source terms consist of fission plus extraneous sources and slowing-down sources from higher energy groups. Note that coefficients for both approximations are independent of the flux and may be computed in advance. Other methods of relating the average slowing-down density to the value at interpolation points are possible.

For each of the schemes illustrated above the calculational procedure for the multi-group method is evident. One makes an initial estimate of the flux at each value of j. From the initial distribution, the source function can be computed from known coefficients and assumed flux values. The inhomogeneous terms f^j are computed by using the initial flux estimate and calculable coefficients. The basic diffusion equation is then solved for the range of values of j. (We discuss the spatial effects in the second section of the report.) The computation proceeds from $j = 1$ to $j = J+1$. After obtaining a new estimate of the flux, the inhomogeneous terms are recomputed, and the iteration continues. Convergence of the iteration is obtained when changes in the value of the flux are negligible. For criticality studies, one can compute successive values of ν by the procedure outlined earlier.

The first step in the derivation of the multi-group method has been the simplification of the lethargy dependence. By computing the slowing-down flux (or density) at a discrete number of points, we may perform the integration over lethargy in a simple manner. Further steps in the derivation are studied in Part II of this report. We now consider forming the multi-group adjoint equations.

1.6 MULTI-GROUP ADJOINT EQUATIONS

The adjoint equations for the age-diffusion model can be written (see section 1.2),

$$-\xi\Sigma_s \frac{\partial\phi^*}{\partial u}(\underline{r},u) = D(u)\nabla^2\phi^*(\underline{r},u) - \Sigma_a(u)\,\phi^*(\underline{r},u) + \\ + \nu\Sigma_f(u)\int_{-\infty}^{\infty}\chi(u')\,\phi^*(\underline{r},u')\,du' + \xi\Sigma_s\phi^*_{th}(\underline{r})\,\delta(u-u_{th}), \tag{1.6.1}$$

and

$$-D_{th}\nabla^2\phi^*_{th}(\underline{r}) + \Sigma_a^{th}\phi^*_{th}(\underline{r}) = \nu\Sigma_f^{th}\int_{-\infty}^{\infty}\chi(u')\,\phi^*(\underline{r},u')\,du'. \tag{1.6.2}$$

We again divide the lethargy into a discrete number of divisions, say j, where the division points are the same as before. Integrating Equation (1.6.1) over the interval Δu_j, we have

$$\phi^*_{j-1}(\underline{r}) - \phi^*_j(\underline{r}) = \int_{u_{j-1}}^{u_j}\frac{D(u)}{\xi\Sigma_s(u)}\nabla^2\phi^*(\underline{r},u)\,du - \int_{u_{j-1}}^{u_j}\frac{\Sigma_a(u)}{\xi\Sigma_s(u)}\phi^*(\underline{r},u)\,du + \\ + \nu\int_{u_{j-1}}^{u_j}\frac{\Sigma_f(u)}{\xi\Sigma_s(u)}G(\underline{r})\,du + \phi^*_{th}(\underline{r})\,\delta_{iJ}, \tag{1.6.3}$$

where

$$G(\underline{r}) = \int_0^{u_{th}}\chi(u)\,\phi^*(\underline{r},u)\,du. \tag{1.6.4}$$

In the absence of leakage, absorption, and sources, Equation (1.6.3) states that

$$\phi^*(\underline{r},u_j) = \phi^*(\underline{r},u_{j-1}), \tag{1.6.5}$$

that is, the adjoint flux is a constant over lethargy. The adjoint slowing-down density is not a constant over lethargy if the scattering cross section varies. Thus, the adjoint flux is a smoother function of lethargy than the adjoint slowing-down density in contrast to the flux and slowing-down density. In order to use the simplest approximation to obtain the multi-group adjoint equations, i.e., constant

coefficients, we must deal with the adjoint flux.

Assuming that $\phi^*(\underline{r}, u)$ is reasonably smooth over the interval Δu_j, we define the average coefficients

$$D^j = \frac{\int_{u_{j-1}}^{u_j} \frac{D(u)}{\xi\Sigma_s(u)}\, du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}}, \tag{1.6.6}$$

$$\Sigma_a^j = \frac{\int_{u_{j-1}}^{u_j} \frac{\Sigma_a(u)}{\xi\Sigma_s(u)}\, du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}}, \tag{1.6.7}$$

$$\Sigma_f^j = \frac{\int_{u_{j-1}}^{u_j} \frac{\Sigma_f(u)}{\xi\Sigma_s(u)}\, du}{\int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}}, \tag{1.6.8}$$

and

$$a^j = \frac{1}{\Delta u_j} \int_{u_{j-1}}^{u_j} \frac{du}{\xi\Sigma_s(u)}. \tag{1.6.9}$$

Notice that the coefficients are the same as computed in section 5, save for the fission term. The multi-group, adjoint equations become

$$\phi^*_{j-1}(\underline{r}) = \phi^*_j(\underline{r}) + a^j \Delta u_j \left[D^j \nabla^2 \overline{\phi^*_j}(\underline{r}) - \Sigma_a^j \overline{\phi^*_j}(\underline{r}) \right] + \nu\Sigma_f^j \Delta u_j G(\underline{r}) + \phi^*_{th}(\underline{r})\, \delta_{jJ}. \tag{1.6.10}$$

Notice that the adjoint thermal flux appears as a source only in the first group above the thermal group. As indicated earlier, the

adjoint flux is computed in the direction of decreasing lethargy. The relations between the average value of the lethargy and the value at the end point of an interval may be chosen as before. In particular, we consider the approximations

$$1)\quad \overline{\phi_j^*} = \phi_{j-1}^*,$$

$$2)\quad \overline{\phi_j^*} = \left[\phi_{j-1}^* + \phi_j^*\right]/2 .$$

For the first approximation, the multi-group equations become

$$D^j \nabla^2 \phi_{j-1}^*(\underline{r}) - \Sigma^j \phi_{j-1}^*(\underline{r}) = -g^j \qquad j = 1, 2, \ldots, J \quad (1.6.11)$$

with

$$\Sigma^j = \Sigma_a^j + \frac{1}{a^j \Delta u_j},$$

$$g^j = \frac{\phi_j^*(\underline{r})}{a^j \Delta u_j} + \frac{\nu \Sigma_f^j}{a^j} G(\underline{r}) + \frac{\phi_{th}^*(\underline{r})}{a^j \Delta u_j} \delta_{jJ} . \qquad (1.6.12)$$

The adjoint flux is not necessarily zero at $j = 0$. However, for $j \leq 0$, there are no sources, save slowing-down sources, and the flux rapidly diminishes. We shall only include terms up to $j = 1$.

The results above are directly comparable to the results of section 5. By performing the algebra, similar equations for the second approximation to the average adjoint flux are readily obtained. The source function $G(\underline{r})$ is readily computed by a series expansion in terms of the $\phi_j^*(\underline{r})$.

The method of successive approximations is applied to the adjoint equations in much the same manner as before, except for the change in direction of progression in lethargy space.

1.7 MATRIX FORM OF MULTI-GROUP EQUATIONS

For later purposes, it is convenient to consider the matrix form of the multi-group equations. We begin by defining the J+1 dimensional vectors

$$\underline{\Psi}(\underline{r}) = \begin{bmatrix} \phi^1(\underline{r}) \\ \phi^2(\underline{r}) \\ \cdot \\ \cdot \\ \cdot \\ \phi^{J+1}(\underline{r}) \end{bmatrix}, \tag{1.7.1}$$

and

$$\underline{F}(\underline{r}) = \begin{bmatrix} f^1(\underline{r}) \\ f^2(\underline{r}) \\ \cdot \\ \cdot \\ \cdot \\ f^{J+1}(\underline{r}) \end{bmatrix}, \tag{1.7.2}$$

The basic diffusion equation (1.5.42) is written

$$\begin{bmatrix} (D^1\nabla^2-\Sigma^1) & 0 & 0 & \cdots & 0 \\ 0 & (D^2\nabla^2-\Sigma^2) & 0 & \cdots & 0 \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ 0 & \cdots & \cdots & 0 & (D^{J+1}\nabla^2-\Sigma^{J+1}) \end{bmatrix} \begin{bmatrix} \phi^1(\underline{r}) \\ \phi^2(\underline{r}) \\ \cdot \\ \cdot \\ \cdot \\ \phi^{J+1}(\underline{r}) \end{bmatrix} = - \begin{bmatrix} f^1(\underline{r}) \\ f^2(\underline{r}) \\ \cdot \\ \cdot \\ \cdot \\ f^{J+1}(\underline{r}) \end{bmatrix} \tag{1.7.3}$$

We factor the diagonal matrix into the form

$$[D-\Sigma] = \begin{bmatrix} D^1\nabla^2 & 0 & \cdots & 0 \\ 0 & D^2\nabla^2 & \cdots & 0 \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 0 & \cdots & \cdots & D^{J+1}\nabla^2 \end{bmatrix} - \begin{bmatrix} \Sigma^1 & 0 & \cdots & 0 \\ 0 & \Sigma^2 & \cdots & 0 \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 0 & \cdots & \cdots & \Sigma^{J+1} \end{bmatrix} \tag{1.7.4}$$

and write Equation (1.7.3) as

$$[D-\Sigma]\underline{\psi} = -\underline{F}. \tag{1.7.5}$$

The vector $\underline{F}$ can be written in terms of the vector $\underline{\psi}$. To this end, we consider the simple approximation $q^j(\underline{r}) = q^j(\underline{r})$. From Equation (1.5.40), we have

$$f^j = \eta^j \phi^{j-1}(\underline{r}) + \nu\kappa^j \left\{ \sum_{j=1}^{J} \beta^j \phi^j(\underline{r}) + \Sigma_f^{th} \phi_{th}(\underline{r}) \right\} + \rho^j S_e(\underline{r}) \tag{1.7.6}$$

with

$$\eta^j = \frac{(\xi\Sigma_s)^{j-1}}{(\xi\Sigma_s)^j \alpha^j \Delta u_j}, \qquad j = 1, 2, \ldots, J \tag{1.7.7}$$

$$\kappa^j = \frac{\chi^j}{(\xi\Sigma_s)^j \alpha^j}, \tag{1.7.8}$$

$$\rho^j = \frac{z^j}{(\xi\Sigma_s)^j \alpha^j}. \tag{1.7.9}$$

The vector $\underline{F}(\underline{r})$ consists of two portions, the flux dependent terms, say $\underline{F}_\phi(\underline{r})$, and the extraneous terms, say $\underline{F}_e(\underline{r})$. From Equation (1.7.6), we have

$$\underline{F}_{\phi}(\underline{r}) = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \eta^2 & 0 & \cdots & 0 \\ 0 & \eta^3 & & \\ \vdots & & & \\ 0 & \cdots & (\Sigma_s)^J & 0 \end{bmatrix} \begin{bmatrix} \phi^1(\underline{r}) \\ \phi^2(\underline{r}) \\ \vdots \\ \phi^{J+1}(\underline{r}) \end{bmatrix} +$$

$$+ \nu \begin{bmatrix} \kappa_1\beta_1 & \kappa_1\beta_2 & \cdots & \kappa_1\Sigma_f^{th} \\ \kappa_2\beta_1 & \kappa_2\beta_2 & \cdots & \\ \vdots & & & \\ 0 & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} \phi^1(\underline{r}) \\ \phi^2(\underline{r}) \\ \vdots \\ \phi^{J+1}(\underline{r}) \end{bmatrix} \qquad (1.7.11)$$

The above can be written

$$\underline{F}_{\phi} = [N+\nu K]\underline{\psi}\,, \qquad (1.7.12)$$

and hence, the entire set of equations are written

$$[D-\Sigma]\underline{\psi} = -[N+\nu K]\underline{\psi} + \underline{F}_e\,. \qquad (1.7.13)$$

For the case of no extraneous sources, we have

$$[\Sigma-D-N]\underline{\psi} = \nu K\underline{\psi}\,, \qquad (1.7.14)$$

which is the generalized eigenvalue problem. Assuming the operator on the left-hand side has an inverse, we define an operator A, such that

$$A = [\Sigma-D-N]^{-1}K \qquad (1.7.15)$$

Equation (1.7.14) is then

$$\frac{\underline{\psi}}{\nu} = A\underline{\psi}\,. \qquad (1.7.16)$$

Notice that this result is similar to the results used in section 4. The important feature is the reduction of the integral equation (over the lethargy variable) into a set of algebraic equations.

The method of successive approximations may be outlined in matrix form very simply. If we have an initial estimate, say $\underline{\psi}_o$, and if we take $\underline{\psi}_1 = A\underline{\psi}_o$, then

$$\frac{1}{\nu} \approx \frac{\underline{\psi}_1}{\underline{\psi}_o} , \tag{1.7.17}$$

and, in general

$$\frac{1}{\nu} \approx \frac{\underline{\psi}_p}{\underline{\psi}_{p-1}} . \tag{1.7.18}$$

A similar result is readily formed for the adjoint.

The result of generating the multi-group equations has been a simplification of the nature of the operator which relates successive estimates of the flux. The operator A above still contains terms involving the derivatives of the flux. We now turn to methods of simplifying the spatial dependence of the flux.

II. NUMERICAL SOLUTION OF MULTI-GROUP EQUATIONS

In the previous section of the report, we obtained a set of simultaneous differential equations from the integro-differential age-diffusion equation. The purpose of deriving the multi-group equations was to present a simplified form of the age-diffusion equation. In effect, the formation of the multi-group equations divided the lethargy interval into a finite set of sub-intervals. We then used simple assumptions to relate the flux (or slowing-down density) within intervals to the flux at interpolation points on the lethargy scale. Thus the original problem in the continuum was reduced to a finite set of equations in the discrete lethargy space.

The next step in obtaining approximate solutions to the age-diffusion equation is to treat the spatial dependence of the flux. As before, we attempt to divide the continuous configuration space into a finite set of interpolation points. The set of equations obtained from a discretization of the space variables are called finite difference equations. In the remainder of the report, we shall be concerned with obtaining the finite difference group equations and in reviewing methods of solving the resultant algebraic equations.

It is important to realize that the purpose of constructing the multi-group equations, and then sets of finite difference equations, is simply to reduce the problem to solving sets of simultaneous algebraic equations. For sets of algebraic equations, large scale computers are most useful.

2.1 CONSTRUCTION OF FINITE DIFFERENCE EQUATIONS

The basic approach to constructing finite difference equations is by the use of the Taylor series. Consider the problem of approximating the function $d^2g(x)/dx^2$. If we assume $g(x)$ can be expanded in a Taylor series about x, then we have

$$g(x+\Delta x) = g(x) + g'(x)\Delta x + g''(x)\frac{\Delta x^2}{2} + \ldots \qquad (2.1.1a)$$

$$g(x-\Delta x) = g(x) - g'(x)\Delta x + g''(x)\frac{\Delta x^2}{2} - \ldots \qquad (2.1.1b)$$

Adding the above equations, we have

$$g(x+\Delta x) + g(x-\Delta x) = 2g(x) + g''(x)(\Delta x)^2 + g^{iv}(x)\frac{(\Delta x)^4}{12} + \ldots \qquad (2.1.2)$$

or

$$g''(x) \approx \frac{g(x+\Delta x) - 2g(x) + g(x-\Delta x)}{(\Delta x)^2} - \frac{g^{iv}(x)(\Delta x)^2}{12} - \ldots \qquad (2.1.3)$$

Thus, we have approximated the second derivative by a second divided difference plus an error term. We denote the divided difference as

$$\frac{g((x+\Delta x) - 2g(x) + g(x-\Delta x)}{(\Delta x)^2} = \frac{\delta^2 g(x)}{(\Delta x)^2} \qquad (2.1.4)$$

The operator δ is called the central difference operator. Equation (2.1.3) is written

$$\frac{d^2 g(x)}{dx^2} = \frac{\delta^2 g(x)}{(\Delta x)^2} + 0(\Delta x^2) \qquad (2.1.5)$$

The term, $0(\Delta x^2)$, states that the second central difference approximates the second derivative to terms within the order of $(\Delta x)^2$. The term, $0(\Delta x^2)$, is the "truncation error" of the expansion.

The simple one-dimensional diffusion equation

$$D^j\nabla^2\phi^j(x) - \Sigma^j\phi^j(x) = - f^j(x) \qquad (2.1.6)$$

can be approximated

$$D^j\left[\frac{\phi^j(x+h) - 2\phi^j(x) + \phi^j(x-h)}{h^2}\right] - \Sigma^j\phi^j(x) = -f^j(x)$$

or

$$D^j\phi^j_{x+h} - (2D^j + h^2\Sigma^j)\,\phi^j_x + D^j\phi^j_{x-h} = -h^2 f^j_x \qquad (2.1.7)$$

where the superscript j denotes the group, and $h = \Delta x$.

In (2.1.7), we have assumed the spacing interval h is constant across the volume. It is useful to have methods of generating the finite difference approximations for non-uniform spacings and also for differential equations with non-constant coefficients. We consider first the case of one-dimensional regions. The basic diffusion equation for a given group is

$$\nabla(D^j \nabla\phi^j) - \Sigma^j\phi^j = -f^j \qquad (2.1.8)$$

where D^j = constant except at interfaces. The differential operator can be written

$$\frac{1}{r^a}\left[\frac{d}{dr}\left[r^a D^j \frac{d\phi^j}{dr}\right]\right], \qquad \begin{cases} a = 0 & \text{plane} \\ a = 1 & \text{cylinder} \\ a = 2 & \text{sphere} \end{cases}$$

Hence the diffusion equation becomes

$$\frac{d}{dr}\left[r^a D^j \frac{\partial\phi^j}{\partial r}\right] = (\Sigma^j\phi^j - f^j)\, r^a \qquad (2.1.9)$$

We take the interval of definition of Equation (2.1.9) from r = 0 to r = a. We divide the interval into K subintervals and denote the interpolation points as r_k, $0 \leq k \leq K$. The spacings between interpolation points are denoted by $\Delta r_k = r_{k+1} - r_k$. The spacings are not necessarily taken to be equal. Furthermore, we assume any boundaries between regions occur at space point r_k. We integrate Equation (2.1.9) from $r_{k-1/2}$ to $r_{k+1/2}$

$$r^a D^j \frac{\partial\phi^j}{\partial r}\Bigg|_{r_{k-1/2}}^{r_{k+1/2}} = \int_{r_{k-1/2}}^{r_{k+1/2}} (\Sigma^j\phi^j - f^j)\, r^a\, dr$$

or

$$r^a D^j \frac{\partial\phi^j}{\partial r}\Bigg|_{r_{k+1/2}} - r^a D^j \frac{\partial\phi^j}{\partial r}\Bigg|_{r_{k-1/2}} = \int_{r_k}^{r_{k+1/2}} (\Sigma^j\phi^j - f^j)\, r^a\, dr + \int_{r_{k-1/2}}^{r_k} (\Sigma^j\phi^j - f^j)\, r^a\, dr \qquad (2.1.10)$$

The right-hand side may be discontinuous at r_k and hence the integral is divided into portions in which the integrands are continuous. Denote the integrand in the interval r_k to $r_{k+1/2}$ by $[\Sigma^j(r_k^+)\,\phi^j(r_k^+) - f^j(r_k^+)]\,r_k^a$. That is, we assume the integrand can be expanded in a one-term Taylor series evaluated at r_k^+; the plus sign denotes the limit approached from the right-hand side of the interval r_k to $r_{k+1/2}$. By similar definitions, we arrive at

$$\int_{r_k}^{r_{k+1/2}} (\Sigma^j\phi^j - f^j)\,r^a\,dr + \int_{r_{k-1/2}}^{r_k} (\Sigma^j\phi^j - f^j)\,r^a\,dr =$$

$$= \left[\Sigma^j(r_k^+)\phi^j(r_k^+) - f^j(r_k^+)\right] r_k^a \frac{\Delta r_k}{2} + \left[\Sigma^j(r_k^-)\phi^j(r_k^-) - f^j(r_k^-)\right] r_k^a \frac{\Delta r_{k-1}}{2}\,, \tag{2.1.11}$$

where $\Delta r_k = r_{k+1} - r_k$. Notice that if the integrand is continuous, the integral becomes

$$[\Sigma^j\phi^j - f^j]_{r_k}\; r_k^a \left(\frac{r_{k+1} - r_{k-1}}{2}\right)$$

which is merely the average over the interval.

The left-hand side of Equation (2.1.10) is evaluated at the half-spacing. To eliminate the first derivative, we take the simple assumption

$$\frac{\partial\phi}{\partial r} = \frac{\phi_{k+1/2} - \phi_{k-1/2}}{r_{k+1/2} - r_{k-1/2}}\,. \tag{2.1.12}$$

We have

$$r_{k+1/2}^a\, D_{k+1/2}^j\, \frac{\partial\phi_{k+1/2}^j}{\partial r} = r_{k+1/2}^a\, D_{k+1/2}^j \left[\frac{\phi_{k+1}^j - \phi_k^j}{r_{k+1} - r_k}\right], \tag{2.1.13a}$$

$$r_{k-1/2}^a\, D_{k-1/2}^j\, \frac{\partial\phi_{k-1/2}^j}{\partial r} = r_{k-1/2}^a\, D_{k-1/2}^j \left[\frac{\phi_k^j - \phi_{k-1}^j}{r_k - r_{k-1}}\right] \tag{2.1.13b}$$

Combining Equations (2.1.11) and (2.1.13a, b), we have

$$\frac{r^a_{k+1/2} D^j_{k+1/2}}{\Delta r_k} \phi^j_{k+1} - \left\{ \frac{r^a_{k+1/2} D^j_{k+1/2}}{\Delta r_k} + \frac{r^a_{k+1/2} D^j_{k-1/2}}{\Delta r_{k-1}} - \right.$$

$$\left. - \frac{\Sigma^j(r^+_k)\, r^a_k \Delta r_k}{2} - \frac{\Sigma^j(r^-_k)\, r^a_k \Delta r_{k-1}}{2} \right\} \phi^j_k + \frac{r^a_{k-1/2} D^j_{k-1/2}}{\Delta r_{k-1}} \phi^j_{k-1} =$$

$$= - \left\{ r^a_k \frac{\Delta r_k}{2} f^j(r^+_k) + r^a_k \frac{\Delta r_{k-1}}{2} f^j(r^-_k) \right\} \qquad (2.1.14)$$

Equation (2.1.14) can also be written

$$a_k \phi^j_{k+1} - \beta_k \phi^j_k + r_k \phi^j_{k-1} = -\omega^j_k \qquad (2.1.15)$$

Notice that for a plane problem with $\Delta r_k = h$ and for a homogeneous region, Equation (2.1.14) reduces to the simple expression (2.1.7) obtained earlier.

The difference relation (2.1.14) can be made more accurate by improving the expansion formulas (2.1.11). We shall not bother with the details here (see Marchuk, ref. 1). It is important to realize that the derivation has produced a 3-point difference equation. If we take $\phi^j_o = \phi^j_K = 0$ (the usual boundary conditions), then Equation (2.1.15) applies for $1 \leq k \leq K - 1$. The various coefficients can be computed once and for all, and hence the entire set of simultaneous equations for the j^{th} group is known. In the next section, we shall consider the matrix form of the equations, but first we consider the two-dimensional form of the multi-group equations.

For the simple case of a one-region rectangular reactor, we can write the diffusion equation for each group as

$$\frac{\partial^2 \phi^j}{\partial x^2} + \frac{\partial^2 \phi^j}{\partial \phi^2} - \Sigma^j \phi^j = - f^j \, . \qquad (2.1.16)$$

We consider a two-dimensional mesh of the form

$$x_k = x_o + kh_x, \qquad k = 0, 1, \ldots K$$

$$x_\ell = y_o + \ell h_y, \qquad \ell = 0, 1, \ldots L$$

where h_x and h_y are constant. Replacing the second derivatives with second central differences, (2.1.16) becomes

$$\frac{\phi^j_{k+1,\,\ell} - 2\phi^j_{k,\,\ell} + \phi^j_{k-1,\,\ell}}{h_x^2} + \frac{\phi^j_{k,\,\ell+1} - 2\phi^j_{k,\,\ell} + \phi^j_{k,\,\ell-1}}{h_y^2} - \frac{\Sigma^j}{D^j}\,\phi^j_{k,\,\ell} = -\frac{f^j}{D^j} \qquad (2.1.17)$$

Equation (2.1.17) is a 5-point difference relation.

We now seek a general method of constructing appropriate difference equations for other geometries and for multi-region problems. The geometries of interest are the rectangle and circular cylinder. The diffusion equation becomes

$$\frac{1}{r^a}\frac{\partial}{\partial r}\left(r^a\,\frac{D^j \partial\phi^j}{\partial r}\right) + \frac{\partial}{\partial z}\left[D^j\,\frac{\partial\phi^j}{\partial z}\right] - \Sigma^j\phi^j = -f^j \qquad (2.1\ 18)$$

As before, we divide the space into a two-dimensional mesh, and we further assume discontinuities occur at the interpolation points. We now multiply by r_k^a and integrate (2.1.18) from $r_{k-1/2}$ to $r_{k+1/2}$ and from $z_{\ell-1/2}$ to $z_{\ell+1/2}$. We have

$$\int_{r_{k-1/2}}^{r_{k+1/2}}\left[\left(r^a D^j\,\frac{\partial\phi^j}{\partial z}\right)_{\ell+1/2} - \left(r^a D^j\,\frac{\partial\phi^j}{\partial z}\right)_{\ell-1/2}\right]dr + \int_{z_{\ell-1/2}}^{z_{\ell+1/2}}\left[\left(r^a D^j\,\frac{\partial\phi^j}{dr}\right)_{r_{k+1/2}} - \left(r^a D^j\,\frac{\partial\phi^j}{\partial r}\right)_{r_{k-1/2}}\right]dz = \int_{k-1/2}^{k+1/2}\int_{\ell-1/2}^{\ell+1/2}\left[\Sigma^j\phi^j - f^j\right]r^a\,dr\,dz \qquad (2.1.19)$$

If we again assume the integrand of the right-hand side a constant in the intervals $\ell-1/2, \ell$; $\ell, \ell+1/2$; $k-1/2, k$; $k, k+1/2$, we have

$$\int_{k-1/2}^{k+1/2}\int_{\ell-1/2}^{\ell+1/2}\left[\Sigma^j\phi^j-f^j\right]r^a\,dr\,dz =$$

$$=\left[\Sigma^j(k^+,\ell^+)\,\phi^j(k^+,\ell^+)-f^j(k^+,\ell^+)\frac{\Delta r_k}{2}\frac{\Delta z_\ell}{2}+\right.$$

$$+\Sigma^j(k^+,\ell^-)\,\phi^j(k^+,\ell^-)-f^j(k^+,\ell^-)\frac{\Delta r_k}{2}\frac{\Delta z_{\ell-1}}{2}+$$

$$+\Sigma^j(k^-,\ell^+)\,\phi^j(k^-,\ell^+)-f^j(k^-,\ell^+)\frac{\Delta r_{k-1}}{2}\frac{\Delta z_\ell}{2}+$$

$$\left.+\Sigma^j(k^-\ \ell^-)\,\phi^j(k^-,\ell^-)-f^j(k^-,\ell^-)\frac{\Delta r_{k-1}}{2}\frac{\Delta z_{\ell-1}}{2}\right]r_k^a \qquad (2.1.20)$$

where the +, - notation is the same as before. From the continuity of flux, we have $\phi_{k,\ell}$ the same for all +, - combinations. For the left-hand sides, we again approximate the derivative by a central difference and assume the integrands constant. We have then

$$\int_{k-1/2}^{k+1/2}\left(r^aD^j\frac{\partial\phi^j}{\partial z}\right)_{\ell+1/2}dr=\left[r_k^aD^j_{k,\ell+1/2}\phi^j_{k,\ell+1}-r_k^aD^j_{k,\ell+1/2}\phi^j_{k,\ell}\right]\frac{r_{k+1}-r_{k-1}}{2\Delta z_\ell}$$

(2.1.21a)

$$\int_{k-1/2}^{k+1/2}\left(r^aD^j\frac{\partial\phi^j}{\partial z}\right)_{\ell-1/2}dr=\left[r_k^aD^j_{k,\ell-1/2}\phi^j_{k,\ell}-r_k^aD_{k,\ell-1/2}\phi^j_{k,\ell-1}\right]\frac{r_{k+1}-r_{k-1}}{2\Delta z_{\ell-1}}$$

(2.1.21b)

$$\int_{\ell-1/2}^{\ell+1/2}\left(r^aD^j\frac{\partial\phi^j}{\partial r}\right)_{r_{k+1/2}}dz=\left[r^a_{k+1/2}D^j_{k+1/2,\ell}\phi^j_{k+1,\ell}-\right.$$

$$\left.-r^a_{k+1/2}D^j_{k+1/2,\ell}\phi^j_{k,\ell}\right]\frac{(z_{\ell+1}-z_{\ell-1})}{2\Delta r_k} \qquad (2.1.21c)$$

(2.1.21c)

$$\int_{\ell-1/2}^{\ell+1/2} \left(r^a D^j \frac{\partial \phi^j}{\partial r}\right)_{r_{k-1/2}} dz = \left[r^a_{k-1/2} D^j_{k-1/2,\,\ell} \phi^j_{k,\,\ell} - \right.$$

$$\left. - r^a_{k-1/2} D^j_{k-1/2,\,\ell} \phi^j_{k-1,\,\ell} \right] \frac{(z_{\ell+1} - z_{\ell-1})}{2\Delta r_{k-1}} \qquad (2.1.22)$$

The results (2.1.20), (2.1.21a-c) and (2.1.22) can be combined to yield the difference equation

$$r^a_{k+1/2} \frac{(z_{\ell+1} - z_{\ell-1})}{2\Delta r_k} D^j_{k+1/2,\,\ell} \phi^j_{k+1,\,\ell} + r^a_{k-1/2} \frac{(z_{\ell+1} - z_{\ell-1})}{2\Delta r_{k-1}} D^j_{k-1/2,\,\ell} \phi^j_{k-1,\,\ell} +$$

$$+ r^a_k \frac{(r_{k+1} - r_{k-1})}{2\Delta z_\ell} D^j_{k,\,\ell+1/2} \phi^j_{k,\,\ell+1} + r^a_k \frac{(r_{k+1} - r_{k-1})}{2\Delta z_{\ell-1}} D^j_{k,\,\ell-1/2} \phi^j_{k,\,\ell-1} -$$

$$- \left\{ \frac{(z_{\ell+1} - z_\ell)}{2} \left[\frac{r^a_{k+1/2} D^j_{k+1/2,\,\ell}}{\Delta r_k} + \frac{r^a_{k-1/2} D^j_{k-1/2,\,\ell}}{\Delta r_{k-1}} \right] + \right.$$

$$+ \frac{(r_{k+1} - r_{k-1})}{2} r^a_k \left[\frac{D^j_{k,\,\ell+1/2}}{\Delta z_\ell} + \frac{D^j_{k,\,\ell-1/2}}{\Delta z_{\ell-1}} \right] + \frac{r^a_k}{4} \left[\Delta r_k \Delta z_\ell \Sigma^j(k^+, \ell^+) + \right.$$

$$\left. \left. + \Delta r_k \Delta z_{\ell-1} \Sigma^j(k^+, \ell^-) + \Delta r_{k-1} \Delta z_\ell \Sigma^j(k^-, \ell^+) + \Delta r_{k-1} \Delta z_{\ell-1} \Sigma^j(k^-, \ell^-) \right] \right\} \phi^j_{k,\,\ell} =$$

$$= - \frac{r^a_k}{4} \left[\Delta r_k \Delta z_\ell f^j(k^+, \ell^+) + \Delta r_k \Delta z_{\ell-1} f^j(k^+, \ell^-) + \Delta r_{k-1} \Delta z_\ell f^j(k^-, \ell^+) + \right.$$

$$\left. + \Delta r_{k-1} \Delta z_{\ell-1} f^j(k^-, \ell^-) \right], \qquad (2.1.23)$$

which can be written

$$r^j_{k,\,\ell} \phi^j_{k+1,\,\ell} + \ell^j_{k,\,\ell} \phi^j_{k-1,\,\ell} + t^j_{k,\,\ell} \phi^j_{k,\,\ell+1} + b^j_{k,\,\ell} \phi^j_{k,\,\ell-1} - c^j_{k,\,\ell} \psi^j_{k,\,\ell} = d^j_{k,\,\ell} \,. \qquad (2.1.24)$$

If we take r = x, z = y, and assume a homogeneous one-region assembly, we recover the simple form (2.1.17). As before, Equation (2.1.24) is a 5-point difference relation. More accurate 5-point formulas may be derived by considering additional terms of the Taylor series expansion of the integrands.

Other difference approximations are obtainable for the diffusion equations; in fact, there is no unique difference equation for a given differential equation. Details of alternative formulations may be found in the references.

2.2 MATRIX FORM OF MULTI-GROUP DIFFERENCE EQUATIONS

In order to simplify the discussion of latter sections, we present the matrix forms of the difference equations in this section. Consider first the one-dimensional problem. For a given group, the relevant difference equation is (2.1.15).

$$a_k \phi^j_{k+1} - \beta_k \phi^j_k + \gamma_k \phi^j_{k-1} = -\omega^j_k \tag{2.2.1}$$

with

$$a_k = \frac{r^a_{k+1/2} D^j_{k+1/2}}{\Delta r_k} \tag{2.2.2a}$$

$$\beta_k = \frac{r^a_{k+1/2} D^j_{k+1/2}}{\Delta r_k} + \frac{r^a_{k-1/2} D^j_{k-1/2}}{\Delta r_{k-1}} - \frac{r^a_k}{2}\left(\Sigma^j(r^+_k)\Delta r_k + \Sigma^j(r^-_k)\Delta r_{k-1}\right) \tag{2.2.2b}$$

$$\gamma_k = \frac{r^j_{k-1/2} D^j_{k-1/2}}{\Delta r_{k-1}} \tag{2.2.2c}$$

$$\omega_k = \frac{r^a_k}{2}\left[f^j(r^+_k)\Delta r_k + f^j(r^-_k)\Delta r_{k-1}\right]. \tag{2.2.2d}$$

We define the vectors $\underline{\psi}^j$, $\underline{F}^j_+$, $\underline{F}^j_-$

$$\underline{\psi}^j = \begin{bmatrix} \phi_1^j \\ \phi_2^j \\ . \\ . \\ \phi_{K-1}^j \end{bmatrix} ; \quad \underline{F}_+^j = \begin{bmatrix} f_1^j(+) \\ f_2^j(+) \\ . \\ . \\ f_{K-1}^j(+) \end{bmatrix} ; \quad \underline{F}_-^j = \begin{bmatrix} f_1^j(-) \\ f_2^j(-) \\ . \\ . \\ f_{K-1}^j(-) \end{bmatrix}$$

The set of equations (2.2.1) becomes

$$\begin{bmatrix} -\beta & a_1 & 0 \ldots & & \\ \gamma_2 & -\beta_2 & a_2 \ldots & & \\ \ldots & & & & \\ \ldots & & & & \\ & & \gamma_{K-1} & \omega\beta_{K-1} \end{bmatrix} \begin{bmatrix} \phi_1^j \\ \phi_2^j \\ . \\ . \\ \phi_{K-1}^j \end{bmatrix} = \begin{bmatrix} r_1^a \Delta r_1 & 0 & \ldots & & \\ 0 & \frac{r_2^a \Delta r_2}{2} & \ldots & 0 & \\ & & & & \\ & & & & \frac{r_{K-1}^a \Delta r_{K-1}}{2} \end{bmatrix}$$

$$\begin{bmatrix} f_1^j(+) \\ . \\ . \\ . \\ f_{K-1}^j(+) \end{bmatrix} + \begin{bmatrix} \frac{r_1^a \Delta r_o}{2} & 0 & \ldots & \ldots & \\ \ldots & & & & \\ \ldots & & & & \\ \ldots & & & & \\ & & & \frac{r_{K-1}^a \Delta r_{K-1}}{2} & \end{bmatrix} \begin{bmatrix} f_1^j(-) \\ f_2^j(-) \\ \ldots \\ \ldots \\ f_{K-1}^j(-) \end{bmatrix} \qquad (2.2.3)$$

which can be written

$$A^j \underline{\psi}^j = B^j \underline{F}_+^j + D^j \underline{F}_-^j \qquad (2.2.4)$$

We have taken $\psi_o^j = \psi_K^j = 0$ (the extrapolated boundary). The continuity conditions on flux and current have been used in deriving the equations. In order to consider the entire set of multi-group difference equations,

we define the super-vectors

$$\underline{\Psi} = \begin{bmatrix} \psi^1 \\ \psi^2 \\ . \\ . \\ . \\ \psi^{th} \end{bmatrix}; \quad \underline{F}_+ = \begin{bmatrix} F_+^1 \\ F_+^2 \\ . \\ . \\ . \\ F_+^{th} \end{bmatrix}; \quad \underline{F}_- = \begin{bmatrix} F_-^1 \\ F_-^2 \\ . \\ . \\ . \\ F_-^{th} \end{bmatrix}$$

Then the entire set of equations becomes

$$A\underline{\Psi} = B\underline{F}_+ + C\underline{F}_- \tag{2.2.5}$$

where A, B, C, are (J+1) + (J+1) partitioned matrices of the form

$$A = \begin{bmatrix} A^1 & 0 & \cdots & \cdots \\ 0 & A^2 & \cdots & 0 \\ & & & A^{th} \end{bmatrix} \quad \text{etc.}$$

In order to examine the equations in more detail, we consider the form of F_+^j and F_-^j. From section 1.5, for a simple multi-group equation, we have (Equation 1.5.40)

$$f^j = \frac{(\xi\Sigma_s)^{j-1}}{(\xi\Sigma_s)^j} \frac{\phi^{j-1}(r)}{a^j \Delta u_j} + \frac{\nu x^j}{(\xi\Sigma_s)^j a^j} \sum_{j=1}^{J} \beta^j \phi^j(r) + \Sigma_f^{th}\phi(r) + \frac{z^j}{(\xi\Sigma_s)^j a^j} S_e(r) \tag{2.2.6}$$

At the k^{th} space point, we then have

$$f_+^j = \frac{(\xi\Sigma_s)^{j-1}}{(\xi\Sigma_s)^j} \frac{\phi_k^{j-1}}{a^j \Delta u_j} + \frac{\nu x^j}{(\xi\Sigma_s)^j a^j} \Sigma_j \beta^j \phi_k^j + \Sigma_f^{th}\phi_k^{th} + \frac{z^j}{(\xi\Sigma_s)^j a^j} S_{e_k} \tag{2.2.7}$$

where the coefficients evaluated at the limit k^+. (We have assumed the reactor homogeneous by regions in obtaining (2. 2. 6); the +, - notation applies only at interfaces.) As an example, if the K^+ boundary were in a pure moderator, then all $z_j = 0$, $x_j = 0$, and f_+^j would consist of slowing down neutrons only. The scattering properties would be those of the moderator, of course.

By rather obvious substitutions, we can write

$$\underline{F}_+^j = G_+^j \underline{\Psi}^j + \nu_j^{\Sigma} H_+^j \underline{\Psi}^j + \Gamma_+^j \underline{\mathcal{S}}_e^{j+}, \qquad (2.2.8)$$

where $\underline{\mathcal{S}}_e^+$ is the discrete vector extraneous source, which may be discontinuous in space.

The matrix G_+^j is the slowing-down term, the matrix H_+^j is the fission source term, and Γ_+^j is the extraneous source term. In similar manner, we have

$$\underline{F}_-^j = G_-^j \underline{\Psi}^j + \nu_j^{\Sigma} H_-^j \underline{\Psi}^j + \Gamma_-^j \underline{\mathcal{S}}_e^{j-} \qquad (2.2.9)$$

Combining (2. 2. 8) and (2. 2. 9) with (2. 2. 4), we have

$$A^j \underline{\Psi}^j = B^j \left[G_+^j \underline{\Psi}^j + \nu_j^{\Sigma} H_+^j \underline{\Psi}^j + \Gamma_+^j \underline{\mathcal{S}}_e^{j+} \right] + C^j \left[G_-^j \underline{\Psi}^j + \nu_j^{\Sigma} H_-^j \underline{\Psi}^j + \Gamma_-^j \underline{\mathcal{S}}_e^{j-} \right]$$

or

$$\left[A^j - B^j G_+^j - C^j G_-^j - \nu_j^{\Sigma} \left(B^j H_+^j + C^j H_-^j \right) \right] \underline{\Psi}^j = B^j \Gamma_+^j \underline{\mathcal{S}}_e^{+} + C^j \Gamma_-^j \underline{\mathcal{S}}_e^{j-}$$

or

$$\left[N^j - \nu P^j \right] \underline{\Psi}^j = R_e^j \qquad (2.2.10)$$

where R_e^j is the composite external source.

By collecting the group equations into super matrices/vectors, we have

$$\left[N - \nu P \right] \underline{\Psi} = \underline{R}_e \qquad (2.2.11)$$

The dimension of the vector $\underline{\Psi}$ and $\underline{R}_e$ is (K-1)*(J+1) while the matrices N and P are (K-1)*(J+1) by (K-1)*(J+1). The operator N depends only upon the slowing down and diffusion properties of the

assembly, and P depends upon the fission properties of the medium.

For the case of the source-free problem, we again recover the eigenvalue problem

$$N\Psi = \nu P\Psi \ , \tag{2.1.12}$$

or

$$\frac{\Psi}{\nu} = N^{-1}P\Psi \ .$$

If we define the starting guess ψ_o and take $N^{-1}P\psi_o = \psi_1$, then ν is approximated in the form

$$\frac{1}{\nu} \approx \frac{\psi_1}{\psi_o} \tag{2.2.13}$$

Notice that this form of the method of successive approximations is reasonably obtained as compared to previous forms of the same approximation. The original integro-differential equation led to an integral definition of the eigenvalue ν. By dividing the lethargy space into finite intervals, we derived a similar approximation where the integral definition was replaced by a differential operator. The finite difference approximation leads to a matrix operator definition. Of course, we cannot expect the results from the three different approaches to be the same, but the intent of the method is to obtain a reasonably accurate approximation with the simplest amount of effort.

The two-dimensional difference equations can also be written in matrix form. We merely outline the step below. Defining the vector ψ_k^j, D_k^j as

$$\psi_k^j = \begin{bmatrix} \phi_{k,1}^j \\ \phi_{k,2}^j \\ . \\ . \\ \phi_{k,L-1}^j \end{bmatrix}; \qquad D_k^j = \begin{bmatrix} d_{k,1}^j \\ d_{k,2}^j \\ . \\ . \\ d_{k,L-1}^j \end{bmatrix}$$

The basic equation, (2.1.24), takes the form

$$A^j_k \underline{\Psi}^j_{k+1} + B^j_k \underline{\Psi}^j_k + C^j_k \underline{\Psi}^j_{k-1} = \underline{D}^j_k \ , \qquad (2.2.14)$$

where the matrices are L-1 by L-1 in dimension. We form super matrices and vectors for the K-1 equations of the form (2.2.14) and have

$$[A^j + B^j + C^j]\, \underline{\Psi}^j = D^j \qquad (2.2.15)$$

The entire J+1 sets of equations can be extended to the form

$$[A + B + C]\, \underline{\Psi} = \underline{D} \qquad (2.2.16)$$

By expanding the right-hand side in terms of fission and extraneous sources plus slowing-down terms, we can then show the two-dimensional problem reduces to an equation of the form

$$[N - \nu P]\, \underline{\Psi} = \underline{R} \qquad (2.2.17)$$

By completely analogous formation of difference equations, the adjoint equations can also be reduced to a set of simultaneous equations. We now turn to methods for solving the sets of simultaneous algebraic equations.

2.3 DIRECT METHODS OF SOLUTION

By direct methods of solutions, we mean techniques of solving the equations in a finite number of steps. We consider only one direct method at this time.

The entire set of multi-group equations can be written in the matrix form

$$A\underline{\Psi} = \underline{R}\,, \qquad (2.3.1)$$

and if the operator A has an inverse, then the solution is

$$\underline{\Psi} = A^{-1}\underline{R}\ . \qquad (2.3.2)$$

There are a number of methods of matrix inversion. The most common is probably the Gauss-Jordan reduction. Consider the set of equations in expanded form

$$
\begin{aligned}
a_{11}\psi_1 + a_{12}\psi_2 + \ldots \quad a_{1n}\psi_n &= R_1 \\
a_{21}\psi_1 + a_{22}\psi_2 + \ldots \quad a_{2n}\psi_n &= R_2 \\
\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & \\
a_{n1}\psi_1 + a_{n2}\psi_2 + \ldots \quad a_{nn}\psi_n &= R_n
\end{aligned}
\tag{2.3.3}
$$

The reduction is begun by dividing the first equation by a_{11}. (We assume $a_{11} \neq 0$; otherwise, re-order the equation so that this is so.) The resultant equation is now multiplied by a_{21}, and then subtracted from the second of the equations. In this manner, ψ_1 is eliminated from the second equation. Similarly, we eliminate ψ_1 from the third, fourth, etc. equations. The set of equations becomes

$$
\begin{aligned}
\psi_1 + a'_{12}\psi_2 + \quad \ldots \quad a'_{1n}\psi_n &= R'_1 \\
a'_{22}\psi_2 + \quad \ldots \quad a'_{2n}\psi_n &= R'_2 \\
a'_{32}\psi_2 + \quad \ldots \quad a'_{3n}\psi_n &= R'_3 \\
\ldots\ldots\ldots\ldots\ldots\ldots & \\
a'_{n2}\psi_2 + \quad \ldots \quad a'_{nn}\psi_n &= R'_n
\end{aligned}
\tag{2.3.4}
$$

where prime denotes a modified coefficient. We now divide the second equation by a'_{22} and multiply the resultant equation by a'_{32}, a'_{42}, etc. to sequentially eliminate ψ_2 from the third, fourth, etc. equations.

Continuing in this manner, we ultimately produce a set of equations in triangular form as

$$
\begin{aligned}
\psi_1 + \bar{a}_{12}\psi_2 + \bar{a}_{13}\psi_3 + \ldots \; \bar{a}_{1n}\psi_n &= \bar{R}_1 \\
\psi_2 + \bar{a}_{23}\psi_3 + \ldots \; \bar{a}_{2n}\psi_n &= \bar{R}_2 \\
\psi_n &= \bar{R}_n
\end{aligned}
\tag{2.3.5}
$$

By back substitution, we obtain the solution. It should be mentioned that the inverse matrix is obtainable in the above process by a little additional labor.

The difficulty with the method outlined above is twofold. First, the operations are all performed with the various coefficients, and, for large arrays, the inevitable round-off may have a serious influence on the accuracy of the solution. Another important aspect is the number of operations required. The rescaling of each equation requires something like n operations. The elimination of any unknown requires on the order of n operations, and the process is repeated for n unknowns; hence, the number of steps required to solve the problem will be proportional to n^3. If we were treating a 10-group, 100-point problem, something on the order of 10^9 operations would be necessary. Even for present-day computers, this becomes an appreciable number of steps. For larger problems, it is necessary to look for other methods of solving the sets of equations. We remark that there are other direct methods of inversion, but, except for special cases, they all have the objectionable features of requiring something like n^3 operations.

2.4 ITERATIVE METHODS

There are many iterative methods for solving sets of algebraic equations. We shall outline a number of methods of broad applicability. As the name implies, iterative methods are analogous to the method of successive approximations as defined earlier. In general, an infinite number of steps is required to solve a problem iteratively. However, it is also true for a convergent iteration that the near asymptotic solution is reached in a finite number of steps. If one is willing to accept an answer which is "reasonably" accurate, then frequently iterative methods are as fast or faster than direct methods.

Before discussing various techniques in detail, let us examine the general conditions under which an iterative process converges. We assume we are solving the matrix equation

$$A\underline{\psi} = \underline{R} \qquad (2.4.1)$$

We further assume that the iteration process can be represented as a matrix of the form

$$B\underline{\psi}^{p-1} + \underline{C} = \underline{\psi}^{p} \tag{2.4.2}$$

where $\underline{\psi}^{p-1}$ and $\underline{\psi}^{p}$ are successive trials for the solution, B is a matrix dependent upon the method of solution, and $\underline{C}$ is a vector. Since B and $\underline{C}$ are independent of p, the iteration is called stationary. If $\underline{\psi}$ is the solution, then a solution must have the property

$$B\underline{\psi} + C = \underline{\psi} = A^{-1}R \tag{2.4.3}$$

and hence

$$C = [I - B]\, A^{-1}\underline{R} = \underline{\psi} - B\underline{\psi} \tag{2.4.4}$$

If we write $\underline{\psi}^{p}$ in the form

$$\underline{\psi}^{p} = \underline{\psi} + \underline{\epsilon}^{p} \tag{2.4.5}$$

and define $\underline{\epsilon}^{p}$ as the error associated with a given trial solution, then from (2.4.2) we have

$$B\underline{\psi} + B\underline{\psi}^{p-1} + \underline{\psi} - B\underline{\psi} = \underline{\psi} + \underline{\epsilon}^{p}$$

or

$$B\underline{\epsilon}^{p-1} = \underline{\epsilon}^{p} \tag{2.4.6}$$

Thus, the error obeys the homogeneous form of the iteration equation. This property is true of all stationary iterations.

We note that for a solution $\underline{\epsilon}^{p} \to 0$ as $p \to \infty$. The elimination of the error depends upon the properties of the matrix B. Let us assume B has a complete set of eigenvectors, say $\underline{e}_r$, and corresponding to each eigenvector, an eigenvalue λ_r. We take the eigenvalues as ordered, so that $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n|$.

The original error vector $\underline{\epsilon}^{o}$ is then expandable in the form

$$\underline{\epsilon}^{o} = \Sigma_r a_r \underline{e}_r \tag{2.4.7}$$

Successive values are

$$\underline{\epsilon}^1 = \Sigma_r a_r \lambda_r \underline{e}_r$$

$$\vdots$$

$$\underline{\epsilon}^p = \Sigma_r a_r \lambda_r^p \underline{e}_r \qquad (2.4.8)$$

Since the eigenvalues are ordered, the asymptotic error is of the form

$$\underline{\epsilon}^p \approx a_1 \lambda_1^p \underline{e}_1 \qquad (2.4.9)$$

In order for the error to vanish, we require that

$$|\lambda_1| < 1 \qquad (2.4.10)$$

This result is quite general and is also applicable to the case where the eigenvectors of B are not complete (for details, see ref. 6, Forsyth and Wasow).

The primary objectives of the various iterative methods are to form iteration operators which converge (i.e., ($\lambda_{max} < 1$)), and the speed of convergence is dependent upon the actual magnitude of the largest eigenvalue. For many of the methods to be discussed, a good deal is known concerning the rates of convergence. For further detail, we refer to the various references.

In discussing the basic properties of iteration methods, we have so far considered only the inhomogeneous equation. Before reviewing iterative methods, we consider the solution of the eigenvalue problems by iterative procedures. In this case, the basic equation is of the form

$$A\underline{\psi} = \lambda\underline{\psi} .$$

By the method of successive approximations, we assume a trial solution, $\underline{\psi}_o$, and if $A\underline{\psi}_o = \underline{\psi}_1$, then

$$\lambda = \frac{\underline{\psi}_1}{\underline{\psi}_o} . \qquad (2.4.11)$$

The generalization is obviously

$$\lambda = \frac{\Psi_p}{\Psi_{p-1}} \tag{2.4.12}$$

Since Ψ is a vector, the comparison of successive values can be made with any component of Ψ. However, such a comparison requires a number of iterations to reach a steady state. A more rapidly attained approximation to the eigenvalue is the so-called Rayleigh quotient. If we consider the iteration of the form

$$\lambda\Psi_{p-1} = A\Psi_{p-1} = \Psi_p \tag{2.4.13}$$

and take the dot product of both sides with respect to Ψ_{p-1}, we have

$$\lambda \approx \frac{(A\Psi_{p-1}, \Psi_{p-1})}{(\Psi_{p-1}, \Psi_{p-1})} = \frac{(\Psi_p, \Psi_{p-1})}{(\Psi_{p-1}, \Psi_{p-1})} \tag{2.4.14}$$

It is easily shown that the algorithm (2.4.14) converges to the largest value of λ. Furthermore, λ can be related to the neutron multiplication ν_e/ν for the multi-group equations, and hence the Rayleigh quotient can be used to find the neutron multiplication factor. To show that the method converges to the largest λ, we expand the vector Ψ in terms of the eigenvectors of A. We have

$$\Psi_o = \Sigma_r a_r \underline{e}_r$$

and hence the Rayleigh quotient is

$$\frac{(A\Psi_o, \Psi_o)}{(\Psi_o, \Psi_o)} = \frac{\Sigma_r \lambda_r a_r^2}{\Sigma_r a_r^2} = \frac{\lambda_1 \Sigma_r (\lambda_r/\lambda_1) a_r^2}{\Sigma_r a_r^2} \tag{2.4.15}$$

where we take the eigenvalues ordered with λ_1 the largest. By induction, we have

$$\frac{(A\Psi_{p-1}, \Psi_{p-1})}{(\Psi_{p-1}, \Psi_{p-1})} = \frac{\lambda_1 \Sigma_r (\lambda_r/\lambda_1)^{2p-1} a_r^2}{\Sigma_r (\lambda_r/\lambda_1)^{2p-2} a_r^2} \tag{2.4.16}$$

Since $\lambda_r/\lambda_1 < 1$ for $r > 1$, the process converges to λ_1.

The Rayleigh quotient method is more rapid than the single component method since the ratio of eigenvalues in the expansion appears quadratically, whereas, in the single component method, the convergence is linear with the number of iterations. Of course, formation of the dot products requires more steps after a single iteration.

An iteration of the form

$$A\underline{\psi}_{p-1} = \underline{\psi}_p \tag{2.4.17}$$

is called the "power method". The use of the Rayleigh quotient to estimate the eigenvalues of a given problem is not limited to the power method. Before considering other iterations, we remark that the adjoint function is useful in obtaining eigenvalues by the Rayleigh method when the operators involved do not have orthogonal eigenvectors. The details are similar to previous discussions.

In order to introduce iterative methods, we consider the general multi-group equations in the form

$$[N - \nu P]\,\underline{\psi} = \underline{R} \tag{2.4.18}$$

which is the general form of the multi-group equations obtained in the previous section. If there are no external sources, $\underline{R} = 0$. To derive the various iterative procedures, we recall that the matrix N related to the diffusion properties of the neutrons within a given group, P related to the fission and slowing-down sources, and $\underline{R}$ the external sources. Let us assume an initial estimate, $\underline{\psi}_o$, and write (2.4.18) in the form

$$N\underline{\psi}_o = \nu P\underline{\psi}_o + \underline{R} = \underline{S}_o \tag{2.4.19}$$

For a given estimate of $\underline{\psi}_o$, the entire right hand can be computed before starting the numerical computation. We now factor N in the form

$$N = L + D + U \tag{2.4.20}$$

where L is a lower triangular matrix, D a diagonal matrix, and U an upper triangular matrix. As an example, the one-dimensional equation given in (2. 2. 3) would give the following

$$L = \begin{bmatrix} 0 & 0 & \cdots & \cdots & 0 \\ \gamma_2 & 0 & \cdots & \cdots & \cdots \\ 0 & \gamma_3 & \cdots & \cdots & \cdots \\ & & & \gamma_{K-1} & 0 \end{bmatrix}, \qquad (2.4.21a)$$

$$D = \begin{bmatrix} -\beta_1 & & 0 \\ & -\beta_2 & \\ 0 & & -\beta_{K-1} \end{bmatrix}, \qquad (2.4.21b)$$

$$U = \begin{bmatrix} 0 & \alpha_1 & 0 & \cdots & \cdots & 0 \\ & 0 & \alpha_2 & \cdots & \cdots & \\ & & & & & \alpha_{K-2} \\ & & & & & 0 \end{bmatrix} \qquad (2.4.21c)$$

A similar expansion in the two dimensional case would replace each of the elements in (2. 4. 21a, b, c) with a submatrix. A matrix consisting of elements along the principal diagonal and the two adjoining diagonals is called "tri-diagonal". A matrix consisting of submatrices along the principal and the two adjoint diagonals is called "block tri-diagonal". We consider first the one-dimensional problem. From (2. 4. 19), we write the basic equation in the form

$$L\underline{\psi}_o + D\underline{\psi}_o + U\underline{\psi}_o = \underline{S}_o \qquad (2.4.21)$$

We now write this in the form

$$D\underline{\psi}_o = \underline{S}_o - L\underline{\psi}_o - U\underline{\psi}_o$$

and finally we define $\underline{\psi}_1$ from the relation

$$\underline{\psi}_1 = D^{-1}\underline{S}_o - D^{-1}[L+U]\,\underline{\psi}_o \qquad (2.4.22)$$

The above relation defines an iterative process known as the "Richardson" method and also the "method of simultaneous displacements". In component forms for a given space point and lethargy group, the equation has the form

$$\phi'_k = \frac{S^o_k + \gamma_k \phi^o_{k-1} + \alpha_k \phi^o_{k+1}}{\beta_k} \qquad (2.4.23)$$

and in general

$$\phi^p_k = \frac{S^{p-1}_k + \gamma_k \phi^{p-1}_{k-1} + \alpha_k \phi^{p-1}_{k-1}}{\beta_k} \qquad (2.4.24)$$

Computationally, this algorithm is very simple and since the original difference relation is a 3-point relation, the equation preserves this property.

By expanding the matrices for the two-dimensional case, it is easily seen that the equation takes the form

$$\phi^p_{k,\ell} = \frac{S^{p-1}_{k,\ell} + r_{k,\ell}\phi^{p-1}_{k+1,\ell} + \ell_{k,\ell}\phi^{p-1}_{k-1,\ell} + b_{k,\ell}\phi^{p-1}_{k,\ell-1} + t_{k,\ell}\phi^{p-1}_{k,\ell+1}}{C_{k,\ell}} \qquad (2.4.25)$$

(See Equation (2.1.24)). For this case, we preserve the 5-point characters of the difference relation.

For either case, the iteration operator can be written

$$\underline{\psi}_p = B\underline{\psi}_{p-1} + \underline{C}$$

as before. Hence, the convergence of the method is again dependent upon the eigenvalues of B.

An alternative method is similarly obtained starting from (2.4.21). We notice that elements of the matrix L operate on values of the flux for which the space index is less than k, the generic point. If the iteration

moves from k = 1 to k = k, then values of the function ϕ_m are computed for m < k before we reach the space point k. Hence, it is possible to use these latest values while computing ϕ_k. Mathematically, the iteration becomes

$$(L+D)\underline{\Psi}_o = \underline{S}_o - U\underline{\Psi}_o$$

and

$$\underline{\Psi}_1 = [L+D]^{-1}\underline{S}_o - (L+D)^{-1}U\underline{\Psi}_o \qquad (2.4.26)$$

For a three-point difference relation, the basic equation can be written

$$\phi_k^p = \frac{S_k^{p-1} + \gamma_k\phi_{k-1}^p + \alpha_k\phi_{k+1}^{p-1}}{\beta_k} \qquad (2.4.27)$$

The similar relation for the two-dimensional equation is

$$\phi_{k,\ell}^p = \frac{S_{k,\ell}^{p-1} + r_{k,\ell}\phi_{k+1,\ell}^{p-1} + t_{k,\ell}\phi_{k,\ell+1}^{p-1} + \ell_{k,\ell}\phi_{k-1,\ell}^p + b_{k,\ell}\phi_{k,\ell-1}^p}{C_{k,\ell}} \qquad (2.4.28)$$

An iteration of the above type is called the "Gauss-Seidel" method and also the "method of successive displacements". Under certain conditions on the matrix operators (usually obeyed for the diffusion equations), it can be shown that the Gauss-Seidel method converges more rapidly than the Richardson method.

The convergence of the method is again dependent upon the nature of the eigenvalues of the iteration operator.

For either of the iterations considered thus far, we note that the change in the function on successive iteration can be written

$$\underline{\Psi}_p - \underline{\Psi}_{p-1} = B\underline{\Psi}_{p-1} + \underline{C} - \underline{\Psi}_{p-1} = (B-I)\underline{\Psi}_{p-1} + \underline{C} \qquad (2.4.29)$$

If we denote $\underline{\Psi}_p - \underline{\Psi}_{p-1}$ as the "residual" vector $\underline{\Delta}_p$, then the iteration can be written

$$\underline{\Psi}_p = \underline{\Psi}_{p-1} + \underline{\Delta}_p \qquad (2.4.30)$$

For the Richardson method, the residual vector Δ_p is

$$\underline{\Delta}_p = D^{-1}\underline{S}_{p-1} - [D^{-1}(L+U) - I]\,\underline{\psi}_{p-1} \qquad (2.4.31)$$

while, for the Gauss-Seidel method, we have

$$\underline{\Delta}_p = (L+D)^{-1}\underline{S}_{p-1} - [(L+D)^{-1}U - I]\,\underline{\psi}_{p-1} \qquad (2.4.32)$$

The residuals are calculable at any stage of the iteration by using the appropriate basic iteration equation (2.4.24), (2.4.25), or (2.4.27), (2.4.28).

The residuals are particularly useful in conjunction with the so-called "extrapolated Liebmann method" or the "method of over-relaxation". If we take (2.4.30) as the basic iteration equation, then an alternative iteration is

$$\psi_p = \psi_{p-1} + \omega\Delta_p \qquad (2.4.33)$$

where ω is some real constant (which may depend upon p). For $\omega > 1$, we "over"-correct a trial solution while for $\omega < 1$, we "under"-correct a trial solution. Under certain restrictive conditions (usually obeyed by the diffusion equation), it can be shown that the extrapolated Liebmann method converges more rapidly than either the Richardson or Gauss-Seidel iteration, <u>provided</u> the factor ω is properly chosen. It is an unfortunate fact that obtaining the proper ω is, in general, a trial and error problem. Nevertheless, for an appropriate selection of the over-relaxation factor, the increase in the speed of convergence is quite large.

For the problems involving three-point difference equations, and hence tri-diagonal matrices, there exists a particularly rapid method of solution called the method of "matrix factorization". Consider a one-dimensional reactor. The set of multi-group equations for a given group is of the form

$$A^j\underline{\psi}^j = \underline{R}^j \qquad (2.4.34)$$

We assume the vector $\underline{R}^j$ has been computed from a given initial estimate of the flux. The equations are of the form (see section 2.2)

$$\begin{bmatrix} -\beta_1 & \alpha_1 & 0 & \cdots & 0 \\ \gamma_2 & -\beta_2 & \alpha_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & \alpha_k & & -\beta_k \end{bmatrix} \begin{bmatrix} \phi_1^j \\ \phi_2^j \\ \cdot \\ \phi_k^j \end{bmatrix} = \begin{bmatrix} R_1^j \\ R_2^j \\ \cdot \\ R_k^j \end{bmatrix} \qquad (2.4.35)$$

The matrix A^j can be factored into the product of two matrices in the form

$$A^j = X^j Y^j \qquad (2.4.36a)$$

or

$$\begin{bmatrix} -\beta_1 & \alpha_1 & 0 & \cdots & 0 \\ \gamma_2 & -\beta_2 & \alpha_2 & \cdots & 0 \\ 0 & & \gamma_k & & -\beta_k \end{bmatrix} = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ b_2 & a_2 & 0 & \cdots \\ & b_k & a_k & \end{bmatrix} \begin{bmatrix} 1 & d_1 & 0 & \cdots \\ 0 & 1 & d_2 & \cdots 0 \\ & & 1 & d_{k-1} \end{bmatrix}$$

(2.4.36b)

In order for the equality to hold, we require

$$\left.\begin{aligned} a_1 &= -\beta_1 \\ a_1 d_1 &= \alpha_1 \end{aligned}\right\} \qquad (2.4.37a)$$

$$\left.\begin{aligned} b_2 &= \alpha_2 \\ b_2 d_1 + a_2 &= -\beta_2 \\ a_2 d_2 &= \alpha_2 \end{aligned}\right\} \qquad (2.4.37b)$$

and in general

$$\left.\begin{aligned} b_n &= \gamma_n \\ b_n d_{n-1} + a_n &= -\beta_n \\ a_n d_n &= \alpha_n \end{aligned}\right\} \qquad (2.4.37c)$$

The above relations can be solved in the form

$$\left.\begin{aligned} a_1 &= -\beta_1 \\ d_1 &= \alpha_1/a_1 \end{aligned}\right\} \tag{2.4.38a}$$

$$\left.\begin{aligned} b_2 &= \gamma_2 \\ a_2 &= -\beta_2 - b_2 d_1 \\ d_2 &= \alpha_2/a_2 \end{aligned}\right\} \tag{2.4.38b}$$

and in general

$$\left.\begin{aligned} b_n &= \gamma_n \\ a_n &= -\beta_n - b_n d_{n-1} \\ d_n &= \alpha_n/a_n \end{aligned}\right\} \tag{2.4.38c}$$

Thus, starting from the original equation, we can compute the elements of the two matrices, X^j and Y^j. Thus far, we have only performed some algebra, but it is important to notice that the two matrices, X and Y, have only two elements per row, rather than three. The next step in the solution by factorization is to write the source vector in the form

$$\underline{R}^j = X^j \underline{E}^j \tag{2.4.39}$$

The set of equations is thus

$$X^j Y^j \underline{\psi}^j = X^j \underline{E}^j \tag{2.4.40}$$

or

$$Y^j \underline{\psi}^j = \underline{E}^j \tag{2.4.41}$$

The advantage of the factorization is now apparent. Since Y^j has only two elements per row, we can solve (2.4.41) recursively without iteration. To illustrate, we first compute the elements of E^j. From (2.4.39), we have

$$
\begin{aligned}
R_1^j &= a_1 E_1^j \\
R_2^j &= b_2 E_1^j + a_2 E_2^j \\
R_3^j &= b_3 E_2^j + a_3 E_3^j \\
&\vdots \\
R_n^j &= b_n E_{n-1}^j + a_n E_n^j
\end{aligned}
\qquad (2.4.42)
$$

The set of equations can easily be solved by successive substitution. Having obtained the E_k^j, we solve (2.4.41) in similar fashion. We have

$$
\begin{aligned}
\phi_1^j + d_1 \phi_2^j &= E_1^j \\
\phi_2^j + d_2 \phi_3^j &= E_2^j \\
&\vdots \\
\phi_k^j &= E_k^j
\end{aligned}
\qquad (2.4.43)
$$

We solve the set (2.4.43) backwards; we compute ϕ_k^j, then ϕ_{k-1}^j, etc. until all the fluxes are computed.

The method of matrix factorization is a "two-pass" computation. Beginning at k = 1 and proceeding to k = k, we compute successively the coefficients a_k, b_k, d_k, and E_k^j. When we have the vector E_k^j and the d_k, we proceed backwards, computing the ϕ_k^j. The method is very rapid and non-iterative.

A similar procedure is possible for two-dimensional problems, except the elements of the factored matrices appear as sub-matrices. To perform the solution, it is necessary to invert these sub-matrices. The two-dimensional method thus has drawbacks not associated with

the one-dimensional problem. Rather than pursue the details of matrix factorization in two-dimension, we introduce an alternative method for such problems.

The method to be considered is the "alternating-direction implicit method" first conceived by D. W. Peaceman and H. H. Rachford. The method is iterative but very rapid. We remark that the advantage of the method in speed of convergence is a result of using rectangular coordinates. Although the technique can also be applied to other geometries, the advantages of the method are subject to some doubt. (For details, see the references.) We consider for illustration a two-dimensional rectangular reactor. The basic diffusion equation can be written in the difference form

$$\{r_{k,\ell}\phi_{k+1,\ell} + \ell_{k,\ell}\phi_{k-1,\ell} - g_{k,\ell}\phi_{k,\ell}\} +$$

$$+ \{t_{k,\ell}\phi_{k,\ell+1} + b_{k,\ell}\psi_{k,\ell-1} - h_{k,\ell}\phi_{k,\ell}\} = d_{k,\ell} \qquad (2.4.44)$$

where the braces are used to separate the x and y dependence. If we denote the iteration subscript by p, then (2.4.44) can be written

$$r_{k,\ell}\phi^{p}_{k+1,\ell} + \ell_{k,\ell}\phi^{p}_{k-1,\ell} - g_{k,\ell}\phi^{p}_{k,\ell} =$$

$$= d_{k,\ell} - t_{k,\ell}\phi^{p-1}_{k,\ell+1} - b_{k,\ell}\phi^{p-1}_{k,\ell-1} + h_{k,\ell}\phi^{p-1}_{k,\ell} \qquad (2.4.45)$$

As written above, the equation is called an "implicit" equation, since we require knowledge of the elements of the left-hand side simultaneously (i.e., the same index p). However, the right-hand side is known and hence (2.4.45) is in reality a 3-point difference relation. The method of matrix factorization can be used to solve for $\phi^{p}_{k,\ell}$ (all k). Therefore, we compute an entire set of lines "ℓ" by a very rapid method.

After solving in one direction, we rotate the direction of solution and solve an equation of the form

$$t_{k,\ell}\phi^{p+1}_{k,\ell+1} + b_{k,\ell}\phi^{p+1}_{k,\ell-1} - h_{k,\ell}\phi^{p+1}_{k,\ell} =$$

$$= d_{k,\ell} - r_{k,\ell}\phi^{p}_{k+1,\ell} - \ell_{k,\ell}\phi^{p}_{k-1,\ell} + g_{k,\ell}\phi^{p}_{k,\ell} \qquad (2.4.46)$$

The method of matrix factorization is again used. The reason for the alternating direction is to insure that the method converges.

There are many other techniques for solving sets of simultaneous equations. Particular mention should be given to the "method of steepest descent" and the "method of conjugate gradients". We shall not examine the procedures in detail here.

2.5 RÉSUMÉ OF NUMERICAL SOLUTIONS OF MULTI-GROUP EQUATIONS

In this section, we review the material of the report and indicate how an actual problem is solved.

The initial steps consist of deciding upon the group sizes for the discretization of the lethargy space. The decision is based upon the element mixtures and the cross sections of the elements. One must then compute the coefficients of the group equations. The process involves integration by machine or graphically.

The finite difference equations are derived and, based upon the net spacing in the assembly, the various spatial dependent coefficients are computed.

The method of solving the simultaneous equation may be direct or iterative. Usually, iterative methods are used for all but the simplest of problems. An initial source estimate is made and the fission source terms are computed. Beginning with the highest energy group, the difference equations are solved. It should be noted that one may have to iterate many times within a group to obtain a consistent flux distribution for a given source configuration. The process of solving the equations within a single group is called an "inner iteration". One proceeds from the higher lethargy groups to the lower groups, iterating within each group until the group fluxes are consistent. After the thermal group equation is satisfied, the source function is recomputed. (For criticality studies, the multiplication factor is computed.) If the source function, (multiplication factor), is not steady, then the entire cycle is begun again. The iteration on the source function (or multiplication factor) is called an "outer iteration".

Variants on the above process are possible; for instance, inner iteration may be bypassed in the computation, etc.

For criticality problems, an additional difficulty is encountered. If the multiplication factor is less than unity, the neutron population will approach zero. The same effect occurs in the numerical process of solving the multi-group equation. In order to avoid generating the trivial solution, one usually "normalizes" the source. That is, one computes the source function to be a given number of neutrons. If the number predicted after an iteration is less than the initial estimate, then the source function is rescaled by a constant factor such that the source is back to its original strength. The rescaling factor is, in fact, just the multiplication predicted. A similar argument holds for super-critical assemblies.

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