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HALF-SPACE MULTIGROUP TRANSPORT THEORY IN PLANE GEOMETRY

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ABSTRACT

In this dissertation exact solutions to the isotropic multigroup neutron transport equation for various half-space problems in plane-geometry are obtained. These solutions are obtained by combining the techniques of Chandrasekhar's principle of invariance and Case's singular eigenfunctions expansion, and extending them to the multigroup case. The main advantage of the present method over previous half-space techniques is that it is less complicated and numerical evaluation, particularly for emergent distributions, is far simpler.

The albedo problem is found to be of fundamental importance for half-space problems, since the solutions of all the other problems can be expressed in of the albedo solution. The albedo problem is solved in two distinct steps. First the emergent distribution is calculated. By considering a singular eigenfunction expansion for the albedo problem, an inhomogeneous Fredholm equation for this emergent distribution is obtained. This equation is, however, difficult to evaluate numerically since it involves computation of the N-group eigenfunctions. By using Chandrasekhar's invariance principle, a nonlinear integral equation for the emergent distribution can be obtained. This equation is easily solved by numerical iteration. Once this emergent distribution is known, the known full range completeness and orthogonality relations of the eigenfunctions are used to obtain the angular flux inside the half-space.

From the albedo problem solution, the solutions of the other half-space problems are obtained. As an example, a computer code has been developed which gives the emergent distribution to the Milne problem and its extrapolation length for any number of energy groups.

Finally for the special case of a symmetric transfer matrix (as is found in thermal neutron transport problems, and certain radiative transfer cases) it is shown how the results for a general transfer matrix can be greatly simplified. For this case, uniqueness of solution of the Fredholm equation, reality of the eigenvalues of the transport equation, and half-range completeness of the eigenfunctions can be easily proven.

CHAPTER I

INTRODUCTION

During the past three decades, much effort has been expended in investigating the neutron transport equation. The interest and importance of the properties of the transport equation are reflected by the vast number of papers and many comprehensive books on the subject. Yet, despite all the extensive research, exact solutions have been obtained only for specially idealized situations. Even with the present generation of high-seed computers, it has not been possible to solve numerically the neutron transport equation in its full generality.

Very few realistic problems are described well by a version of the transport equation which is sufficiently simplified to permit an exact analytical solution. For instance, reactor design requires the solution of an energy-dependent transport equation in a medium with often rapidly varying material properties; on the other hand, exact solutions of the transport equation have been obtained primarily for the one-speed approximation and physical situations no more complicated than adjacent half-spaces.[1-4]

In the past few years the energy-dependent transport equation has begun to receive much attention. The present situation in the energy-dependent theory, however, is far less satisfactory than in the one-speed case. Analytic solutions have been obtained only for a very few idealized situations and for grossly oversimplified physical models. Whenever these analytic

methods are applied to realistic problems of practical technical interest, they usually become untractable or so time-consuming as to become worthless as a practical computational technique.[5] As a result engineers have come to rely upon very crude approximations together with elaborate computational schemes. For example, reactor designers use almost exclusively the multi-group diffusion approximation for finding the neutron flux distribution in fast and intermediate reactors.[6]

However, investigation of the energy-dependent transport equation does have some valid justification, aside from its own inherent beauty. The exact solution of idealized problems serves as useful standards against which the rougher methods used in engineering can be compared. Further, the analytic study of the transport equation in a form which only roughly models some physical situation, may give some previously unknown information about the physics of the actual problem. This is particularly true of problems which traditionally are treated by techniques that "hide" the inherent physics (e.g., computer simulations, Monte Carlo calculations, etc.). Finally, there is always the hope that one of the exact methods can in some approximate way be extended to an area of practical importance.

One of the most successful techniques in the monoenergetic treatment of the transport equation is the singular eigenfunction expansion method of Case.[7] The generalization of this method to the continuous energy-dependent case in plane geometry has been done by Bednarz and Mika,[8] and while quite general, it is highly formalistic and limited to infinite medium problems. To extend the

singular eigenfunction method to energy-dependent half-space problems, two different approximations have come into wide use.

The first maintains the continuous energy dependence in the transport equation but assumes very special forms of the energy dependence of the cross sections. Exact solutions have so far been limited to non-multiplying media with degenerate scattering kernels,[5,9,10] or to the constant cross section case.[11] For these cases, with two exceptions, the analytic solutions and the reduction of these solutions to numerics are highly non-trivial. These two special half-space problems are the constant cross section case,[11] and the completely seperable kernel model.[12-14] Both of these problems can be handled is a manner similar to the one-speed case.

An alternative approach for solving half-space problems is to use the multigroup formulation which splits the continuous energy range into N distinct regions over which the cross sections are assumed constant. The eigenfunctions to the N-group isotropic transport equation and their "full-range completeness" property (whereby the solution of any infinite medium problem can be expanded uniquely in terms of these eigenfunctions) have been known for several years.[15,16] Recently their full-range orthogonality relations and the solution of the infinite medium Green's function have been obtained for the two-group[17] and N-group[16] cases. Until now, however, the solution of half-space problems has been limited to special cases. Several two-group problems have been investigated.[18,19] In a paper on radiative transfer by Siewert and Zweifel full-range and "half-range completeness" of the eigenfunctions (whereby the solution to any half-space problem can be expanded uniquely in terms of only half of the eigenfunctions)

for the N-group case were proved with the specific restriction that the determinants of the transfer matrix, $\underset{\sim}{C}$, and all its minors vanished.[20] Finally, Leonard and Ferziger have shown that the N-term degenerate kernel for thermal neutrons in a nonmultiplying medium can be reduced to the N-group transport equation with a symmetric transfer matrix.[9,10] For this symmetric $\underset{\sim}{C}$ case half-range completeness can be proved and, in principle, closed form solutions to half-range problems be obtained although thus far none have been.

The purpose of this work, therefore, is to consider half-space problems of the N-group isotropic transport equation with a completely arbitrary transfer matrix. All previous energy-dependent half-space investigations have depended fundamentally upon a half-range completeness theorem. Furthermore this theorem has always been constructive in the sense that it explicitly demonstrated how the expansion coefficients could be calculated from the given boundary conditions. For energy-dependent problems, such constructive theorms tend to be exceedingly complex. In view of this situation several authors have tried various alternative schemes to avoid the half-range formalism. Fuchs and Collatz[21] and Zelazny[22] have favoured an iteration scheme for slab problems based on full-range rather than on half-range expansions. Case also has developed a very general method which when applied to half-space problems, completely avoids eigenfunction expansions altogether.[23] In this method all that is required is a knowledge of the infinite medium Green's function.

Recently a different approach has been used by Pahor to circumvent the half-range expansion difficulties.[24,25] By applying the invariance principles of Ambarzumian[26] and Chandrasekhar[27] to the singular eigenfunction of the thermal

neutron degenerate kernel case, he derived the emergent angular distribution for half-space problems from a nonlinear integral equation. Once the emergent distribution is known, then the simpler full-range singular eignefunction expansions can be used to obtain the complete solution. It is this approach which here is extended to the general multigroup situation.

The plan of the present research is as follows: Chapter II reviews the known results of the N-group infinite medium eigenfunctions and the adjoint eigenfunctions as developed by Zelazny[15] and Yoshimura.[16] The full-range orthogonality and completness properties of these eigenfunctions are then used to solve the infinite medium Green's function problem.

The next two chapters deal with the emergent distribution of the albedo problem. Consideration of the N different albedo problems (one for source neutrons belonging to each energy group) leads to a generalized $\underset{\sim}{S}$-function. This matrix function assumes the same important role in multigroup theory as does the scalar Ambarzumian-Chandrasekhar $\underset{\sim}{S}$-function in the one-speed situation.[27] From use of the principle of invariance, a non-linear integral equation for the $\underset{\sim}{S}$-matrix is derived. This equation demonstrates that the $\underset{\sim}{S}$-matrix, a function of two variables, can be decomposed into a product of two other matrices, $\underset{\sim}{U}$ and $\underset{\sim}{V}$, each of which is a function of only one variable. The nonlinear integral equations for these, $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices, which are analogous to the $\underset{\sim}{H}$-function in the one-speed case, are amenable to solution by numerical means. Once the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices are known the emergent distribution for the albedo problem can then easily be found.

An alternative approach to the albedo problem is then considered. From a full-range eigenfunction expansion of the albedo problem and the adjoint albedo problem, a pair of regular inhomogeneous Fredholm equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices are obtained. These Fredholm equations, along with associated singular integral equations, have been solved analytically only for the one-speed case.[23] Nevertheless standard numerical techniques can be applied to solve for $\underset{\sim}{U}$ and $\underset{\sim}{V}$. For a certain class of problems, namely for systems near criticality, these equations can yield a good analytic approximation for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions.

Chapter IV shows how for the special case of symmetric transfer, as is found in certain thermal systems for example, the results of the previous chapter are greatly simplified. In particular, the $\underset{\sim}{V}$-matrix becomes simply the transpose of the $\underset{\sim}{U}$-matrix. Hence only one nonlinear integral equation or Fredholm equation need be solved. For symmetric $\underset{\sim}{C}$, other very useful results can be derived. It can be shown that all the eigenvalues are real (a requirement, which while physically necessary, had to be assumed for the general case). The reality of the eigenvalues then permits one to prove the existence and uniqueness of solution of the Fredholm equation for $\underset{\sim}{U}$. This uniqueness property implies that the eigenvectors are half-range complete—a result recently proved by Leonard and Ferziger in a much more complicated fashion.[10]

In Chapter V it is demonstrated how the emergent distribution of other half-space problems (Milne's and Green's function) can be expressed directly in terms of the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions (or equivalently the generalized $\underset{\sim}{S}$-function.) Then once the emergent distributions have been calculated, the complete solutions

inside the half-space are readily obtained from application of the full-range orthogonality and completeness of the eigenfunctions.

To demonstrate the usefulness of the $\underset{\sim}{U}$ and $\underset{\sim}{V}$-matrices and the ease with which they are computed from the nonlinear integral equations, Chapter VI presents several numerical examples. The Milne problem is considered for several different media and the emergent distributions and extrapolation lengths are explicitly evaluated. To this end, a series of computer programs for general N and arbitrary $\underset{\sim}{C}$ have been written. The listings of these programs are given in the Appendix.

To summarize, it is the purpose of this work to demonstrate how various half-space problems encountered in multigroup theory can be solved without recourse to a half-range completeness property of the infinite medium eigenfunctions. The overall approach has been to show that these problems may be solved in two distinct steps. First the emergent distribution can be expressed with the help of two fundamental matrix functions; and then full-range expansions can be used to generate the complete angular density.

CHAPTER II

MULTIGROUP TRANSPORT EQUATION EIGENFUNCTIONS

The time-independent multigroup neutron transport equation for isotopic scattering in plane geometry can be written in the form

$$\mu \frac{\partial}{\partial x} \underset{\sim}{\psi}(x,\mu) + \underset{\sim}{\Sigma}\, \underset{\sim}{\psi}(x,\mu) = \underset{\sim}{C} \int_{-1}^{1} d\mu' \; \underset{\sim}{\psi}(x,\mu') \quad . \tag{2.1}$$

The vector $\underset{\sim}{\psi}(x,\mu)$ is an N-component vector (where N is the number of energy groups), of which the ith component, $\psi_i(x,\mu)$, is the angular flux of the ith group. The components of the matrix, $\underset{\sim}{\Sigma}$, are given by $\sigma_i \, \delta_{ij}$, σ_i being the total interaction cross section for the ith group. Finally, the elements, c_{ij}, of the transfer matrix, $\underset{\sim}{C}$, describe the transfer of neutrons from the jth group to the ith group. For an isotropically scattering and fissioning medium the c_{ij}'s are given by

$$c_{ij} = \frac{1}{2} \sigma^{s}_{j\to i} + \frac{1}{2} \chi_i \, \nu_j \, \sigma^{f}_{j} \tag{2.2}$$

where $\sigma^{s}_{j\to i}$ is the scattering cross section (both elastic and inelastic) for the transfer of neutrons from the jth group to the ith group, σ^{f}_{j} is the fission cross section for the jth group, ν_j the number of fission neutrons produced by an incident jth group neutron, and χ_i is the fission spectrum fraction of the ith group.

It is always possible to order the groups such that (see Section 4.1)

$$\sigma_1 > \sigma_2 > \ldots > \sigma_N \tag{2.3}$$

and by dividing Eq. (2.1) by σ_N and measuring distance in units of the smallest mean free path, $1/\sigma_N$, one may set $\sigma_N = 1$.[20] In the following discussion it will be assumed that the normalizing factor $1/\sigma_N$ is included in the σ_i's and c_{ij}'s.

In this chapter the infinite medium eigenfunctions and eigenvectors to the transport equation (2.1), and its adjoint, are reviewed. The orthogonality and full-range completeness properties of these eigenvectors are then discussed. Finally as an example of the application of these eigenvectors, the infinite medium Green's function problem is solved.

2.1 INFINITE MEDIUM EIGENVECTORS AND ADJOINT EIGENVECTORS

Using the analogy of the one-speed problem,[1] a set of eigenfunctions solutions, $\underset{\sim}{\psi}(\nu,x,\mu)$ to Eq. (2.1) of the form

$$\underset{\sim}{\psi}(\nu,x,\mu) = e^{-x/\nu}\, \underset{\sim}{\phi}(\nu,\mu) \tag{2.4}$$

is sought. Substituting this ansatz into Eq. (2.1), the following equation for the eigenvectors, $\underset{\sim}{\phi}(\nu,\mu)$ is obtained:

$$(\underset{\sim}{\Sigma} - \frac{\mu}{\nu}\underset{\sim}{E})\,\underset{\sim}{\phi}(\nu,\mu) = \underset{\sim}{C}\int_{-1}^{1} d\mu'\, \underset{\sim}{\phi}(\nu,\mu') \quad , \tag{2.5}$$

where $\underset{\sim}{E}$ is the unit matrix. Different but equivalent forms for these eigenvectors have been obtained by several authors.[16-18] In this thesis the simple notation (with slight changes) and approach of Yoshimura[16] will be used.

The eigenvectors can be written in the form

$$\underset{\sim}{\phi}(\nu,\mu) = P\,\underset{\sim}{F}(\nu,\mu)\,\underset{\sim}{b}(\nu) + \underset{\sim}{G}(\nu,\mu)\,\underset{\sim}{\lambda}(\nu) \quad , \tag{2.6}$$

where P indicates the Cauchy principal value. The matrices $\underset{\sim}{F}$ and $\underset{\sim}{D}$ are defined as

$$[\underset{\sim}{F}(z,\mu)]_{ij} = \frac{z}{\sigma_i z - \mu}\,\delta_{ij} \quad , \tag{2.7}$$

and

$$[\underset{\sim}{G}(z,\mu)]_{ij} = \delta(\sigma_i z - \mu)\,\delta_{ij} \quad , \tag{2.8}$$

and the vector $\underset{\sim}{b}(\nu)$, which has yet to be determined, satisfies

$$\underset{\sim}{b}(\nu) = \underset{\sim}{C}\int_{-1}^{1} d\mu'\ \underset{\sim}{\phi}(\nu,\mu') \equiv \underset{\sim}{C}\ \underset{\sim}{a}(\nu) \tag{2.9}$$

Substitution of Eq. (2.6) into Eq. (2.9) yields the following simultaneous equation for the unknown vectors $\underset{\sim}{b}(\nu)$ and $\underset{\sim}{\lambda}(\nu)$:

$$\underset{\sim}{\Omega}(\nu)\,\underset{\sim}{b}(\nu) = \int_{-1}^{1} d\mu\ \underset{\sim}{G}(\nu,\mu)\,\underset{\sim}{\lambda}(\nu) \quad , \tag{2.10}$$

where

$$\underset{\sim}{\Omega}(z) = \underset{\sim}{C}^{-1} - P\int_{-1}^{1} \underset{\sim}{F}(z,\mu)\,d\mu \quad . \tag{2.11}$$

To solve for $\underset{\sim}{b}(\nu)$ and $\underset{\sim}{\lambda}(\nu)$ it is necessary to divide the eigenvalue spectrum into two regions.

Region I: $\nu \notin (-1,1)$—Discrete spectrum

On this region the eigenvalues are denoted by ν_o, and Eq. (2.10) immediately yields

$$\underset{\sim}{\Omega}(\nu_o)\,\underset{\sim}{b}(\nu_o) = 0 \quad . \tag{2.12}$$

For this equation to have a nontrivial solution, the following condition must be satisfied:

$$\det \underset{\sim}{\Omega}(\nu_o) = 0 \quad . \tag{2.13}$$

Equation (2.13) is the general N-group dispersion relation which gives an even number, say 2M, of discrete eigenvalues. For simplicity it will be assumed all these eigenvalues are distinct. For each root, ν_o, the vector $\underset{\sim}{b}(\nu_o)$ is determined from Eq. (2.12) and a normalization condition $|\underset{\sim}{b}(\nu_o)| = 1$. The $\underset{\sim}{\lambda}(\nu_o)$ vector is completely arbitrary with the provision it has a finite norm. For convenience the null vector will be chosen for $\underset{\sim}{\lambda}(\nu_o)$. Thus, in component form, the discrete eigenvectors may be written as

$$\phi_i(\nu_o,\mu) = \frac{\nu_o\, b_i(\nu_o)}{\sigma_i \nu_o - \mu} \quad , \; i = 1 \sim N, \; |\nu_o| > 1 \quad . \tag{2.14}$$

From Eq. (2.11) it is easily verified that if ν_o is an eigenvalue then $-\nu_o$ and ν_o^* (complex conjugate) are eigenvalues with

$$\underset{\sim}{b}(\nu_o) = \underset{\sim}{b}(-\nu_o) = \underset{\sim}{b}^*(\nu_o^*) \quad . \tag{2.15}$$

For the special case of symmetric $\underset{\sim}{C}$, it can be proved (Chapter IV) that all the eigenvalues are real or imaginary, and in Appendix A it is shown for any subcritical system the eigenvalues are always real. For a general system, on the other hand, there is no a priori reason to suspect that all the discrete eigenvalues are necessarily real. However, from physical grounds, a subcritical infinite medium must not have any imaginary discrete roots, and the dominant root (defined as the root with the largest real part) must be real. An eigenfunction expansion for a realistic problem which has imaginary

eigenvalues or a complex dominant root would produce an oscillatory behavior at large source distances and hence negative fluxes.

For the purposes of this thesis, it will be assumed that the medium is subcritical, and that all the discrete eigenvalues are nonmultiple and finite.

Region II: $\nu\epsilon(-1,1)$ Continuum Spectrum

This region is divided into N subintervals, ν_j, $j = 1 \sim N$ such that for $\nu\epsilon\nu_j$, $\eta_{j-1} < |\nu| \leq \eta_j$ where η_j is defined as $1/\sigma_j$ and $\eta_o = 0$. Without loss of generality, one may consider only the jth subinterval. First decompose the $\underset{\sim}{\Omega}(\nu)$ matrix and $\underset{\sim}{b}(\nu)$ and $\underset{\sim}{\lambda}(\nu)$ vectors as shown below:

$$\underset{\sim}{\Omega}(\nu) = \begin{array}{|c|c|}\hline \underset{\sim}{\Omega}_1 & \underset{\sim}{\Omega}_2 \\ \hline \underset{\sim}{\Omega}_3 & \underset{\sim}{\Omega}_4 \\ \hline \end{array} \quad \begin{array}{l} 1 \\ j \\ N \end{array} \qquad \underset{\sim}{b}(\nu) = \begin{array}{|c|}\hline \underset{\sim}{b}_1 \\ \hline \underset{\sim}{b}_2 \\ \hline \end{array} \quad \begin{array}{l} 1 \\ j \\ N \end{array} \qquad \underset{\sim}{\lambda}(\nu) = \begin{array}{|c|}\hline \underset{\sim}{\lambda}_1 \\ \hline \underset{\sim}{\lambda}_2 \\ \hline \end{array} \quad \begin{array}{l} 1 \\ j \\ N \end{array} \tag{2.16}$$

The vectors $\underset{\sim}{b}_1$ and $\underset{\sim}{\lambda}_1$ are (j-1) component vectors, $\underset{\sim}{b}_2$ and $\underset{\sim}{\lambda}_2$ are (N-j+1) component vectors, and $\underset{\sim}{\Omega}_1$ and $\underset{\sim}{\Omega}_4$ are square matrices of size (j-1) and (N-j+1) respectively. The matrices $\underset{\sim}{\Omega}_2$ and $\underset{\sim}{\Omega}_3$ are rectangular of size (N-j+1) x (j-1) and (j-1) x (N-j+1), respectively. With these definitions. Eq. (2.10) can be written as

$$\underset{\sim}{\Omega}_1(\nu)\,\underset{\sim}{b}_1(\nu) + \underset{\sim}{\Omega}_2\,\underset{\sim}{b}_2(\nu) = 0 \ , \tag{2.16a}$$

$$\underset{\sim}{\Omega}_3 \underset{\sim}{b}_1(\nu) + \underset{\sim}{\Omega}_4(\nu) \underset{\sim}{b}_2(\nu) = \underset{\sim}{\lambda}_2(\nu) \quad . \tag{2.16b}$$

This system of N equations has (2N-j+1) unknowns [(N-j+1) λ's and N b's]. Thus one must specify the values of (N-j+1) of these unknowns to obtain a solution. Let these be the (N-j+1) components of the vector $\underset{\sim}{b}_2(\nu)$. But there are (N-j+1) linearly independent choices of $\underset{\sim}{b}_2(\nu)$ which satisfy Eqs. (2.16a) and (2.16b), and hence there is an (N-j+1) fold degeneracy in the eigenvectors for the jth region. An obvious choice for the (N-j+1) $\underset{\sim}{b}_2$'s is[16]

$$\underset{\sim}{b}_2^m(\nu) = \underset{\sim}{e}_{(m-j+1)} \quad , \; m = j \sim N \quad , \tag{2.17}$$

where $\underset{\sim}{e}_i$ is an (N-j+1) dimensional vector all of whose components are zero, except the ith which is equal to unity.

Corresponding to each vector $\underset{\sim}{b}_2^m$ there is a vector $\underset{\sim}{\lambda}^m(\nu)$. From Eqs. (2.16a) and (2.16b) one obtains

$$\underset{\sim}{b}_1^m(\nu) = -\underset{\sim}{\Omega}^{-1}(\nu) \underset{\sim}{\Omega}_2 \underset{\sim}{b}_2^m \quad , \tag{2.18}$$

and

$$\underset{\sim}{\lambda}_2^m(\nu) = [\underset{\sim}{\Omega}_4 - \underset{\sim}{\Omega}_3 \Omega_1^{-1}(\nu) \underset{\sim}{\Omega}_2] \underset{\sim}{b}_2^m \quad . \tag{2.19}$$

where it is assumed $\underset{\sim}{\Omega}^{-1}(\nu)$ exists for $\nu\epsilon(-1,1)$. Since $\underset{\sim}{\lambda}_1^m(\nu)$ can be choosen arbitrarily, it is set equal to the null vector. Then from Eqs. (2.16a) and (2.16b), $\underset{\sim}{\lambda}^m(\nu)$ is determined completely from

$$\underset{\sim}{\lambda}^m(\nu) = \underset{\sim}{\Omega}(\nu) \underset{\sim}{b}^m(\nu) \quad . \tag{2.20}$$

Thus for the jth subinterval, the eigenvectors, in component form, may be written as

$$[\underset{\sim}{\phi}_j^m(\nu,\mu)]_i = P\frac{\nu[\underset{\sim}{b}^m(\nu)]_i}{\sigma_i\nu - \mu} + (\sigma_i\nu - \mu)[\underset{\sim}{\lambda}^m(\nu)]_i \quad , \qquad (2.21)$$

$$j = 1 \sim N,\ m = j \sim N,$$

where $\underset{\sim}{b}^m(\nu)$ and $\underset{\sim}{\lambda}^m(\nu)$ are determined from Eqs. (2.18) and (2.20), respectively. In passing, it should be noted that $\underset{\sim}{b}^m(\nu)$ and $\underset{\sim}{\lambda}^m(\nu)$ are even functions of ν and hence the eigenvectors $\underset{\sim}{\phi}(\nu,\mu)$ have the property

$$\underset{\sim}{\phi}(\nu,-\mu) = \underset{\sim}{\phi}(-\nu,\mu) \quad . \qquad (2.22)$$

Before discussing the orthogonality and completeness properties of the infinite medium eigenfunctions, it is necessary to introduce the adjoint eigenvectors. The adjoint equation of Eq. (2.1) is defined to be[16,17]

$$-\mu\frac{\partial}{\partial x}\underset{\sim}{\psi}^\dagger(x,\mu) + \underset{\sim}{\Sigma}\underset{\sim}{\psi}^\dagger(x,\mu) = \underset{\sim}{\tilde{C}}\int_{-1}^{1} d\mu'\ \underset{\sim}{\psi}^\dagger(x,\mu') \qquad (2.23)$$

where $\underset{\sim}{\psi}^\dagger(x,\mu)$ is the adjoint angular flux and the tilde denotes the transpose matrix operator. As before, the adjoint eigenfunctions, $\underset{\sim}{\psi}^\dagger(\nu,x,\mu)$, are defined as

$$\underset{\sim}{\psi}^\dagger(\nu,x,\mu) = e^{+x/\nu}\,\underset{\sim}{\phi}^\dagger(\nu,\mu) \quad . \qquad (2.24)$$

The adjoint eigenvector equation becomes

$$(\underset{\sim}{\Sigma} - \frac{\mu}{\nu}\underset{\sim}{E})\,\underset{\sim}{\phi}^\dagger(\nu,\mu) = \underset{\sim}{\tilde{C}}\int_{-1}^{1} d\mu\ \phi^\dagger(\nu,\mu) \quad . \qquad (2.25)$$

This eigenvector equation is precisely the same as Eq. (2.5) with $\underset{\sim}{C}$ replaced by $\underset{\sim}{\tilde{C}}$. The adjoint equation has exactly the same spectrum as that obtained for the infinite medium direct eigenvalues. Thus one has

$$\underset{\sim}{\phi}^{\dagger}(\nu,\mu,\underset{\sim}{C}) = \underset{\sim}{\phi}(\nu,\mu,\underset{\sim}{\tilde{C}}) \quad , \tag{2.26}$$

i.e., the adjoint eigenvectors are obtained by simply replacing c_{ij} by c_{ji} in the ordinary infinite medium eigenvectors.

In this work these adjoint eigenvectors are denoted by

$$\phi_i^{\dagger}(\nu_o,\mu) = \frac{\nu_o[\underset{\sim}{b}^{\dagger}(\nu_o)]_i}{\sigma_i\nu_o - \mu}, \quad \nu_o \in (-1,1), \tag{2.27}$$

and

$$[\underset{\sim}{\phi}_j^{\dagger_m}(\nu,\mu)]_i = P\frac{\nu\left[\underset{\sim}{b}^{\dagger_m}(\nu)\right]_i}{\sigma_i\nu - \mu} + \delta(\sigma_i\nu - \mu)\left[\underset{\sim}{\lambda}^{\dagger_m}(\nu)\right]_i \quad , \quad \nu \in (-1,1). \tag{2.28}$$

Their normalization is written as

$$\underset{\sim}{a}^{\dagger}(\nu_o) = \int_{-1}^{1} d\mu\, \underset{\sim}{\phi}^{\dagger}(\nu_o,\mu) \tag{2.29a}$$

$$\underset{\sim}{a}_j^{\dagger_m}(\nu) = \int_{-1}^{1} d\mu\, \underset{\sim}{\phi}_j^{\dagger_m}(\nu,\mu) \quad . \tag{2.29b}$$

Finally, one can verify that these adjoint eigenvectors satisfy the relationship

$$\underset{\sim}{\phi}^{\dagger}(\nu,-\mu) = \underset{\sim}{\phi}^{\dagger}(-\nu,\mu) \quad . \tag{2.29c}$$

2.2 FULL-RANGE COMPLETENESS

The eigenvectors, $\underset{\sim}{\phi}(\nu,\mu)$, discussed in Section 2.1 have the very useful

property that they are "full-range complete." This property may be stated in the form of the following theorem.

Theorem. The set of functions $\underset{\sim}{\phi}(\nu,\mu)$ for all $\nu\epsilon$ to the eigenvalue spectrum is complete, in the sense that an arbitrary function $\underset{\sim}{\psi}(\mu)$ defined for $\mu\epsilon[-1,1]$ can be expanded in the form

$$\underset{\sim}{\psi}(\mu) = \sum_{s=1}^{M} a_{+s}\, \underset{\sim}{\phi}(\nu_{os},\mu) + \sum_{s=1}^{M} a_{-s}\, \underset{\sim}{\phi}(-\nu_{os},\mu)$$

$$+ \sum_{j=1}^{N} \int_{\nu_j} d\nu \left\{ \sum_{m=j}^{N} A_j^m(\nu)\, \underset{\sim}{\phi}_j^m(\nu,\mu) \right\} , \qquad (2.30)$$

where a_{+s}, a_{-s} and $A_j^m(\nu)$ are uniquely determined expansion coefficients.

This theorem has been proved in various forms by several authors. Zelazny and Kuszell[18] tried to prove it by obtaining a set of Fredholm equations for the expansion coefficients. However it was not shown that the solution of these Fredholm equations existed or was unique. Special proofs of completeness for particular cases of the transfer matrix have been obtained—e.g., symmetric $\underset{\sim}{C}$,[9] two-group case,[17] and $\det|\underset{\sim}{C}| = 0$.[20] A proof by the method of construction[6] for general N-dimensional $\underset{\sim}{C}$ has been recently obtained by Yoshimura,[16] and it is his proof, with some modification and correction which will be given here. First consider the vector $\underset{\sim}{\psi}'(\mu)$ defined as

$$\underset{\sim}{\psi}'(\mu) = \underset{\sim}{\psi}(\mu) - \sum_{s=1}^{M} \left\{ a_{+s}\, \underset{\sim}{\phi}(\nu_{os},\mu) - a_{-s}\, \underset{\sim}{\phi}(-\nu_{os},\mu) \right\} , \qquad (2.31)$$

where M is the number of discrete pairs of roots. To prove this theorem it is sufficient to show that the function $\underset{\sim}{\psi}'(\mu)$ can be expanded solely in terms of the continuum modes, i.e.,

$$\underset{\sim}{\psi}'(\mu) = \sum_{j=1}^{N} \int_{\nu_j} d\nu \left\{ \sum_{m=j}^{N} A_j^m(\nu) \underset{\sim}{\phi}_j^m(\nu,\mu) \right\} . \tag{2.32}$$

If the coefficients $A_j^m(\nu)$ exist, then one can define the two vectors $\underset{\sim}{\eta}(\nu)$ and $\underset{\sim}{\zeta}(\nu)$ such that for $\nu \epsilon \nu_j$

$$\underset{\sim}{\eta}(\nu) = \sum_{m=j}^{N} A_j^m(\nu) \underset{\sim}{b}_j^m(\nu) , \tag{2.33}$$

and

$$\underset{\sim}{\zeta}(\nu) = \sum_{m=j}^{N} A_j^m(\nu) \underset{\sim}{\lambda}_j^m(\nu) . \tag{2.34}$$

From Eq. (2.20) one has

$$\underset{\sim}{\zeta}(\nu) = \underset{\sim}{\Omega}(\nu) \underset{\sim}{\eta}(\nu) , \tag{2.35}$$

and using the explicit form of $\phi_j^m(\nu,\mu)$, Eq. (2.25) becomes

$$\psi_i'(\mu) = \sum_{j=1}^{N} \int_{\nu_j} d\nu \left\{ P \frac{\nu}{\sigma_i \nu - \mu} \eta_i(\nu) + \delta(\sigma_i \nu - \mu) \zeta_i(\nu) \right\} , \tag{2.36}$$

or equivalently

$$\psi_i'(\mu) = \int_{-1}^{1} d\nu \left\{ P \frac{\nu}{\sigma_i \nu - \mu} \eta_i(\nu) + \delta(\sigma_i \nu - \mu) \zeta_i(\nu) \right\} . \tag{2.36a}$$

Replacement of μ by $\sigma_i \mu'$ in Eq. (2.36a) yields

$$\sigma_i \psi_i'(\sigma_i \mu') = \int_{-1}^{1} d\nu \left\{ \frac{P\nu}{\nu - \mu'} \eta_i(\nu) + \delta(\nu - \mu') \zeta_i(\nu) \right\} , \tag{2.37}$$

$$-\frac{1}{\sigma_i} \leq \mu' \leq \frac{1}{\sigma_i} ,$$

or in vector form

$$\underset{\sim}{\Sigma}\,\underset{\sim}{\psi}'(\sigma\mu') = P\int_{-1}^{1} d\nu\,\frac{\nu}{\nu-\mu'}\,\underset{\sim}{\eta}(\nu) + \underset{\sim}{\zeta}(\mu') \quad . \tag{2.38}$$

Now introduce the vector

$$\underset{\sim}{N}(z) = \frac{1}{2\pi i}\int_{-1}^{1}\frac{\nu d\nu}{\nu - z}\,\underset{\sim}{\eta}(\nu) \quad , \tag{2.39}$$

which has the following three properties:[28]

$$\text{(i)}\ \underset{\sim}{N}(z) \in A \text{ in the complex plane cut from } (-1,1), \tag{2.40}$$

$$\text{(ii)}\ \underset{\sim}{N}(z) \sim 1/z \text{ as } |z| \to \infty, \tag{2.41}$$

$$\text{(iii)}\ N^{\pm}(\mu) = \frac{1}{2\pi i}\,P\int_{-1}^{1} d\nu\,\frac{\nu}{\nu-\mu}\,\underset{\sim}{\eta}(\nu) \pm \frac{1}{2}\,\mu\,\underset{\sim}{\eta}(\mu),\ -1 \le \mu \le 1. \tag{2.42}$$

If one could solve for $\underset{\sim}{N}(z)$, then the vector $\underset{\sim}{\eta}(\mu)$ could be found from Eq. (2.40), and the expansion for $\underset{\sim}{\psi}'(\mu)$ would be determined. With this in mind define the matrix

$$\underset{\sim}{\Omega}'(z) = \underset{\sim}{C}^{-1} - \int_{-1}^{1} d\mu\,\underset{\sim}{F}(z,\mu) \quad . \tag{2.43}$$

(Note that $\underset{\sim}{\Omega}'(z)$ differs from the $\underset{\sim}{\Omega}(z)$ of Eq. (2.11) in which the integral is a principle value.) Applying the Plemelj formulae[29] to $\underset{\sim}{\Omega}'(z)$ one finds

$$\underset{\sim}{\Omega}'^{\pm}(\mu') = \underset{\sim}{\Omega}(\mu') \pm i\pi\mu'\,\underset{\sim}{E} \quad , \ (-1, \le \sigma\mu' \le 1). \tag{2.44}$$

Upon substitution from Eqs. (2.40) and (2.42), Eq. (2.36) may now be reduced to a Hilbert equation for the unknown vector $\underset{\sim}{N}(z)$,

$$\mu' \underset{\sim}{\Sigma} \underset{\sim}{\psi}'(\sigma\mu') = \underset{\sim}{\Omega}^{+}(\mu') \underset{\sim}{N}^{+}(\mu') - \underset{\sim}{\Omega}^{-}(\mu') \underset{\sim}{N}^{-}(\mu') \quad . \tag{2.45}$$

Since the vector $\underset{\sim}{\Omega}'(z)\underset{\sim}{N}(z)$ is analytic in the complex plane cut from (-1,1) and is required to vanish like $1/z$ as $|z| \to \infty$, the Cauchy integral theorem can be applied to prove that

$$\underset{\sim}{N}(z) = -\frac{1}{2\pi i} [\underset{\sim}{\Omega}'(z)]^{-1} \frac{1}{z} \int_{-1}^{1} d\mu \, \mu \, \underset{\sim}{F}(z,\mu) \, \underset{\sim}{\psi}'(\mu) \quad . \tag{2.46}$$

This function $\underset{\sim}{N}(z)$ has the required behavior except for $z = \pm\nu_{os}$, $s = 1 \sim M$ where $[\underset{\sim}{\Omega}'(z)]^{-1}$ does not exist. One can write

$$[\underset{\sim}{\Omega}'(z)]^{-1} = \frac{1}{\det|\underset{\sim}{\Omega}'(z)|} \underset{\sim}{\Omega}'_{c}(z) \tag{2.47}$$

where $\underset{\sim}{\Omega}'_{c}(z)$ is the matrix whose elements are the cofactors of $\underset{\sim}{\Omega}'(z)$. Then

$$\underset{\sim}{N}(z) = -\frac{1}{2\pi i} \frac{1}{z \det|\underset{\sim}{\Omega}'(z)|} \underset{\sim}{\Omega}'_{c}(z) \int_{-1}^{1} d\mu \, \mu \, \underset{\sim}{F}(z,\mu) \, \underset{\sim}{\psi}'(\mu) \quad , \tag{2.48}$$

and to remove the difficulty at $\pm\nu_{os}$, $s = 1 \sim M$ where $\det|\underset{\sim}{\Omega}'(z)|$ has single zeroes, one requires that the numerator also vanish. In component form this requirement is

$$\left[\int_{-1}^{1} d\mu \, \mu \, \underset{\sim}{F}(\pm\nu_{os},\mu) \, \underset{\sim}{\psi}'(\mu) \right]_{i} = 0 \quad , \; i = 1 \sim N, \; s = 1 \sim M. \tag{2.49}$$

Of course this condition is not true for an arbitrary $\underset{\sim}{\psi}'(\mu)$; however there are 2M unspecified conditions on $\underset{\sim}{\psi}'(\mu)$, namely the 2M $a_{\pm s}$, $(s = 1 \sim M)$. It can be verified, Eq. (2.44) will be satisfied if one chooses

$$a_{\pm s} = \frac{\int_{-1}^{1} d\mu\, \mu\, \tilde{\underset{\sim}{\phi}}^{\dagger}(\pm\nu_{os},\mu)\, \underset{\sim}{\psi}(\mu)}{\int_{-1}^{1} d\mu\, \mu\, \tilde{\underset{\sim}{\phi}}^{\dagger}(\pm\nu_{os},\mu)\, \underset{\sim}{\phi}(\pm\nu_{os},\mu)} \quad . \tag{2.50}$$

Hence $\underset{\sim}{N}(z)$ as given by Eq. (2.48) has all the required analytic properties. Therefore $\underset{\sim}{\eta}(\mu)$ exists and can be determined from Eq. (2.42).

2.3 ORTHOGONALITY AND NORMALIZATION OF EIGENVECTORS

The eigenvectors and adjoint eigenvectors are orthogonal to each other in the sense

$$\int_{-1}^{1} d\mu\, \mu\, \tilde{\underset{\sim}{\phi}}^{\dagger}(\nu,\mu)\, \underset{\sim}{\phi}(\nu',\mu) = 0 \quad , \quad \nu \neq \nu' . \tag{2.51}$$

This result immediately follows from Eqs. (2.5) and (2.25). Multiply Eq. (2.5) from the left by $\mu\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu,\mu)$ and the transpose of Eq. (2.25) from the right by $\mu\underset{\sim}{\phi}(\nu',\mu)$. Integrating these two scalar equations and subtracting one obtains

$$\left(\frac{1}{\nu'} - \frac{1}{\nu}\right)\int_{-1}^{1} d\mu\, \mu\, \tilde{\underset{\sim}{\phi}}^{\dagger}(\nu,\mu)\, \underset{\sim}{\phi}(\nu',\mu) = 0 \quad , \tag{2.52}$$

from which Eq. (2.29) follows.

Since this orthogonality property of the eigenvectors is to be used to determine the expansion coefficients in an eigenfunction expansion, one must determine the normalization intergrals. For Region I, $\nu \notin (-1,1)$, the normalization is defined as

$$\int_{-1}^{1} d\mu\ \mu\ \tilde{\phi}^{\dagger}(\pm\nu_{os},\mu)\ \tilde{\phi}(\pm\nu_{os'},\mu) = N_{\pm s}\delta_{ss'},\quad s',s = 1 \sim M \quad . \tag{2.53}$$

Straightforward integration of Eqs. (2.14) and (2.27) yields

$$N_{\pm s} = \pm\nu_{os}^{2} \sum_{i=1}^{N} b_i^{\dagger}(\nu_{os}) \left[\ell n \frac{\sigma_i \nu_{os} - 1}{\sigma_i \nu_{os} + 1} + \frac{2\sigma_i \nu_{os}}{\sigma_i^{2}\nu_{os}^{2} - 1} \right] b_i(\nu_{os}) \tag{2.54}$$

For Region II, $\nu\epsilon\nu_j$ defining,

$$\int_{-1}^{1} d\mu\ \mu\ \tilde{\phi}_j^{\dagger m'}(\nu,\mu)\ \tilde{\phi}_j^{m}(\nu',\mu) = N_j^{mm'}(\nu)\ \delta(\nu - \nu') \tag{2.55}$$

and using the Poincaré-Bertrand formula,[29] one obtains (after much algebra)[16]

$$N_j^{mm'}(\nu) = \pi^{2}\nu^{3}\ \tilde{b}_{j2}^{\dagger m'}\ \tilde{b}_{j2}^{m} + \nu\ \tilde{\lambda}_{j2}^{\dagger m'}(\nu)\ \tilde{\lambda}_{j2}^{m}(\nu) \quad , \tag{2.56}$$

or:

$$= \nu\ \tilde{b}_{j2}^{\dagger m'}\ \tilde{M}(\nu)\ \tilde{b}_{j2}^{m} \quad , \ m',m = j \sim N, \tag{2.57}$$

where the (N-j+1) dimensional matrix is defined as

$$\tilde{M}(\nu) = \{\pi^{2}\nu^{2}\tilde{E} + [\tilde{\Omega}_4(\nu) - \tilde{\Omega}_3\tilde{\Omega}^{-1}(\nu)\tilde{\Omega}_2]^{2}\} \quad . \tag{2.58}$$

Thus for the jth subinterval there are $(N-j+1)^{2}$ different $N_j^{mm'}(\nu)$ since the (N-j+1) fold degenerate eigenvectors of the jth region are not mutually orthogonal.

It would be convenient for theoretical purposes if these degenerate eigenvectors could be made mutually orthogonal. It the (N-j+1) eigenvectors of the matrix $\underset{\sim}{M}(\nu)$ had been chosen for the $\underset{\sim}{b}_2$'s and $\underset{\sim}{b}_2^+$'s instead of those given by Eq. (2.17), one would have

$$N_j^{mm'}(\nu) = N_j^m \delta_{mm'} \quad . \tag{2.59}$$

For the remainder of this work, it will be assumed that the degenerate "continuum" eigenvectors, $\underset{\sim}{\phi}_j^m(\nu,\mu)$ are also orthogonal.

2.4 INFINITE MEDIUM GREEN'S FUNCTION

An immediate application of the full-range completeness and orthogonality properties of the infinite medium eigenfunctions is to solve the infinite medium Green's function problem. Consider a unit plane source at the origin emitting q_i ith group neutrons per unit area per unit time in the direction μ_o. The angular density $\underset{\sim}{G}^\infty(o,\mu_o \to x,\mu) \equiv \underset{\sim}{G}^\infty(x,\mu)$ satisfies the homogeneous transport equation (2.1) except at the origin where the source can be replaced by the "jump condition"

$$[\underset{\sim}{G}^\infty(0^+,\mu) - \underset{\sim}{G}^\infty(0^-,\mu)] = \frac{1}{4\pi\mu} \delta(\mu - \mu_o) \underset{\sim}{q} \quad . \tag{2.60}$$

If the system is subcritical one has the boundary condition

$$\lim_{x \to \pm\infty} \underset{\sim}{G}^\infty(x,\mu) = \underset{\sim}{0} \quad . \tag{2.61}$$

Expansion of the solution in terms of the eigenfunctions which satisfy boundary condition (2.61), gives

$$\pm\underset{\sim}{G}^{\infty}(x,\mu) = \sum_{s=1}^{M} a_{\pm s}\, \underset{\sim}{\phi}(\pm\nu_{os},\mu)\, e^{\pm x/\nu_{os}}$$

$$+ \sum_{j=1}^{N} \int_{\pm\eta_{j-1}}^{\pm\eta_j} d\nu\, e^{-x/\nu} \left\{ \sum_{m=j}^{N} A_j^m(\nu)\, \underset{\sim}{\phi}_j^m(\nu,\mu) \right\} \quad , \; x \gtrless 0. \qquad (2.62)$$

Application of Eq. (2.60) yields

$$\frac{\delta(\mu - \mu_o)}{4\pi\mu}\, \underset{\sim}{q} = \sum_{s=1}^{M} \left\{ a_{+s}\, \underset{\sim}{\phi}(\nu_{os},\mu) + a_{-s}\, \underset{\sim}{\phi}(-\nu_{os},\mu) \right\}$$

$$+ \sum_{j=1}^{N} \int_{\nu_j} d\nu \left\{ \sum_{m=j}^{N} A_j^m(\nu)\, \phi_j^m(\nu,\mu) \right\} \quad , \qquad (2.63)$$

which is simply a full-range expansion of $(\delta(\mu-\mu_o)/4\pi\mu)\underset{\sim}{q}$. For simplicity, it will be assumed the $\underset{\sim}{\phi}_j^m$'s for $m = j \sim N$ have been constructed such that they are mutually orthogonal. Then the orthogonality results of the previous section immediately give for the expansion coefficients

$$a_{\pm s} = \frac{1}{N_{\pm s}} \int_{-1}^{1} d\mu\, \frac{\delta(\mu - \mu_o)}{4\pi}\, \underset{\sim}{\phi}^{\dagger}(\pm\nu_{os},\mu)\, \underset{\sim}{q} = \frac{\underset{\sim}{\phi}^{\dagger}(\pm\nu_{os},\mu_o)\underset{\sim}{q}}{4\pi\, N_{\pm s}} \quad , \qquad (2.64)$$

and

$$A_j^m(\nu) = \frac{1}{N_j^m(\nu)} \int_{-1}^{1} d\mu\, \frac{\delta(\mu - \mu_o)}{4\pi}\, \underset{\sim}{\phi}_j^{m\dagger}(\nu,\mu)\, \underset{\sim}{q} = \frac{\underset{\sim}{\phi}_j^{m\dagger}(\nu,\mu_o)\underset{\sim}{q}}{4\pi\, N_j^m(\nu)} \quad . \qquad (2.65)$$

CHAPTER III

THE ALBEDO PROBLEM

In many problems in transport theory, only the angular flux at the surface of a medium is needed. To this end, the half-space albedo problem will be considered in this chapter, since the emergent distribution of this particular problem turns out to be of fundamental importance in determing the emergent distributions of all other half-space problems. Once the emergent fluxes have been found, the interior distributions, if desired, can be obtained from these surface quantities by applying the full-range completeness and orthogonality properties of the infinite medium eigenfunctions which were obtained in Chapter II.[24]

The emergent distribution of the multigroup albedo problem can be expressed directly in terms of a generalized $\underset{\sim}{S}$-function matrix. To determine this $\underset{\sim}{S}$-function, two different approaches can be used to obtain equations suitable for its evaluation.

The first method derives a nonsingular, nonlinear integral equation for $\underset{\sim}{S}$ by using Chandrasekhar's "principle of invariance".[27] This equation demonstrates how the $\underset{\sim}{S}$-matrix, which is a function of two angular variables, can be decomposed into a product of two matrices, $\underset{\sim}{U}$ and $\underset{\sim}{V}$, each of which is a function of only one variable. The second technique obtains from an eigenfunction expansion of the albedo problem, a Fredholm and a singular integral equation for the $\underset{\sim}{S}$-matrix.

From the decomposition of the $\underset{\sim}{S}$-matrix and the introduction of the adjoint albedo problem, Fredholm and nonlinear integral equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices are obtained. These $\underset{\sim}{U}$ and $\underset{\sim}{V}$ integral equations yield readily to numerical solution and hence the emergent albedo distribution can easily be obtained.

3.1 GENERALIZED $\underset{\sim}{S}$-FUNCTION

Consider an albedo problem for which the incident neutron beam belongs to the ith energy group. The angular flux of this "ith albedo problem", $\underset{\sim}{\psi}_i(o,\mu_o;x,\mu)$, is the solution of Eq. (2.1) with the boundary conditions,

$$\text{(i)}\ \underset{\sim}{\psi}_i(o,\mu_o;o,\mu) = \underset{\sim}{e}_i\delta(\mu-\mu_o),\ \mu > o,\ \mu_o > o, \tag{3.1}$$

and

$$\text{(ii)}\ \lim_{x\to\infty} \underset{\sim}{\psi}_i(o,\mu_o;x,\mu) = 0\ . \tag{3.2}$$

The N distinct albedo problems (one for each group) can be handled collectively by introducing the "albedo matrix" $\underset{\sim}{\Psi}(o,\mu_o;x,\mu)$ defined as

$$\underset{\sim}{\Psi}(o,\mu_o;x,\mu) = [\underset{\sim}{\psi}_1(o,\mu_o;x,\mu)\ \underset{\sim}{\psi}_2(o,\mu_o;x,\mu)\ \ldots\ \underset{\sim}{\psi}_N(o,\mu_o;x,\mu)] \tag{3.3}$$

This matrix is the solution of the transport equation

$$(\mu\frac{\partial}{\partial x}\underset{\sim}{E} + \underset{\sim}{\Sigma})\ \underset{\sim}{\Psi}(o,\mu_o;x,\mu) = \underset{\sim}{C}\int_{-1}^{1} d\mu\ \underset{\sim}{\Psi}(o,\mu_o;x,\mu) \tag{3.4}$$

with the boundary conditions

$$\text{(i)}\ \underset{\sim}{\Psi}(o,\mu_o;o,\mu) = \underset{\sim}{E}\,\delta(\mu-\mu_o)\ ,\ \mu > o,\ \mu_o > o\ , \tag{3.5}$$

$$\text{(ii)}\ \lim_{x\to\infty} \underset{\sim}{\Psi}(o,\mu_o;x,\mu) = o \quad . \tag{3.6}$$

One can think of the albedo matrix as a type of Green's function for a delta-like incident distribution. If the incident distribution is given as $\underset{\sim}{\psi}^{inc}(\mu)$, $o \le \mu \le 1$, then the angular flux, $\underset{\sim}{\psi}(x,\mu)$, everywhere in the half-space is simply

$$\underset{\sim}{\psi}(x,\mu) = \int_o^1 d\mu' \ \underset{\sim}{\Psi}(o,\mu';x,\mu)\ \underset{\sim}{\psi}^{inc}(\mu') \quad . \tag{3.7}$$

In particular if the generalized S-function is defined as

$$\underset{\sim}{S}(\mu_o,\mu) = \mu\ \underset{\sim}{\Psi}(o,\mu_o;o,-\mu) \quad , \quad o \le \mu,\mu_o \le 1 \ , \tag{3.8}$$

the reflected distribution at the interface is

$$\underset{\sim}{\psi}(o,-\mu) = \frac{1}{\mu}\int_o^1 d\mu' \ \underset{\sim}{S}(\mu';\mu)\underset{\sim}{\psi}^{inc}(\mu') \quad . \tag{3.9}$$

In the one-speed case this $\underset{\sim}{S}$-matrix degenerates to the well known Ambarzumian-Chandrasekhar $\underset{\sim}{S}$-function. (except for a normalization factor of 2).[26,27]

With these definitions of the albedo matrix and the $\underset{\sim}{S}$-function, a non-singular, nonlinear integral equation for this latter quantity will be derived. By using the "principle of invariance,"[27] it is possible to express at some point, x, inside the half-space, the outwardly moving flux vector in terms of the inwardly directed flux vector and the albedo matrix.

The principle of invariance states that the reflected flux from a half-space is unchanged by the addition (or subtraction) of layers of arbitrary thickness to (or from) the medium. This means that at any point, x, inside the half-space, neutrons moving in the positive x direction are reflected in

the same manner as if they were incident upon the surface. If $\underset{\sim}{\psi}(x,\mu)$ is the flux at a distance x inside the half-space, the outwardly moving flux can then be expressed in terms of the inward flux as

$$\underset{\sim}{\psi}(x,\mu) = \int_0^1 d\mu' \underset{\sim}{\Psi}(0,\mu';0,-\mu)\underset{\sim}{\psi}(x,\mu'). \tag{3.10}$$

In particular, Eq. (3.10) gives for the ith albedo problem

$$\underset{\sim}{\psi}_i(0,\mu_0;x,-\mu) = \int_0^1 d\mu' \, \underset{\sim}{\Psi}(0,\mu';0,-\mu) \, \underset{\sim}{\psi}_i(0,\mu_0;x,\mu') \ . \tag{3.11}$$

Finally if the N albedo problems are treated collectively, Eq. (3.11) yields the following important relation for the albedo matrix

$$\underset{\sim}{\Psi}(0,\mu_0;x,-\mu) = \int_0^1 d\mu' \, \underset{\sim}{\Psi}(0,\mu';0,-\mu) \, \underset{\sim}{\Psi}(0,\mu_0;x,\mu'), \ \mu > 0 \ . \tag{3.12}$$

From this equation and Eqs. (3.4)-(3.6) a nonlinear integral equation for $\underset{\sim}{\Psi}(0,\mu';0,-\mu)$ can be obtained. Differentiation of Eq. (3.12) with respect to x at x = 0 yields

$$\frac{\partial}{\partial x} \underset{\sim}{\Psi}(0,\mu_0;x,-\mu)\Big|_{x=0} = \int_0^1 d\mu' \, \underset{\sim}{\Psi}(0,\mu';0,-\mu) \, \frac{\partial}{\partial x} \underset{\sim}{\Psi}(0,\mu_0,x,\mu')\Big|_{x=0} \ . \tag{3.13}$$

Using the transport equation (3.4) to evaluate these derivatives together with the boundary condition (3.5), Eq. (3.13) becomes

$$\frac{1}{\mu} \underset{\sim}{\sum}\underset{\sim}{\Psi}(0,\mu_0;0,-\mu) + \frac{1}{\mu_0} \underset{\sim}{\Psi}(0,\mu_0;0,-\mu)\underset{\sim}{\sum} = \frac{1}{\mu} \underset{\sim}{\mathfrak{C}} + \frac{1}{\mu} \underset{\sim}{C} \int_0^1 d\mu' \underset{\sim}{\Psi}(0,\mu_0;0,\mu')$$

$$+ \int_0^1 \frac{d\mu'}{\mu'} \underset{\sim}{\Psi}(0,\mu';0,-\mu)\underset{\sim}{C} + \int_0^1 \frac{d\mu'}{\mu'} \underset{\sim}{\Psi}(0,\mu';0,-\mu)\underset{\sim}{C} \int_0^1 d\mu'' \, \underset{\sim}{\Psi}(0,\mu\ ;0,-\mu'').$$

(3.14)

Multiplication by μ, and the use of the $\underset{\sim}{S}$-matrix definition, gives the result

$$\frac{1}{\mu}\underset{\sim}{\Sigma}\underset{\sim}{S}(\mu_o,\mu) + \frac{1}{\mu_o}\underset{\sim}{S}(\mu_o,\mu)\underset{\sim}{\Sigma}$$

$$= [\underset{\sim}{E} + \int_0^1 \frac{d\mu'}{\mu'}\underset{\sim}{S}(\mu',\mu)]\underset{\sim}{C}[\underset{\sim}{E} + \int_0^1 \frac{d\mu'}{\mu'}\underset{\sim}{S}(\mu_o,\mu')] \ . \qquad (3.15)$$

Since each bracket on the right hand side of this equation is a function of only one angular variable, Eq. (3.15) can be written as

$$\frac{1}{\mu}\underset{\sim}{\Sigma}\underset{\sim}{S}(\mu_o,\mu) + \frac{1}{\mu_o}\underset{\sim}{S}(\mu_o,\mu)\underset{\sim}{\Sigma} = \underset{\sim}{U}(\mu)\underset{\sim}{C}\underset{\sim}{V}(\mu_o) \ . \qquad (3.16)$$

where

$$\underset{\sim}{U}(\mu) = \underset{\sim}{E} + \int_0^1 \frac{d\mu'}{\mu'}\underset{\sim}{S}(\mu',\mu) \qquad (3.17)$$

and

$$\underset{\sim}{V}(\mu) = \underset{\sim}{E} + \int_0^1 \frac{d\mu'}{\mu'}\underset{\sim}{S}(\mu,\mu') \ . \qquad (3.18)$$

For the special case when N = 1, Eq. (3.15) is just Chandrasekhar's S-equation, and both $\underset{\sim}{U}$ and $\underset{\sim}{V}$ become the well-known H-function.[27]

Unfortunately $\underset{\sim}{\Sigma}$ and $\underset{\sim}{S}$ do not commute, and to obtain an equation more amenable to numerical solution, the definition of a "matrix direct product" is introduced. If $\underset{\sim}{D}$ is the direct product (denoted by the symbol *) of $\underset{\sim}{A}$ and $\underset{\sim}{B}$, i.e., $\underset{\sim}{D} = \underset{\sim}{A} * \underset{\sim}{B}$ then in component form

$$\underset{\sim}{D}_{ij} = \underset{\sim}{A}_{ij}\underset{\sim}{B}_{ij} \ , \qquad i,j = 1 \sim N \ . \qquad (3.19)$$

This direct product operator has associative and distributive properties with other direct operators. However, it is neither associative nor distributive with the conventional product, e.g.,

$$(\underset{\sim}{A}\ \underset{\sim}{B})*\underset{\sim}{C} \neq A(\underset{\sim}{B}*C) . \tag{3.20}$$

Equation (3.15) can then be written as

$$\underset{\sim}{R}(\mu_o,\mu) = [\underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{R}(\mu',\mu)*\underset{\sim}{A}(\mu,\mu')$$

$$(x)\ \underset{\sim}{C}[\underset{\sim}{E} + \mu_o \int_0^1 d\mu' \underset{\sim}{R}(\mu_o,\mu')*\underset{\sim}{A}(\mu',\mu_o)], \tag{3.21}$$

where the matrix A is given by

$$[\underset{\sim}{A}(\mu,\mu')]_{ij} = \frac{1}{\sigma_i\mu'+\sigma_j\mu} , \tag{3.22}$$

and the associated $\underset{\sim}{R}$-matrix is related to the $\underset{\sim}{S}$-matrix by

$$\underset{\sim}{S}(\mu',\mu) = \mu\mu'\underset{\sim}{A}(\mu,\mu')*\underset{\sim}{R}(\mu',\mu) . \tag{3.23}$$

Further, the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices expressed in terms of the $\underset{\sim}{R}$-matrix are

$$\underset{\sim}{U}(\mu) = \underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{R}(\mu',\mu)*\underset{\sim}{A}(\mu,\mu') \tag{3.24}$$

and

$$\underset{\sim}{V}(\mu) = \underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{R}(\mu,\mu')*\underset{\sim}{A}(\mu',\mu) . \tag{3.25}$$

To obtain a system of equations equivalent to Eq. (3.21) involving only $\underset{\sim}{U}$ and $\underset{\sim}{V}$, take the direct product of Eq. (3.21) and $\mu_o\ \underset{\sim}{A}(\mu,\mu_o)$, and integrate with resepct to μ. The result is

$$\underset{\sim}{V}(\mu_o) = \underset{\sim}{E} + \mu_o \int_o^1 d\mu' \underset{\sim}{A}(\mu',\mu_o)*[\underset{\sim}{U}(\mu')\underset{\sim}{\sim}\underset{\sim}{V}(\mu_o)] \ . \tag{3.26}$$

Similarly, by taking the direct product of Eq. (3.29) and $\mu\ \underset{\sim}{A}(\mu,\mu_o)$, and integrating with respect to μ_o, an equation for $\underset{\sim}{U}$ is obtained:

$$\underset{\sim}{U}(\mu) = \underset{\sim}{E} + \mu \int_o^1 d\mu' \underset{\sim}{A}(\mu,\mu')*[\underset{\sim}{U}(\mu)\underset{\sim}{\sim}\underset{\sim}{V}(\mu')] \ . \tag{3.27}$$

Equations (3.26) and (3.27) are two simultaneous nonlinear integral equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrix functions. They correspond to Chandrasekhar's one-speed nonlinear H-function equation.[27] In fact, if one takes the one-speed limit (N=1) and lets $H(\mu) = U(\mu) = V(\mu)$, the nonlinear integral H-function equation, which is so often used, is obtained; namely

$$H(\mu) = 1 + c\mu H(\mu) \int_o^1 d\mu' \frac{H(\mu')}{\mu+\mu'} \ . \tag{3.28}$$

The equations for $\underset{\sim}{U}$ and $\underset{\sim}{V}$, as they stand, can be solved numerically by the method of successive iterations, which is commonly called the "power method."[6] A computer code using this technique has been written to solve these equations (see Chapter 6). However, it is possible to cast the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ equations into a different form whose iterative solution converges faster than that of Eqs. (3.26) and (3.24). This modification is discussed in Section (3.3).

From Eq. (3.16) a useful identity for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices can be obtained. Integrating this equation over μ from o to 1, and using the definition of $\underset{\sim}{U}(\mu)$, Eq. (3.17), one obtains

$$\underset{\sim}{\Sigma}(\underset{\sim}{V}(\mu_o)-\underset{\sim}{E}) + \frac{1}{\mu_o} \int_o^1 d\mu \underset{\sim}{S}(\mu_o,\mu)\underset{\sim}{\Sigma} = \int_o^1 d\mu\ \underset{\sim}{U}(\mu)\underset{\sim}{\sim}\underset{\sim}{V}(\mu_o) \ . \tag{3.29}$$

Rearrangement of this equation gives

$$[\underset{\sim}{\Sigma} - \int_0^1 d\mu \underset{\sim}{U}(\mu)\underset{\sim}{C}]\underset{\sim}{V}(\mu_o) = [\underset{\approx}{E} - \frac{1}{\mu_o}\int_0^1 d\mu \underset{\approx}{S}(\mu_o,\mu)]\underset{\sim}{\Sigma} . \tag{3.30}$$

Finally, integrating this result over μ_o, rearranging and using Eq. (3.17), the following relation is obtained:

$$2\underset{\sim}{\Sigma} = \int_0^1 d\mu \underset{\sim}{U}(\mu)\underset{\sim}{\Sigma} + \underset{\approx}{\Sigma}\int_0^1 d\mu_o \underset{\sim}{V}(\mu_o) - \int_0^1 d\mu \underset{\sim}{U}(\mu)\underset{\approx}{C}\int_0^1 d\mu_o \underset{\sim}{V}(\mu_o) . \tag{3.31}$$

This identity for $\underset{\sim}{U}$ and $\underset{\sim}{V}$ is most useful in giving a measure of the convergence of the iterated $\underset{\sim}{U}$ and $\underset{\sim}{V}$ equations. It can be easily and quickly evaluated in any computer code which is used to obtain a numerical solution for $\underset{\sim}{U}$ and $\underset{\sim}{V}$.

3.2 THE ADJOINT ALBEDO PROBLEM

In the previous section, it was found that the generalized $\underset{\sim}{S}$-function could be decomposed into two matrices of a single variable, $\underset{\sim}{U}$ and $\underset{\sim}{V}$. However, these matrices are not independent, but are related in a simple manner through corresponding adjoint equations.

Consider now, the adjoint albedo matrix, $\underset{\sim}{\Psi}^\dagger(o,\mu_o;x,\mu)$, which is a solution of the adjoint transport equation

$$(-\mu\frac{\partial}{\partial x}\underset{\approx}{E} + \underset{\approx}{\Sigma})\underset{\sim}{\Psi}^\dagger(o,-\mu_o';x,\mu) = \underset{\approx}{\tilde{C}}\int_{-1}^1 d\mu' \underset{\sim}{\Psi}^\dagger(o,-\mu_o';x,\mu') \tag{3.32}$$

with the adjoint boundary conditions

$$\text{(i)}\quad \underset{\sim}{\Psi}^\dagger(o,-\mu_o';x,-\mu) = \underset{\sim}{E}\,\delta(\mu_o'-\mu), \quad \mu_o' > 0, \quad \mu > 0 , \tag{3.33}$$

and

$$\text{(ii)} \quad \lim_{x\to\infty} \underset{\sim}{\Psi}^{\dagger}(o,-\mu_o';x,\mu) = 0 \; . \tag{3.34}$$

The ith column of the adjoint albedo matrix is simply the ith adjoint albedo problem solution $\underset{\sim}{\psi}_i^{\dagger}(o,-\mu_o';x,\mu)$, which is uniquely defined by taking the ith column of the matrix equations (3.32)-(3.34). A generalized $\underset{\sim}{S}^{\dagger}$-function may be defined in an analogous manner as was the $\underset{\sim}{S}$-function, namely,

$$\underset{\sim}{S}^{\dagger}(\mu_o,\mu) = \mu\underset{\sim}{\Psi}^{\dagger}(o,-\mu_o;o,\mu) \; . \tag{3.35}$$

The adjoint albedo matrix gives the response of an albedo adjoint transport solution for a forced delta-like emergent distribution. In particular if a solution of the adjoint equation has a forced emergent distribution, $\underset{\sim}{\psi}^{\dagger em}(-\mu)$, $\mu > 0$, the resultant incident distribution must be

$$\underset{\sim}{\psi}^{\dagger inc}(\mu) = \int_o^1 d\mu' \underset{\sim}{\Psi}^{\dagger}(o,-\mu';o,\mu)\underset{\sim}{\psi}^{\dagger em}(\mu') \tag{3.36}$$

or terms of the adjoint $\underset{\sim}{S}^{\dagger}$-matrix

$$\underset{\sim}{\psi}^{\dagger inc}(\mu) = \frac{1}{\mu}\int_o^1 d\mu' \underset{\sim}{S}^{\dagger}(\mu',\mu)\underset{\sim}{\psi}^{\dagger em}(\mu') \; . \tag{3.37}$$

To find the relationship between the emergent distribution of the albedo matrix, $\underset{\sim}{\Psi}(o,\mu_o;o,-\mu)$, $\mu > 0$, and the incident distribution of the adjoint albedo matrix, $\underset{\sim}{\Psi}^{\dagger}(o,-\mu_o;o,\mu)$, first multiply Eq. (3.4) from the left by $\underset{\sim}{\Psi}^{\dagger}(o,-\mu_o';x,\mu)$. Then multiply the transpose of Eq. (3.32) from the right by $\underset{\sim}{\Psi}(o,\mu_o;x,\mu)$. Subtraction of these two results and integration over μ from -1 to 1, and over x from 0 to ∞, yields the identity

$$\int_{-1}^{1} d\mu \int_{0}^{\infty} dx \Big\{ \tilde{\underset{\sim}{\Psi}}^{\dagger}(o,-\mu_o';x,\mu) \Big[\mu \frac{\partial}{\partial x} \underset{\sim}{\Psi}(o,\mu_o;x,\mu) + \underset{\sim}{\Sigma}\underset{\sim}{\Psi}(o,\mu_o;x,\mu) - \underset{\sim}{C} \int_{-1}^{1} d\mu' \underset{\sim}{\Psi}(o,\mu_o;x,\mu') \Big]$$

$$- \Big[-\mu \frac{\partial}{\partial x} \tilde{\underset{\sim}{\Psi}}^{\dagger}(o,-\mu_o';x,\mu) + \tilde{\underset{\sim}{\Psi}}^{\dagger}(o,-\mu_o';x,\mu)\underset{\sim}{\Sigma}$$

$$- \int_{-1}^{1} d\mu' \tilde{\underset{\sim}{\Psi}}^{\dagger}(o,-\mu_o';x,\mu)\underset{\sim}{C} \Big] \underset{\sim}{\Psi}(o,\mu_o;x,\mu) \Big\} = 0 . \tag{3.38}$$

This immediately reduces to

$$\int_{-1}^{1} d\mu \int_{0}^{\infty} dx \; \mu \frac{\partial}{\partial x} \Big\{ \tilde{\underset{\sim}{\Psi}}^{\dagger}(o,-\mu_o';x,\mu)\underset{\sim}{\Psi}(o,\mu_o;x,\mu) \Big\} = 0 . \tag{3.39}$$

Use of the boundary conditions of Eqs. (3.5), (3.6), (3.33) and (3.34) and integration by parts of the above equation gives

$$\mu_o \tilde{\underset{\sim}{\Psi}}^{\dagger}(o,-\mu_o';o,\mu_o) = \mu_o' \underset{\sim}{\Psi}(o,\mu_o;o,-\mu_o'), \qquad \mu_o,\mu_o' > 0 . \tag{3.40}$$

Finally, from the definitions of the $\underset{\sim}{S}$-function and the adjoint $\underset{\sim}{S}^{\dagger}$-function the above identity immediately shows the relationship between these two functions, i.e.,

$$\tilde{\underset{\sim}{S}}^{\dagger}(\mu_o,\mu) = \underset{\sim}{S}(\mu,\mu_o) . \tag{3.41}$$

A nonlinear integral equation for $\underset{\sim}{S}^{\dagger}(\mu_o,\mu)$ may be written by taking the transpose of Eq. (3.15) and using the identity (3.38). The result:

$$\frac{1}{\mu} \underset{\sim}{\Sigma}\underset{\sim}{S}^{\dagger}(\mu_o,\mu) + \frac{1}{\mu_o} \underset{\sim}{S}^{\dagger}(\mu_o,\mu)\underset{\sim}{\Sigma} = \underset{\sim}{U}^{\dagger}(\mu)\underset{\sim}{C}\underset{\sim}{V}^{\dagger}(\mu_o) , \tag{3.42}$$

where the adjoint $\underset{\sim}{U}^{\dagger}(\mu)$ and $\underset{\sim}{V}^{\dagger}(\mu)$ matrices are defined as

$$\underset{\sim}{U}^{\dagger}(\mu) = \underset{\sim}{E} + \int_{0}^{1} \frac{d\mu'}{\mu'} \underset{\sim}{S}^{\dagger}(\mu',\mu) \tag{3.43}$$

and

$$\underset{\sim}{V}^{\dagger}(\mu) = \underset{\sim}{E} + \int_0^1 \frac{d\mu'}{\mu'} \underset{\sim}{S}^{\dagger}(\mu,\mu') \tag{3.44}$$

Finally from (3.17), (3.18) and (3.41) the relationship between the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices is obtained, namely

$$\underset{\sim}{U}^{\dagger}(\mu) = \tilde{\underset{\sim}{V}}(\mu); \quad \underset{\sim}{V}^{\dagger}(\mu) = \tilde{\underset{\sim}{U}}(\mu) . \tag{3.45}$$

These $\underset{\sim}{U}^{\dagger}$ and $\underset{\sim}{V}^{\dagger}$-functions will be used later to derive a Fredholm equation for $\underset{\sim}{V}^{\dagger}(\mu)$, and therefore, in view of the above relation, a Fredholm equation for $\underset{\sim}{U}(\mu)$.

3.3 REDUCTION OF THE NONLINEAR $\underset{\sim}{U}$ AND $\underset{\sim}{V}$ EQUATIONS

It is possible to put the nonlinear equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices, Eqs. (3.26) and (3.27), into a form which does not involve the direct matrix products. This modification yields a system of equations which not only simplifies the computational schemes, but improves the iteration convergence.

Let us consider first the $\underset{\sim}{V}$-equation (3.26),

$$\underset{\sim}{V}(\mu) = \underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{A}(\mu',\mu) * [\underset{\sim}{U}(\mu') \underset{\sim}{C} \underset{\sim}{V}(\mu)] . \tag{3.46}$$

Becasue of the direct product, the term $\underset{\sim}{V}(\mu)$ cannot be factored outside of the integral in the above equation. Substituting explicitly for $\underset{\sim}{A}(\mu',\mu)$, and denoting summation by the repeated index notation (where a repeated lower case Greek subscript signifies summation of the indexed quantity from 1 to N), the integrand in Eq. (3.46) can be written in component form as

$$[\underset{\sim}{A}(\mu',\mu)*(\underset{\sim}{U}(\mu')\underset{\sim}{\underset{\sim}{C}}\underset{\sim}{V}(\mu))]_{ij} = \frac{\underset{\sim}{U}_{i\nu}(\mu')\underset{\sim}{\underset{\sim}{C}}_{\nu\eta}\underset{\sim}{V}_{\eta j}(\mu)}{\sigma_i\mu+\sigma_j\mu'} \quad . \tag{3.47}$$

Now define the matrix $\underset{\sim}{V}_k(\mu)$ all of whose elements are zero except the kth column which equals the kth column of the $\underset{\sim}{V}(\mu)$ matrix, i.e.,

$$[\underset{\sim}{V}_k(\mu)]_{ij} = [\underset{\sim}{V}(\mu)]_{ij}\delta_{jk} \equiv \begin{pmatrix} 0 & \cdots & 0 & \overset{k}{V_{1k}} & 0 & \cdots & 0 \\ & & & V_{2k} & & & \\ & & & \vdots & & & \\ 0 & \cdots & 0 & V_{Nk} & 0 & \cdots & 0 \end{pmatrix} . \tag{3.48}$$

With this definition the integrand (3.47) becomes

$$\underset{\sim}{D}_\eta(\mu,\mu')\underset{\sim}{U}(\mu')\underset{\sim}{\underset{\sim}{C}}\underset{\sim}{V}_\eta(\mu) \quad ,* \tag{3.49}$$

where the diagonal matrix $\underset{\sim}{D}_k(\mu,\mu')$ is defined as

$$[\underset{\sim}{D}_k(\mu,\mu')]_{ij} = \frac{1}{\sigma_i\mu+\sigma_k\mu'}\,\delta_{ij} \quad . \tag{3.50}$$

Using this notation, Eq. (3.46) can be written in the form

$$\underset{\sim}{V}(\mu) = \sum_{i=1}^{N} \underset{\sim}{V}_i(\mu) = \underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{D}_\eta(\mu,\mu')\underset{\sim}{U}(\mu')\underset{\sim}{\underset{\sim}{C}}\underset{\sim}{V}_\eta(\mu) \quad . \tag{3.51}$$

*For example with N = 2 the integrand is

$$\begin{bmatrix} \frac{1}{\sigma_1\mu+\sigma_1\mu'} & 0 \\ 0 & \frac{1}{\sigma_2\mu+\sigma_1\mu'} \end{bmatrix} \underset{\sim}{U}(\mu')\underset{\sim}{\underset{\sim}{C}} \begin{bmatrix} V_{11}(\mu) & 0 \\ V_{21}(\mu) & 0 \end{bmatrix} + \begin{bmatrix} \frac{1}{\sigma_1\mu+\sigma_2\mu'} & 0 \\ 0 & \frac{1}{\sigma_2\mu+\sigma_2\mu'} \end{bmatrix} \underset{\sim}{U}(\mu')\underset{\sim}{\underset{\sim}{C}} \begin{bmatrix} 0 & V_{12}(\mu) \\ 0 & V_{22}(\mu) \end{bmatrix}$$

Similarly the transpose of the $\underset{\sim}{U}$ equation, Eq. (3.27), can be written without the direct product. The equation for $\tilde{\underset{\sim}{U}}(\mu)$ is

$$\tilde{\underset{\sim}{U}}(\mu) = \underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{A}(\mu',\mu) * [\tilde{\underset{\sim}{V}}(\mu') \tilde{\underset{\sim}{C}} \tilde{\underset{\sim}{U}}(\mu)] \quad . \tag{3.52}$$

By explicitly expanding the integrand this equation, it can be verified to be equal to

$$\underset{\sim}{D}_\eta(\mu,\mu') \tilde{\underset{\sim}{V}}(\mu') \tilde{\underset{\sim}{C}} \tilde{\underset{\sim}{U}}_\eta(\mu) \quad , \tag{3.53}$$

where the matrix $\tilde{\underset{\sim}{U}}_k$ is defined by

$$[\tilde{\underset{\sim}{U}}_k(\mu)]_{ij} = [\underset{\sim}{U}(\mu)]_{ji} \delta_{jk} \equiv \begin{pmatrix} 0 & \cdots & 0 & U_{k1} & 0 & \cdots & 0 \\ \cdot & & & U_{k2} & & & \cdot \\ \cdot & & & \cdot & & & \cdot \\ \cdot & & & \cdot & & & \cdot \\ & & & \cdot & & & \\ 0 & \cdots & 0 & U_{kN} & 0 & \cdots & 0 \end{pmatrix} \quad . \tag{3.54}$$

Eq. (3.52) becomes with this notation

$$\tilde{\underset{\sim}{U}}(\mu) = \sum_{i=1}^{N} \tilde{\underset{\sim}{U}}_k(\mu) = \underset{\sim}{E} + \mu \int_0^1 d\mu' \underset{\sim}{D}_\eta(\mu,\mu') \tilde{\underset{\sim}{V}}(\mu') \tilde{\underset{\sim}{C}} \tilde{\underset{\sim}{U}}_\eta(\mu) \quad . \tag{3.55}$$

The two new matrix equations for $\underset{\sim}{U}$ and $\underset{\sim}{V}$, Eqs. (3.51) and (3.55), can be reduced to systems of N vector equations. This is possible because of the particularly simple forms of the matrices $\underset{\sim}{V}_k$ and $\underset{\sim}{U}_k$. If one defines the vector v_i and $\tilde{u}_i$ as

$$\underset{\sim}{V}_i(\mu) = \begin{bmatrix} V_{1i}(\mu) \\ V_{2i}(\mu) \\ \cdot \\ \cdot \\ \cdot \\ V_{Ni}(\mu) \end{bmatrix} \quad \text{and} \quad \underset{\sim}{u}_i(\mu) = \begin{bmatrix} U_{i1}(\mu) \\ U_{i2}(\mu) \\ \cdot \\ \cdot \\ \cdot \\ U_{iN}(\mu) \end{bmatrix} \tag{3.56}$$

then Eqs. (3.51) and (3.55) become (for $i = 1 \sim N$)

$$\underset{\sim}{V}_i(\mu) = \underset{\sim}{e}_i + \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu') \underset{\sim}{U}(\mu') \underset{\sim\sim}{C} \underset{\sim}{V}_i(\mu) , \tag{3.57}$$

and

$$\underset{\sim}{u}_i(\mu) = \underset{\sim}{e}_i + \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu') \underset{\sim}{V}(\mu') \underset{\sim\sim}{\tilde{C}} \underset{\sim}{u}_i(\mu). \tag{3.58}$$

This set of vector equations is exactly equivalent to the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrix equations which involved direct products (Eqs. (3.26) and (3.27)). The convergence of an iterated solution of Eqs. (3.57) and (3.58) will be exactly the same as that of the Eqs. (3.26) and (3.27). So far nothing new has been gained--save some practice in matrix manipulation. However these vector equations can yield a better iteration scheme, which should converge faster, and require less storage space in the computer.

Equations (3.57) and (3.58) may now be written, upon factoring $\underset{\sim}{V}_i(\mu)$ or $\underset{\sim}{u}_i(\mu)$, as

$$\underset{\sim}{e}_i = [\underset{\sim}{E} - \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu')\underset{\sim}{U}(\mu')\underset{\sim}{C}]\underset{\sim}{v}_i(\mu) \tag{3.59}$$

and

$$\underset{\sim}{e}_i = [\underset{\sim}{E} - \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu')\tilde{\underset{\sim}{V}}(\mu')\tilde{\underset{\sim}{C}}]\underset{\sim}{u}_i(\mu) \ . \tag{3.60}$$

Then solving for $\underset{\sim}{u}_i$ and $\underset{\sim}{v}_i$, one obtains

$$\underset{\sim}{v}_i(\mu) = [\underset{\sim}{F}_i(\mu)]^{-1}\underset{\sim}{e}_i \ , \tag{3.61}$$

and

$$\underset{\sim}{u}_i(\mu) = [\underset{\sim}{G}_i(\mu)]^{-1}\underset{\sim}{e}_i, \quad i = 1 \sim N, \tag{3.62}$$

where the matrices $\underset{\sim}{F}_i(\mu)$ and $\underset{\sim}{G}_i(\mu)$ are defined as

$$\underset{\sim}{F}_i(\mu) = \underset{\sim}{E} - \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu')\underset{\sim}{U}(\mu')\underset{\sim}{C} \ , \tag{3.63}$$

and

$$\underset{\sim}{G}_i(\mu) = \underset{\sim}{E} - \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu')\tilde{\underset{\sim}{V}}(\mu')\underset{\sim}{C} \ . \tag{3.64}$$

Several three group cases for different values of the transfer matrix, $\underset{\sim}{C}$, have been solved numerically for $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ both from the above equations and from Eqs. (3.26) and (3.27). In all instances not only was the time required for the convergence of $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ less for Eqs. (3.61) and (3.64), but the "convergence rate,"[30] defined as the negative of the logarithm of the asymptotic reduction in error per iteration, was better by a factor of 3 or 4. These differences and the method of solution are discussed in detail in Chapter VI.

Finally, before ending this section, the question of the uniqueness of solution of the nonlinear integral equation for the $\underset{\sim}{S}$-function (and hence for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$-functions) should be discussed. As previously mentioned Eq. (3.16) for the generalized $\underset{\sim}{S}$-function corresponds to Chandrasekhar's one-speed S-function equation. Since this nonlinear equation for Chandrasekhar's S-function does not have a unique solution,[31-32] one suspects that Eq. (3.16) (and its associated $\underset{\sim}{U}$ and $\underset{\sim}{V}$ equations) also may not have a unique solution. It is possible to give, however, a set of necessary conditions which the required $\underset{\sim}{S}$-function must satisfy.

The discrete eigenfunctions $\underset{\sim}{\phi}(\nu_{0s},\mu)e^{-x/\nu_{0s}}, s = 1 \sim M$, are solutions to the transport equation; and since they tend to zero for large x, they are solutions to half-space albedo problems with incident distributions given by $\underset{\sim}{\phi}(\nu_{0s},\mu)$, $\mu > 0$. Thus from Eq. (3.9), the $\underset{\sim}{S}$-function must satisfy

$$\underset{\sim}{\phi}(\nu_{0s},-\mu) = \frac{1}{\mu}\int_0^1 d\mu' \underset{\sim}{S}(\mu',\mu)\underset{\sim}{\phi}(\nu_{0s},\mu'), \quad \mu > 0, \quad s = 1 \sim M . \tag{3.67}$$

Integrating this condition over μ from 0 to 1 and using the definition of the $\underset{\sim}{V}$-matrix, Eq. (3.18), one finds

$$\int_0^1 d\mu \underset{\sim}{\phi}(\nu_{0s},-\mu) + \int_0^1 d\mu \underset{\sim}{\phi}(\nu_{0s},\mu) = \int_0^1 d\mu' \underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu_{0s},\mu'), \tag{3.68}$$

or from Eq. (2.23)

$$\int_{-1}^1 d\mu \underset{\sim}{\phi}(\nu_{0s},\mu) \equiv \underset{\sim}{a}(\nu_{0s}) = \int_0^1 d\mu' \underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu_{0s},\mu') . \tag{3.69}$$

Similarly, consideration of the discrete adjoint eigenfunctions $\underset{\sim}{\phi}^{\dagger}(-\nu_{os},\mu)e^{-x/\nu_{os}}$, $s = 1 \sim M$, as half-space adjoint albedo problem solutions, Eq. (3.37) gives as a necessary condition for the $\underset{\sim}{S}^{\dagger}$-matrix

$$\underset{\sim}{\phi}^{\dagger}(-\nu_{os},\mu) = \frac{1}{\mu}\int_0^1 d\mu' \underset{\sim}{S}^{\dagger}(\mu',\mu)\underset{\sim}{\phi}^{\dagger}(-\nu_{os},-\mu'), \quad \mu > 0, \quad s = 1 \sim M . \tag{3.70}$$

Using the relation between $\underset{\sim}{S}$ and $\underset{\sim}{S}^{\dagger}$, (Eq. (3.41)), the above condition becomes

$$\underset{\sim}{\phi}^{\dagger}(-\nu_{os},\mu) = \frac{1}{\mu}\int_0^1 d\mu' \underset{\sim}{S}(\mu,\mu')\underset{\sim}{\phi}^{\dagger}(-\nu_{os},-\mu') . \tag{3.71}$$

Integration over μ from 0 to 1 together with definition (3.17) gives a condition on $\underset{\sim}{U}$

$$\int_{-1}^1 d\mu \underset{\sim}{\phi}^{\dagger}(-\nu_{os},\mu) \equiv \underset{\sim}{a}^{\dagger}(-\nu_{os}) = \int_0^1 d\mu \underset{\sim}{\tilde{U}}(\mu)\underset{\sim}{\phi}^{\dagger}(-\nu_{os},-\mu) . \tag{3.72}$$

Equations (3.67) and (3.71) are 2M conditions which the generalized $\underset{\sim}{S}$-function must satisfy. Equations (3.69) and (3.72) similarly place necessary conditions on the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices. In the one-speed case Eqs. (3.67) and (3.71) become identical, and it has been proved that these equations are a sufficient condition to specify uniquely the real physical $\underset{\sim}{S}$-function of the nonlinear $\underset{\sim}{S}$-equation.[24,34] Also for the degenerate kernel approximation, Pahor, using a corresponding set of discrete eigenfunction conditions, proved that these conditions were sufficient for uniquely specifying his generalized $\underset{\sim}{S}$-function.[25] Although it has not been possible to show that the discrete root conditions for the multigroup case are a set of sufficient conditions, it is felt that they are a severe restriction on the possible solutions (if

indeed there be more than one solution), and in all likelihood they are sufficient.

3.4 FREDHOLM EQUATIONS FOR THE $\underset{\sim}{U}$ AND $\underset{\sim}{V}$-FUNCTIONS

In this section Fredholm equations are derived for the $\underset{\sim}{S}$, $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions. These equations, while not soluble in closed form, are of a type which usually do not suffer from the shortcomings of nonlinear integral equations (e.g., possible nonuniqueness of solution).

A Fredholm equation for $\underset{\sim}{S}(\mu,\mu_o)$ can easily be obtained by considering an eigenvector expansion for the ith albedo problem. Since the eigenvectors are full-range complete, the solution to the ith albedo problem can be expanded in terms of the eigenfunctions which satisfy the boundary condition at infinity, Eq. (3.2):

$$\underset{\sim}{\psi}_i(o,\mu_o;x,\mu) = \sum_{s=1}^{M} \alpha(\nu_{os})\underset{\sim}{\phi}(\nu_{os},\mu)e^{-x/\nu_{os}}$$

$$+ \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu \left\{ \sum_{m=j}^{N} \underset{\sim}{A}_j^m(\nu)\underset{\sim}{\phi}_j^m(\nu,\mu) \right\} e^{-x/\nu} \quad . \tag{3.73}$$

Here it has been assumed that the half-space has such a composition that all the roots ν_{os}, $s = 1 \sim M$, are finite and distinct. Setting $x = 0$ in Eq. (3.73) and using the full-range orthogonality relations plus boundary condition (3.1), the expansion coefficients are:

$$\alpha(\nu_{os}) = \frac{\mu_o}{N_s}\underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu_o)\underset{\sim}{e}_i - \frac{1}{N_s}\int_o^1 d\mu\mu\underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},-\mu)\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu) \quad , \tag{3.74}$$

and

$$A_j^m(\nu) = \frac{\mu_o}{N_j^m(\nu)}\underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,\mu)\underset{\sim}{e}_i - \frac{1}{N_j^m(\nu)}\int_o^1 d\mu\mu\underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,-\mu)\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu) \quad . \tag{3.75}$$

When these coefficients are substituted into Eq. (3.73), with x = 0, the following non-homogeneous Fredholm equation for the emergent distribution is obtained:

$$\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu) = \mu_o\underset{\sim}{F}(\mu_o,\mu)\underset{\sim}{e}_i - \int_o^1 d\mu'\mu'\underset{\sim}{K}(\mu',\mu)\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu'), \quad \mu > 0. \tag{3.76}$$

The matrices $\underset{\sim}{F}(\mu_o,\mu)$ and $\underset{\sim}{K}(\mu',\mu)$ have been defined as:

$$\underset{\sim}{F}(\mu_o,\mu) = \sum_{s=1}^{M} \frac{1}{N_s}\underset{\sim}{\phi}(\nu_{os},-\mu)\underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu_o) + \sum_{j=1}^{N}\int_{\eta_{j-1}}^{\eta_j} d\nu\left\{\sum_{m=j}^{N}\frac{1}{N_j^m(\nu)}\underset{\sim}{\phi}_j^m(\nu,-\mu)\underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,\mu_o)\right., \tag{3.77}$$

and

$$\underset{\sim}{K}(\mu',\mu) = \sum_{s=1}^{M}\frac{1}{N_s}\underset{\sim}{\phi}(\nu_{os},-\mu)\underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},-\mu') + \sum_{j=1}^{N}\int_{\eta_{j-1}}^{\eta_j} d\nu\left\{\sum_{m=j}^{N}\frac{1}{N_j^m(\nu)}\underset{\sim}{\phi}_j^m(\nu,-\mu)\underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,-\mu')\right\}. \tag{3.78}$$

Both of these matrices can be verified to be continuous functions when their arguments are positive.

It is also possible to obtain a singular integral equation for the emergent distribution by considering the incident distribution as given by Eqs. (3.73), (3.74), and (3.75); explicitly

$$\delta(\mu-\mu_o)\underset{\sim}{e}_i = \mu_o F(\mu_o,-\mu)\underset{\sim}{e}_i - \int_o^1 d\mu'\mu'\underset{\sim}{K}(\mu',-\mu)\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu'), \quad \mu > 0. \tag{3.79}$$

Recently Case has proposed a new method for obtaining solutions to transport problems,[23] with which he derives the same pair of equations for the emergent distribution expressed in terms of the infinite medium Green's function. When the explicit expression for the Green's function (Chapter II, Sec. 4) is substituted into his equations, Eqs. (3.76) and (3.79) are obtained.

In the one-speed case, the singular integral equation (3.79) and the Fredholm equation (3.76) may be solved together in closed form.[23] However, for the multigroup situation no closed form solutions have been obtained, and to determine the emergent distribution numerical procedures must be used.

Finally the N albedo problems may be treated collectively by using the generalized $\underset{\sim}{S}$-function. From the definition of the $\underset{\sim}{S}$-matrix, Eq. (3.8), the Fredholm equation (3.76) yields

$$\frac{1}{\mu}\underset{\sim}{S}(\mu_o,\mu) = \mu_o\underset{\sim}{F}(\mu_o,\mu) - \int_0^1 d\mu'\underset{\sim}{K}(\mu',\mu)\underset{\sim}{S}(\mu_o,\mu'), \qquad \mu,\mu_o > 0 . \tag{3.80}$$

This equation may be solved numerically by standard techniques. However a simpler set of Fredholm equations may be obtained by decomposing the $\underset{\sim}{S}$-function into the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions.

The Fredholm equation for the $\underset{\sim}{U}$-function can be obtained from Eq. (3.80) very readily. Multiply (3.80) by μ/μ_o, integrate over μ_o from o to 1, and use the definition of $\underset{\sim}{U}$, Eq. (3.17): the result is

$$\underset{\sim}{U}(\mu) - \underset{\sim}{E} = \mu \sum_{s=1}^{M} \frac{1}{N_s} \underset{\sim}{\phi}(\nu_{os},-\mu) \left[\int_0^1 d\mu_o \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu_o) + \int_0^1 d\mu' \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},-\mu') \right]$$

$$+ \mu \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu \left\{ \sum_{m=j}^{N} \frac{1}{N_j^m(\nu)} \underset{\sim}{\phi}_j^m(\nu,-\mu) \left[\int_0^1 d\mu_o \underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,\mu_o) \right. \right.$$

$$\left. \left. + \int_0^1 d\mu' \underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,-\mu') \right] \right\} - \mu \int_0^1 d\mu' \underset{\sim}{K}(\mu',\mu) \underset{\sim}{U}(\mu') \ . \qquad (3.81)$$

Combining the terms in the square brackets, Eq. (3.81) becomes

$$\underset{\sim}{U}(\mu) = \underset{\sim}{E} + \mu \int_{-1}^{1} d\mu' \underset{\sim}{K}(\mu',\mu) - \mu \int_0^1 d\mu' \underset{\sim}{K}(\mu',\mu) \underset{\sim}{U}(\mu') . \qquad (3.82)$$

To find a corresponding Fredholm equation for $\underset{\sim}{V}(\mu)$, the adjoint albedo problem must be considered. We expand the ith adjoint albedo problem in terms of the decaying adjoint eigenfunctions (which also are full-range complete) as

$$\underset{\sim}{\psi}_i^{\dagger}(o,-\mu_o;o,\mu) = \sum_{s=1}^{M} \alpha^{\dagger}(\nu_{os}) \underset{\sim}{\phi}^{\dagger}(\nu_{os},-\mu) e^{-x/\nu_{os}}$$

$$+ \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu \left\{ \sum_{m=j}^{N} A_j^{\dagger m}(\nu) \underset{\sim}{\phi}_j^{\dagger m}(\nu,-\mu) \right\} e^{-x/\nu} \qquad (3.83)$$

Proceeding as before in the ordinary albedo problem, one solves for the expansion coefficients, uses the boundary conditions (3.33), and treats the N-adjoint albedo problems collectively. The result expressed in terms of the adjoint $\underset{\sim}{S}^{\dagger}$-function is

$$\frac{1}{\mu} \underset{\sim}{S}^{\dagger}(\mu_o,\mu) = \mu_o \underset{\sim}{F}^{\dagger}(\mu_o,\mu) - \int_0^1 d\mu' \underset{\sim}{\tilde{K}}(\mu,\mu') \underset{\sim}{S}^{\dagger}(\mu_o,\mu'), \quad \mu,\mu_o > 0 \ , \qquad (3.84)$$

where

$$\underset{\sim}{F}^{\dagger}(\mu_o,\mu) = \sum_{s=1}^{M} \frac{1}{N_s} \underset{\sim}{\phi}^{\dagger}(\nu_{os},-\mu)\underset{\approx}{\tilde{\phi}}(\nu_{os},\mu_o)$$

$$+ \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu \left\{ \sum_{m=j}^{N} \frac{1}{N_j^m(\nu)} \underset{\sim}{\phi}_j^{\dagger m}(\nu,-\mu)\underset{\sim}{\tilde{\phi}}_j^{m}(\nu,\mu_o) \right\} . \qquad (3.85)$$

Multiplying by μ/μ_o and integrating over μ_o from 0 to 1 an equation for $\underset{\sim}{U}^{\dagger}(\mu)$ is obtained. Since $\underset{\sim}{\tilde{U}}^{\dagger}(\mu) = \underset{\sim}{V}(\mu)$, this last result can be written as

$$\underset{\sim}{V}(\mu) = \underset{\sim}{E} + \mu \int_{-1}^{1} d\mu' \underset{\sim}{K}(\mu,\mu') - \mu \int_{0}^{1} d\mu' \underset{\sim}{V}(\mu')\underset{\sim}{K}(\mu,\mu') . \qquad (3.86)$$

Equations (3.81) and (3.86) are a pair of nonsingular Fredholm integral equations which could, in principle, be used to evaluate the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices by the standard methods of Fredholm equations.[35] However, the matrix $\underset{\sim}{K}(\mu,\mu')$ involved in these equations is quite difficult to evaluate numerically since all the eigenvectors must first be calculated. Although once evaluated, the norm of $\underset{\sim}{K}(\mu,\mu')$ is readily found; and the uniqueness of solution and the uniform convergence of the Neumann series of successive approximations can be assured by a check on the necessary convergence condition[35]

$$1 < \left\{ \max_{1\le i\le N} \sum_{j=1}^{N} \sqrt{\int_0^1 d\mu \int_0^1 d\mu' |K_{ij}(\mu,\mu')|^2} \right\}^{-1} . \qquad (3.87)$$

3.5 AN APPROXIMATE EQUATION FOR $\underset{\sim}{U}$ AND $\underset{\sim}{V}$

In the previous section two Fredholm equations were derived for the $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ functions. From these equations a first order approximation for $\underset{\sim}{U}$ and $\underset{\sim}{V}$ can be obtained by considering only the asymptotic or dominant eigenfunction in the matrix $\underset{\sim}{K}(\mu',\mu)$. Eqs. (3.81) and (3.86) become upon retaining

only terms containing the largest eigenvalue, ν_ℓ,

$$\underset{\sim}{U}(\mu) \doteq \underset{\sim}{E} + \frac{\mu}{N_\ell}\ \underset{\sim}{\phi}(\nu_\ell,-\mu)\tilde{\underset{\sim}{a}}^{\dagger}(\nu_\ell) - \frac{\mu}{N_\ell}\int_0^1 d\mu'\underset{\sim}{\phi}(\nu_\ell,-\mu)\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu')\underset{\sim}{U}(\mu'), \quad (3.88)$$

and

$$\underset{\sim}{V}(\mu) \doteq \underset{\sim}{E} + \frac{\mu}{N_\ell}\ \underset{\sim}{a}(\nu_\ell)\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu) - \frac{\mu}{N_\ell}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu_\ell,-\mu')\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu). \quad (3.89)$$

First consider Eq. (3.88). If the constant row vector, $\tilde{\underset{\sim}{h}}$ is defined as

$$\tilde{\underset{\sim}{h}} = \int_0^1 d\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu')\underset{\sim}{U}(\mu') , \quad (3.90)$$

multiplication of Eq. (3.88) from the left by $\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell-\mu)$ and integration over μ from 0 to 1 yields for $\tilde{\underset{\sim}{h}}$

$$\tilde{\underset{\sim}{h}} \doteq \frac{\int_0^1 d\mu\ \tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu)[\underset{\sim}{E} + \frac{\mu}{N_\ell}\ \underset{\sim}{\phi}(\nu_\ell,-\mu)\tilde{\underset{\sim}{a}}^{\dagger}(\nu_\ell)]}{1 + \frac{1}{N_\ell}\ \int_0^1 d\mu\mu\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu)\underset{\sim}{\phi}(\nu_\ell,-\mu)} \quad (3.91)$$

Substituting this quantity into Eq. (3.88), collecting terms, and recalling

$$\tilde{\underset{\sim}{a}}^{\dagger}(\nu_\ell) = \int_0^1 d\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,\mu') + \int_0^1 d\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu') , \quad (3.92)$$

one finds

$$\underset{\sim}{U}(\mu) \doteq \underset{\sim}{E} + \mu\underset{\sim}{\phi}(\nu_\ell,-\mu)\left[\frac{\int_0^1 d\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,\mu')}{N_\ell + \int_0^1 d\mu'\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu')\underset{\sim}{\phi}(\nu_\ell,-\mu')}\right] . \quad (3.93)$$

However

$$N_\ell = \int_0^1 d\mu'\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,\mu')\underset{\sim}{\phi}(\nu_\ell,\mu') - \int_0^1 d\mu'\mu'\tilde{\underset{\sim}{\phi}}^{\dagger}(\nu_\ell,-\mu')\underset{\sim}{\phi}(\nu_\ell,-\mu'). \quad (3.94)$$

Thus Eq. (3.92) becomes

$$\underset{\sim}{U}(\mu) \doteq \underset{\sim}{E} + \mu\underset{\sim}{\phi}(\nu_\ell,-\mu)\left[\frac{\int_0^1 d\mu'\underset{\sim}{\tilde{\phi}}^\dagger(\nu_\ell,\mu')}{\int_0^1 d\mu'\mu'\underset{\sim}{\tilde{\phi}}^\dagger(\nu_\ell,\mu')\underset{\sim}{\phi}(\nu_\ell,\mu')}\right] \tag{3.95}$$

By using a similar analysis on Eq. (3.89) a first order approximation for $\underset{\sim}{V}(\mu)$ is obtained:

$$\underset{\sim}{V}(\mu) = \underset{\sim}{E} + \mu\left[\frac{\int_0^1 d\mu'\underset{\sim}{\phi}(\nu_\ell,\mu')}{\int_0^1 d\mu'\mu'\underset{\sim}{\tilde{\phi}}^\dagger(\nu_\ell,\mu')\underset{\sim}{\phi}(\nu_\ell,\mu')}\right]\underset{\sim}{\tilde{\phi}}^\dagger(\nu_\ell,-\mu) \ . \tag{3.96}$$

These approximations for $\underset{\sim}{U}$ and $\underset{\sim}{V}$ have been found to work well only for a very large discrete eigenvalue ($\nu_\ell > 10$). This is not surprising since if ν_ℓ is large enough the continuum, $\nu\epsilon(-1,1)$, becomes "lost." These values of large ν_ℓ are thought to occur in media which are close to being critical—i.e., either the absorption is very weak (pure water) or the fission almost compensates for the absorption. And it precisely for those systems characterized by large descrete roots that the iterative solution of the nonlinear integral for $\underset{\sim}{U}$ and $\underset{\sim}{V}$ is very slow in converging.* Thus it is important that the initial guess for the starting iteration be a "good" one; and Eqs. (3.95) and (3.96) provide such a starting point.

*Recall that in the one-speed case, the nonlinear integral equation was very slow in converging for $2c \ (\equiv \sigma_s/\sigma_t) \to 1$. But taking the limit of Eq. (2.93) as $\nu_\ell \to \infty$, yields for the one-speed case, $H(\mu) \doteq 1 + 2\mu$. This approximate expression has a maximum deviation from the correct value of the H-function of less than 3%.

CHAPTER IV

SYMMETRIC TRANSFER

In this chapter, the case of a symmetric transfer matrix is considered. This particular form of $\underset{\sim}{C}$ is not so restrictive as it may appear at first glance. For instance, all two-group problems may be transformed into such a case. Also the N-group thermal neutron problem and the thermal N-term degenerate kernel approximation[10] for a nonmultiplying medium can be cast into a form with a symmetric transfer matrix. This symmetric $\underset{\sim}{C}$ also appears in the special astrophysical situation of radiative transfer with local thermodynamic equilibrium, the generalized picket fence model for the absorption coefficient, and isotropic scattering.[20]

A symmetric transfer matrix greatly simplifies the results of the preceeding chapter. In particular, all the equations for $\underset{\sim}{U}$ and $\underset{\sim}{V}$ becomes self-adjoint, and thus there is no need to consider an associated adjoint problem. It is possible also to show that for this case all the discrete eigenvalues are either real or imaginary—never complex. Finally a proof is given in Section 4.3 that the solution of the resultant Fredholm equation for the $\underset{\sim}{U}(\mu)$ (or $\underset{\sim}{V}(\mu)$) matrix exists and that this solution is unique. This uniqueness proof in turn can be shown to imply the half-range completeness of the infinite medium eigenvectors.

4.1 MULTIGROUP EQUATIONS FOR THERMAL NEUTRONS

Before discussing the properties of the multigroup transport equation, a brief derivation of this equation for the case of thermal neutrons in a non-multiplying medium will be given. Thermal neutron transport theory is usually handled in two ways. The first method which is probably more familiar to the reactor physicist, involves defining effective group constants and directly reducing the energy dependent transport equation to a set of "multigroup" equations without any explicit energy dependence.[6] The second approach involves an expansion of the energy dependence of the flux into an N-term polynomial expansion.[36] This equation in energy polynomials can then be cast into the form of a multigroup equation with a symmetric transfer matrix.[11]

For the case of plane geometry, and isotropic scattering, the source-free energy-dependent Boltzmann equation can be written as follows:

$$(\mu \frac{\partial}{\partial x} + \Sigma_t(E))\psi(x,\mu,E) = \frac{1}{2} \int_{-1}^{1} d\mu' \int_{0}^{\infty} dE' \Sigma_s(E' \to E)\psi(x,\mu',E') , \qquad (4.1)$$

where $\Sigma_s(E' \to E)$ is the scattering kernel for scattering from energy E' to E. Using the usual multigroup technique,[6,37] the energy variable is split into N regions. Integration of Eq. (4.1) over the ith region, the ith multigroup equation is obtained

$$(\mu \frac{\partial}{\partial x} + \sigma_i)\psi_i(x,\mu) = \sum_{j=1}^{N} c_{ij} \int_{-1}^{1} d\mu' \psi_j(x,\mu'), \qquad (4.2)$$

where the group parameters are defined as

$$\psi_i(x,\mu) = \int_{\Delta E_i} dE\, \psi(x,\mu,E) , \qquad (4.3)$$

$$\sigma_i = \frac{1}{\psi_i(x,\mu)} \int_{\Delta E_i} dE\, \Sigma_t(E)\psi(x,\mu,E), \tag{4.4}$$

$$c_{ij} = \frac{1}{2\psi_i(x,\mu)} \int_{\Delta E_i} dE \int_{\Delta E_j} dE' \Sigma_s(E'\to E)\psi(x,\mu,E') \ . \tag{4.5}$$

To make the multigroup constants σ_i, and c_{ij} independent of x and μ it is usual to assume that the energy dependence of the angular flux is separable. Further for a system in thermal equilibrium a good first approximation is to assume this energy dependence is Maxwellian with an effective temperature T. With these assumptions the multigroup parameters are given by

$$c_{ij} = \alpha_j \int_{\Delta E_i} dE \int_{\Delta E_j} dE' \Sigma_s(E'\to E)M(E',T) \ , \tag{4.6}$$

$$\sigma_i = \alpha_i \int_{\Delta E_i} dE\ \Sigma_t(E)M(E,T) \ , \tag{4.7}$$

$$\frac{1}{\alpha_i} = \int_{\Delta E_i} dE\ M(E,T) \ . \tag{4.8}$$

The cross section $\Sigma_s(E'\to E)$ must obey the detailed balance relation:[38]

$$\Sigma_s(E'\to E)M(E',T) = \Sigma_s(E\to E')M(E,T) \ , \tag{4.9}$$

or

$$\frac{1}{\alpha_j} c_{ij} = \frac{1}{\alpha_i} c_{ji} \ . \tag{4.10}$$

Finally defining the symmetric matrix

$$[\underset{\sim}{A}]_{ij} = \frac{1}{\alpha_j} c_{ij} \ , \tag{4.11}$$

the transfer matrix can be written in the special form

$$\underset{\sim}{C} = \underset{\sim}{A}\,\underset{\sim}{D} \tag{4.12}$$

where $\underset{\sim}{D}$ is a diagonal matrix with elements, α_i.

To show that this form of the multigroup equation can be reduced to the required form (i.e., ordered $\underset{\sim}{\Sigma}$ matric and symmetric $\underset{\sim}{C}$), consider the case where the transfer matrix $\underset{\sim}{C}$ is written as $\underset{\sim}{C} = \underset{\sim}{D}_1\underset{\sim}{A}\underset{\sim}{D}_2$ where $\underset{\sim}{D}_1$ and $\underset{\sim}{D}_2$ are diagonal matrices with positive diagonal elements and $\underset{\sim}{A}$ is a symmetric matrix. Clearly this is a slightly more general case than that for thermal neutrons derived above.

The elements of the $\underset{\sim}{\Sigma}$-matrix generally will not be ordered but will be arranged as

$$\sigma_k \geq \sigma_\ell \geq \ldots \geq \sigma_m > 0, \quad 1 \geq k,\ell,\ldots,m \leq N\ . \tag{4.13}$$

To order them, construct a permutation matrix, $\underset{\sim}{P}$, such that

$$\begin{aligned} P_{1i} &= \delta_{ik}, \quad i = 1 \sim N \\ P_{2\ell} &= \delta_{i\ell}, \quad i = 1 \sim N \\ &\vdots \\ P_{Nm} &= \delta_{im}, \quad i = 1 \sim N \end{aligned} \tag{4.14}$$

By multiplying Eq. (4.2) from the left by $\underset{\sim}{P}$, one obtains

$$(\mu \frac{\partial}{\partial x}\underset{\sim}{E} + \underset{\sim}{\Sigma}')\underset{\sim}{\psi}'(x,\mu) = \underset{\sim}{D}_1'\underset{\sim}{A}'\underset{\sim}{D}_2' \int_{-1}^{1} d\mu \underset{\sim}{\psi}'(x,\mu')\ , \tag{4.15}$$

where

$$\begin{aligned}
\underset{\sim}{\psi}'(x,\mu) &= \underset{\sim}{P}\underset{\sim}{\psi}(x,\mu) \\
\underset{\sim}{\Sigma}' &= \underset{\sim}{P}\underset{\sim}{\Sigma}\underset{\sim}{P}^{-1} \\
\underset{\sim}{A}' &= \underset{\sim}{P}\underset{\sim}{A}\underset{\sim}{P}^{-1} \\
\underset{\sim}{D}_i' &= \underset{\sim}{P}\underset{\sim}{D}_i\underset{\sim}{P}^{-1}, \quad i = 1,2 \ .
\end{aligned} \tag{4.16}$$

Since $\underset{\sim}{P}^{-1} = \underset{\sim}{\tilde{P}}$, it follows by inspection that $\underset{\sim}{\Sigma}'$ is diagonal with ordered elements,

$$\sigma_1' \geq \sigma_2' \geq \ldots \geq \sigma_N' \ . \tag{4.17}$$

Further, $\underset{\sim}{D}_1'$ and $\underset{\sim}{D}_2'$ are diagonal matrices, with positive diagonal elements, and $\underset{\sim}{A}'$ is symmetric.

Now, define the diagonal matrice $\underset{\sim}{D}_i^{\pm(1/2)}$ as

$$[\underset{\sim}{D}_i^{\pm 1/2}]_{jk} = \{[\underset{\sim}{D}_i]_{jk}\}^{\pm 1/2}, \quad i = 1,2. \tag{4.18}$$

Multiplying Eq. (4.18) from the left by $\underset{\sim}{D}_1^{-1/2}\underset{\sim}{D}_2^{1/2}$, the desired form of the transport equation is obtained:

$$[\mu \frac{\partial}{\partial x}\underset{\sim}{E} + \underset{\sim}{\Sigma}'']\underset{\sim}{\psi}''(x,\mu) = \underset{\sim}{A}'' \int_{-1}^{1} d\mu \underset{\sim}{\psi}''(x,\mu') \ , \tag{4.19}$$

where

$$\begin{aligned}
\underset{\sim}{\psi}''(x,\mu) &= \underset{\sim}{D}_1^{-1/2}\underset{\sim}{D}_2^{1/2}\underset{\sim}{\psi}'(x,\mu) \\
\underset{\sim}{\Sigma}'' &= \underset{\sim}{\Sigma}' \\
\underset{\sim}{A}'' &= \underset{\sim}{D}_1^{1/2}\underset{\sim}{D}_2^{1/2}\underset{\sim}{A}'\underset{\sim}{D}_1^{1/2}\underset{\sim}{D}_2^{1/2} = \underset{\sim}{\tilde{A}}'' \ .
\end{aligned} \tag{4.20}$$

Thus the thermal neutron problem can be put into a form with a symmetric transfer matrix.

If instead of using the multigroup approach, the energy dependence of $\psi(x,\mu,E)$ in Eq. (4.1) is approximated by a finite sum of Laguerre polynomials of order one, i.e.,

$$\psi(x,\mu,E) \doteq M(E,T) \sum_{i=1}^{N} f_i(x,\mu)L_i(E) , \tag{4.21}$$

a symmetric transfer matrix form of the multigroup equation can also be obtained. Substitution of (4.21) in Eq. (4.1) yields

$$\sum_{i=1}^{N} \left[\left(\mu \frac{\partial}{\partial x} + \Sigma_t(E) \right) M(E,T)L_i(E)f_i(x,\mu) - \frac{1}{2} \int_{-1}^{1} d\mu' f_i(x,\mu') \int_0^\infty dE' \Sigma_s(E' \to E)M(E',T)L_i(E') \right] = 0. \tag{4.22}$$

Explicit appearance of the energy variable is now removed by multiplying Eq. (4.22) by $L_j(E)$ and integrating the result over energy. Assuming the normalization

$$\int_0^\infty dE\, M(E)L_i(E)L_j(E) = \delta_{ij} , \tag{4.23}$$

the result is

$$\sum_{i=1}^{N} \left[\left(\mu\delta_{ij} \frac{\partial}{\partial x} + V_{ij} \right) f_i(x,\mu) - A_{ij} \int_{-1}^{1} d\mu' f_i(x,\mu') \right] = 0 , \tag{4.24}$$

where

$$V_{ij} = V_{ji} = \int_0^\infty dE\, M(E)\Sigma_t(E)L_i(E)L_j(E) , \tag{4.25}$$

and

$$A_{ij} = \frac{1}{2}\int_0^\infty dE\, L_j(E) \int_0^\infty dE' \Sigma_s(E'\to E) M(E') L_i(E') \ . \tag{4.26}$$

By virtue of detailed balance (which $\Sigma_s(E'\to E)$ is assumed to satisfy), $A_{ij} = A_{ji}$.

Eq. (4.24) may be written in the matrix form

$$\left[\mu \frac{\partial}{\partial x} \underset{\sim}{E} + \underset{\sim}{V}\right] \underset{\sim}{f}(x,\mu) = \underset{\sim}{A} \int_{-1}^{1} d\mu' \underset{\sim}{f}(x,\mu) \tag{4.27}$$

where the matrices $\underset{\sim}{V}$ and $\underset{\sim}{A}$ have elements V_{ij} and A_{ij} respectively, and the vector $\underset{\sim}{f}(x,\mu)$ has components $f_i(x,\mu)$. The real symmetric $\underset{\sim}{V}$-matrix can be diagonalized by an orthogonal transformation, $\underset{\sim}{O}$, as[39]

$$\underset{\sim}{\tilde{O}}\underset{\sim}{V}\underset{\sim}{O} = \underset{\sim}{\Sigma} = \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_N \end{pmatrix}, \tag{4.28}$$

where $\underset{\sim}{\tilde{O}}$ is the transpose (and inverse) of $\underset{\sim}{O}$, and σ_i are the eigenvalues of $\underset{\sim}{V}$. Since $\Sigma_t(E) > 0$ for all energy, it can be shown[11] that $\sigma_i > 0$, $i = 1 \sim N$, and for finite N they are bounded from above because all the V_{ij} are finite.[11]

Multiplying Eq. (4.27) by $\underset{\sim}{O}$ one then has

$$\left(\mu \frac{\partial}{\partial x} \underset{\sim}{E} + \underset{\sim}{\Sigma}\right) \underset{\sim}{\psi}(x,\mu) = \underset{\sim}{C} \int d\mu' \underset{\sim}{\psi}(x,\mu') \ , \tag{4.29}$$

where

$$\underset{\sim}{\psi}(x,\mu) = \underset{\sim}{\tilde{O}}\underset{\sim}{f}(x,\mu) \tag{4.30}$$

$$\underset{\sim}{C} = \underset{\sim}{\tilde{O}}\, \underset{\sim}{A}\, \underset{\sim}{O} = \underset{\sim}{\tilde{C}} \ . \tag{4.31}$$

Finally, the σ_i's may be order in exactly the same manner as was done in Eqs. (4.13)-(4.17). Thus once again one has to solve a multigroup equation with a symmetric transfer matrix.

Before ending this section, it is noted that any two group problem—even those including fission—can always be reduced to the symmetric $\underset{\sim}{C}$ situation. The similarity transformation

$$\underset{\sim}{S} = \begin{bmatrix} 0 & \sqrt{c_{12}} \\ \sqrt{c_{21}} & 0 \end{bmatrix} \tag{4.32}$$

will symmetrize any strictly positive $\underset{\sim}{C}$ and leave $\underset{\sim}{\Sigma}$ diagonal. On the other hand, if one or both off-diagonal elements of $\underset{\sim}{C}$ are zero, the resultant multigroup equations can be solved consecutively by applying one-speed theory.

4.2 DISCRETE EIGENVALUE SPECTRUM

Although it is suspected from physical requirements that all the discrete eigenvalues, ν_{os}, s = 1 ~ M, of any subcritical medium must necessarily be real, it has not been possible to prove mathematically that they are never complex. However for the case of symmetric $\underset{\sim}{C}$, it can be shown that the discrete eigenvalues are always real.

To prove this result, multiply the eigenvector equation for $\underset{\sim}{\Phi}(\nu_{os},\mu)$, Eq. (2.5), by $\underset{\sim}{\tilde{\Phi}}^*(\nu_{os},\mu)$ and integrate over μ from 0 to 1. In this manner the following equation involving ν_{os} is obtained:

$$\frac{1}{\nu_{os}}\int_{-1}^{1} d\mu\mu\tilde{\underset{\sim}{\phi}}^{*}(\nu_{os},\mu)\underset{\sim}{\phi}(\nu_{os},\mu) = \int_{-1}^{1} d\mu\tilde{\underset{\sim}{\phi}}^{*}(\nu_{os},\mu)\underset{\sim}{\underset{\sim}{\Sigma}}\underset{\sim}{\phi}(\nu_{os},\mu) - \int_{-1}^{1} d\mu\tilde{\underset{\sim}{\phi}}^{*}(\nu_{os},\mu)\underset{\sim}{C}\int_{-1}^{1}d\mu'\underset{\sim}{\phi}(\nu_{os},\mu'), \quad s = 1\sim M. \tag{4.33}$$

The right hand side Eq. (4.33) is equal to

$$\text{RHS} = \int_{-1}^{1}d\mu \sum_{i=1}^{N} \sigma_i\phi_i^{*}(\nu_{os},\mu)\phi_i(\nu_{os},\mu) - \sum_{i,j=1}^{N}\int_{-1}^{1}d\mu\phi_i^{*}(\nu_{os},\mu)c_{ij}\int_{-1}^{1}d\mu'\phi_j(\nu_{os},\mu'). \tag{4.34}$$

Using the fact $c_{ij} = c_{ji}$, Eq. (4.34) becomes upon decomposing the last term

$$\text{RHS} = \int_{-1}^{1} d\mu \sum_{i=1}^{N} \sigma_i\phi_i^{*}(\nu_{os},\mu)\phi_i(\nu_{os},\mu) - \sum_{i=1}^{N}\int_{-1}^{1} d\mu\phi_i^{*}(\nu_{os},\mu)c_{ii}\int_{-1}^{1} d\mu'\phi_i(\nu_{os},\mu') - \sum_{i=1}^{N}\sum_{j=i+1}^{N} c_{ij}\left\{\int_{-1}^{1} d\mu\phi_i^{*}(\nu_{os},\mu)\int_{-1}^{1}d\mu'\phi_j(\nu_{os},\mu')+\int_{-1}^{1}d\mu\phi_j^{*}(\nu_{os},\mu)\int_{-1}^{1}d\mu'\phi_i(\nu_{os},\mu')\right\}. \tag{4.35}$$

Clearly every term in the above expansion must be real, regardless of ν_{os}, and hence the left hand side of Eq. (4.33) must be real. The integral on the left hand side of Eq. (4.33), which in veiw of Eq. (2.14) can be written as

$$\int_{-1}^{1} d\mu\mu\tilde{\underset{\sim}{\phi}}^{*}(\nu_{os},\mu)\underset{\sim}{\phi}(\nu_{os},\mu) = \sum_{i=1}^{N} \nu_{os}\nu_{os}^{*}b_i(\nu_{os})b_i^{*}(\nu_{os})\int_{-1}^{1}\frac{\mu d\mu}{(\nu_{os}^{*}\sigma_i-\mu)(\nu_{os}\sigma_i-\mu)} \tag{4.36}$$

is also real since it is a sum of products of complex conjugate terms.

If the integral of Eq. (4.36) is not zero, it follows then that the eigenvalue, ν_{os}, must be real! It will now be shown that this integral can vanish only for purely imaginary eigenvalues.

Assume, for the sake of argument, that ν_{os} is complex and $\text{Re}\{\nu_{os}\} > 0$. It is easily verified that in this case

$$0 < (\nu_{os}\sigma_i-\mu)(\nu_{os}^*\sigma_i-\mu) < (\nu_{os}\sigma_i+\mu)(\nu_{os}^*\sigma_i+\mu), \quad \mu > 0, \quad i = 1\sim N. \quad (4.37)$$

Hence each integral in the sum on the right hand side of Eq. (4.45) is strictly positive, and since at least one of the terms $b_i(\nu_{os})\ b_i^*(\nu_{os})$ is also strictly positive, the sum is strictly positive for $\mathrm{Re}\{\nu_{os}\} > 0$. Similarly it can be proved that for $\mathrm{Re}\{\nu_{os}\} < 0$ the sum is strictly negative. Thus the integral (4.36) never vanishes if $\mathrm{Re}\{\nu_{os}\} \neq 0$.

However, if ν_{os} is purely imaginary, one has

$$(\nu_{os}\sigma_i-\mu)(\nu_{os}^*\sigma_i-\mu) = (\nu_{os}\sigma_i+\mu)(\nu_{os}^*\sigma_i+\mu) , \quad (4.38)$$

and each integral in the right hand side of Eq. (4.36) is zero.

Thus one concludes the discrete eigenvalues, ν_{os}, $s = 1 \sim M$, lie solely on the real or imaginary axis. However, in Appendix A it is proved that for a finite medium to have a stationary solution (i.e., be subcritical) there can be no imaginary eigenvalues. This result is apparent also from the following physical argument.

A transport equation solution for an infinite subcritical medium with some source (not at infinity) must physically tend towards zero at large source distances. Since this solution could be expanded in terms of all the eigenfunctions, the imaginary roots would lead to modes which oscillate at large source distances and in turn lead to negative fluxes. Thus it must be concluded, for a subcritical infinite medium, the eigenvalues must be real. If a particular value of $\underset{\sim}{C}$ and $\underset{\sim}{\Sigma}$ yields an imaginary (or infinite) eigenvalue, ν_o, then a stationary solution for a medium characterized by this $\underset{\sim}{C}$ and $\underset{\sim}{\Sigma}$ does

not exist, i.e., the system must be critical or supercritical. For the remainder of this chapter it will be assumed that any medium under consideration has only real eigenvalues.

4.3 SIMPLIFICATION OF THE $\underset{\sim}{U}$ AND $\underset{\sim}{V}$ EQUATIONS

It is not surprising that the results of the preceding chapters are greatly simplified for the symmetric transfer case, since many of the equations become self-adjoint. In particular the eigenvector equation, Eq. (2.5), becomes self-adjoint and from Eq. (2.27)

$$\underset{\sim}{\phi}^{\dagger}(\nu,\mu) \equiv \underset{\sim}{\phi}(\nu,\mu) \qquad \nu\epsilon(-1,1) \text{ or } \nu_{0s}, \quad s = 1\sim M . \tag{4.39}$$

Using this simplification the Fredholm equation for the $\underset{\sim}{U}$-matrix, Eq. (3.81), becomes

$$\underset{\sim}{U}(\mu) = \underset{\sim}{E} + \mu \int_{-1}^{1} \underset{\sim}{K}^{s}(\mu',\mu)d\mu' - \mu \int_{0}^{1} d\mu' \underset{\sim}{K}^{s}(\mu',\mu)\underset{\sim}{U}(\mu') , \tag{4.40}$$

where

$$\underset{\sim}{K}^{s}(\mu',\mu) = \sum_{s=1}^{M} \frac{1}{N_s} \underset{\sim}{\phi}(\nu_{0s},-\mu)\underset{\sim}{\tilde{\phi}}(\nu_{0s},-\mu') + \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu \left\{ \sum_{m=j}^{N} \frac{1}{N_j^m(\nu)} \underset{\sim}{\phi}_j^m(\nu,-\mu)\underset{\sim}{\tilde{\phi}}_j^m(\nu,-\mu') \right\} . \tag{4.41}$$

The transpose of the Fredholm equation for $\underset{\sim}{V}(\mu)$, Eq. (3.86), becomes, for symmetric $\underset{\sim}{C}$, identical to Eq. (4.40)! It will be shown in the next section that the solution of Eq. (4.40) is unique, and hence from Eq. (3.45) the relation between the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices becomes quite direct, namely

$$\underset{\sim}{U}(\mu) = \underset{\sim}{\tilde{V}}(\mu) . \tag{4.42}$$

This result demonstrates that for this symmetric case there is only one fundamental matrix quantity, $\underset{\sim}{U}(\mu)$, which need be computed to obtain the $\underset{\sim}{S}$-function. Thus only one equation (either a Fredholm or a nonlinear integral equation for the $\underset{\sim}{U}$-matrix) need be evaluated.

The generalized $\underset{\sim}{S}$-function, in view of Eqs. (3.21)-(3.25), and (4.42) then is given in component form as

$$[\underset{\sim}{S}(\mu_o,\mu)]_{ij} = \frac{\mu\mu_o}{\sigma_i\mu_o+\sigma_j\mu} [\underset{\sim}{U}(\mu)\underset{\sim}{C}\,\underset{\sim}{\tilde{U}}(\mu_o)]_{ij} , \tag{4.43}$$

The effect on the $\underset{\sim}{S}$-function upon interchanging variables is easily determined from Eq. (4.43) as

$$\underset{\sim}{S}(\mu_o,\mu) = \underset{\sim}{\tilde{S}}(\mu,\mu_o) . \tag{4.44}$$

The symmetric $\underset{\sim}{C}$ approximation also greatly reduces the computational work for the solution of the nonlinear integral equation. From Eq. (3.58) the nonlinear integral equation for $\underset{\sim}{U}(\mu)$ becomes, employing the vectors $\underset{\sim}{u}_i$ of Eq. (3.56),

$$\underset{\sim}{u}_i(\mu) = \underset{\sim}{e}_i + \mu \int_0^1 d\mu' \underset{\sim}{D}_i(\mu,\mu')\underset{\sim}{U}(\mu')\underset{\sim}{C}\,\underset{\sim}{u}_i(\mu), \quad i = 1\sim N . \tag{4.45}$$

As is expected, the nonlinear integral equation for $\underset{\sim}{V}(\mu)$ becomes equal to the transpose of Eq. (4.45), and once again there is only one equation to solve.

For the one-speed case, Eq. (4.44) immediately yields the important result that the $S(\mu_o,\mu)$ function is symmetric with respect to the interchange of its

arguments. Ambarzumian assumed this result in the original derivation of the S-equation (one-speed version of Eq. (3.15)).[26] This result was first proved by Minnaert[40] using physical arguments and later by Chandrasekhar.[27] This invariance result is important in decomposing the one-speed S-function into a product of two identical functions (i.e., $\underset{\sim}{U} \to H$ and $\underset{\sim}{V} \to H$).

4.4 UNIQUENESS OF SOLUTION OF THE $\underset{\sim}{U}$-EQUATION

In this section it will be shown that the solution of the Fredholm equation for $\underset{\sim}{U}(\mu)$, Eq. (4.40), exists and is unique. This uniqueness for $\underset{\sim}{U}(\mu)$ in turn implies that the eigenvectors are half-range complete.

Consider first, the homogeneous equation

$$\underset{\sim}{U}(\mu) = -\mu \int_0^1 d\mu' \underset{\sim}{K}^S(\mu',\mu)\underset{\sim}{U}(\mu') \ . \tag{4.46}$$

Assume for sake of argument, the above equation has a nontrivial solution. Eq. (4.46) can be written as a system of vector equations using the vector $\underset{\sim}{u}_i(\mu)$ which is the ith column of the $\underset{\sim}{U}(\mu)$ matrix (see Eq. (3.56)), namely

$$\underset{\sim}{u}_i(\mu) = -\mu \int_0^1 d\mu' \underset{\sim}{K}^S(\mu',\mu)\underset{\sim}{u}_i(\mu'), \quad i = 1\sim N \ . \tag{4.47}$$

Define now, the vector $\underset{\sim}{\chi}_i(\mu)$ as $\underset{\sim}{u}_i(\mu) = \sqrt{\mu}\ \underset{\sim}{\chi}_i(\mu)$. Multiplying Eq. (4.47) by $\underset{\sim}{\chi}_i^*(\mu)$ and integrating over μ, one obtains upon explicit substitution of $\underset{\sim}{K}^S(\mu',\mu)$

$$\int_0^1 d\mu \tilde{\chi}_i^*(\mu)\chi_i(\mu) = -\sum_{s=1}^{M}\frac{1}{N_s}\int_0^1 d\mu\sqrt{\mu}\,[\widetilde{\Phi(\nu_{os},-\mu)\chi_i^*(\mu)}]\int_0^1 d\mu'\sqrt{\mu'}\,\tilde{\Phi}(\nu_{os},-\mu')$$

$$(x)\ \chi_i(\mu') - \sum_{j=1}^{N}\int_{\eta_{j-1}}^{\eta_j} d\nu\left\{\sum_{m=j}^{N}\frac{1}{N_j^m(\nu)}\int_0^1 d\mu\sqrt{\mu}\right.$$

$$\left.(x)\ [\tilde{\Phi}_j^m(\nu,-\mu)\chi_i^*(\mu)]\int_0^1 d\mu'\sqrt{\mu'}\,\tilde{\Phi}_j^m(\nu,-\mu')\chi_i(\mu')\right\} . \qquad (4.48)$$

Since all the eigenvalues are real, all the eigenvectors $\Phi(\nu,-\mu)$ are also real. Hence both sides of Eq. (4.48) are composed of terms which are products of complex conjugates. Thus there is an apparent contradiction in that the right hand side of Eq. (4.48) must be real and negative, while the left hand side is strictly positive. This result proves that $\chi_i(\mu)$, $i = 1 \sim N$, must be identically zero, or equivalently the homogeneous Eq. (4.47) has only the trivial null vector as a solution.

The inhomogenous Eq. (4.40) for the $U(\mu)$-matrix also can be written as a vector equation for $u_i(\mu)$,

$$u_i(\mu) = k_i(\mu) - \mu\int_0^1 d\mu' K^s(\mu',\mu)u_i(\mu'), \quad i = 1\sim N, \qquad (4.49)$$

where $k_i(\mu)$ is ith column of the matrix $E + \mu\int_{-1}^{1} d\mu'\, K^s(\mu',\mu)$. Such a vector Fredholm equation can be reduced to the usual scalar Fredholm equation[35]

$$f(\mu) = g(\mu) + \int_a^b d\mu' K(\mu',\mu)f(\mu) . \qquad (4.50)$$

Consider the variables μ and μ' ranging over the interval $(0,N)$. Then define the scalar functions $f(\mu)$, $g(\mu)$, and $K(\mu',\mu)$ in the new interval by the following perscription:

$$f(\mu) = [\underset{\sim}{u}_i(\mu-(j-1)N)]_j \ , \tag{4.51}$$

$$g(\mu) = [\underset{\sim}{k}_i(\mu-(j-1)N)]_j \ , \tag{4.52}$$

$$K(\mu',\mu) = [\underset{\approx}{K}^S(\mu'-)j-1)N,\mu-(\ell-1)N]_{j\ell} \ , \tag{4.53}$$

for μ and μ' in the intervals

$$(j-1)N \leq \mu < jN \ , \tag{4.54}$$

and

$$(\ell-1)N \leq \mu' < \ell N \ . \tag{4.55}$$

Here the subscripts j and ℓ refer to various components of the vectors $\underset{\sim}{u}_i$, $\underset{\sim}{k}_i$ and the matrix $\underset{\approx}{K}^S(\mu',\mu)$. With these definitions the vector equation, Eq. (4.49), takes the form of the scalar equation, Eq. (4.50), with a = 0, and b = N.

One of the well known properties of Fredholm integral equations of the form of Eq. (4.50) may be stated as follows: the inhomogeous equation for any arbitrary $g(\mu)$ has one and only one solution, $f(\mu)$, whenever the corresponding homogeneous equation ($g(\mu) \equiv 0$) has only the trival $f(\mu) = 0$ solution.[41] Thus the solution of $\underset{\sim}{U}(\mu)$ from Eq. (4.40) exists and is unique since, as was shown in the previous section, the inhomogeneous equation has only a trivial zero solution.

An immediate consequence of the uniqueness of solution of Eq. (4.40) for $\underset{\sim}{U}(\mu)$ is that the coefficients of the ith albedo problem eigenvector expansion in Eq. (3.73) are also uniquely determined. This in turn implies that the

eigenvectors $\underset{\sim}{\phi}(\nu,\mu)$, $\nu > 0$, are half-range complete in the sense of Case.[1] This half-range completeness has also recently been proved by Leonard and Ferziger by using a more complicated technique.[11]

CHAPTER V

VARIOUS HALF-SPACE PROBLEMS

One common technique for obtaining the complete solution of a particular half-space problem is to expand the angular flux in terms of singular eigenfunctions.[1] Generally the emergent distribution of the half-space problem is unknown, and to determine uniquely the expansion coefficients, half-range completeness of the eigenfunctions must be employed. For the degenerate kernel approximation and the symmetric $\underset{\sim}{C}$ case, such a half-range completeness proof, which shows explicitly how to obtain the coefficients, has been obtained.[11] However application of such theorems to obtain closed formed solutions is considerably more difficult than in the one speed-case,[5] and to calculate explicit numerical results is highly nontrivial.[19]

To evade such half-range formalism, a different approach can be used. The solution of any problem is obtained in two distinct steps. First the emergent distribution at the interface is obtained. It will be shown that the emergent distributions for all half-space problems can be expressed directly in terms of the generalized $\underset{\sim}{S}$-function of the preceding chapters. Once the emergent distribution is known, the use of full-range completeness and orthogonality properties of the eigenvectors readily yield the coefficients of an eigenfunction expansion of the flux.

In this chapter the complete solution to the half-space Milne, albedo, and Green's function problems are obtained in terms of the $\underset{\sim}{S}$-function or $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices.

5.1 THE MILNE PROBLEM

For every positive eigenvalue $\nu\epsilon(0,1)$ or $\nu=\nu_{os}$, s = 1 ~ M, a Milne problem can be defined. Denoting its solution by $\underset{\sim}{\psi}_\nu(x,\mu)$, it is defined as the solution of the transport equation, Eq. (2.1), with the following boundary conditions:

$$\text{(i)}\quad \underset{\sim}{\psi}_\nu(o,\mu) = 0, \quad \mu > 0, \tag{5.1}$$

$$\text{(ii)}\quad \lim_{x\to\infty} \underset{\sim}{\psi}_\nu(x,\mu) = \underset{\sim}{\phi}(-\nu,\mu)e^{x/\nu}, \quad \nu > 0, \tag{5.2}$$

where $\underset{\sim}{\phi}(-\nu,\mu)$ may be any of the eigenvectors—regular or singular.

The first step in obtaining the solution is to find the emergent distribution, $\underset{\sim}{\psi}_\nu(o,-\mu)$, $\mu>0$. Consider a solution of the transport equation, $\underset{\sim}{\psi}(x,\mu)$, defined as

$$\underset{\sim}{\psi}(x,\mu) = \underset{\sim}{\psi}_\nu(x,\mu) + \underset{\sim}{\psi}_a(x,\mu) \tag{5.3}$$

where $\underset{\sim}{\psi}_a(x,\mu)$ is an albedo problem solution with the boundary conditions

$$\text{(i)}\quad \underset{\sim}{\psi}_a(o,\mu) = \underset{\sim}{\phi}(-\nu,\mu), \quad \mu > 0\ , \tag{5.4}$$

$$\text{(ii)}\quad \lim_{x\to\infty} \underset{\sim}{\psi}_a(x,\mu) = 0\ . \tag{5.5}$$

Hence from Eq. (5.3), $\underset{\sim}{\psi}(x,\mu)$ must have the boundary conditions :

$$\text{(i)}\quad \underset{\sim}{\psi}(o,-\mu) = \underset{\sim}{\phi}(-\nu,\mu), \quad \mu > 0 \tag{5.6}$$

$$\text{(ii)}\quad \lim_{x\to\infty} \underset{\sim}{\psi}(x,\mu) = \underset{\sim}{\phi}(-\nu,\mu)e^{x/\nu}\ . \tag{5.7}$$

Clearly the unique solution for $\underset{\sim}{\psi}(x,\mu)$ is

$$\underset{\sim}{\psi}(x,\mu) = \underset{\sim}{\phi}(-\nu,\mu)e^{x/\nu} . \tag{5.8}$$

Equations (5.3) and (5.8) then yield for the emergent Milne distribution

$$\underset{\sim}{\psi}_{\nu}(o,-\mu) = \underset{\sim}{\phi}(-\nu,-\mu) - \underset{\sim}{\psi}_{a}(o,-\mu), \quad \mu > 0 . \tag{5.9}$$

The emergent albedo distribution, $\underset{\sim}{\psi}_{a}(o,-\mu)$, can be expressed in terms of the $\underset{\sim}{S}$-function. From Eqs. (3.9) and (5.4)

$$\underset{\sim}{\psi}_{a}(o,-\mu) = \frac{1}{\mu}\int_{o}^{1} d\mu' \underset{\sim}{S}(\mu',\mu)\underset{\sim}{\phi}(-\nu,\mu') ; \tag{5.10}$$

and hence the emergent Milne distribution in terms of the S-function is

$$\underset{\sim}{\psi}_{\nu}(o,-\mu) = \underset{\sim}{\phi}(\nu,\mu) - \frac{1}{\mu}\int_{o}^{1} d\mu' \underset{\sim}{S}(\mu',\mu)\underset{\sim}{\phi}(-\nu,\mu') . \tag{5.11}$$

Once the $\underset{\sim}{S}$-function has been determined, this equation could be used to obtain numerical values for the emergent Milne distribution. However in any computational scheme only the $\underset{\sim}{U}$ and $\underset{\sim}{V}$-functions would be obtained, and thus this emergent distribution should be expressed in terms of these single variable functions. This reduction of Eq. (5.11) leads to a far simpler equation for numerical evaluation.

By comparing Eqs. (3.17), (3.24), (3.51) and (3.53) it is seen that the $\underset{\sim}{S}(\mu_{o},\mu)$ matrix may be written in the form

$$\underset{\sim}{S}(\mu',\mu) = \mu\mu'\underset{\sim}{U}_{\eta}(\mu)\underset{\sim}{C}\,\underset{\sim}{V}(\mu')\underset{\sim}{D}_{\eta}(\mu,\mu') , \tag{5.12}$$

where the double index notation is again used to denote summation. Recall also that the eigenvector, $\underset{\sim}{\phi}(\nu,-\mu')$, $\nu > 0$, $\mu' > 0$, in view of Eqs. (2.6) and (2.9), can be expressed as

$$\underset{\sim}{\phi}(\nu,-\mu') = \underset{\sim}{F}(\nu,-\mu')\underset{\sim}{C}\,\underset{\sim}{a}(\nu), \quad \nu > 0, \ \mu' > 0 . \tag{5.13}$$

If the diagonal matrix $\underset{\sim}{M}_k(\nu,\mu,\mu_o)$ is defined as

$$\underset{\sim}{M}_k(\nu,\mu,\mu') = \underset{\sim}{D}_k(\mu,\mu')\underset{\sim}{F}(\nu,-\mu') , \tag{5.14}$$

then the integrand of (5.11) is

$$\frac{1}{\mu}\,\underset{\sim}{S}(\mu',\mu)\underset{\sim}{\phi}(\nu,-\mu) = \mu'\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\,\underset{\sim}{V}(\mu')\underset{\sim}{M}_\eta(\nu,\mu,\mu')\underset{\sim}{C}\,\underset{\sim}{a}(\nu). \tag{5.15}$$

This expression can be considerably simplified by considering the explicit form of $\underset{\sim}{M}_k(\nu,\mu,\mu')$. Substitution of $\underset{\sim}{F}$ and $\underset{\sim}{D}_k$ from Eqs. (2.7) and (3.50) yields (in component form)

$$[\underset{\sim}{M}_k(\nu,\mu,\mu')]_{ij} = \frac{\nu}{(\sigma_i\nu+\mu')(\sigma_i\mu+\sigma_k\mu')}\,\delta_{ij} . \tag{5.16}$$

The identity

$$\frac{1}{(\sigma_i\mu+\sigma_k\mu')(\sigma_i\nu+\mu')} = \frac{1}{\sigma_i}\,\frac{1}{\sigma_k\nu-\mu}\left[\frac{\sigma_k}{\sigma_i\mu+\sigma_k\mu'} - \frac{1}{\sigma_i\nu+\mu'}\right] \tag{5.17}$$

may be written as

$$\frac{1}{(\sigma_i\mu+\sigma_k\mu')(\sigma_i\nu+\mu')} = \frac{1}{\sigma_i}\,\frac{P}{\sigma_k\nu-\mu}\,\frac{\sigma_k}{\sigma_i\mu+\sigma_k\mu'} - \frac{1}{\sigma_i}\,\frac{P}{\sigma_k\nu-\mu}\,\frac{1}{\sigma_i\nu+\mu'} . \tag{5.18}$$

This result transforms Eq. (5.16) to

$$[\underset{\sim}{M}_k(\nu,\mu,\mu')]_{ij} = \frac{1}{\sigma_k\nu-\mu}\left\{\frac{\sigma_k}{\sigma_i}\frac{1}{\sigma_i\mu+\sigma_k\mu'}\delta_{ij} - \frac{1}{\sigma_i}\frac{1}{\sigma_i\nu+\mu'}\delta_{ij}\right\}; \tag{5.19}$$

and since

$$\frac{\mu'}{b\mu+d\mu'} = \frac{1}{d}\left[1 - b\frac{\mu}{b\mu+d\mu'}\right], \tag{5.20}$$

Eq. (5.19) yields

$$\mu'[\underset{\sim}{M}_k(\nu,\mu,\mu')]_{ij} = \frac{1}{\sigma_k\nu-\mu}\left\{\frac{1}{\sigma_i}\delta_{ij} - \frac{\mu}{\sigma_i\mu+\sigma_k\mu'}\delta_{ij} - \frac{1}{\sigma_i}\delta_{ij} + \frac{\nu}{\sigma_i\nu+\mu'}\delta_{ij}\right\}, \tag{5.21}$$

or equivalently

$$\mu'[\underset{\sim}{M}_k(\nu,\mu,\mu')]_{ij} = \frac{1}{\sigma_k\nu-\mu}\left\{\frac{\nu}{\sigma_i\nu+\mu'}\delta_{ij} - \mu[\underset{\sim}{D}_k(\mu,\mu')]_{ij}\right\}. \tag{5.22}$$

Substitution of this result into (5.15) and use of (5.13) gives

$$\frac{1}{\mu}\underset{\sim}{S}(\mu',\mu)\underset{\sim}{\phi}(\nu,-\mu') = \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu,-\mu') - \frac{P\mu\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\underset{\sim}{V}(\mu')\underset{\sim}{D}_\eta\underset{\sim}{C}\underset{\sim}{a}(\nu). \tag{5.23}$$

Thus the emergent distribution is

$$\underset{\sim}{\psi}_\nu(\sigma,-\mu) = \underset{\sim}{\phi}(\nu,\mu) - \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu,-\mu') + \frac{P\mu\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{D}_\eta(\mu,\mu')\underset{\sim}{C}\underset{\sim}{a}(\nu). \tag{5.24}$$

This last term may be further simplified by considering the nonlinear integral equation for the $\underset{\sim}{U}$-function. The transpose of Eq. (3.55) is

$$\underset{\sim}{U}(\mu) = \underset{\sim}{E} + \mu\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{D}_\eta(\mu,\mu'), \tag{5.25}$$

or solely in terms of $\underset{\sim}{U}_k(\mu)$

$$\underset{\sim}{U}_k(\mu) = \underset{\sim}{E}_k + \mu\underset{\sim}{U}_k(\mu)\underset{\sim}{C}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{D}_k(\mu,\mu') , \tag{5.26}$$

where $[\underset{\sim}{E}_k]_{ij} = \delta_{ij}\delta_{ik}$.

Hence the emergent distribution is

$$\underset{\sim}{\psi}_\nu(o,-\mu) = \underset{\sim}{\phi}(\nu,\mu) - \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu,-\mu')$$

$$+ \frac{P\nu}{\sigma_\eta\nu-\mu}(\underset{\sim}{U}_\eta(\mu)-\underset{\sim}{E}_\eta)\underset{\sim}{C}\underset{\sim}{a}(\nu) . \tag{5.27}$$

However from Eq. (2.6)

$$\underset{\sim}{\phi}(\nu,\mu) = P\underset{\sim}{F}(\nu,\mu)\underset{\sim}{C}\underset{\sim}{a}(\nu) + \underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu) , \tag{5.28}$$

or substituting for $\underset{\sim}{F}(\nu,\mu)$

$$\underset{\sim}{\phi}(\nu,\mu) = \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{E}_\eta\underset{\sim}{C}\underset{\sim}{a}(\nu) + \underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu). \tag{5.29}$$

Combining the last term in (5.27) with $\underset{\sim}{\phi}(\nu,\mu)$ the emergent distribution simplifies to

$$\underset{\sim}{\psi}_\nu(o,-\mu) = \underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu) + \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\underset{\sim}{a}(\nu)$$

$$- \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{\phi}(\nu,-\mu'), \tag{5.30}$$

or from (5.28)

$$\underset{\sim}{\psi}_\nu(o,-\mu) = \underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu) + \frac{P\nu}{\sigma_\eta\nu-\mu}\underset{\sim}{U}_\eta(\mu)\underset{\sim}{C}\left[\underset{\sim}{E} - \int_0^1 d\mu'\underset{\sim}{V}(\mu')\underset{\sim}{F}(\nu,-\mu')\underset{\sim}{C}\right]\underset{\sim}{a}(\nu). \tag{5.31}$$

Finally writing this equation completely in terms of the matrix $\underset{\sim}{U}(\mu)$, the emergent distribution of the generalized Milne problem is given by the very simple equation

$$\underset{\sim}{\psi}_{\nu}(o,-\mu) = \underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu) + P\underset{\sim}{F}(\nu,\mu)\underset{\sim}{U}(\mu)\underset{\sim}{h}(\nu), \quad \nu > 0, \quad \mu > 0, \tag{5.32}$$

where the constant vector $\underset{\sim}{h}(\nu)$ is

$$\underset{\sim}{h}(\nu) = \underset{\sim}{C}\left\{\underset{\sim}{E} - \int_{o}^{1} d\mu' \underset{\sim}{V}(\mu')\underset{\sim}{F}(\nu,-\mu')\underset{\sim}{C}\right\}\underset{\sim}{a}(\nu). \tag{5.33}$$

Now that the emergent distribution for the generalized Milne problem has been obtained, the angular flux inside the half-space can be obtained. The solution may be expanded in the eigenfunctions which satisfy boundary condition (5.2) as

$$\begin{aligned}\underset{\sim}{\psi}_{\nu}(x,\mu) = {} & \underset{\sim}{\phi}(-\nu,\mu)e^{x/\nu} + \sum_{s=1}^{M} \alpha(\nu_{os})\underset{\sim}{\phi}(\nu_{os},\mu)e^{-x/\nu_{os}} \\ & + \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu' \left\{ \sum_{m=j}^{N} \underset{\sim}{A}_j^m(\nu')\underset{\sim}{\phi}_j^m(\nu',\mu) \right\} e^{-x/\nu'} .\end{aligned} \tag{5.34}$$

Full-range orthogonality immediately gives the expansion coefficients:

$$\begin{aligned}\alpha(\nu_{os}) &= -\frac{1}{N_s} \int_{o}^{1} d\mu\mu \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu)\underset{\sim}{\psi}_{\nu}(o,-\mu) \\ &= -\frac{1}{N_s} \int_{o}^{1} d\mu\mu \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu)\{\underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu) + P\underset{\sim}{F}(\nu,\mu)\underset{\sim}{U}(\mu)\underset{\sim}{h}(\nu)\}\end{aligned} \tag{5.35}$$

and

$$\underset{\sim}{A}_j^m(\nu') = -\frac{1}{N_j^m(\nu')} \int_{o}^{1} d\mu\mu \underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu',\mu)\{\underset{\sim}{G}(\nu,\mu)\underset{\sim}{\lambda}(\nu) + P\underset{\sim}{F}(\nu,\mu)\underset{\sim}{U}(\mu)\underset{\sim}{h}(\nu)\} . \tag{5.36}$$

Often the Milne problem of most interest is the one related to the largest discrete eigenvalue, ν_ℓ. The asymptotic behavior of this particular problem for large x is

$$\underset{\sim}{\psi}^{as}_{\nu_\ell}(x,\mu) = \underset{\sim}{\phi}(-\nu_\ell,\mu)e^{x/\nu_\ell} + \alpha(\nu_\ell)\underset{\sim}{\phi}(\nu_\ell,\mu)e^{-x/\nu_\ell} . \tag{5.37}$$

A quantity of interest for this problem is the extrapolated end point, x_o, defined such that

$$\rho^{as}(x_o) = \int_{-1}^{1} d\mu\psi^{as}_{\nu_\ell}(x_o,\mu) = \underset{\sim}{a}(\nu_\ell)e^{x_o/\nu_\ell} + \alpha(\nu_\ell)\underset{\sim}{a}(\nu_\ell)e^{-x_o/\nu_\ell} = 0 \tag{5.38}$$

Solving for x_o and substituting for $\alpha(\nu_\ell)$ from Eq. (5.35), the extrapolated end point is

$$x_o = -\frac{\nu_\ell}{2} \ln\left\{\frac{1}{N_\ell}\int_o^1 d\mu\mu\underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_\ell,\mu)\underset{\sim}{\psi}_{\nu}(o,-\mu)\right\} , \tag{5.39}$$

or in terms of the $\underset{\sim}{U}(\mu)$ matrix

$$x_o = -\frac{\nu_\ell}{2} \ln\left\{\frac{1}{N_\ell}\int_o^1 d\mu\mu\underset{\sim}{\tilde{a}}^{\dagger}(\nu_\ell)\underset{\sim}{C}\,\underset{\sim}{F}^2(\nu_\ell,\mu)\underset{\sim}{U}(\mu)\underset{\sim}{h}(\nu_\ell)\right\} . \tag{5.40}$$

5.2 THE ALBEDO PROBLEM

In Chapter III the albedo problem was discussed, and the complete solution obtained. For sake of completeness the general results briefly are reviewed. The generalized $\underset{\sim}{S}$-function was defined in terms of the emergent distributions of the N albedo problems. From Eqs. (3.1), (3.3), and (3.9), the emergent distribution for the ith problem, $\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu)$, is

$$\underset{\sim}{\psi}_i(o,\mu_o;o,-\mu) = \frac{1}{\mu}\underset{\sim}{S}(\mu_o,\mu)\underset{\sim}{e}_i, \quad \mu > 0. \tag{5.41}$$

The complete solution, $\psi_i(o,\mu\ ;x,\mu)$, can be expanded in an eigenfunction expansion as was done in Eq. (3.73).

$$\underset{\sim}{\psi}_i(o,\mu_o,x,\mu) = \sum_{s=1}^{M} \alpha(\nu_{os})\underset{\sim}{\phi}(\nu_{os},\mu)e^{-x/\nu_{os}}$$

$$+ \sum_{j=1}^{N} \int_{\eta_{j-1}}^{\eta_j} d\nu \left\{ \sum_{m=j}^{N} A_j^m(\nu)\underset{\sim}{\phi}_j^m(\nu,\mu) \right\} e^{-x/\nu} . \qquad (5.42)$$

From Eqs. (5.1) and (3.1) full-range orthogonality gives for these expansion coefficients

$$\alpha(\nu_{os}) = \frac{\mu_o}{N_{os}} \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu_o)\underset{\sim}{e}_i - \frac{1}{N_{os}} \int_o^1 d\mu \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},-\mu)\underset{\sim}{S}(\mu_o,\mu)\underset{\sim}{e}_i , \qquad (5.43)$$

and

$$A_j^m(\nu) = \frac{\mu_o}{N_j^m(\nu)} \underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,\mu)\underset{\sim}{e}_i - \frac{1}{N_j^m(\nu)} \int_o^1 d\mu \underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,-\mu)\underset{\sim}{S}(\mu_o,\mu)\underset{\sim}{e}_i . \qquad (5.44)$$

These results can be expressed more simply when the transfer matrix of the problem becomes symmetric. In this case the expansion coefficients can be expressed in terms of the emergent distribution of the generalized Milne problem. The transpose of this emergent distribution is, from Eq. (5.11),

$$\underset{\sim}{\tilde{\psi}}_\nu(o,-\mu) = \underset{\sim}{\tilde{\phi}}(\nu,\mu) - \frac{1}{\mu} \int_o^1 d\mu' \underset{\sim}{\tilde{\phi}}(\nu,-\mu')\underset{\sim}{\tilde{S}}(\mu',\mu) , \qquad (5.45)$$

or in view of Eq. (4.53)

$$\underset{\sim}{\tilde{\psi}}_\nu(o,-\mu) = \underset{\sim}{\tilde{\phi}}(\nu,\mu) - \frac{1}{\mu} \int_o^1 d\mu' \underset{\sim}{\tilde{\phi}}(\nu,-\mu')\underset{\sim}{S}(\mu,\mu') . \qquad (5.46)$$

Comparison of this equation with Eqs. (5.43) and (5.44) shows that the expansion coefficients can be written in the simple form

$$\alpha(\nu_{os}) = \frac{\mu_o}{N_{os}} \tilde{\underset{\sim}{\psi}}_{\nu_{os}}(o,-\mu_o)\underset{\sim}{e}_i \ , \tag{5.47}$$

and

$$A_j^m(\nu) = \frac{\mu_o}{N_j^m(\nu)} \tilde{\underset{\sim}{\psi}}^m_{\nu_j}(o,-\mu_o)\underset{\sim}{e}_i \ , \tag{5.48}$$

where $\underset{\sim}{\psi}_{\nu j}{}^m(x,\mu)$ is the generalized Milne problem solution associated with continuum eigenvector $\underset{\sim}{\phi}_j{}^m(-\nu,\mu)$. Finally using Eqs. (5.32) and (4.51), these coefficients in terms of the $\underset{\sim}{U}(\mu)$ matrix are

$$\alpha(\nu_{os}) = \frac{\mu_o}{N_{os}} \underset{\sim}{F}(\nu_{os},\mu_o)\underset{\sim}{U}(\mu_o)\underset{\sim}{C}\left\{\underset{\sim}{E} - \int_o^1 d\mu' \tilde{\underset{\sim}{U}}(\mu')\underset{\sim}{F}(\nu_{os},-\mu')\underset{\sim}{C}\right\}\underset{\sim}{a}(\nu_{os}), \tag{5.49}$$

and

$$A_j^m(\nu) = \frac{\mu_o}{N_j^m(\nu)} \underset{\sim}{G}(\nu,\mu_o)\underset{\sim}{\lambda}_j^m(\nu) + \frac{\mu_o P}{N_j^m(\nu)} \underset{\sim}{F}(\nu,\mu_o)\underset{\sim}{U}(\mu_o)\underset{\sim}{C}\left\{\underset{\sim}{E} - \int_o^1 d\mu' \tilde{\underset{\sim}{U}}(\mu')\underset{\sim}{F}(\nu,-\mu')\underset{\sim}{C}\right\}a_j^m(\nu). \tag{5.50}$$

For the nonsymmetric $\underset{\sim}{C}$ situation, the expansion coefficients for the albedo problem could be expressed in terms of a generalized adjoint Milne problem. However since this latter problem has no immediate physical meaning this approach will not be pursued further.

5.3 HALF-SPACE GREEN'S FUNCTION

As a final example of the use of the generalized $\underset{\sim}{S}$-function technique, the half-space Green's function problem will be solved. This problem is the most general half-space problem in the sense that all other half-space problems can, in principle, be generated from this function. The half-space Green's function, with the source neutrons belonging solely to the ith energy group, $\underset{\sim}{G}_i(x_o,\mu_o;x,\mu)$, is defined by the equation

$$(\mu \frac{\partial}{\partial x} \underset{\sim}{E} + \underset{\sim}{\Sigma})\underset{\sim}{G}_i(x_o,\mu_o;x,\mu) = C \int_{-1}^{1} d\mu' \underset{\sim}{G}_i(x_o,\mu_o;x,\mu') + \delta(\mu-\mu_o)\delta(x-x_o)\underset{\sim}{e}_i, \quad x_o>0, \tag{5.51}$$

with the boundary conditions

$$\text{(i)} \quad \underset{\sim}{G}_i(x_o,\mu_o;o,\mu) = 0, \quad \mu > 0 , \tag{5.52}$$

$$\text{(ii)} \quad \lim_{x\to\infty} \underset{\sim}{G}_i(x_o,\mu_o;x,\mu) = 0 . \tag{5.53}$$

The first step towards obtaining the solution, is to determine the emergent distribution, $\underset{\sim}{G}_i(x_o,\mu_o;o,-\mu)$, $\mu > 0$. Consider the Green's function to be composed of two parts:

$$\underset{\sim}{G}_i(x_o,\mu_o;x,\mu) = \underset{\sim}{G}_i^{\infty}(x_o,\mu_o;x,\mu) + \underset{\sim}{\psi}_a(x,\mu), \quad x_o > 0 , \tag{5.54}$$

where $\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;x,\mu)$ is the known infinite medium Green's function discussed in Section 2.4. The albedo problem solution, $\underset{\sim}{\psi}_a(x,\mu)$, satisfies the homogeneous transport equation with the boundary conditions

$$\left.\begin{aligned} &\text{(i)} \quad \underset{\sim}{\psi}_a(o,\mu) = -\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,\mu), \quad \mu > 0, \\ &\text{(ii)} \quad \lim_{x\to\infty} \underset{\sim}{\psi}_a(x,\mu) = 0 . \end{aligned}\right\} \tag{5.55}$$

Clearly $\underset{\sim}{G}_i(x_o,\mu_o;x,\mu)$ defined by Eq. (5.54) satisfies Eq. (5.51) and has the required boundary conditions.

The emergent distribution of the albedo solution, $\underset{\sim}{\psi}_a(o,-\mu)$, can be expressed in terms of its incident distribution from Eq. (3.9). Hence from Eq. (5.54) the emergent distribution $\underset{\sim}{G}_i(x_o,\mu_o;o,-\mu)$ is

$$\underset{\sim}{G}_i(x_o,\mu_o;o,-\mu) = \underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,-\mu) - \frac{1}{\mu}\int_o^1 d\mu' \underset{\sim}{S}(\mu',\mu)\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,\mu'). \qquad (5.56)$$

Since the angular flux for the half-space Green's function is now known at $x = 0$, for all μ, the complete solution can be found by using the full range completeness and orthogonality properties of the infinite medium eigenfunctions. Explicitly

$$\underset{\sim}{G}_i(x_o,\mu_o;x,\mu) = \underset{\sim}{G}_i^{\infty}(x_o,\mu_o;x,\mu) + \sum_{s=1}^{M}\alpha(\nu_{os})\underset{\sim}{\phi}(\nu_{os},\mu)e^{-x/\nu_{os}} + \sum_{j=1}^{N}\int_{\eta_{j-1}}^{\eta_j} d\nu\left\{\sum_{m=j}^{N} A_j^m(\nu)\underset{\sim}{\phi}_j^m(\nu,\mu)\right\}e^{-x/\nu}, \qquad (5.57)$$

where

$$\alpha(\nu_{os}) = -\frac{1}{N_s}\int_o^1 d\mu\mu\underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_{os},\mu)\left\{\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,\mu) - \frac{1}{\mu}\int_o^1 d\mu'\underset{\sim}{S}(\mu',\mu)\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,\mu')\right\} \qquad (5.58)$$

and

$$A_j^m(\nu) = -\frac{1}{N_j^m(\nu)}\int_o^1 d\mu\mu\underset{\sim}{\tilde{\phi}}_j^{\dagger m}(\nu,\mu)\left\{\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,\mu) - \frac{1}{\mu}\int_o^1 d\mu'\underset{\sim}{S}(\mu',\mu)\underset{\sim}{G}_i^{\infty}(x_o,\mu_o;o,\mu')\right\}. \qquad (5.59)$$

CHAPTER VI

NUMERICAL RESULTS

In most analytical treatments of transport theory, the extension of results to numerical evaluation is far from trivial. To obtain numerical values for a particular half-space solution, the singular eigenfunction expansion coefficients must be evaluated. This evaluation can be quite difficult since it involves principle value integrals and functions which vary rapidly. Even to calculate the emergent distribution (which often is all that is required), methods based on half-range eigenfunction expansions still require evaluation of the expansion coefficients.[2,19] However, the emergent distributions are readily evaluated from the present $\underset{\sim}{S}$-function formulation without recourse to complicated numerical techniques.

When the solution is needed inside the half-space, the present method is still thought to be superior to half-range methods even though expansion coefficients must also be evaluated. The difference is that the $\underset{\sim}{S}$-function method uses a full-range expansion which allows the use of the known full-range orthogonality relations, while half-space methods must use the more complicated half-range orthogonality properties or constructive half-range completeness theorems to obtain the coefficients.

To demonstrate the feasibility of solving multigroup problems in terms of the generalized $\underset{\sim}{S}$-function, five different examples are considered. The first four are for light water thermal systems. The first case, Case I, is for ordinary water and Cases II, III and IV are for borated water with con-

centrations of 1.025, 2.99 and 6.35 barns per hydrogen atom respectively. Three broad energy groups were chosen and defined as

$$\begin{aligned} &\text{Group 1:} \quad 0 \leq E_1 \leq .0253 \text{ eV} \\ &\text{Group 2:} \quad .0253 \leq E_2 < .5320 \text{ eV} \\ &\text{Group 3:} \quad .5320 \leq E_3 \leq 2.38 \text{ eV} \end{aligned} \tag{6.1}$$

The thermal spectra evaluation and cross section averaging to determine the group constants were performed by the INCITE code,[42] using the McMurry-Russell[43] H_2O kernel at room temperature (293°K). The group constants for the four cases are listed in Table I.

As a final example, Case V, a half-space of uranium-238 enriched with 2% uranium-235 is considered. This case, which includes fission in the transfer matrix, was broken into six energy groups. The group constants for this 2% enriched case were calculated from the 6-group constant tables originally developed for highly enriched pure uranium systems such as Godiva and Topsy.[37,44] The energy groups and the group constants for Case V are listed in Table II.

6.1 ITERATIVE SOLUTION FOR THE $\underset{\sim}{U}$ AND $\underset{\sim}{V}$-FUNCTIONS

In Chapter III two sets of nonlinear integral equations for the $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ matrices were derived. Both of these sets, Eqs. (3.26) and (3.27) and Eqs. (3.61) and (3.62), can be solved readily by numerical methods. In this section the numerical procedures and results of the computational schemes for both sets are discussed briefly.

TABLE I

THREE-GROUP MACROSCOPIC CROSS SECTIONS FOR WATER (cm^{-1})

CASE I: Pure Water

$\sigma_1 = 4.8824$, $\sigma_2 = 3.2345$, $\sigma_3 = 1.7467$

$$2\underset{\sim}{C} = \begin{pmatrix} 3.8180 & .35242 & .012285 \\ 1.0326 & 2.8669 & .65299 \\ 1.145\times10^{-9} & .0002069 & 1.07789 \end{pmatrix}$$

CASE II: Borated Water, 1.025 barns/hydrogen atom

$\sigma_1 = 4.9270$, $\sigma_2 = 3.1692$, $\sigma_3 = 1.7493$

$$2\underset{\sim}{C} = \begin{pmatrix} 3.7953 & .32387 & .012239 \\ 1.0345 & 2.8005 & .65012 \\ 1.143\times10^{-9} & .0005813 & 1.0763 \end{pmatrix}$$

CASE III: Borated Water, 2.99 barns/hydrogen atom

$\sigma_1 = 5.0914$, $\sigma_2 = 3.0720$, $\sigma_3 = 1.7696$

$$2\underset{\sim}{C} = \begin{pmatrix} 3.7659 & .27047 & .012204 \\ 1.0454 & 2.6828 & .64697 \\ 1.140\times10^{-9} & .001379 & 1.0796 \end{pmatrix}$$

CASE IV: Borated Water, 6.35 barns/hydrogen atom

$\sigma_1 = 5.3220$, $\sigma_2 = 2.9760$, $\sigma_3 = 1.7853$

$$2\underset{\sim}{C} = \begin{pmatrix} 3.7901 & .21636 & .012019 \\ 1.0481 & 2.5341 & .63509 \\ 1.132\times10^{-9} & .002291 & 1.0737 \end{pmatrix}$$

TABLE II

SIX GROUP URANIUM CROSS SECTIONS

(98% U-238, 2% U-235)

Group i	Energy (Mev)	σ_i (cm^{-1})	Transfer Cross Sections (cm^{-1})					
			σ_{i1}	σ_{i2}	σ_{i3}	σ_{i4}	σ_{i5}	σ_{i6}
1	3.0-∞	.1917	.0761	.0123	.00163	.000584	.000686	.00112
2	1.4-3.0	.2105	.0448	.1079	.00276	.000982	.00115	.00188
3	0.9-1.4	.2164	.0361	.0267	.1399	.000480	.000564	.000916
4	0.4-0.9	.2512	.0528	.0563	.0395	.2163	.000605	.000985
5	0.1-0.4	.3919	.0328	.0358	.0266	.0240	.3797	.000492
6	0-0.1	.5655	.00452	.00512	.00487	.00387	.00387	.5432

$N^{U-235} = 9.56 \times 10^{-28}$ atoms/cm^3.

$N^{U-238} = 4.69 \times 10^{-26}$ atoms/cm^3.

In any numerical scheme, integration of some function $f(\mu)$ over μ, must be approximated by some summation procedure. In all of the present work a 16 point Gauss quadrature technique was employed, i.e.,

$$\int_a^b d\mu f(\mu) \doteq \sum_{k=1}^{16} w(\mu_k) f(\mu_k) \tag{6.2}$$

where μ_k are the quadrature ordinates for the range (a,b), and $w(\mu_k)$ are the corresponding Christoffel numbers.[45]

With this integration approximation, the iterative schemes for the set of nonlinear integral equations, Eqs. (3.26)-(3.27) can be written as:

$$\underset{\sim}{V}^{(n+1)}(\mu_k) = \underset{\sim}{E} + \mu_k \sum_{\ell=1}^{16} w(\mu_\ell) \underset{\sim}{A}(\mu_\ell, \mu_k) * [\underset{\sim}{U}^{(n)}(\mu_\ell) \underset{\sim}{C} \underset{\sim}{V}^{(n)}(\mu_k)], \quad k = 1 \sim 16, \tag{6.3}$$

and

$$\underset{\sim}{U}^{(n+1)}(\mu_k) = \underset{\sim}{E} + \mu_k \sum_{\ell=1}^{16} w(\mu_\ell) \underset{\sim}{A}(\mu_k, \mu_\ell) * [\underset{\sim}{U}^{(n)}(\mu_k) \underset{\sim}{C} \underset{\sim}{V}^{(n+1)}(\mu_\ell)], \quad k = 1 \sim 16, \tag{6.4}$$

where the superscripts on $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ are the iteration index. Similarly the iteration scheme for the equations for $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ without direct products, Eqs. (3.61)-(3.64) can be represented as,

$$\underset{\sim}{v}_i^{(n+1)}(\mu_k) = \left[\underset{\sim}{E} - \mu_k \sum_{\ell=1}^{16} w(\mu_\ell) \underset{\sim}{D}_i(\mu_k, \mu_\ell) \underset{\sim}{U}^{(n)}(\mu_\ell) \underset{\sim}{C}\right]^{-1} \underset{\sim}{e}_i, \quad k = 1 \; 16, \tag{6.5}$$

$$\underset{\sim}{u}_i^{(n+1)}(\mu_k) = \left[\underset{\sim}{E} - \mu_k \sum_{\ell=1}^{16} w(\mu_\ell) \underset{\sim}{D}_i(\mu_k, \mu_\ell) \underset{\sim}{\tilde{V}}^{(n+1)}(\mu_\ell) \underset{\sim}{C}\right]^{-1} \underset{\sim}{e}_i, \quad k = 1 \sim 16. \tag{6.6}$$

For both these schemes a good starting point is to take $\underset{\sim}{U}^{(o)}(\mu) = \underset{\sim}{V}^{(o)}(\mu) = \underset{\sim}{E}$.

For a large number of groups, Eqs. (6.5) and (6.7) as they stand, require per iteration considerably more computation than Eqs. (6.3) and (6.4). This

follows the fact that to evaluate the matrix inverse of Eq. (6.5) or Eq. (6.6) involves finding N^2 cofactors of an N x N matrix. A more efficient, but equivalent, technique would be to use Cramer's method.[46] From Eqs. (3.54) and (3.60) one obtains

$$[\underset{\sim}{v}_i^{(n+1)}(\mu_k)]_j = \frac{\det|\underset{\sim}{F}_j(\mu_k)|}{\det|\underset{\sim}{F}(\mu_k)|} , \tag{6.7}$$

and

$$[\underset{\sim}{u}_i^{(n+1)}(\mu_k)]_j = \frac{\det|\underset{\sim}{G}_j(\mu_k)|}{\det|\underset{\sim}{G}(\mu_k)|} , \quad j = 1 \sim N . \tag{6.8}$$

where the N x N matrices $\underset{\sim}{F}$ and $\underset{\sim}{G}$ are given by

$$\underset{\sim}{F}(\mu_k) = \underset{\sim}{E} - \mu_k \sum_{\ell=1}^{16} w(\mu_\ell)\underset{\sim}{D}_i(\mu_k,\mu_\ell)\underset{\sim}{U}^{(n)}(\mu_\ell)\underset{\sim}{C} , \tag{6.9}$$

and

$$\underset{\sim}{G}(\mu_k) = \underset{\sim}{E} - \mu_k \sum_{\ell=1}^{16} w(\mu_\ell)\underset{\sim}{D}_i(\mu_k,\mu_\ell)\underset{\sim}{V}^{(n+1)}(\mu_\ell)\underset{\sim}{C} . \tag{6.10}$$

The matrices $\underset{\sim}{F}_j(\mu_k)$ and $\underset{\sim}{G}_j(\mu_k)$ are obtained by replacing the jth row by the vector $\underset{\sim}{e}_i$. Because $\underset{\sim}{e}_i$ has a particularly simple form, evaluation of Eqs. (6.7) or (6.8) involves calculating only N cofactors of an $\underset{\sim}{N}$ x $\underset{\sim}{N}$ matrix. For a large number of groups this savings can be appreciable.

Two computer programs in the FORTRAN IV language[47] have been written to solve by iteration Eqs. (6.3)-(6.4) and Eq. (6.7)-(6.8) for the $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ matrices. These programs, called GENUV and MILNE respectively, are listed in Appendix B. To investigate the properties of these two computational schemes,

the four three-group cases of water (discussed at the beginning of this chapter) were solved for $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ on The University of Michigan's IBM-360 system.

Instead of storing successive iterations of $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ to measure convergence, identity (3.31) is used to a given measure of the error in $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$. Every five iterations the matrix

$$\frac{1}{2}\sum_{\ell=1}^{16} w(\mu_\ell)\left\{ \underset{\sim}{U}^{(n)}(\mu_\ell)\underset{\sim}{\Sigma} + \underset{\sim}{\Sigma}\,\underset{\sim}{V}(\mu_\ell) - \underset{\sim}{U}(\mu_\ell)\underset{\sim}{C}\sum_{m=1}^{16} w(\mu_m)\underset{\sim}{V}(\mu_m)\right\} \tag{6.11}$$

is evaluated. The maximum deviation of the elements of (6.11) from the elements of the known $\underset{\sim}{\Sigma}$ matrix is then used as a measure of the error for each iteration. With this definition of the error in $\underset{\sim}{U}^{(n)}(\mu)$ and $\underset{\sim}{V}^{(n)}(\mu)$ at the nth iteration, a plot of error versus iteration index can be made.

In Fig. 1 the iteration error versus the iteration index is given for both iteration schemes for the four cases of water. It is quickly seen that as the absorption decreases the convergence rate correspondingly decreases. This result is not too surprising for in the one speed case it is well known that iteration of the nonlinear integral equation (3.28), for $H(\mu)$, which is a specialization of the $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ equations, converges extremely slowly as $c \to 1/2$ (the angular averaging factor of 2 has been absorbed into the present definition of c).[27,48]

However from Fig. 1, the convergence of the "Cramer's" scheme (Eqs. (6.7)-(6.10)) is far superior to the direct scheme of Eqs. (6.3) and (6.4). In fact, the convergence rate of the Cramer's scheme is a factor of 3 to 3-1/2 times greater.

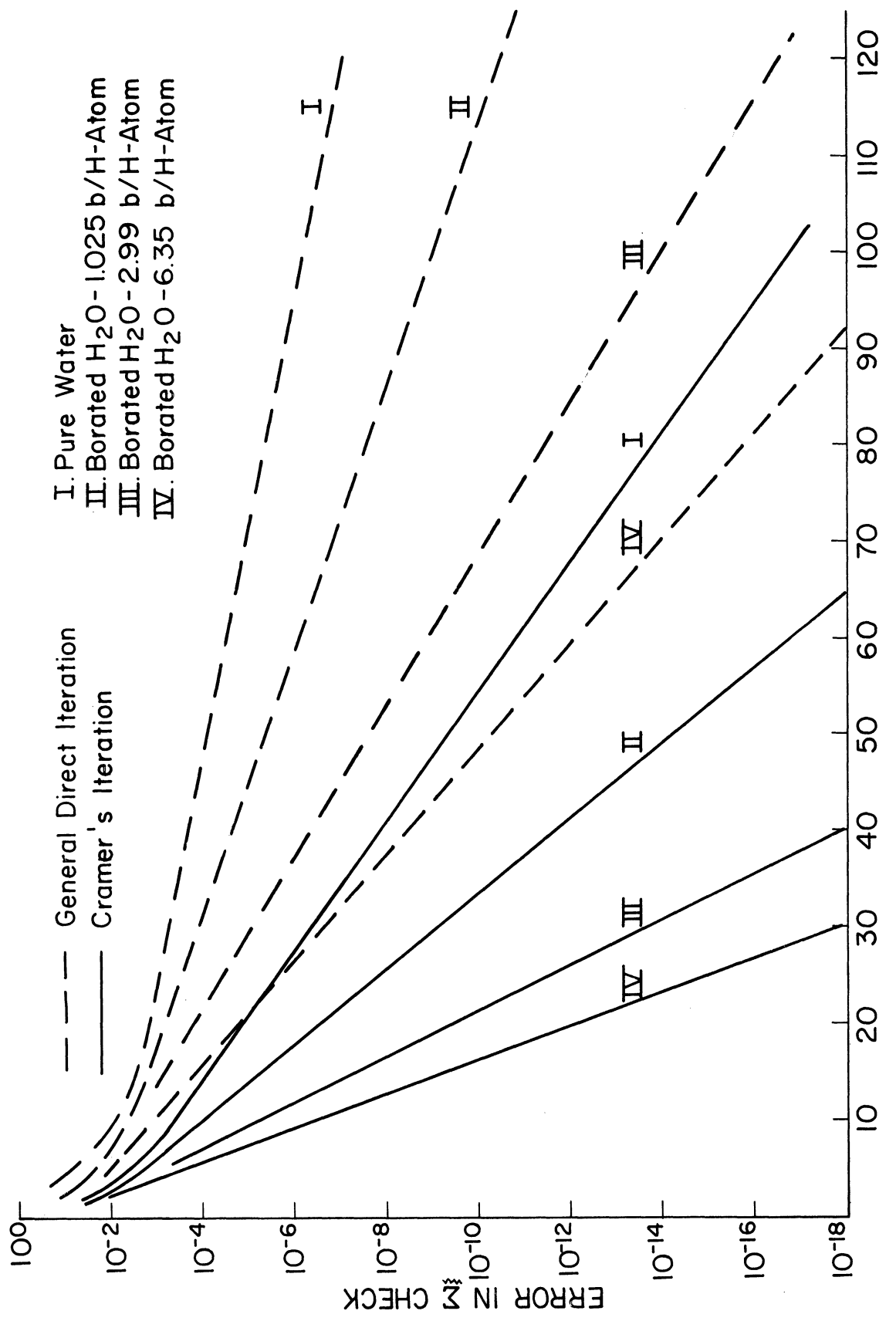

Fig. 6.1. Convergence of $\underset{\sim}{U}$-$\underset{\sim}{V}$ iteration schemes.

From Fig. 1, it may appear that even this Cramer's method is slow to converge. But it should be noted that the four cases presented as examples were all for relatively weakly absorbing situations. The INCITE code which generated the group parameters for these cases, also gave effective one group constants. The effective one-speed multiplication factors, 2c, for Case I through IV are .995, .984, .958, and .920, respectively. For other cases which have more absorption or are farther removed from criticality, the Cramer's iteration scheme converges quite rapidly. In those situations, which are close to criticality, the approximations of the Fredholm equations for $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$, given by Eqs. (3.42) and (3.93), can be used to give a good initial starting point to the iteration scheme. A program to calculate these Fredholm approximations, called FRED, is listed in Appendix B.

Although the Cramer's scheme does converge relatively quickly, the computational time required for a large number of groups is appreciable. For example, the six-group calculation required approximately ten minutes on the IBM-360 Model 70 computer. To improve the convergence rate when a large number of groups is involved, various well-known schemes for accelerating the convergence could be used (e.g., successive overrelaxation, residual polynomials, etc).[6,30]

6.2 MILNE PROBLEM

To demonstrate the ease with which emergent distributions for half-space problems can be numerically evaluated from the $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ functions, the classical Milne problem (i.e., $\nu = \nu_\ell$, largest of ν_{os}, $s = 1 \sim M$) is considered for the five multigroup cases previously mentioned. This particular problem

first requires knowledge of the discrete eigenvalue spectrum, and a method by which the discrete eigenvector, $\underset{\sim}{\phi}(\nu_\ell,\mu)$, can be evaluated. Once these quantities have been found, straight forward evaluation of Eqs. (5.32) and (5.39) gives the emergent flux and extrapolated endpoint. Unlike the computations done by others for this problem, no difficult mathematical techniques such as principle value integrals are encountered in the present technique. In this section the computer programs used to evaluate this problem are briefly described, and the results presented. These programs, written in FORTRAN IV for the IBM 360, are all listed in Appendix B.

To find the discrete eigenvalues of the dispersion relation, Eq. (2.13), a series of three subprograms were written, DISP, MINV, and ROOT. The first evaluates the matrix $\underset{\sim}{\Omega}(1/y)$ for any $y \in (0,1)$, and MINV then evaluates the determinant. The program ROOT then searches for the values y_o for which $\det|\underset{\sim}{\Omega}(1/y_o)| = 0$. This search is accomplished by calculating the quantity $\det|\Omega(1/y)|$ for successively decreasing values of y and watching for a change in sign in $\det|\Omega(1/y)|$. The use of increasingly finer grids whenever a change of sign is encountered, allows the zero to be evaluated as accurately as desired. In the present case all zeros were calculated to within an accuracy of one part in 10^7, although ROOT allows accuracy to within one part in 10^{16}. The only major limitations on the above procedure is that it will not always find successfully multiple zeros, or if the initial search grid is too coarse it may pass over zeros which are very closely spaced. This latter restriction is easily circumvented for a difficult situation by making the search grid finer

For all five cases, two discrete roots were found. The first four cases for water were also investigated recently by Metcalf, who used two group constants for the same four cases.[19] The results for all five cases are tabulated below along with Metcalf's two-group results. For the classical Milne problem $\nu_\ell = \nu_{o_1}$.

TABLE III

DISCRETE EIGENVALUES

Case	ν_{o_1} (cm)	ν_{o_2} (cm)	Two Group Result[19] ν_o (cm)
I Pure Water	2.22151	.638781	2.2221
II borated Water	1.31951	.636656	1.3190
III borated Water	.847391	.625854	.84534
IV borated Water	.659514	.610169	.65105
V 2% enriched Uranium	12.3793	5.21725	

The evaluation of the discrete eigenvector $\underset{\sim}{\phi}(\nu_\ell, \mu)$ and its normalization $\underset{\sim}{a}(\nu_\ell)$ is calculated by the subprogram AVEC. From Eqs. (2.9), (2.11) and (2.12) the normalization vector is given by

$$[\underset{\sim}{E}-\underset{\sim}{T}(\nu_\ell)\underset{\sim}{C}]\underset{\sim}{a}(\nu_\ell) = 0 \quad , \tag{6.12}$$

where $\underset{\sim}{T}(\nu_\ell)$ is the diagonal matrix

$$[\underset{\sim}{T}(\nu_\ell)]_{ij} = 2\nu_\ell \tanh^{-1}\left(\frac{1}{\sigma_i \nu_\ell}\right) \quad . \tag{6.13}$$

Equation (6.12) is readily solved by matrix inversion (MINV) by using only the first N-1 equations in (6.12) and setting $a_N(\nu_\ell) \equiv 1$. The subroutine entry

EIGEN of this subroutine allows calculation of $\underset{\sim}{\phi}^{\dagger}(\nu_\ell,\mu)$ or $\underset{\sim}{\phi}(\nu_\ell,\mu)$ for the positive Gaussian integration ordinates, μ_k, k = 1 ~ 16 for an input parameter of $\underset{\sim}{\tilde{C}}$ or $\underset{\sim}{C}$ respectively. From these evaluations of the discrete eigenvectors, the full-range orthogonality normalization, N_ℓ, is readily calculated by

$$N_\ell \equiv \int_{-1}^{1} d\mu \underset{\sim}{\tilde{\phi}}^{\dagger}(\nu_\ell,\mu)\underset{\sim}{\phi}(\nu_\ell,\mu) \doteq \sum_{k=1}^{16} \mu_k w(\mu_k)[\underset{\sim}{\tilde{\phi}}_k^{\dagger}(\nu_\ell,\mu_k)\underset{\sim}{\phi}(\nu_\ell,\mu_k) + \underset{\sim}{\tilde{\phi}}^{\dagger}(-\nu_\ell,\mu_k)\underset{\sim}{\phi}(-\nu_\ell,\mu_k)]. \tag{6.14}$$

Once the quantities ν_ℓ and $\underset{\sim}{a}(\nu_\ell)$, together with the $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ matrices have been calculated, the emergent Milne problem distribution $\underset{\sim}{\psi}_{\nu_\ell}(o,-\mu)$ is readily evaluated from Eq. (5.32) for $\nu = \nu_\ell$, i.e.,

$$\underset{\sim}{\psi}_{\nu_\ell}(o,-\mu) = \underset{\sim}{F}(\nu_\ell,\mu)\underset{\sim}{U}(\mu)\underset{\sim}{C}\{\underset{\sim}{E} - \int_{o}^{1} d\mu' \underset{\sim}{V}(\mu')\underset{\sim}{F}(\nu_\ell,-\mu')\underset{\sim}{C}\}\underset{\sim}{a}(\nu_\ell) \tag{6.15}$$

The above calculation is performed by the main program MILNE which used Cramer's scheme for finding $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$. This program is listed in Appendix B.

Since the vector $\underset{\sim}{a}(\nu_\ell)$ was arbitrarily normalized in the subroutine AVEC such that $a_N(\nu_\ell) = 1$, it is not possible to directly compare results for different $\underset{\sim}{C}$'s and ν_ℓ's. To aid comparison the program MAIN also gives the emergent distribution normalized to unit density; namely,

$$\sum_{i=1}^{N} \int_{-1}^{1} d\mu [\underset{\sim}{\psi}_{\nu_\ell}(o,\mu)]_i = \sum_{i=1}^{N} \int_{o}^{1} d\mu [\underset{\sim}{\psi}_{\nu_\ell}(o,-\mu)]_i = 1 . \tag{6.16}$$

In Fig. 6.2 to 6.5 the emergent distributions for the Milne problem corresponding to the largest discrete eigenvalues for the four three-group water cases. Fig. 6.6 is a polar plot of the normalized emergent Milne distribution

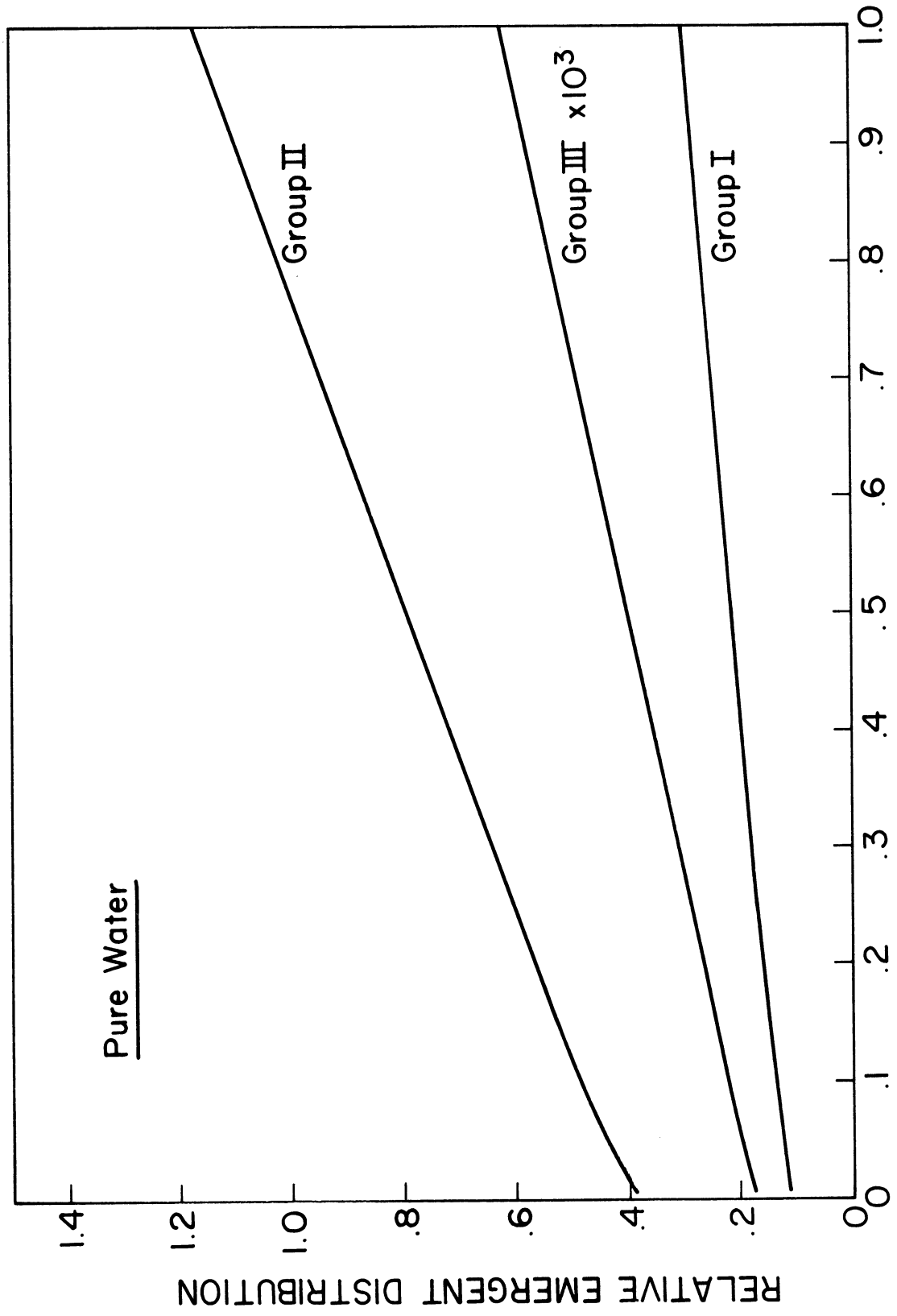

Fig. 6.2. Emergent Milne distribution (normalized to unit density) for Case I.

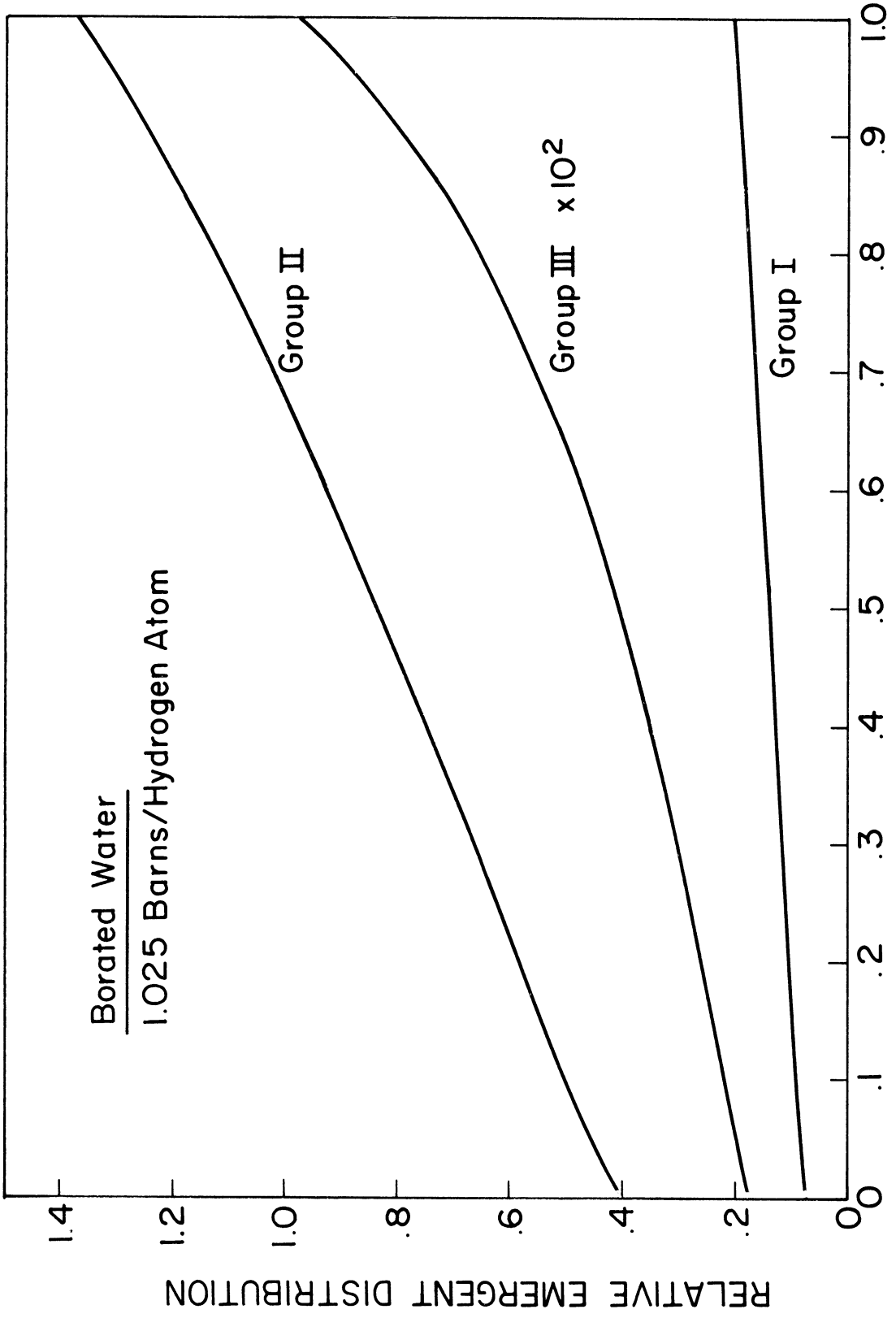

Fig. 6.3. Emergent Milne distribution (normalized to unit density) for Case II.

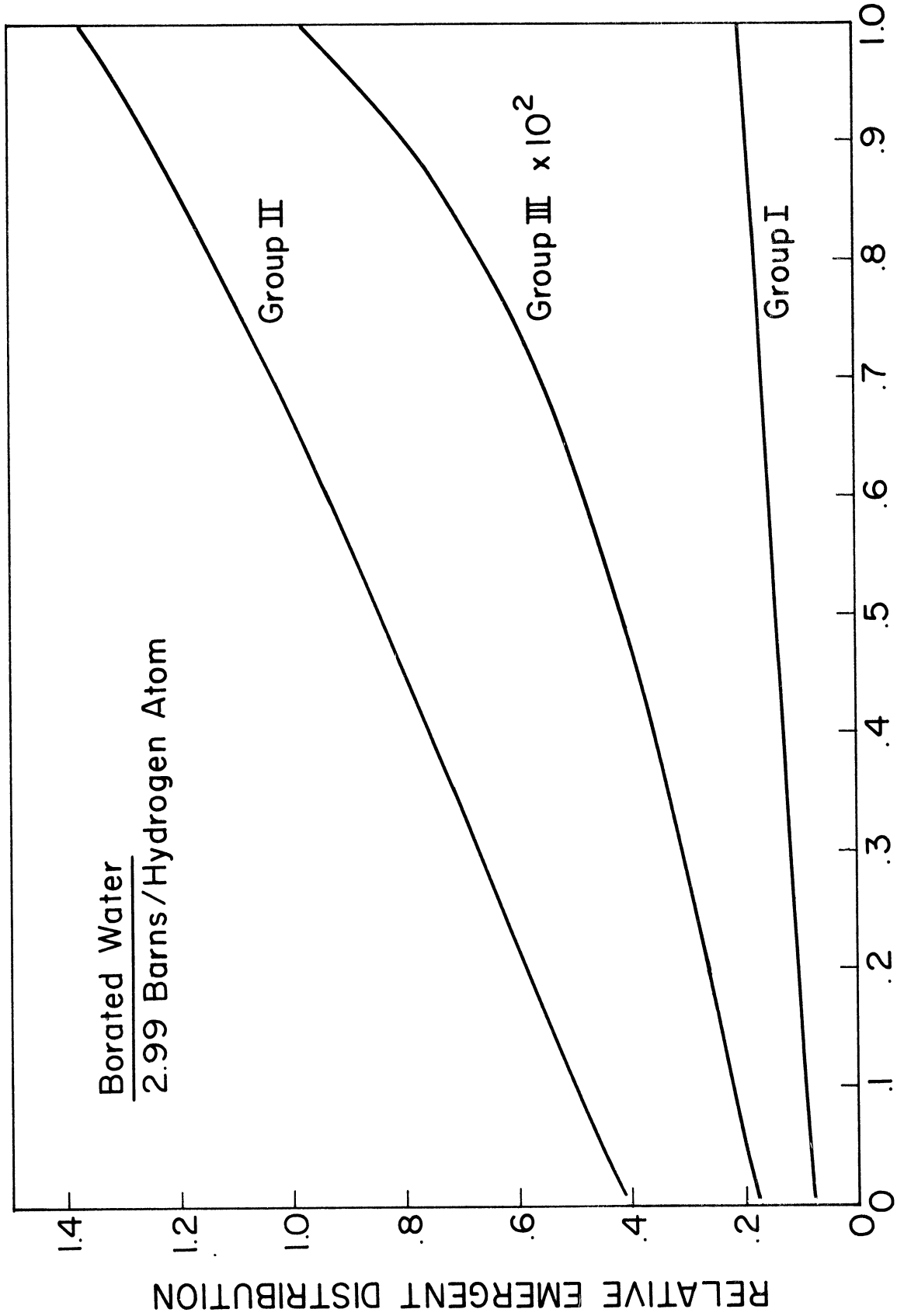

Fig. 6.4. Emergent Milne distribution (normalized to unit density) for Case III.

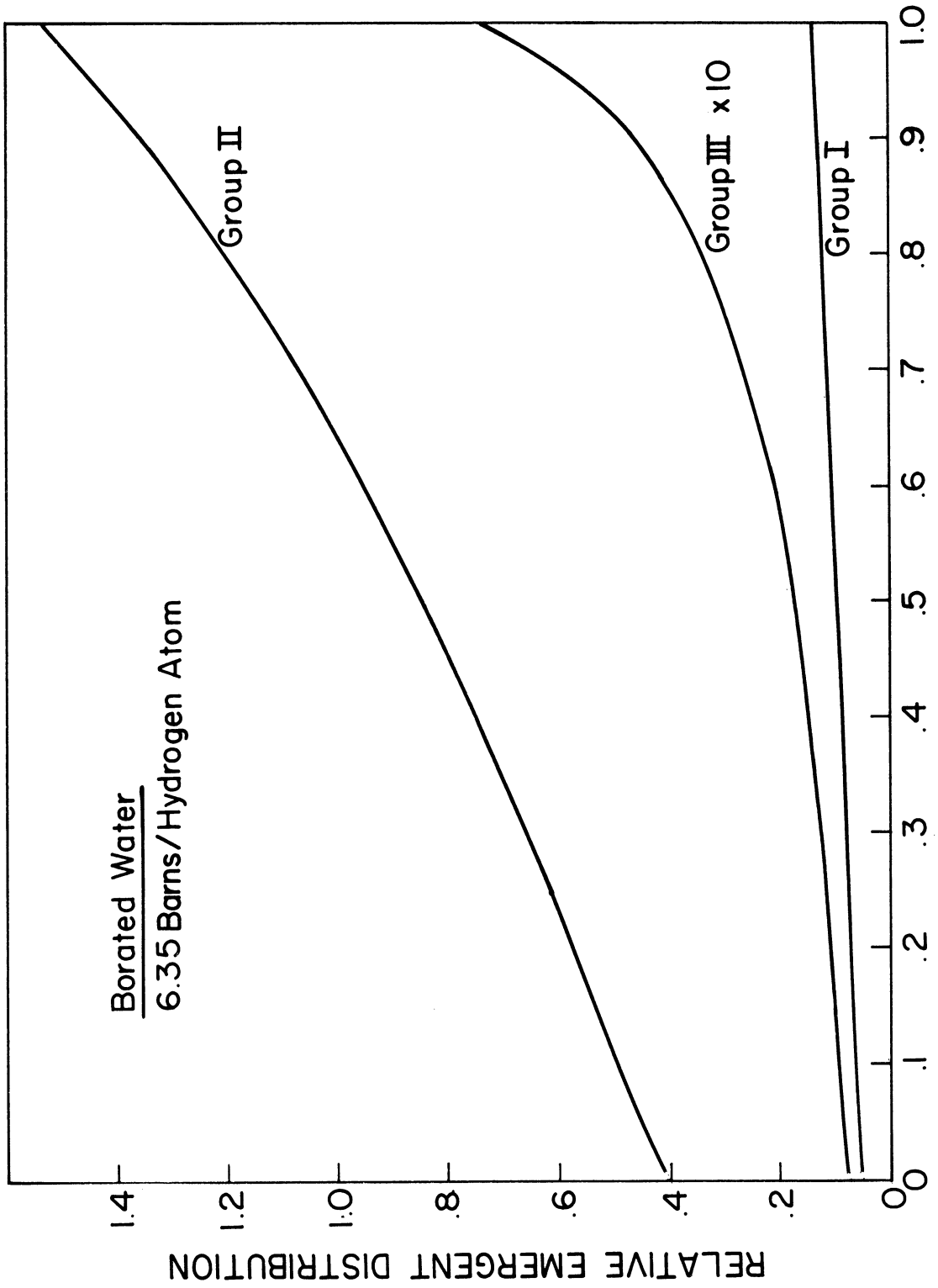

Fig. 6.5. Emergent Milne distribution (normalized to unit density) for Case IV.

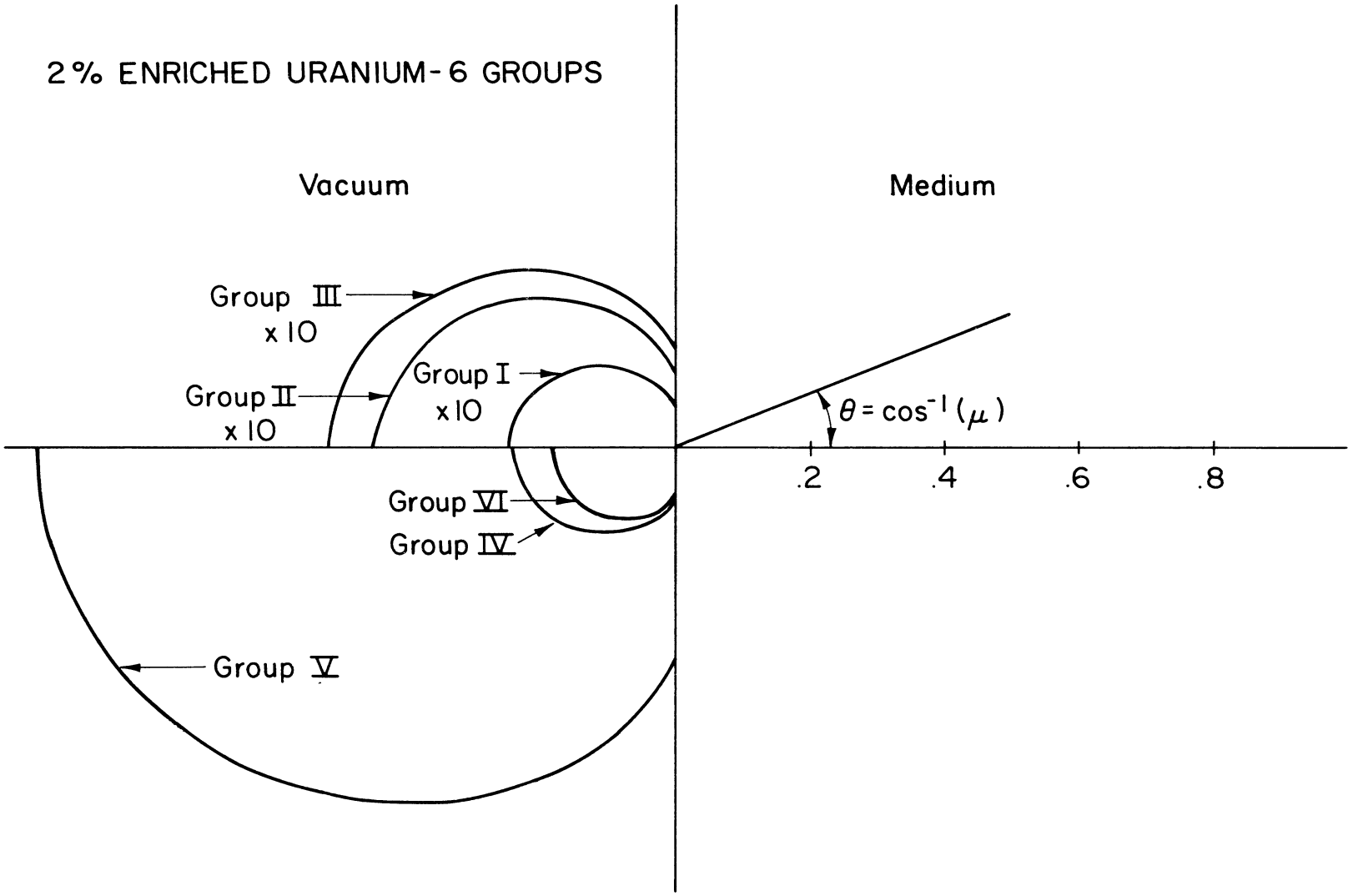

Fig. 6.6. Normalized emergent Milne distribution for Case V.

for the six-group uranium case, Case V. In this latter figure only half the emergent distribution is plotted since the distribution is symmetric about $\mu = 0$.

In the four cases for pure and borated water, two interesting results are noted. For pure water (a system close to criticality) the emergent distribution is almost linear with the cosine of the emergent angle, i.e., $-\mu$. Then as absorption is increased the emergent flux becomes increasingly more anisotropic. This result was also noted by Metcalf.[19]

As a final numerical example for these five cases, the extrapolation length was calculated (performed by the MILNE program). This quantity is calculated by straightforward evaluation of Eq. (3.59). The results for the five cases are shown in Table IV, and as before the four water cases are compared with the results Metcalf obtained using a two group analysis.

TABLE IV

EXTRAPOLATION LENGTHS

Case	Extrapolation Length (cm) calculated by MILNE	Calculated by Metcalf
I pure water	-.205947	-.2058
II borated water	-.214407	-.2140
III borated water	-.233944	-.2319
IV borated water	-.294657	-.2560
V 2% enriched	-2.21798	

These three-group calculations agree quite well with the two group results in the first three cases. However there is an appreciable difference for the most heavily borated water case. This is at first surprising since the discrete eigenvalues for this case agreed reasonably well. To investigate this discrepancy all the two group calculations were performed by the MILNE

program, and Metcalf's results were confirmed. Hence one is led to believe that the introduction of the third high energy group has become quite significant. In fact from Figs. 6.2 and 6.5 it is seen that the flux at the interface for the third group is one hundred times larger for Case IV than for the pure water situation.

As a final check on the accuracy of the emergent distribution, MILNE calculates the coefficient of the asymptotically increasing mode. This quantity should be unity. From Eq. (5.34) this coefficient is

$$\frac{1}{N_\ell}\int_0^1 d\mu\mu\tilde{\underset{\sim}{\Phi}}^\dagger(\nu_\ell,\mu)\underset{\sim}{\psi}_{\nu_\ell}(o,-\mu) = \frac{1}{N_\ell}\sum_{k=1}^{16}\mu_k w(\mu_k)\tilde{\underset{\sim}{\Phi}}^\dagger(\nu_\ell,\mu_k)\underset{\sim}{\psi}_{\nu_\ell}(o,-\mu_k) \quad (6.17)$$

In all cases the difference from unity was less than 10^{-5}.

CHAPTER VII

CONCLUSIONS

In this work the solutions of various half-space N-group transport problems in plane geometry were found. These solutions were obtained by combining the techniques of Chandrasekhar's principle of invariance and Case's singular eigenfunction expansions, and extending them to the multigroup case. In particular, it was shown that the expansion coefficients of a multigroup eigenfunction expansion for any given problem could be expressed directly in terms of a "generalized $\underset{\sim}{S}$-function."

To obtain equations for this generalized $\underset{\sim}{S}$-function, which is closely related to the emergent distribution of the half-space albedo problem, two different approaches were used. The first, obtained from Chandrasekhar's principle of invariance a nonsingular, nonlinear integral equation for this function. Furthermore, this method demonstrated that the $\underset{\sim}{S}$-function, which has two angular arguments, could be decomposed into two auxiliary functions, $\underset{\sim}{U}$ and $\underset{\sim}{V}$, each of which depends on only a single variable. Although it was not possible to solve analytically the nonlinear integral equation for the $\underset{\sim}{S}$-function (or the corresponding nonlinear integral equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions), numerical solution by iteration was found to be quite straightforward. However this approach does appear to have one defficiency. From analogy to the one speed equations, it is suspected that the nonlinear integral equations may not have a unique solution. As a result, a set of necessary conditions for

$\underset{\sim}{S}$ (and for $\underset{\sim}{U}$ and $\underset{\sim}{V}$) were derived; and, again from the one-speed analogy, it is expected that these necessary conditions may indeed be sufficient. However, a proof of sufficiency is still lacking.

The second approach obtained, from an eigenfunction expansion of the albedo and adjoint albedo problems, Fredholm equations for the functions $\underset{\sim}{S}$, $\underset{\sim}{U}$, and $\underset{\sim}{V}$. These equations also could not be solved analytically; and although they generally do not have the short-comings of the nonlinear integral equations (i.e., possible nonuniqueness), their solution by numerical techniques, while also straightforward, is more difficult since all the infinite medium eigenfunctions must first be evaluated to calculate the Fredholm kernel. In the specific situation of a near-critical system, the Fredholm equations gave a good approximate analytic expression for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions by neglecting all but the dominant mode entirely.

Throughout this research great emphasis was placed on techniques amenable to numerical evaluation. This reduction, of analytic results to numerics has, until quite recently, been decidedly neglected for energy-dependent problems. This work demonstrated how emergent distributions for any half-space problem are readily calculated. Although evaluation of the eigenfunction expansion coefficients (from which the iterior distribution may be calculated) is still a difficult problem because the explicit forms of the eigenfunctions must first be calculated, the method described here is still felt to be superior to other half-space methods. The simplification arises from the fact that full-range expansions can be employed rather than the more difficult half-range techniques.

As an example of the ease with which the nonlinear integral equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions can be computed, a series of computer codes were written in the widely-used FORTRAN IV language to solve for the emergent distribution of the general N-group Milne problem. These programs are designed for any number of groups and arbitrary cross section data (with the proviso the data represent a subcritical system).

Finally for the special case of symmetric transfer (as is found in thermal neutron transport problems) it was shown how the results for a general transfer matrix are greatly simplified. For this case many interesting results can be proved: uniqueness of solution of the Fredholm equations, reality of the eigenvalues, and half-range completeness of the infinite medium eigenfunctions can be demonstrated.

As in any research of this nature, many related extensions and areas of further investigation suggest themselves. Among those areas which deserve further attention are the nonlinear integral equations for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions. Although these equations are readily evaluated numerically for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions, the determination of their uniqueness (or sufficient conditions for uniqueness) would put the present theory on a much firmer mathematical basis.

For the symmetric transfer case it was shown that subcritical systems must have real eigenvalues. In the general case, however, this was not possible, and an investigation of the relation between the group parameters, subcriticality and the eigenvalues would be quite interesting.

It is felt that the present method for solving multigroup half-space problems with isotropic scattering can be readily extended to other transport problems. In particular, the anisotropic scattering situation seems quite amenable to the generalized $\underset{\sim}{S}$-function approach. More useful perhaps—would be an extension to slab problems. Again using the analogy of the one-speed case, it should be possible to derive nonlinear matrix integral equations for the reflected and transmitted flux. Thus while the main effort of this work has been to multigroup, isotropic, half-space transport problems, it is expected that the techniques explored and developed here will be found useful in exploring both the numerical and analytic treatments of other energy dependent transport problems.

APPENDIX A

DISCRETE EIGENVALUES FOR SYMMETRIC TRANSFER

In Chapter VI, the eigenvalues, $\pm\nu_{os}$, s = 1 ~ M for symmetric transfer were shown to be either purely real or purely imaginary. From physical arguments, it was then demonstrated that for subcritical systems, ν_{os} could not be imaginary. This appendix will present a more rigorous derivation of this fact.[49]

Consider a half-space which at time, t = 0, has some arbitrary angular flux distribution, $\underset{\sim}{\psi}(x,\mu,o)$. The resultant flux for t > 0, $\underset{\sim}{\psi}(x,\mu,t)$, is given by the time-dependent multigroup equation

$$\left(\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial t} + \underset{\sim}{\Sigma}\right)\underset{\sim}{\psi}(x,\mu,t) = \underset{\sim}{C}\int_{-1}^{1} d\mu'\underset{\sim}{\psi}(x,\mu',t) \quad . \tag{A.1}$$

If the system is "subcritical", this flux must tend to zero after a long time, i.e., $\lim_{t\to\infty}\underset{\sim}{\psi}(x,\mu,t) = 0$. This requirement will be shown to imply that the discrete eigenvalues, ν_{os}, cannot be imaginary.

Taking the Laplace Transform of Eq. (A.1) one obtains

$$\left(s + \mu\frac{\partial}{\partial x} + \underset{\sim}{\Sigma}\right)\underset{\sim}{\psi}_{\ell}(x,\mu,x) = \underset{\sim}{C}\int_{-1}^{1} d\mu'\,\underset{\sim}{\psi}_{\ell}(x,\mu',s) + \underset{\sim}{\psi}(x,\mu,o), \tag{A.2}$$

where

$$\underset{\sim}{\psi}_{\ell}(x,\mu,s) = \int_{o}^{\infty} ds\, e^{-st}\underset{\sim}{\psi}(x,\mu,t) \quad . \tag{A.3}$$

Then taking the Fourier Transform of (A.2) one has

$$(s + ik\mu + \underset{\sim}{\Sigma})\,\underset{\sim}{\psi}_{f}(k,\mu,s) = \underset{\sim}{C}\,\underset{\sim}{h}(k,s) + \underset{\sim}{\chi}(k,\mu,o) \quad , \tag{A.4}$$

where

$$\underset{\sim}{\psi}_f(k,\mu,s) = \int_{-\infty}^{\infty} dx\, e^{-ikx}\, \underset{\sim}{\psi}_\ell(x,\mu,s) \quad , \tag{A.5}$$

$$\underset{\sim}{\chi}(k,\mu,o) = \int_{-\infty}^{\infty} dx\, e^{-ikx}\, \underset{\sim}{\psi}(x,\mu,o) \quad , \tag{A.6}$$

and

$$\underset{\sim}{h}(k,s) = \int_{-1}^{1} d\mu'\, \underset{\sim}{\psi}_f(k,\mu',s) \quad . \tag{A.7}$$

Integration of Eq. (A.4) with respect to μ, yields for $\underset{\sim}{h}(k,s)$

$$\underset{\sim}{h}(k,s) = [\underset{\sim}{E} - \underset{\sim}{\Lambda}(k,s)]^{-1}\underset{\sim}{C}^{-1}\, \underset{\sim}{\chi}(k,\mu,o) \quad . \tag{A.8}$$

The matrix $\underset{\sim}{\Lambda}(k,s)$ is defined by

$$\underset{\sim}{\Lambda}(k,s) = \int_{-1}^{1} d\mu'(s + ik\mu' + \underset{\sim}{\sum})^{-1}\, \underset{\sim}{C} \quad . \tag{A.9}$$

From Eq. (A.4) and (A.8) the Fourier transformed flux, $\underset{\sim}{\psi}_f(k,\mu,s)$, is

$$\underset{\sim}{\psi}_f(k,\mu,s) = (s+ik\mu+\underset{\sim}{\sum})^{-1}\underset{\sim}{C}\{[\underset{\sim}{E}-\underset{\sim}{\Lambda}(k,s)]^{-1}+\underset{\sim}{E}\}\underset{\sim}{C}^{-1}\underset{\sim}{\chi}(k,\mu,o) \quad . \tag{A.10}$$

This equation may be simplified by noting

$$\{[\underset{\sim}{E} - \underset{\sim}{\Lambda}(k,s)]^{-1} + \underset{\sim}{E}\} = [\underset{\sim}{E} - \underset{\sim}{\Lambda}(k,s)]^{-1}\{2\underset{\sim}{E} - \Lambda(\underset{\sim}{k},s)\}$$

$$= \frac{\underset{\sim}{M}'(k,s)}{\det|\underset{\sim}{E}-\underset{\sim}{\Lambda}(k,s)|}\{2\underset{\sim}{E} - \Lambda(\underset{\sim}{k},s)\} \quad , \tag{A.11}$$

where $\underset{\sim}{M}'(k,s)$ is the matrix formed by the cofactors of the matrix $[\underset{\sim}{E} - \underset{\sim}{\Lambda}(k,s)]$.

If another matrix $M(k,s)$ is defined as

$$\underset{\sim}{M}(k,s) = \underset{\sim}{M}'(k,s)\{2\underset{\sim}{E} - \underset{\sim}{\Lambda}(k,s)\} \quad , \tag{A.12}$$

then Eq. (A.10) becomes

$$\underset{\sim}{\psi}_f(k,\mu,s) = \frac{1}{\det|\underset{\sim}{E}-\underset{\sim}{\Lambda}(k,s)|}\,(s + ik\mu + \underset{\sim}{\Sigma})^{-1}\,\underset{\sim}{C}\,\underset{\sim}{M}(k,s)\underset{\sim}{C}^{-1}\,\underset{\sim}{X}(k,\mu,o). \tag{A.13}$$

To obtain the Laplace transform of the flux, $\underset{\sim}{\psi}_\ell(x,\mu,s)$, the inverse Fourier transform of Eq. (A.13) is taken.

$$\underset{\sim}{\psi}_\ell(x,\mu,s) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx}\,\underset{\sim}{\psi}_f(k,\mu,s)$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx}\,\frac{1}{\det|\underset{\sim}{E}-\underset{\sim}{\Lambda}(k,s)|}(s + i\mu k + \underset{\sim}{\Sigma})^{-1}\underset{\sim}{C}\,\underset{\sim}{M}(k,s)\underset{\sim}{C}^{-1}\underset{\sim}{\chi}(k,\mu,o)\ . \tag{A.14}$$

From this quantity the asymptotic time behaviour of the angular flux may be determined by application of the "final value theorem," of Laplace transforms.[50] This theorem states

$$\lim_{t\to\infty}\underset{\sim}{\psi}(x,\mu,t) = \lim_{s\to\infty} s\underset{\sim}{\psi}_\ell(x,\mu,s) \quad . \tag{A.15}$$

Hence from Eq. (A.14) the asymptotic flux is

$$\lim_{t\to\infty}\underset{\sim}{\psi}(x,\mu,t) = \lim_{s\to o}\int_{-\infty}^{\infty} dk\, e^{ikx}\,(i\mu k+\underset{\sim}{\Sigma})^{-1}\underset{\sim}{C}\,\underset{\sim}{M}(k,o)\underset{\sim}{C}^{-1}\underset{\sim}{\chi}(k,\mu,o)\frac{s}{\det|\underset{\sim}{E}-\underset{\sim}{\Lambda}(k,s)|} \tag{A.16}$$

For k belonging to the real axis, the matrix $\underset{\sim}{M}(k,o)$ never vanishes; and hence the subcriticality requirement that the asymptotic flux be zero depends on whether the following quantity vanishes:

$$\lim_{s\to o} \frac{s}{\det|\underset{\sim}{E}-\underset{\sim}{\Lambda}(k,s)|} \quad , \quad k \in(-\infty,\infty) \quad . \tag{A.16}$$

To find the behaviour of this quantity for small s, consider the time independent transport equation, Eq. (2.1), and look for solutions of the form $e^{ikx}\underset{\sim}{\phi}(k,\mu)$. These solutions are identical to the eigenvectors of Chapter II, $\underset{\sim}{\phi}(\nu,\mu)$ with ν replaced by $1/ik$. The dispersion relation for the discrete eigenvalues, ν_{os}, Eq. (2.13), in terms of the k parameter (denoted by k_o), becomes in view of Eq. (A.9)

$$\det|\underset{\sim}{E}- \underset{\sim}{\Lambda}(k_o,o)| \;=\; o \;,\quad k_o \notin(-i,i) \quad . \tag{A.17}$$

Further from Chapter IV, these discrete eigenvalues, k_o, are either real or imaginary.

Since the root ν_o (and hence k_o) was assumed nonmultiple, a Taylor series expansion for $\det|\underset{\sim}{E} - \Lambda(k_o,s)|$ for small s gives

$$\det|\underset{\sim}{E} - \underset{\sim}{\Lambda}(k_o,s)| \approx \alpha_1 s + \alpha_2 s^2 + \ldots \tag{A.18}$$

where α_1, α_2, ... are constants independent of s. Thus if k_{os} is real (or ν_{os} imaginary) the quantity (A.16) does not vanish as $s \to o$ and the asymptotic flux does not decay to zero. Therefore for imaginary eigenvalues, ν_{os}, the system cannot be subcritical. If on the other hand, the k_o's are confined to the imaginary axis (ν_{os} on the real axis), Eq. (A.16) goes to zero as required for subcritiality.

APPENDIX B

COMPUTER CODE LISTINGS

In this appendix several programs which were used to calculate the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ functions and the emergent Milne problem distribution are listed. All these codes were written in the FORTRAN IV language for the IBM-360 computer. In listing these codes, attempts have been made to organize the programs and to include pertinent "comment" cards so that the program flow is readily apparent. It is not expected that anyone familiar with FORTRAN will have difficulty in understanding these codes.

Throughout these codes, "double precision" length variables have been used (which allow accuracies of up to sixteen significant figures). Finally each listing is prefaced by a brief description of the program's purpose and restrictions and by a list of the principal symbols.

B.1 PROGRAM MILNE

Purpose

This main program calculates first the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ matrices from the Cramer's scheme for given $\underset{\sim}{C}$ and $\underset{\sim}{\sum}$ matrices. Then after all the discrete roots, ν_{0s}, $s = 1 \sim M$, are found, the emergent distribution for the Milne problem corresponding to the largest discrete eigenvalue is evaluated. Finally the extrapolation length is calculated, and the emergent distribution normalized to unit density.

Restrictions

(i) This program calls the subroutines GAUX, ROOT, DIS, MINV, AVEC, PRT, and these must be supplied.

(ii) The dimension statements 3-7 must be changed for problems with different number of groups.

List of Principal Symbols

Program Symbol	Definition
IG	N (number of groups)
IPR	Printing parameter for ouput every 5 iterations.
EE(IG,IG)	$\underset{\sim}{E}$ (unit matrix)
X(16)	μ_k, k = 1~16 (Gaussian ordinates)
SIG(I)	σ_i
C(I,J)	c_{ij}
RT(IG)	Holds discrete eigenvalues, ν_{os}, in descending size.
IMU, IMUP	Counter used to specify integration ordinate.
U(16,IG,IG)	$\underset{\sim}{U}(\mu)$
V(16,IG,IG)	$\underset{\sim}{V}(\mu)$
ITER	Iteration counter
IEQ	Denotes subscript of $\underset{\sim}{u}_i(\mu)$ and $\underset{\sim}{v}_i(\mu)$.
SMAX	Maximum deviation of Eq. (3.31) from the $\underset{\sim}{\sum}$-matrix
NUO	ν_ℓ (largest discrete eigenvalue)
EIG(K,I)	$\underset{\sim}{\phi}_i(\nu_o,\mu_k)$
EIGN(K,I)	$\underset{\sim}{\phi}_i(\nu_o,-\mu_k)$
ADEIG(K,I)	$\underset{\sim}{\phi}_i^\dagger(\nu_o,\mu_k)$
ADEIGN(K,I)	$\underset{\sim}{\phi}_i^\dagger(\nu_o,-\mu_k)$
NPLUS	N_{o_ℓ}
EXTRAP	Extrapolation length.

MILNE

```
      C  THIS PROGRAM SOLVES THE U AND V EQUATIONS BY CRAMMER'S METHOD AND THEN
      C  SOLVES FOR THE EMERGENT MILNE DISTRIBUTION USING SIMPLE APPROACH
      C NO DISCRETE CONDITONS ARE USED-- SOLVES ONLY THE GENERAL EQUATIONS
0001        IMPLICIT REAL*8(A-H,M-Z)
0002        COMMON/GAU/X(16)
      C  THE FOLLOWING FIVE (5) CARDS ARE TO BE CHANGED WHEN THE NUMBER OF
      C   GROUPS ARE CHANGED
0003          REAL*8 AA(16,3,3),B(3,3),SIG(3),C(3,3),U(16,3,3),V(16,3,3)
0004          REAL*8 EE(3,3)/9*0.0D0/,ASCR(3),BSCR(3),S(16,16,3,3),VET(16,3)
0005          REAL*8 D(3,3),DSCR(3,3),RT(3)
0006          REAL*8 EIG(16,3),EIGN(16,3),ADEIG(16,3),ADEIGN(16,3),VEC(16)
0007          DIMENSION LLL(3),LLLL(3)
0008          EXTERNAL DIS
      C  CALCULATION OF THE MU ORDINATES FOR INTEGRATION FROM 0 TO 1
0009          SUM=GAUX(0.0D0,1.D0)
0010        5 FORMAT('0THE ORDINATES FOR THE MU INTEGRATION ARE'/(' ',8G15.7))
0011          WRITE(6,5) (X(I),I=1,16)
      C  READ IN THE INPUT DATA
0012        1 FORMAT(I2)
0013       35 READ(5,1) IG
0014          IF (IG.EQ.0) RETURN
0015          DO 8 J=1,IG
0016        8 EE(J,J)=1.D0
0017          IPR=1
0018        2 FORMAT(8G10.7)
0019          READ(5,2) (SIG(J),J=1,IG)
0020          READ(5,2) ((C(J,K),K=1,IG),J=1,IG)
0021          WRITE(6,311)
0022      311 FORMAT('1NOW NORMALIZE THE SIGMA AND C MATRICES')
0023          DO 9 J=1,IG
0024          DO 7 K=1,IG
0025          C(J,K)=C(J,K)/(2.D0*SIG(IG))
0026        7 D(J,K)=C(J,K)
0027        9 SIG(J)=SIG(J)/SIG(IG)
      C  PRINT THE INPUT DATA
0028        3 FORMAT('0THE SIGMA MATRIX IS'/(' ',8G15.7))
0029          WRITE(6,3) (SIG(J),J=1,IG)
0030        4 FORMAT('0THE C MATRIX IS'/(' ',8G15.7))
0031          WRITE(6,4) ((C(J,K),K=1,IG),J=1,IG)
      C  CALCULATE THE DISCRETE ROOT
0032          DO 33 J=1,IG
0033       33 RT(J)=1.D0
0034          DELX=.1D0
0035          DO 34 J=1,IG
0036          IF (J-1) 39,39,30
0037       30 JJ=J-1
0038          XST=1.D0/RT(JJ) +.1D-7
0039          IF ((XST+.1D-7).GT.1.D0) GO TO 38
0040          DEL=1.D0-(1.D0/RT(JJ))
0041          IF (DEL.LE..1D0) DELX=DEL/2.D0
0042          GO TO 34
0043       39 XST=.1D-5
0044       34 RT(J)=1.D0/ROOT(DIS,C,SIG,IG,XST,1.D0,DELX,.1D-7,DSCR,BSCR)
0045       38 WRITE(6,36) (RT(J),J=1,IG)
0046       36 FORMAT('0THE DISCRETE ROOTS FOR THE ABOVE C AND SIGMA MATRICES ARE
```

MILNE

```
     1'/(6G15.8))
C  START WITH APPROXIMATION ONLY FOR U  NAMELY U=EE
0047       DO 6 IMU=1,16
0048       DO 6 J=1,IG
0049       DO 6 K=1,IG
0050     6 U(IMU,J,K)=EE(J,K)
0051       WRITE(6,11)
0052     1 FORMAT('1THE ZERO-TH APPROXIMATION FOR THE U AND V MATRICES IS THE
     1 UNIT MATRIX')
C  ITERATE THE V EQUATION FIRST---INVOLVES ONLY THE U MATRIX
0053       ITER=1
0054    10 DO 17 IMU=1,16
0055       AMU=X(IMU)
C   CALCULATE U.C=S(1,IMU,J,K)
0056       DO 12 IMUP=1,16
0057       DO 12 J=1,IG
0058       DO 12 K=1,IG
0059       SUM=0.0D0
0060       DO 13 L=1,IG
0061    13 SUM=SUM+U(IMUP,J,L)*C(L,K)
0062    12 S(1,IMUP,J,K)=SUM
C
C   IF IEQ=I  WE DO THE I-TH EQUATION
0063       DO 17 IEQ=1,IG
C  NOW EVALUATE D(MU,MUP)=F(IEQ).U.C==AA(IMUP,J,K)
0064       DO 14 IMUP=1,16
0065       AMUP=X(IMUP)
0066       DO 14 J=1,IG
0067       DO 14 K=1,IG
0068    14 AA(IMUP,J,K)=S(1,IMUP,J,K)*AMU/(SIG(J)*AMU+SIG(IEQ)*AMUP)
C  DO INTEGRAL OF F(IEQ).U.C OVER MUP, AND CALCULATE (EE-INTEGRAL)
0069       SUM=GAUMAT(AA,DSCR,IG)
0070       DO 15 J=1,IG
0071       DO 15 K=1,IG
0072    15 DSCR(J,K)=EE(J,K)-DSCR(J,K)
C NOW CALCULATE DETERMINANT OF DSCR, AND SOLVE THE V EQUATIONS
C  SOLVE THE V EQUATIONS
0073       CALL MINV(DSCR,IG,DETD,LLL,LLLL,IG)
0074       IF (DETD) 19,16,19
0075    16 WRITE(6,18) ITER
0076       GO TO 35
0077    18 FORMAT ('0A SINGULAR MATRIX HAS BEEN ENCOUNTERED AT ITERATION',I5)
0078    19 DO 17 J=1,IG
0079    17 V(IMU,J,IEQ)=DSCR(J,IEQ)
C
CTHE BEGINNING OF THE U EQUATION CALCULATION
0080    20 DO 27 IMU=1,16
0081       AMU=X(IMU)
C  FIRST CALCULATE S(2,IMUP,J,K)=(TRANS V(MUP)).(TRANS C)
0082       DO 22 IMUP=1,16
0083       DO 22 J=1,IG
0084       DO 22 K=1,IG
0085       SUM=0.0D0
0086       DO 23 L=1,IG
0087    23 SUM=SUM+V(IMUP,L,J)*C(K,L)
```

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```
0088          22 S(2,IMUP,J,K)=SUM
              C
              CIF IEQ=I, WE DO THE I-TH U EQUATION
0089               DO 27 IEQ=1,IG
              C  NOW CALCULATE D(MU,MUP)=F(IEQ).(TRANS U).(TRANS C)
0090               DO 24 IMUP=1,16
0091               AMUP=X(IMUP)
0092               DO 24 J=1,IG
0093               DO 24 K=1,IG
0094          24 AA(IMUP,J,K)=S(2,IMUP,J,K)*AMU/(SIG(J)*AMU+SIG(IEQ)*AMUP)
              C  DO INTEGRAL OF D(MU,MUP) OVER MUP
0095               SUM=GAUMAT(AA,DSCR,IG)
0096               DO 25 J=1,IG
0097               DO 25 K=1,IG
0098          25 DSCR(J,K)=EE(J,K)-DSCR(J,K)
              C NOW CALCULATE DETERMINANT OF DSCR, AND SOLVE FOR THE U EQUATIONS
              C  SOLVE THE U EQUATIONS
0099               CALL MINV(DSCR,IG,DETD,LLL,LLLL,IG)
0100               IF (DETD) 29,26,29
0101          26 WRITE(6,18) ITER
0102               GO TO 35
0103          29 DO 27 J=1,IG
0104          27 U(IMU,IEQ,J)=DSCR(J,IEQ)
0105               IF (IPR-5) 32,31,32
0106          31 WRITE(6,77) ITER
0107          77 FORMAT('0WE HAVE JUST FINISHED ITERATION NUMBER ',I5)
0108               IPR=0
              C
              C  TEST ON U AND V
0109               UINT=GAUMAT(V,B,IG)
0110               VINT=GAUMAT(U,D,IG)
0111               DO 71 J=1,IG
0112               DO 71 K=1,IG
0113               DSCR(J,K)=0.0D0
0114               DO 71 L=1,IG
0115          71 DSCR(J,K)=DSCR(J,K)+C(J,L)*B(L,K)
0116               DO 72 J=1,IG
0117               DO 72 K=1,IG
0118               VET(J,K)=0.0D0
0119               DO 72 L=1,IG
0120          72 VET(J,K)=VET(J,K)+D(J,L)*DSCR(L,K)
0121               DO 74 J=1,IG
0122               DO 74 K=1,IG
0123               B(J,K)=SIG(J)*B(J,K)
0124               D(J,K)=SIG(K)*D(J,K)
0125          74 B(J,K)=.5D0*(B(J,K)+D(J,K)-VET(J,K))
0126               WRITE(6,75)((B(J,K),K=1,IG),J=1,IG)
0127          75 FORMAT (' CHECK ON U AND V'/(' ',8G15.7))
              C  CONVERGENCE TEST
0128               SMAX=0.0D0
0129               DO 62 J=1,IG
0130               DO 63 K=1,IG
0131          63 DSCR(J,K)=0.0D0
0132               DSCR(J,J)=SIG(J)
0133               DO 62 K=1,IG
```

MILNE

```
0134              DEV=DABS(DSCR(J,K)-B(J,K))
0135              IF (DEV.GT.SMAX) SMAX=DEV
0136           62 CONTINUE
0137              WRITE(6,67) SMAX
0138           67 FORMAT('0MAXIMUM DEVIATION FROM THE SIGMA MATRIX IS',G15.7)
0139              IF (SMAX.LT..1D-8) GO TO 40
               C  CHECK ON THE NUMBER OF ITERATIONS--IF GREATER THAN 50 IT DOES NOT
               C  CONVERGE.  THUS GO ON THE NEXT DATA SET
0140           32 IPR=IPR+1
0141              IF (ITER.EQ.75) GO TO 64
0142              ITER=ITER+1
0143              GO TO 10
0144           64 WRITE(6,65)
0145           65 FORMAT('0U AND V HAVE NOT CONVERGED AFTER 75 ITERATIONS-THUS GO ON
                 1 TO THE NEXT DATA SET')
0146           66 GO TO 35
               C
               C  CALCULATON OF THE EMERGENT DISTRIBUTION FOR MILNE PROBLEM USING SIMPLE
               C TECHNIQUE
0147           40 NUO=RT(1)
0148              CALL PRT(U,V,IG,ITER)
0149              WRITE(6,67) SMAX
0150              WRITE(6,97) NUO
0151           97 FORMAT('1THE LARGEST DISCRETE ROOT IS',G15.8)
               C  CALCULATE THE INTEGRAL OF THE DISCRETE EIGENFUNCTION   VECTOR A
0152              CALL AVEC(ASCR,NUO,C,SIG,IG,DSCR,BSCR,LLL,LLLL)
0153              WRITE(6,28) (ASCR(J),J=1,IG)
0154           28 FORMAT('0INTEGRAL OF DISCRETE EIGENVECTOR FOR LARGEST NUO'/
                 1(' ',8G15.7))
               C
               C  CALCULATE THE CONSTANT VECTOR B
0155              DO 81 J=1,IG
0156              BSCR(J)=0.0D0
0157              DO 81 L=1,IG
0158           81 BSCR(J)=BSCR(J)+C(J,L)*ASCR(L)
0159              DO 84 JMUP=1,16
0160              DO 83 J=1,IG
0161              DO 83 K=1,IG
0162           83 AA(JMUP,J,K)=V(JMUP,J,K)/(SIG(K)*NUO+X(JMUP))
0163              DO 84 J=1,IG
0164              VET(JMUP,J)=0.0D0
0165              DO 84 L=1,IG
0166           84 VET(JMUP,J)=AA(JMUP,J,L)*BSCR(L)+VET(JMUP,J)
0167              VINT=GAUVEC(VET,ASCR,IG)
0168              DO 82 J=1,IG
0169              D(1,J)=0.0D0
0170              DO 89 L=1,IG
0171           89 D(1,J)=D(1,J)+C(J,L)*ASCR(L)
0172           82 BSCR(J)=(BSCR(J)-NUO*D(1,J))*NUO
0173              WRITE(6,85) (BSCR(J),J=1,IG)
0174           85 FORMAT ('0CONSTANT VECTOR B IS',(4G15.7))
               C  CALCULATED THE EMERGENT DISTRIBUTION
0175              DO 88 JMU=1,16
0176              DO 88 J=1,IG
0177              VET(JMU,J)=0.0D0
```

```
0178              DO 87 L=1,IG
0179           87 VET(JMU,J)=VET(JMU,J)+U(JMU,J,L)*BSCR(L)
0180           88 VET(JMU,J)=VET(JMU,J)/(SIG(J)*NUO-X(JMU))
               C  PRINT OUT THE UNNORMALIZED EMERGENT DISTRIBUTION
0181              WRITE(6,45)
0182           45 FORMAT('0THE UNNORMALIZED MILNE EMERGENT DISTRIBUTION,PSI(0,-MU),
                  1 FOR ASCENDING MU IS'/)
0183              DO 47 J=1,IG
0184              WRITE(6,46) J
0185           47 WRITE(6,48) (VET(JMU,J),JMU=1,16)
0186           46 FORMAT ('0GROUP NUMBER IS',I3)
0187           48 FORMAT (' ',8G15.7)
               C
               C  CALCULATION OF THE DISCRETE EIGENFUNCTIONS
0188              CALL AVEC(ASCR,NUO,C,SIG,IG,DSCR,BSCR,LLL,LLLL)
0189              CALL EIGEN(EIG,NUO,IG)
0190              CALL EIGEN(EIGN,-NUO,IG)
0191              DO 117 J=1,IG
0192              DO 117 K=1,IG
0193          117 D(J,K)=C(K,J)
0194              CALL AVEC(ASCR,NUO,D,SIG,IG,DSCR,BSCR,LLL,LLLL)
0195              CALL EIGEN(ADEIG,NUO,IG)
0196              CALL EIGEN(ADEIGN,-NUO,IG)
0197              WRITE(6,100)
0198              WRITE(6,102)((EIG(JMU,J),JMU=1,16),J=1,IG)
0199              WRITE(6,102)((EIGN(JMU,J),JMU=1,16),J=1,IG)
0200              WRITE(6,102)((ADEIG(JMU,J),JMU=1,16),J=1,IG)
0201              WRITE(6,102)((ADEIGN(JMU,J),JMU=1,16),J=1,IG)
0202          100 FORMAT('1THE EIGENFUNCTIONS FOR ASCENDING MU ARE')
0203          102 FORMAT (2(' ',8G15.7/)/2(' ',8G15.7/)/)
               C  CALCULATION OF THE NORMALIZATION BY INTEGRATION
0204              DO 105 JMU=1,16
0205              FST=0.0D0
0206              DO 104 J=1,IG
0207          104 FST=FST+EIG(JMU,J)*ADEIG(JMU,J)
0208          105 VEC(JMU)=X(JMU)*FST
0209              FST=GAUS(VEC,IG)
0210              DO 106 JMU=1,16
0211              TST=0.0D0
0212              DO 107 J=1,IG
0213          107 TST=TST+ADEIGN(JMU,J)*EIGN(JMU,J)
0214          106 VEC(JMU)=X(JMU)*TST
0215              TST=GAUS(VEC,IG)
0216              NPLUS=FST-TST
0217              WRITE(6,109) NPLUS
0218          109 FORMAT ('0NPLUS BY DIRECT INTEGRATION IS ',G15.7)
              C CALCULATION OF ASYMPTOTIC COEFFICIENT
0219              DO 110 JMU=1,16
0220              SS=0.0D0
0221              DO 111 J=1,IG
0222          111 SS=SS+VET(JMU,J)*ADEIG(JMU,J)
0223          110 VEC(JMU)=X(JMU)*SS
0224              SS=GAUS(VEC,IG)/NPLUS
0225              WRITE(6,112) SS
0226          112 FORMAT('0ASYMPTOTIC COEFFICIENT IN MILNE PROBLEM EIGENVECTOR EXPAN
```

```
     1SION IS (SHOULD BE UNITY)',G15.8)
C  CALCULATION OF THE EXTRAPOLATION LENGTH
0227       DO 113 JMU=1,16
0228       SS=0.0D0
0229       DO 114 J=1,IG
0230     114 SS=SS+VET(JMU,J)*ADEIGN(JMU,J)
0231     113 VEC(JMU)=SS*X(JMU)
0232       EXTRAP=-GAUS(VEC,IG)/NPLUS
0233       EXTRAP=.5D0*NUO*DLOG(-EXTRAP)
0234       WRITE(6,115) EXTRAP
0235     115 FORMAT ('0EXTRAPOLATION LENGTH IS',G15.7)
C  NOW NORMALIZE EMERGENT DISTRIBUTION TO UNIT DENSITY
0236       VINT=GAUVEC(VET,BSCR,IG)
0237       WRITE(6,48) (BSCR(J),J=1,IG)
0238       NORM=0.0D0
0239       DO 116 J=1,IG
0240     116 NORM=NORM+BSCR(J)
0241       DO 51 J=1,IG
0242       DO 51 JMU=1,16
0243      51 VET(JMU,J)=VET(JMU,J)/NORM
C  PRINT OUT NORMALIZED FLUX
0244       WRITE(6,52)
0245      52 FORMAT('1THE EMERGENT DISTRIBUTION,NORMALIZED TO UNIT DENSITY AT T
     1HE INTERFACE,IS'/)
0246       DO 53 J=1,IG
0247       WRITE(6,46) J
0248      53 WRITE(6,48) (VET(JMU,J),JMU=1,16)
0249       GO TO 35
0250     999 FORMAT(1H0)
0251       END
```

B.2 PROGRAM GENUV

Purpose

This main program iterates Eqs. (6.3) and (6.4) for $\underset{\sim}{U}(\mu)$ and $\underset{\sim}{V}(\mu)$ for arbitrary $\underset{\sim}{C}$ and $\underset{\sim}{\Sigma}$ matrices. This method has previously been called the "direct iteration" scheme (see Section 6.1).

Restrictions

(i) This program calls the subroutines PRT and GAUX, and they must be supplied.

(ii) The dimension statements 3-5 must be changed if the number of groups is changed.

List of Principal Symbols

Program Symbol	Definition
IG	N (number of groups)
IPR	Printing iteration counter
EE(IG,IG)	$\underset{\sim}{E}$ (unit matrix)
SIG(I)	σ_i
C(I,J)	c_{ij}
V(I,J,K)	$[\underset{\sim}{V}(\mu_i)]_{jk}$
U(I,J,K)	$[\underset{\sim}{U}(\mu_i)]_{jk}$
VINT	$\int_0^1 d\mu \underset{\sim}{V}(\mu)$
UINT	$\int_0^1 d\mu \underset{\sim}{U}(\mu)$

GENUV

```
      C THIS PROGRAM CALCULATES VARIOUS TWO GROUP PROBLEMS
      C NO DISCRETE CONDITION IS USED--SOLVES ONLY THE GENERAL EQUATIONS
0001        IMPLICIT REAL*8(A-H,M-Z)
0002        COMMON/GAU/X(16)
      C  THE FOLLOWING CARD IS TO BE CHANGED WHEN THE NUMBER OF GROUPS IS CHANGED
0003        REAL*8 AA(16,2,2),B(2,2),SIG(2),C(2,2),U(16,2,2),V(16,2,2)
0004        REAL*8 EE(2,2)/4*0.0D0/, ASCR(2), BSCR(2), S(16,16,2,2), VET(16,2)
0005        REAL*8 D(2,2)
      C  READ IN THE INPUT DATA
0006      1 FORMAT(I2)
0007     35 READ(5,1) IG
0008        IF (IG.EQ.0) RETURN
0009        IPR=1
0010        DO 8 J=1,IG
0011      8 EE(J,J)=1.D0
0012      2 FORMAT(8G10.7)
0013        READ(5,2) (SIG(J),J=1,IG)
0014        READ(5,2) ((C(J,K),K=1,IG),J=1,IG)
      C  PRINT THE INPUT DATA
0015      3 FORMAT('1THE SIGMA MATRIX IS'/(' ',8G15.7))
0016        WRITE(6,3) (SIG(J),J=1,IG)
0017      4 FORMAT('0THE C MATRIX IS'/(' ',8G15.7))
0018        WRITE(6,4) ((C(J,K),K=1,IG),J=1,IG)
      C  CALCULATION OF THE MU ORDINATES FOR INTEGRATION FROM 0 TO 1
0019        SUM=GAUX(0.0D0,1.D0)
0020      5 FORMAT('0THE ORDINATES FOR THE MU INTEGRATION ARE'/(' ',8G15.7))
0021        WRITE(6,5) (X(I),I=1,16)
      C  INITIALIZE U AND V TO THE UNIT MATRIX
0022        DO 6 IMU=1,16
0023        DO 6 J=1,IG
0024        DO 6 K=1,IG
0025        V(IMU,J,K)=EE(J,K)
0026      6 U(IMU,J,K)=EE(J,K)
      C  ITERATE THE U AND V EQUATIONS
0027        ITER=1
0028     10 DO 17 IMU=1,16
0029        AMU=X(IMU)
      C THE V EQUATION---FIRST CALCULATE  C.V(MU)
0030        DO 12 J=1,IG
0031        DO 12 K=1,IG
0032        SUM=0.0D0
0033        DO 13 L=1,IG
0034     13 SUM=SUM+ C(J,L)*V(IMU,L,K)
0035     12 B(J,K)=SUM
      C  NOW CALCULATE AA(MUPRIME)=B.U(MUPRIME).C.V(MU)
0036        DO 15 IMUP=1,16
0037        AMUP=X(IMUP)
0038        DO 15 J=1,IG
0039        DO 15 K=1,IG
0040        SUM=0.0D0
0041        DO 14 L=1,IG
0042     14 SUM=SUM+ U(IMUP,J,L)*B(L,K)
0043     15 AA(IMUP,J,K)=SUM*AMU/(SIG(J)*AMU+SIG(K)*AMUP)
      C  NOW INTEGRATE OVER MUPRIME  AND GET V(MU)
0044        SUM=GAUMAT(AA,B,IG)
```

GENUV

```
0045            DO 17 J=1,IG
0046            DO 17 K=1,IG
0047         17 V(IMU,J,K)=B(J,K)+EE(J,K)
             C  DO THE U EQUATION-- FIRST CALCULATE U(MU).C
0048            DO 30 IMU=1,16
0049            AMU=X(IMU)
0050            DO 22 J=1,IG
0051            DO 22 K=1,IG
0052            SUM=0.0D0
0053            DO 23 L=1,IG
0054         23 SUM=SUM+ U(IMU,J,L)*C(L,K)
0055         22 B(J,K)=SUM
             C  NOW CALCULATE  A.U(MU).C.V(MUPRIME)
0056            DO 25 IMUP=1,16
0057            AMUP=X(IMUP)
0058            DO 25 J=1,IG
0059            DO 25 K=1,IG
0060            SUM=0.0D0
0061            DO 24 L=1,IG
0062         24 SUM=SUM+ B(J,L)*V(IMUP,L,K)
0063         25 AA(IMUP,J,K)=SUM*AMU/(SIG(J)*AMUP+SIG(K)*AMU)
             C  NOW INTEGRATE OVER MUPRIME AND GET U(MU)
0064            SUM=GAUMAT(AA,B,IG)
0065            DO 27 J=1,IG
0066            DO 27 K=1,IG
0067         27 U(IMU,J,K)=B(J,K)+EE(J,K)
0068         30 CONTINUE
0069            IF (IPR-5) 32,31,32
0070         31 CALL PRT(U,V,IG,ITER)
0071            IPR=0
             C   TEST ON U AND V
0072            VINT=GAUMAT(V,B,IG)
0073            UINT=GAUMAT(U,D,IG)
0074            WRITE(6,81)((B(J,K),K=1,2),J=1,2)
0075            WRITE(6,81)((D(J,K),K=1,2),J=1,2)
0076            DO 71 J=1,IG
0077            DO 71 K=1,IG
0078            AA(1,J,K)=0.0D0
0079            DO 71 L=1,IG
0080         71 AA(1,J,K)=AA(1,J,K)+C(J,L)*B(L,K)
0081            DO 73 J=1,IG
0082            DO 73 K=1,IG
0083            VET(J,K)=0.0D0
0084            DO 73 L=1,IG
0085         73 VET(J,K)=VET(J,K)+D(J,L)*AA(1,L,K)
0086            WRITE(6,81)((VET(J,K),K=1,2),J=1,2)
0087         81 FORMAT ('0',4G15.7)
0088            DO 74 K=1,IG
0089            DO 74 J=1,IG
0090            B(K,J)= SIG(K)*B(K,J)
0091            D(K,J)= SIG(J)*D(K,J)
0092         74 B(K,J)= .5D0*(B(K,J)+D(K,J)-VET(K,J))
0093            WRITE(6,75) ((B(K,J),J=1,IG),K=1,IG)
0094         75 FORMAT (' CHECK ON U AND V'/(' ',8G15.7))
0095         32 IPR=IPR+1

             C THERE IS NO CONVERGENCE TEST--JUST WHETHER U AND V HAVE BEEN
             C ITERATED TEN TIMES
0096            IF (ITER.EQ.100) GO TO 35
0097            ITER=ITER+1
0098            GO TO 10
0099            END
```

B.3 SUBROUTINE: AVEC(A,NUO,C,SIG,IG,AA,AX,LLL,LLLL)

Purpose

This subroutine calculates the normalization of a discrete eigenvector, $\underset{\sim}{a}(\nu_o) = \int_{-1}^{1} d\mu \underset{\sim}{\phi}(\nu_o,\mu)$ by evaluating Eq. (6.12).

Dummy Variables

Program Symbol	Definition
A(IG)	Vector where $\underset{\sim}{a}(\nu_o)$ is stored.
NUO	Discrete eigenvalue, ν_o.
C(IG,IG)	$\underset{\sim}{C}$ matrix
SIG(IG)	Stores matrix elements σ_i.
IG	Number of groups.
AA(IG,IG),AX(IG),LLL(IG),LLLL(IG)	Temporary storage for quantities generated by the subroutine.

ENTRY EIGEN (EIG,NUO,IG)

Purpose

This entry calculates the discrete eigenvectors $\underset{\sim}{\phi}(\nu_o,\mu,\underset{\sim}{C})$, $\mu > 0$, for the Gaussian ordinates, μ_k, k = 1~16.

Dummy Variables

Program Symbol	Definition
EIG(K,I)	$\underset{\sim}{\phi}_i(\nu_o,\mu_k,\underset{\sim}{C})$
NUO	ν_o
IG	Number of groups.

Restrictions

(i) $|\nu_o|$ must be greater than unity.

(ii) AVEC must be called before EIGEN is used.

(iii) The subroutine MINV must be supplied.

(iv) The external function GAUX must be called before using AVEC to generate the correct Gaussian ordinates.

AVEC

```
0001                SUBROUTINE AVEC(A,NUC,C,SIG,IG,AA,AX,LLL,LLLL)
0002                IMPLICIT REAL*8(A-H,M-Z)
0003                REAL*8 A(1),NUC,C(IG,IG),SIG(1)
0004                REAL*8 AA(IG,IG),AX(1)
0005                DIMENSION LLL(1),LLLL(1)
0006                T(X)=DLOG((1.D0+X*NUC)/(X*NUC-1.D0))*NUC
0007                IN=IG-1
0008                DO 13 J=1,IN
0009                SG=SIG(J)
0010                SG=T(SG)
0011                DO 12 K=1,IN
0012             12 AA(J,K)=C(J,K)*SG
0013                AA(J,J)=AA(J,J)-1.D0
0014             13 AX(J)=C(J,IG)*SG
0015                CALL MINV(AA,IN,DETAX,LLL,LLLL,IG)
0016                DO 14 J=1,IN
0017                A(J)=0.0D0
0018                DO 14 L=1,IN
0019             14 A(J)=A(J)-AA(J,L)*AX(L)
0020                A(IG)=1.D0
0021                RETURN
0022                ENTRY EIGEN(EIG,NUC,IG)
0023                REAL*8 EIG(16,IG)
0024                COMMON/GAU/X(16)
0025                DO 16 J=1,IG
0026                AX(J)=0.0D0
0027                DO 16 L=1,IG
0028             16 AX(J)= AX(J)+C(J,L)*A(L)
0029             17 DO 19 JMU=1,16
0030                AMU=X(JMU)
0031                DO 19 J=1,IG
0032             19 EIG(JMU,J)=NUC*AX(J)/(SIG(J)*NUC-AMU)
0033                RETURN
0034                END
```

B.4 SUBROUTINE: ROOT(FN,C,SIG,IG,XST,XEND,EPS1,EPS2,DSCR,BSCR)

Purpose

This subroutine finds the simple zero, x_o, of an arbitrary function f(x), in the interval x_1 to x_2. The method of calculation used in this subroutine is discussed in detail in Section 6.2.

Dummy Variables

Program Symbol	Definition
FN	f(x)
C(IG,IG)	$\underset{\sim}{C}$
SIG(IG)	$\underset{\sim}{\Sigma}$
IG	N (number of groups)
XST	x_1
XEND	x_2
EPS1	Rough grid size.
EPS2	Allowable error in x_o.
DSCR,BSCR	Are scratch files used for temporary storage.

Restrictions

(i) There must be only one zero between XST and SEND.

(ii) |XST+EPS1| must be less than |XEND|.

(iii) EPS1 and EPS2 have the same sign.

(iv) An external function, FN, is required.

ROOT

```
0001              REAL FUNCTION ROOT*8(FN,C,SIG,IG,XST,XEND,EPS1,EPS2)
0002              IMPLICIT REAL*8(A-H,M-Z)
0003              REAL*8 FN,XST,XEND,EPS1,EPS2,C(IG,IG),SIG(IG)
0004              EP=EPS1
0005              S=DABS(EP)/EP
0006              Y=XST
0007           10 Y1=FN(C,SIG,IG,Y)
0008           11 Y2=FN(C,SIG,IG,Y+EP)
0009              IF (Y1*Y2) 12,15,14
0010           14 IF (S*(Y+2.D0*EP).GE.XEND*S) GO TO 12
0011              Y=Y+EP
0012              Y1=Y2
0013              GO TO 11
0014           12 IF (S*EP.LT.EPS2*S) GO TO 13
0015              EP=EP/10.D0
0016              GO TO 11
0017           15 IF (Y2.EQ.0.0D0) Y=Y+EP
0018           13 ROOT=Y
0019              RETURN
0020              END
```

B.5 EXTERNAL FUNCTION: DIS(C,SIG,IG,Y,A,TN)

Purpose

This subroutine calculates the determinant of the dispersion matrix for any value of the argument.

Dummy Variables

Program Symbols	Definition
C(IG,IG)	$\underset{\sim}{C}$
SIG(IG)	$\underset{\sim}{\Sigma}$
IG	N (number of groups).
Y	$1/\nu$ (argument of dispersion matrix).
A(IG,IG)	$\underset{\sim}{\Omega}(\nu)$ (dispersion matrix).
TN(IG)	Scratch vector used temporary storage.
DIS	$\det\|\underset{\sim}{\Omega}(\nu)\|$

Restriction

(i) The subroutine MINV is called and must be supplied.

DIS

```
0001            REAL FUNCTION DIS*8(C,SIG,IG,Y,A,TN)
0002            IMPLICIT REAL*8 (A-H,M-Z)
0003            REAL*8 Y,C(IG,IG),SIG(IG),A(IG,IG),TN(IG)
              C   CHANGE THE FOLLOWING CARD WHEN THE NUMBER OF GROUPS IS CHANGED
0004            DIMENSION LLL(3),LLLL(3)
              C  CONSTRUCT THE DISPERSION MATRIX
0005            DO 11 J=1,IG
0006            TN(J)=DLOG((SIG(J)+Y)/(SIG(J)-Y))
0007            DO 11 K=1,IG
0008         11 A(J,K)=C(J,K)*TN(J)/Y
0009            DO 12 J=1,IG
0010         12 A(J,J)=A(J,J)-1.D0
0011            CALL MINV(A,IG,DETD,LLL,LLLL,IG)
0012            DIS=DETD
0013            RETURN
0014            END
```

B.6 SUBROUTINE: PRT(U,V,IG,ITER)

Purpose

This subroutine points out the value of the U and V matrices.

Dummy Variables

Program Symbol	Definition
U(K,I,J)	$[\underset{\sim}{U}(\mu_k)]_{ij}$
V(K,I,J)	$[\underset{\sim}{V}(\mu_k)]_{ij}$
IG	N (number of groups).
ITER	Iteration index for $\underset{\sim}{U}$ and $\underset{\sim}{V}$.

PRT

```
0001            SUBROUTINE PRT(U,V,IG,ITER)
0002            IMPLICIT REAL*8(A-H,M-Z)
0003            REAL*8 U(16,IG,IG), V(16,IG,IG)
0004          10 FORMAT('1AT ITERATION NUMBER',I4,'VALUES OF V(MU,J,K)AND U(MU,J,K)
                1 ARE LISTED BELOW'/)
0005            WRITE(6,10) ITER
0006          11 FORMAT(8G15.7)
0007          12 FORMAT('0U(MU',I2,',',I2,') FOR ASCENDING VALUES OF MU')
0008          13 FORMAT(' V(MU',I2,',',I2,') FOR ASCENDING VALUES OF MU')
0009            DO 20 J=1,IG
0010            DO 20 K=1,IG
0011            WRITE(6,12) J,K
0012            WRITE(6,11) (U(I,J,K),I=1,16)
0013            WRITE(6,13) J,K
0014          20 WRITE(6,11) (V(I,J,K),I=1,16)
0015            RETURN
0016            END
```

B.7 EXTERNAL FUNCTION: GAUX(AA,BB)

Purpose

This initial entry calculates the sixteen Gaussian integration ordinates, μ_k, k = 1~16, for the interval (AA,BB). The resultant ordinates are stored in the COMMON storage |GAU|-vector X(16). The following entry points then integrate matrix functions, vector functions, and scalar functions.

Entries

(1) GAUMAT (A,B,IG)

Program Symbol	Definition
A(K,I,J)	$[\underset{\sim}{A}(\mu_k)]_{ij}$, k = 1~16 ($\underset{\sim}{A}(\mu)$ is some arbitrary matrix function.
B(I,J)	$\int_{AA}^{BB} d\mu[\underset{\sim}{A}(\mu)]_{ij} \doteq \sum_{k=1}^{16} w(\mu_k)[\underset{\sim}{A}(\mu_k)]_{ij}$
IG	N (dimension of $\underset{\sim}{A}$ and $\underset{\sim}{B}$)

(2) GAUVEC (AV,BV,IG)

Program Symbol	Definition
AV(I,J)	$[\underset{\sim}{AV}(\mu_k)]_i$, k = 1~16, ($\underset{\sim}{AV}(\mu)$ is some arbitrary vector function).
BV(I)	$\int_{AA}^{BB} d\mu[\underset{\sim}{AV}(\mu)]_i \doteq \sum_{k=1}^{16} w(\mu_k)[\underset{\sim}{AV}(\mu_k)]_i$
IG	N (dimension of vectors $\underset{\sim}{AV}$ and $\underset{\sim}{BV}$).

(3) GAUS (AS,IG)

Program Symbol	Definition
AS(K)	$f(\mu_k)$ where $f(\mu)$ is an arbitrary scalar function.
GAUS	$\int_{AA}^{BB} d\mu f(\mu) \doteq \sum_{k=1}^{16} w(\mu_k)f(\mu_k)$.
IG	Any integer.

Restriction

(i) GAUS must be called before any of the entry points are called.

GAUX

```
0001              REAL FUNCTION GAUX*8(AA,BB)
0002              IMPLICIT REAL*8(A-H,M-Z)
0003              REAL*8 AA,BB
0004              COMMON/GAU/XI(16)
0005              REAL*8 ZI(8)/.0950125098,.2816035508, .4580167777, .6178762444,
                 1 .7554044084, .8656312024, .9445750231, .9894009350/,
                 2WT(8)/.1894506105, .1826034150, .1691565194,  .1495959888,
                 3 .1246289713, .0951585117, .0622535239, .0271524594/
0006              C=.5D0*(BB-AA)
0007              D=.5D0*(BB+AA)
0008              DO 9 J=1,8
0009              K=9-J
0010            9 XI(J)=-C*ZI(K)+D
0011              DO 8 J=9,16
0012              K=J-8
0013            8 XI(J)=C*ZI(K)+D
0014              GAUX=XI(1)
0015              RETURN
                C
0016              ENTRY GAUMAT(A,B,IG)
0017              REAL*8 A(16,IG,IG), B(IG,IG)
0018              DO 20 K=1,IG
0019              DO 20 J=1,IG
0020              SUM=0.0D0
0021              DO 21 I=1,8
0022              L=9-I
0023           21 SUM=SUM+ A(L,J,K)*WT(I)
0024              DO 22 I=9,16
0025              L=I-8
0026           22 SUM=SUM+ A(I,J,K)*WT(L)
0027           20 B(J,K)=SUM*C
0028              GAUMAT=1.D0
0029              RETURN
                C
0030              ENTRY GAUVEC(AV,BV,IG)
0031              REAL*8 AV(16,IG),BV(1)
0032              DO 30 K=1,IG
0033              SUM=0.0D0
0034              DO 31 I=1,8
0035              L=9-I
0036           31 SUM=SUM+AV(L,K)*WT(I)
0037              DO 32 I=9,16
0038              L=I-8
0039           32 SUM=SUM+AV(I,K)*WT(L)
0040           30 BV(K)=SUM*C
0041              GAUVEC=1.D0
0042              RETURN
                C
0043              ENTRY GAUS(AS,IG)
0044              REAL*8AS(16)
0045              GAUS=0.0D0
0046              DO 41 I=1,8
0047              L=9-I
0048           41 GAUS=GAUS+AS(L)*WT(I)
0049              DO 42 I=9,16
0050              L=I-8
0051           42 GAUS=GAUS+AS(I)*WT(L)
0052              GAUS=GAUS*C
0053              RETURN
0054              END
```

B.8 SUBROUTINE: MINV(A,N,D,L,M,NC)

Purpose

This subroutine calculates the determinant and inverse of an arbitrary square matrix.

Dummy Variables

Program Symbols	Definition
A(N,N)	Arbitrary square matrix which is replaced by its inverse.
N	Dimension of matrix $\underset{\sim}{A}$.
D	Determinant of $\underset{\sim}{A}$.
L,M	Scratch vectors used in calculating the inverse.
NC	An integer which allow evaluation of the determinant of a minor of A. For example if NC = N-1 the inverse and determinant of the minor of element $[\underset{\sim}{A}]_{11}$ is calculated.

MINV

```
0001            SUBROUTINE MINV(A,N,D,L,M,NC)
0002            DIMENSION A(1),L(1),M(1)
0003            DOUBLE PRECISION A,D,BIGA,HOLD
                C       SPECIAL CASE FOR A DEGENERATE MATRIX  N=1
0004            IF (N.GT.1) GO TO 11
0005            D=A(1)
0006            A(1)=1.D0/D
0007            RETURN
                C                       INITIALIZATION
0008         11 ICOUNT=0
0009            D=1.D0
0010            DO 10 I=1,N
0011         10 L(I)=I
0012            K=1
                C       SEARCH FOR LARGEST ELEMENT IN THE RESIDUAL MATRIX
0013         15 BIGA=0.0
0014            DO 30 J=K,N
0015            IJBASE=NC*(L(J)-1)
0016            DO 30 I=K,N
0017            IJ=IJBASE+L(I)
0018            IF (DABS(BIGA)-DABS(A(IJ))) 20,30,30
0019         20 BIGA=A(IJ)
0020            IZ=L(I)
0021            JZ=L(J)
0022            KSUB=J
0023         30 CONTINUE
0024            IF (BIGA) 50,40,50
0025         40 D=0.0
0026            RETURN
                C       PERFORM ROW INTERCHANGE AND MODIFY RESIDUAL SUBSCRIPTS
0027         50 L(KSUB)=L(K)
0028            IF (IZ-JZ) 60,80,60
0029         60 ICOUNT=ICOUNT+1
0030            L(ICOUNT)=IZ
0031            M(ICOUNT)=JZ
0032            DO 70 J=1,N
0033            HOLD=A(IZ)
0034            A(IZ)=A(JZ)
0035            A(JZ)=HOLD
0036            IZ=IZ+NC
0037         70 JZ=JZ+NC
0038            JZ=M(ICOUNT)
0039            D=-D
                C               REPLACE PIVOT BY RECIPROCAL AND DIVIDE PIVOT ROW
0040         80 IZ=NC*(JZ-1)
0041            A(IZ+JZ)=1.0
0042            I=JZ
0043            DO 90 J=1,N
0044            A(I)=A(I)/BIGA
0045         90 I=I+NC
                C                       REDUCE THE MATRIX
0046            DO 110 I=1,N
0047            IF (I-JZ) 100,110,100
0048        100 HOLD=-A(IZ+I)
0049            A(IZ+I)=0.
```

MINV

```
0050                IJ=I
0051                KSUB=JZ
0052                DO 110 J=1,N
0053                A(IJ)=A(IJ)+HOLD*A(KSUB)
0054                IJ=IJ+NC
0055                KSUB=KSUB+NC
0056          110   CONTINUE
                  C
0057                D=D*BIGA
0058                K=K+1
0059                IF (N-K) 120,15,15
                  C               PERFORM COMPENSATIOG COLUMN INTERCHANGES
0060          120   IF (ICOUNT) 150,150,130
0061          130   IZ=NC*(L(ICOUNT)-1)
0062                JZ=NC*(M(ICOUNT)-1)
0063                DO 140 I=1,N
0064                IZ=IZ+1
0065                JZ=JZ+1
0066                HOLD=A(IZ)
0067                A(IZ)=A(JZ)
0068          140   A(JZ)=HOLD
0069                ICOUNT=ICOUNT-1
0070                GO TO 120
                  C
0071          150   RETURN
0072                END
```

B.9 PROGRAM FRED

Purpose

This program evaluates the analytic approximations Eqs. (3.95) and (3.96) for the $\underset{\sim}{U}$ and $\underset{\sim}{V}$ function. The program symbols are the same as those in MILNE and hence will not be repeated here.

FRED

```
      C  THIS PROGRAM TESTS THE FREDHOLM EQUATION APPROXIMATION
0001        IMPLICIT REAL*8(A-H,M-Z)
0002        COMMON/GAU/X(16)
      C  WHEN PUTTING INTO MAIN MUST INCLUDE NEWLY DEFINED MATRICES ESCR,CSRC
0003        REAL*8 U(16,2,2),V(16,2,2),AA(16,2,2),EE(2,2)/4*0.0D0/
0004        REAL*8 EIG(16,2),ADEIG(16,2),EIGN(16,2),ADEIGN(16,2)
0005        REAL*8 VEC(16),ESCR(2),ASCR(2),BSCR(2),C(2,2),D(2,2),DSCR(2,2)
0006        REAL*8 SIG(2),CSCR(2)
0007        DIMENSION LLL(2),LLLL(2)
      C  CALCULATE THE MU ORDINATES AND READ IN INPUT DATA
0008        SUM=GAUX(0.0D0,1.D0)
0009        5 FORMAT ('0THE ORDINATES FOR THE MU INTEGRATION ARE',/(' ',8G15.7))
0010        WRITE(6,5) (X(I),I=1,16)
0011        4 FORMAT(I2,G18.8)
0012        6 READ(5,4) IG,NUO
0013        2 FORMAT (8G10.7)
0014        READ(5,2) (SIG(J),J=1,IG)
0015        IF (SIG(1).EQ.0.0D0) RETURN
0016        READ(5,2) ((C(J,K),K=1,IG),J=1,IG)
0017        DO 8 J=1,IG
0018        EE(J,J)=1.D0
0019        DO 8 K=1,IG
0020        8 D(J,K)=C(K,J)
      C
0021        3 FORMAT ('1NEXT SET OF DATA')
0022        WRITE(6,3)
      C
      C CALCULATION OF THE EIGENFUNCTION NORMALIZATION--VECTOR A
0023        CALL AVEC(ASCR,NUO,C,SIG,IG,DSCR,BSCR,LLL,LLLL)
0024        WRITE(6,201) (ASCR(J),J=1,IG)
0025      201 FORMAT(' INTEGRAL OF DISCRETE EIGENFUNCTION IS',(' ',5G15.8))
0026        CALL EIGEN(EIG,NUO,IG)
0027        CALL EIGEN(EIGN,-NUO,IG)
0028        CALL AVEC(BSCR,NUO,D,SIG,IG,DSCR,CSCR,LLL,LLLL)
0029        WRITE(6,202) (BSCR(J),J=1,IG)
0030      202 FORMAT(' INTEGRAL OF ADJOINT EIGENFUNCTION IS',(' ',5G15.8))
0031        CALL EIGEN(ADEIG,NUO,IG)
0032        CALL EIGEN(ADEIGN,-NUO,IG)
0033        WRITE(6,102) ((EIG(JMU,J),JMU=1,16),J=1,IG)
0034        WRITE(6,102) ((EIGN(JMU,J),JMU=1,16),J=1,IG)
0035        WRITE(6,102) ((ADEIG(JMU,J),JMU=1,16),J=1,IG)
0036        WRITE(6,102) ((ADEIGN(JMU,J),JMU=1,16),J=1,IG)
0037      102 FORMAT (2(' ',8G15.7/)/2(' ',8G15.7/)/)
      C   CALCULATION OF THE DISCRETE EIGENFUNCTION NORMALIZATION--NPLUS
0038        DO 105 JMU=1,16
0039        FST=0.0D0
0040        DO 104 J=1,IG
0041      104 FST=FST+EIG(JMU,J)*ADEIG(JMU,J)
0042      105 VEC(JMU)=X(JMU)*FST
0043        FST=GAUS(VEC,IG)
0044        DO 106 JMU=1,16
0045        TST=0.0D0
0046        DO 107 J=1,IG
0047      107 TST=TST+ADEIGN(JMU,J)*EIGN(JMU,J)
0048      106 VEC(JMU)=X(JMU)*TST
```

FRED

```
0049            TST=GAUS(VEC,IG)
0050            NPLUS=FST-TST
0051            WRITE(6,109) NPLUS
0052          109 FORMAT('0NPLUS BY DIRECT INTEGRATION IS',G15.8)
              C
              C  CALCULATE U AND V APPROXIMAYIONS
              C CALCULATE THE SCALAR DIVISOR
0053            DO 212 JMU=1,16
0054            SUM=0.0D0
0055            DO 211 J=1,IG
0056          211 SUM=SUM+ADEIG(JMU,J)*EIG(JMU,J)
0057          212 VEC(JMU)=SUM*X(JMU)
0058            SCALAR=GAUS(VEC,IG)
0059            WRITE(6,213)
0060          213 FORMAT('0THE SCALAR INTEGRAND AND THE RESULTANTINTEGRAL ARE')
0061            WRITE(6,217) (VEC(J),J=1,16)
0062          217 FORMAT (' ',8G15.7)
0063            WRITE(6,218) SCALAR
0064          218 FORMAT(G16.8)
0065            CALL GAUVEC(EIG,ESCR,IG)
0066            CALL GAUVEC(ADEIG,CSCR,IG)
0067            WRITE(6,214) (CSCR(J),J=1,IG),(ESCR(J),J=1,IG)
0068          214 FORMAT('0INTEGRALS OF EIGN AND ADEIGN ARE',(' ',2G15.7))
              C CALCULATE U AND V
0069            DO 215 JMU=1,16
0070            DO 215 J=1,IG
0071            DO 216 K=1,IG
0072            U(JMU,J,K)=(X(JMU)*EIGN(JMU,J)*CSCR(K))/SCALAR
0073          216 V(JMU,J,K)=(X(JMU)*ESCR(J)*ADEIGN(JMU,K))/SCALAR
0074            U(JMU,J,J)=U(JMU,J,J) +1.D0
0075          215 V(JMU,J,J)=V(JMU,J,J) +1.D0
0076            CALL PRT(U,V,IG,0)
0077            GO TO 6
0078            END
```

REFERENCES

1. Case, K. M., and Zweifel, P. F., Linear Transport Theory, Addison-Wesley, Reading, Mass. (1967).

2. Mendelson, M. R., Doctoral Thesis, University of Michigan, Ann Arbor, (1964).

3. Kuščer, I., McCormick, N.J., and Summerfield, G. C., Ann. Phys., 30 (1964) 411.

4. Mitsis, G. J., Argonne National Laboratory Report, ANL-6787, (1963).

5. Kuščer, I., Proc. Symposium on Neutron Thermalization and Reactor Spectra, Ann Arbor, (1967) (to be published).

6. Ferziger, J. and Zweifel, P. F., The Theory of Neutron Slowing Down in Nuclear Reactors, MIT Press. Cambridge, Mass. (1966).

7. Case, K. M., Ann. Phys. 9 (1960) 1.

8. Bednarz, R. J., and Mika, J. R., J. Math. Phys., 4 (1963) 1285.

9. Leonard, A., and Ferziger, J. H., Nucl. Sci. Eng., 26 (1966) 170.

10. Leonard, A., and Ferziger, J. H., Nucl. Sci. Eng., 26 (1966) 181.

11. Leonard, A., and Ferziger, J. H., Ann. Phys., 22 (1963) 192.

12. Mika, J. R., Nucl. Sci. Eng., 22 (1965) 235.

13. Steward, J. C., Kuščer, I., McCormick, N. J., Ann. Phys., 40 (1966) 321.

14. McCormick, N. J., Kuščer, I., Trans. Amer. Nucl. Soc., 9 (1966) 444.

15. Zelazny, R., and Kuszell, A., Proc. Seminar on the Physics of Fast and Intermediate Reactors, Vol. II, IAEA, Vienna (1962).

16. Yoshimura, T., (submitted to Nucl. Sci. Eng.).

17. Siewert, C. E., and Shiek, P. S., J. Nucl. Eng., 21 (1967) 383.

18. Zelazny, R., and Kuszell, A., Ann. Phys., 16 (1961) 81.

19. Metcalf, D., Doctoral Thesis, The University of Michigan (1968).

20. Siewert, C. E., and Zweifel, P. F., J. Math. Phys., 7 (1966) 2092.

21. Fuchs, K., and Collatz, S., Kernenergie, 7 (1964) 386.

22. Zelazny, R., Proc. 3rd UN Int. Conf. PUAE (1964).

23. Case, K. M., Proc. Symp. on Transport Theory, Am. Math. Soc., April (1967) (to be published).

24. Pahor, S., Nucl. Sci. Eng., 26 (1966) 192.

25. Pahor, S., Nucl. Sci. Eng., 29 (1967) 248.

26. Ambarzumian, V. A., Astr. J. Sov. Union, 19 (1942) 30.

27. Chandrasekhar, S., Radiative Transfer, Dover, New York (1960).

28. Gel'Fand, I. M., and Shilov, G. E., Generalized Functions, Academic Press, New York (1964).

29. Muskhelishvili, N. I., Singular Integral Equations, Noordhoff Groningen, Holland, (1946).

30. Wachspress, E. L., Iterative Solution of Elliptic Systems, Prentice-Hall, Englewood, (1966).

31. Mullikin, T. W., Astrophys. J., 136 (1962) 627.

32. Mullikin, T. W., Astrophys. J., 139 (1964) 379.

33. Mullikin, T. W., Astrophys. J., 139 (1964) 1267.

34. Pahor, S., and Kuscer, I., Astrophys. J., 143 (1966) 888.

35. Mikhlin, S. G., Integral Equations, Pergamon, New York, (1964).

36. Shapiro, C., and Corngold, N., Trans. Am. Nucl. Soc., 6 (1963) 26.

37. Reactor Physics Constants, 2nd ed., Argonne National Laboratory Report, ANL 5800, (1963).

38. Williams, M.M.R., The Slowing Down and Thermalization of Neutrons, Interscience, New York, (1966).

39. Perlis, F., Theory of Matrices, Addison-Wesley, New York (1962).

40. Minnaert, Astrophys. J., 93, 403.

41. Courant, R., and Hilbert, D., Methods of Mathematical Physics, Interscience, New York, (1953) 116.

42. Curtis, R. L., and Grimesey, R. A., "INCITE A Fortran IV Program to Generate Neutron Spectra and Multigroup Constants Using Arbitrary Scattering Kernels," IN-1062, Idaho Nuclear Corporation (to be published).

43. McMurry, H. L., Russell, G. J., and Brugger, R. M., Nucl. Sci. Eng., 25 (1966) 248.

44. Hansen, G. E., "Properties of Elementary, Fast-neutron Critical Assemblies", Prov. Geneva Conf. (1958).

45. Abramowitz, M., and Stegun, I. A., Handbook of Mathematical Functions, National Bureau of Standards, AMS 55 (1964) 916.

46. Margenau, H., and Murphy, G. M., Mathematics of Physics and Chemistry, Van Nostrand, New York (1956).

47. FORTRAN IV Language, IBM Systems Library, C28-6515-N (1968).

48. Shure, F. C., and Natelson, M., Ann. Phys., 26 (1964) 274.

49. Case, K. M., (private communication) February, (1968).

50. Savant, C. J., Fundamentals of the Laplace Transformation, McGraw-Hill, New York (1962).