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SOLUTIONS OF THE TWO-GROUP TRANSPORT EQUATION IN PLANE GEOMETRY

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TABLE OF CONTENTS

TABLE OF CONTENTS (Concluded)

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

The main objective of this thesis is to obtain exact solutions to the two-group neutron transport equation utilizing the singular eigenfunction approach. By this method exact solutions to a limited set of problems can be obtained against which the accuracy of conventional approximations may be tested.

A detailed study was made of the singular eigenfunctions of the two-group transport equation. A convenient linear combination of the continuum eigenfunctions was selected to simplify later analysis. Using these eigenfunctions, a full-range completeness proof for infinite medium applications is presented. For the half-range case, reliance is placed on a half-range theorem proved several years ago and (with this as authority) the general half-range problem is rederived in a form convenient for numerical analysis. Explicitly, two coupled equations are obtained where the unknowns are the discrete and one continuum mode expansion coefficients. Finally, the remaining continuum mode expansion coefficient is expressed directly in terms of the other two coefficients. This general result is then applied to the solution of two typical half-space problems, the Milne and constant source problems. For comparison purposes the solutions of the two-group Milne and constant source problems are also obtained in the P_1, P_3, and DP_1 approximations.

Special numerical methods developed for the computer solution to the exact problem are discussed in detail. Of particular importance is the development of a relatively fast and accurate method for calculating singular integrals.

Computer codes are written in the Michigan Algorithm Decoder (MAD) language and a complete listing is given. With these codes anyone can (with different cross section sets) test the accuracy of conventional approximation methods.

Calculations are performed for four light water systems with varying amounts of absorption. These calculations show that although the P_1 approximation yields fairly good results for the total flux and current, the angular distribution is not so well represented especially at the interface. The P_3 approximation continues to give negative inward angular fluxes but of a reduced magnitude. The DP_1 method improves significantly on the P_1 and P_3 angular fluxes as well as on the total flux and current. The boundary condition at the vacuum-medium interface can be specified exactly in the DP_1 approximation; therefore, the exit angular distribution at the boundary is well represented.

An interesting result from this study was in the constant source case the exit angular distribution becomes less pronounced in the forward direction with increased absorption in the medium. This is in contrast to the Milne problem where the opposite effect is noted. Also of interest is the fact that the P_1 approximation in two-group theory yields two eigenvalues in the con-

tinuum (as well as two outside the continuum) while in the one-group case both eigenvalues are outside the continuum. This means that in two-group theory more than just the asymptotic solution is obtained even in the lowest order approximation.

In two-group neutron transport theory, the P_3 and DP_1 approximations present essentially the same computational difficulty. We conclude that in reactor physics design analysis (with reactor parameters similar to those studied here) the DP_1 approximation is much to be preferred over the P_3.

I. INTRODUCTION

Essentially all of the (static) physical properties of a nuclear reactor are determined by a knowledge of the velocity and space dependent neutron flux. This quantity obeys to a very high approximation the neutron transport equation.[1] In its full generality, this equation is too difficult to solve even for the present generation of digital computers. For this reason various approximation techniques have been developed through the years to determine the flux in nuclear reactor systems.[2] The usual criterion for assessing the accuracy of the calculations has been to compare the results with critical experiments.[3] The three main sources of error in these comparisons are the cross sections used, the geometric model of the reactor, and the simplification of the transport equation to a tractable approximate form. The calculations have often given results that compare quite well with critical experiments.[3] But there remains a certain amount of justified skepticism in the calculations when one attempts to study a new and different system on which no experimental data exist. Furthermore, the current requirements for economic performance of power reactors entail a great deal more than a simple knowledge of the static criticality factor. It has been well-documented that calculation of temperature coefficients, burnup, etc., require more sophisticated treatments of the transport equation.[4]

In the absence of detailed experimental information, it is possible to use exact solutions of the transport equation as test cases to assess the validity of various approximation schemes. Needless to say, the physical model involved must be grossly simplified, but it is still possible to interpret the accuracy obtainable from the approximate methods when they are then applied to practical systems.

The first detailed numerical efforts along these lines were made by Mendelson[5] who treated the one-speed model in some detail. Our purpose is to extend these results to the "two-speed" (or as it is generally called the "two-group") approximation. This is the next logical extension to the grossly inadequate treatment of the neutron energy spectrum in a reactor yielded by the one-speed approximation. In fact, many reactors are treated reasonably well with two-group theory.[3] For those systems which do require more groups (fast and intermediate systems particularily) the present work serves as a guide for the extension to a multigroup approximation.

As a matter of fact, although there has been considerable effort expended in recent years to obtain exact analytical solutions to the transport equation (as is described in detail in Ref. 1), the reduction of these results to numerics has lagged. Obtaining numbers from the analytical formulae is far from a trivial problem, the major reason being the different and unusual nature of the functions involved. This point is clearly made in Mendelson's work.[5]

Thus, two contributions are made in this thesis. First, the (singular) eigenmodes of the two-group transport equation are studied in some detail and the two-group equations are reduced to a form convenient for numerical analysis. Then, the numerical analysis is carried through and comparisons are made to standard approximation methods. Some attempt is made to draw general conclusions as to the range of reactor parameters for which the common approximation schemes are valid.

The two-group case has been studied previously by Żelazny and Kuszell.[6] They succeeded in proving a "completeness theorem" which in effect tells us that the normal modes which we develop are adequate to solve all infinite and semi-infinite medium problems. We depend upon this theorem, but because the results of Ref. 6 are not presented in a form convenient for numerical or analytical computation much of their analysis is redone. Siewert and Zweifel[7] have obtained analytical solutions to a very special two-group problem, but their restrictions upon the parameters involved are invalid in the neutron transport case. (This work was applied to the problem of radiative transport.) Siewert and Shieh[8] have carried out some preliminary work on the more general problem considered here, but their results can be applied directly only to infinite medium problems. Recently some unpublished work along similiar lines to that described here has come to our attention and we are able to incorporate some of these results into our work.[9]

Aside from these very little work similiar to that presented here appears in the literature. Most of the effort expended upon the exact energy-dependent transport equation has been applied to neutron thermalization problems.[10]

Specifically, we treat the one-dimensional two-group transport equation with isotropic scattering. The method, based on Case's singular eigenfunction approach[1,11] is a logical extension of that described in Ref. 7.

In Chapter II we develop the appropriate eigenvectors and eigenvalues. In Chapter III we present a full-range completeness proof such as is necessary in infinite medium applications. As we have mentioned, similiar theorems have been proved in Refs. 6 and 7, so our treatment is brief, and is presented only because we use a different (and we believe more convenient) notation. In Chapter IV we re-derive the half-space problem in a form convenient for numerical analysis. Želazny and Kuszell[6] have proved completeness and we do not repeat their work. (Anyway, the completeness theorem is not constructive[12] so its utility is more or less academic.) In our final equation the presence of a nondegenerate Fredholm term prevents the usual Weiner-Hopf factorization. We develop a pair of coupled equations where the unknowns are the discrete and one continuum mode expansion coefficients. These equations can readily be solved with a computer program which is presented in Appendix D. In Chapter V we solve the two-group Milne and constant source problems. Some important simplifications are developed by using the X-function identities listed in Appendix A. Some of the special, unique numerical methods which were developed for the computer solution are discussed in Chapter VI. In particular, a relatively fast and accurate method for the evaluation of singular integrals is presented. In Chapter VII we develop the spherical harmonic solutions to the two-group Milne and constant source problems. These solutions are developed in the P_1, P_3, and DP_1 approximations.[13] To solve the Milne and constant source problems in these approximations most efficiently, a series of computer programs were written. A listing of these computer programs is given in Appendix D. Some special problems, which are not of great importance to the overall goals of this thesis, are discussed in Appendices B and C.

II. EIGENFUNCTIONS AND EIGENVALUES

The two-group transport equations with isotropic scattering in plane geometry can be written[7]

$$\mu \frac{\partial\psi_1(x,\mu)}{\partial x} + \sigma_1\psi_1(x,\mu) = \frac{\sigma_{11}}{2}\int_{-1}^{1}\psi_1(x,\mu)d\mu + \frac{\sigma_{12}}{2}\int_{-1}^{1}\psi_2(x,\mu)d\mu \qquad (2.1a)$$

$$\mu \frac{\partial\psi_2(x,\mu)}{\partial x} + \sigma_2\psi_2(x,\mu) = \frac{\sigma_{21}}{2}\int_{-1}^{1}\psi_1(x,\mu)d\mu + \frac{\sigma_{22}}{2}\int_{-1}^{1}\psi_2(x,\mu)d\mu \qquad (2.1b)$$

$\psi_1(x,\mu)$ and $\psi_2(x,\mu)$ are the angular fluxes in groups one and two respectively, σ_1 and σ_2 are the total macroscopic cross sections for each group and the σ_{ij} are the macroscopic scattering transfer cross sections which describe the transfer of neutrons from group j to group i. All σ's are assumed to be spatially independent.

We make the nonrestrictive assumption that $\sigma_2 < \sigma_1$ and we divide Eqs. (2.1) by σ_2. By defining $\sigma = \sigma_1/\sigma_2$ and using the optical length $z = \sigma_2 x$, we write Eqs. (2.1) in the same convenient matrix form as in Ref. 6:

$$\mu \frac{\partial}{\partial z}\underline{\psi}(z,\mu) + \underline{\underline{\Sigma}}\,\underline{\psi}(z,\mu) = \underline{\underline{C}}\int_{-1}^{1}\underline{\psi}(z,\mu)d\mu \qquad (2.2)$$

where

$$\underline{\underline{\Sigma}} = \begin{pmatrix}\sigma & 0\\ 0 & 1\end{pmatrix}, \qquad \underline{\psi}(z,\mu) = \begin{pmatrix}\psi_1(z,\mu)\\ \psi_2(z,\mu)\end{pmatrix},$$

$$\underline{\underline{C}} = \begin{pmatrix}C_{11} & C_{12}\\ C_{21} & C_{22}\end{pmatrix} \text{ and } C_{ij} = \frac{\sigma_{ij}}{2\sigma_2}.$$

As usual we assume solutions of the form

$$\underset{\sim}{\psi}(z,\mu) = e^{-z/\eta}\,\underline{F}(\eta,\mu) \quad . \tag{2.3}$$

This ansatz when substituted into Eq. (2.2), and after cancellation of the space dependence, yields the eigenvalue equation (η is the eigenvalue),

$$\underline{\underline{A}}\,\underline{F}(\eta,\mu) = \eta\underline{\underline{C}}\int_{-1}^{1}\underline{F}(\eta,\mu)d\mu \tag{2.4a}$$

where

$$\underline{\underline{A}} = \begin{pmatrix} \sigma\eta-\mu & 0 \\ 0 & \eta-\mu \end{pmatrix}. \tag{2.4b}$$

In contrast to the one-speed case where two eigenvalue spectrum consisting of the discrete eigenvalues of magnitude $|\eta| > 1$ and a continuous spectrum in the range $\eta\epsilon[-1,1]$,[1] we must here consider three separate regions for the spectrum since in Eq. (2.4b) the term $\sigma\eta-\mu$ does not vanish in the intervals $\eta\epsilon[-1, \frac{1}{\sigma}]$ and $\eta\epsilon[\frac{1}{\sigma},1]$. (Recall that $\sigma > 1$.)

Following Siewert and Zweifel,[7] we consider Region 1 of the continuous spectra as $\eta\epsilon[-\frac{1}{\sigma}, \frac{1}{\sigma}]$. The eigensolutions in this region are twofold degenerate and will be denoted by $\underline{F_1}^{(1)}(\eta,\mu)$ and $\underline{F_2}^{(1)}(\eta,\mu)$. To obtain linearly independent eigensolutions, we first normalize by

$$\int_{-1}^{1}\underline{F_1}^{(1)}(\eta,\mu')d\mu' = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{2.5a}$$

where

$$\underline{F_1}^{(1)}(\eta,\mu) = \begin{pmatrix} F_{1,1}^{(1)}(\eta,\mu) \\ F_{1,2}^{(1)}(\eta,\mu) \end{pmatrix}. \tag{2.5b}$$

We substitute Eq. (2.5a) into Eq. (2.4a) and solve for $\underline{F}_1^{(1)}(\eta,\mu)$. Explicitly

$$F_{1,1}^{(1)}(\eta,\mu) = \frac{\eta C_{11} P}{\sigma\eta-\mu} + \lambda_1(\eta)\delta(\sigma\eta-\mu) \tag{2.6a}$$

and

$$F_{1,2}^{(1)}(\eta,\mu) = \frac{\eta C_{21} P}{\eta-\mu} + \lambda_2(\eta)\delta(\eta-\mu) \tag{2.6b}$$

where

$$\underline{\lambda}(\eta) = \begin{pmatrix} \lambda_1(\eta) \\ \lambda_2(\eta) \end{pmatrix}$$

is to be determined from Eq. (2.5a).

By integrating Eqs. (2.6) over $d\mu$ and using Eq. (2.5a), we find

$$\lambda_1(\eta) = 1 - 2C_{11}\eta\tau(\sigma\eta) \tag{2.7a}$$

$$\lambda_2(\eta) = -2C_{21}\eta\tau(\eta) \tag{2.7b}$$

where

$$P\int_{-1}^{1} \frac{d\mu}{\sigma\eta-\mu} = \ell n\left(\frac{1+\sigma\eta}{1-\sigma\eta}\right) = 2\tanh^{-1}(\sigma\eta) \equiv 2\tau(\sigma\eta) \,. \tag{2.7c}$$

The symbol P in Eqs. (2.6) indicates that the integrals are to be interpreted in the sense of the Cauchy principal value.

With Eqs. (2.7) inserted into Eqs. (2.6), we have

$$\underline{F}_1^{(1)}(\eta,\mu) = \begin{pmatrix} \dfrac{C_{11}\eta P}{\sigma\eta-\mu} + [1-2\eta C_{11}\tau(\sigma\eta)]\delta(\sigma\eta-\mu) \\ \\ \dfrac{C_{21}\eta P}{\eta-\mu} - 2C_{21}\eta\tau(\eta)\delta(\eta-\mu) \end{pmatrix}. \tag{2.8}$$

A similar procedure with the normalization

$$\int_{-1}^{1} \underline{F_2}^{(1)}(\eta,\mu)d\mu = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (2.9)$$

leads to the result

$$\underline{F_2}^{(1)}(\eta,\mu) = \begin{pmatrix} \frac{C_{12}\eta P}{\sigma\eta-\mu} - 2C_{12}\eta\tau(\sigma\eta)\delta(\sigma\eta-\mu) \\ \frac{C_{22}\eta P}{\eta-\mu} + [1-2\eta C_{22}\tau(\eta)]\delta(\eta-\mu) \end{pmatrix}. \quad (2.10)$$

Thus the two linearly independent eigenvectors for $\eta\epsilon[-\frac{1}{\sigma}, \frac{1}{\sigma}]$ are given by Eq. (2.8) and Eq. (2.10).

Next we consider $\eta\epsilon[-1, -\frac{1}{\sigma}]$ and $\eta\epsilon[\frac{1}{\sigma},1]$, (Region 2). Defining the eigenvector as $\underline{F}^{(2)}(\eta,\mu)$ and noting that the normalization is arbitrary, we use

$$\int_{-1}^{1} \underline{F}^{(2)}(\eta,\mu)d\mu = \begin{pmatrix} a_1(\eta) \\ a_2(\eta) \end{pmatrix} = \begin{pmatrix} 2\eta C_{12}\tau(1/\sigma\eta) \\ 1-2C_{11}\eta\tau(1/\sigma\eta) \end{pmatrix} \quad (2.11)$$

where

$$\underline{F}^{(2)}(\eta,\mu) = \begin{pmatrix} F_1^{(2)}(\eta,\mu) \\ F_2^{(2)}(\eta,\mu) \end{pmatrix}.$$

From Eq. (2.4), we have

$$F_1^{(2)}(\eta,\mu) = \frac{C_{11}\eta a_1(\eta)}{\sigma\eta-\mu} + \frac{C_{12}\eta a_2(\eta)}{\sigma\eta-\mu} \quad (2.12a)$$

$$F_2^{(2)}(\eta,\mu) = \frac{C_{21}\eta a_1(\eta)P}{\eta-\mu} + \frac{C_{22}\eta a_2(\eta)P}{\eta-\mu} + \lambda(\eta)\delta(\eta-\mu). \quad (2.12b)$$

We integrate each term in Eqs. (2.12) over $d\mu$ and use the normalization given by Eq. (2.11) to derive

$$\lambda(\eta) = 1 - 2\eta C_{22}\tau(\eta) - 2\eta C_{11}\tau(1/\sigma\eta) + 4C\eta^2\tau(\eta)\tau(1/\sigma\eta) \qquad (2.13)$$

where

$$C = \det \underline{\underline{C}} \ .$$

Equations (2.11) and (2.13) are inserted into Eqs. (2.12) to derive the following eigenvector for Region 2:

$$\underline{F}^{(2)}(\eta,\mu) = \begin{pmatrix} C_{12}\eta/\sigma\eta-\mu \\ \dfrac{\eta t(\eta)P}{\eta-\mu} + \delta(\eta-\mu)\lambda(\eta) \end{pmatrix} \ . \qquad (2.14)$$

Here $t(\eta) = C_{22}-2\eta C\tau(1/\sigma\eta)$ and $\lambda(\eta)$ is given by Eq. (2.13).

Next we consider $\eta \notin [-1,1]$ and define the associated eigenvector as

$$\underline{F}(\eta,\mu) = \begin{pmatrix} F_1(\eta,\mu) \\ F_2(\eta,\mu) \end{pmatrix} .$$

In this case, Eq. (2.4) can be solved directly to give

$$F_1(\eta,\mu) = \frac{\eta}{\sigma\eta-\mu}\left[C_{11}\int_{-1}^{1} F_1(\eta,\mu')d\mu' + C_{12}\int_{-1}^{1} F_2(\eta,\mu')d\mu'\right] \qquad (2.15a)$$

$$F_2(\eta,\mu) = \frac{\eta}{\eta-\mu}\left[C_{21}\int_{-1}^{1} F_1(\eta,\mu')d\mu' + C_{22}\int_{-1}^{1} F_2(\eta,\mu')d\mu'\right] \ . \qquad (2.15b)$$

We integrate Eqs. (2.15) over $d\mu$ to obtain the following secular determinant whose zeros yield the discrete eigenvalues:

$$\begin{vmatrix} 1-2C_{11}\eta\tau(1/\sigma\eta) & 2C_{12}\eta\tau(1/\sigma\eta) \\ 2C_{21}\eta\tau(1/\eta) & 1-2C_{22}\eta\tau(1/\eta) \end{vmatrix} = 0. \qquad (2.16)$$

By defining the dispersion function $\Omega(z)$, we have

$$\Omega(z) \equiv 1-2c_{11}z\tau(1/\sigma z)-2C_{22}z\tau(1/z)+4Cz^2\tau(1/z)\tau(1/\sigma z) = 0 \quad . \qquad (2.17)$$

We have replaced η by the complex variable z to indicate that the roots can be real and/or complex. We can easily see from Eq. (2.17) that if η_i is the positive root then $-\eta_i$ is also. And if η_i is a complex root of Eq. (2.17), η_i^* is also. We have

$$\Omega(-\eta_i) = \Omega(\eta_i) = 0 \qquad (2.18)$$

$$\Omega(\eta_i) = \Omega(\eta_i^*) = 0 \quad . \qquad (2.19)$$

Żelazny and Baran[9] have made a detailed study of Eq. (2.17) to determine the number and type of discrete roots as a function of the C_{ij}'s and σ. We reproduce in Table 2.1 their results which take into account all possibilities. For the two-group problems considered in this thesis we have only two discrete eigenvalues. By virtue of Eqs. (2.18) and (2.19) these must be real or imaginary. In fact from Table 2.1 we note that the discrete roots are either real and/or purely imaginary. Therefore the eigenvalues occur in $\pm$ pairs and we denote these by $\pm\eta_i$ with associated eigenvectors $\underline{F}_{i\pm}(\mu)$.

The normalization in Eqs. (2.15) is arbitrary. If we use the same normalization as in Region 2 (with $\eta_i \to \eta$), we derive the discrete eigenvectors for $\eta \notin [-1,1]$; namely

$$\underline{F}_{i\pm}(\mu) = \begin{pmatrix} C_{12}\eta_i/\sigma\eta_i \mp \mu \\ \eta_i t(\eta_i)/\eta_i - \mu \end{pmatrix} = \begin{pmatrix} \underline{F}_{i\pm,1}(\mu) \\ \underline{F}_{i\pm,2}(\mu) \end{pmatrix} \qquad (2.20)$$

TABLE 2.1

THE ZEROS OF THE DISPERSION FUNCTION

Conditions			Roots
$C = 0$		$C_{11}+\sigma C_{22} < \sigma/2$	2 Real
		$C_{11}+\sigma C_{22} > \sigma/2$	2 Imaginary
		$C_{11}+\sigma C_{22} = \sigma/2$	2 Infinite
$C < 0$		$C_{11}+\sigma C_{22}-2C < \sigma/2$	2 Real
		$C_{11}+\sigma C_{22}-2C > \sigma/2$	2 Imaginary
		$C_{11}+\sigma C_{22}-2C = \sigma/2$	2 Infinite
$C > 0$ $C_{22} > 2C\tau(1/\sigma)$		$C_{11}+\sigma C_{22}-2C < \sigma/2$	2 Real
		$C_{11}+\sigma C_{22}-2C > \sigma/2$	2 Imaginary
		$C_{11}+\sigma C_{22}-2C = \sigma/2$	2 Infinite
$C > 0$ $C_{22} \leq 2C\tau(1/\sigma)$	$C_{11} \leq \sigma/2$ and $C_{22} \geq 1/2$ or $C_{11} \geq \sigma/2$ and $C_{22} \leq 1/2$		2 Real and 2 Imaginary
	$C_{11} < \sigma/2$ and $C_{22} < 1/2$	$C_{11}+\sigma C_{22}-2C < \sigma/2$	4 Real
		$C_{11}+\sigma C_{22}-2C > \sigma/2$	2 Real and 2 Imaginary
		$C_{11}+\sigma C_{22}-2C = \sigma/2$	2 Real and 2 Infinite
	$C_{11} > \sigma/2$ and $C_{22} > 1/2$	$C_{11}+\sigma C_{22}-2C < \sigma/2$	4 Imaginary
		$C_{11}+\sigma C_{22}-2C > \sigma/2$	2 Real and 2 Imaginary
		$C_{11}+\sigma C_{22}-2C = \sigma/2$	2 Imaginary and 2 Infinite

where

$$t(\eta_i) \;=\; C_{22}-2\eta_i C\tau(1/\sigma\eta_i) \;.$$

We note that $\Omega(z)$ is analytic in the complex plane cut along the real axis from -1 to 1. Introducing the notation

$$\begin{aligned} \theta_i(\eta) &= 1, \quad \eta\epsilon \text{ Region } i \\ &= 0, \quad \text{otherwise,} \end{aligned}$$

we easily find

$$\begin{aligned} \Omega^{\pm}(\mu) \;=\; & 1-2C_{22}\mu\tau(\mu)-2C_{11}\mu\tau(\sigma\mu)\theta_1(\mu)-2C_{11}\mu\tau(1/\sigma\mu)\theta_2(\mu)+4C\mu^2\tau(\mu)\tau(\sigma\mu)\theta_1(\mu) \\ & +4C\mu^2\tau(\mu)\tau(1/\sigma\mu)\theta_2(\mu)-\pi^2\mu^2 C\theta_1(\mu)\pm\pi i\mu[C_{22}+C_{11}\theta_1(\mu)-2C\mu\tau(\sigma\mu)\theta_1(\mu) \\ & -2C\mu\tau(\mu)\theta_1(\mu)-2C\mu\tau(1/\sigma\mu)\theta_2(\mu)] \;. \end{aligned} \tag{2.21}$$

Here $\Omega^{\pm}$ represent the boundary values of $\Omega(z)$ as the branch cut is approached from $\binom{\text{above}}{\text{below}}$. That is, $\Omega^{\pm}(\mu) = \lim_{\epsilon\to 0} \Omega(\mu\pm i\epsilon)$.

It is convenient to use the following linear combination of Region 1 eigenvectors:

$$\underline{\phi}_1(\eta,\mu) \;=\; \frac{1}{C_{11}}\,\underline{F}_1^{(1)}(\eta,\mu) - \frac{1}{C_{12}}\,\underline{F}_2^{(1)}(\eta,\mu). \tag{2.22}$$

Explicitly,

$$\underline{\phi}_1(\eta,\mu) \;=\; \begin{pmatrix} \dfrac{1}{C_{11}}\,\delta(\sigma\eta-\mu) \\ -\dfrac{C\eta P}{C_{11}C_{12}(\eta-\mu)} - \dfrac{\delta(\eta-\mu)}{C_{12}C_{11}}\,[C_{11}-2C\eta\tau(\eta)] \end{pmatrix} . \tag{2.23}$$

The following linear combination is a convenient eigenvector valid over the full range, $\eta\epsilon[-1,1]$:

$$\underline{\phi}_2(\eta,\mu) = 2C_{12}\eta\tau(\sigma\eta)\Theta_1(\eta)\underline{F}_1^{(1)}(\eta,\mu) + [1-2C_{11}\eta\tau(\sigma\eta)]\Theta_1(\eta)\cdot\underline{F}_2^{(1)}(\eta,\mu)$$
$$+ \underline{F}^{(2)}(\eta,\mu)\Theta_2(\eta) \quad . \tag{2.24}$$

Again the explicit form is

$$\underline{\phi}_2(\eta,\mu) = \begin{pmatrix} C_{12}\eta P/\sigma\eta-\mu \\ \dfrac{\eta g(\eta)P}{\eta-\mu} + \lambda(\eta)\delta(\eta-\mu) \end{pmatrix} . \tag{2.25}$$

Here we define

$$g(\eta) = C_{22}-2C\eta\tau(\sigma\eta)\Theta_1(\eta)-2C\eta\tau(1/\sigma\eta)\Theta_2(\eta), \tag{2.26}$$

$$\lambda(\eta) = 1-2C_{22}\eta\tau(\eta)-2C_{11}\eta\tau(\sigma\eta)\Theta_1(\eta)-2C_{11}\eta\tau(1/\sigma\eta)\Theta_2(\eta)+4C\eta^2\tau(\eta)\tau(\sigma\eta)\Theta_1(\eta)$$
$$+4C\eta^2\tau(\eta)\tau(1/\sigma\eta)\Theta_2(\eta) \quad . \tag{2.27}$$

In comparing Eq. (2.27) with Eq. (2.21), we note that we can write Eq. (2.27) in the compact form

$$\lambda(\eta) = \frac{\Omega^+(\eta)+\Omega^-(\eta)}{2} + \pi^2\eta^2 C\Theta_1(\eta) \quad . \tag{2.28}$$

Also (for later use) we have from Eq. (2.21)

$$f(\mu) \equiv \frac{\Omega^+(\mu)-\Omega^-(\mu)}{2\pi i\mu} = C_{22}+C_{11}\Theta_1(\mu)-2C\mu\tau(\mu)\Theta_1(\mu)$$
$$- 2C\mu\tau(\sigma\mu)\Theta_1(\mu)-2C\mu\tau(1/\sigma\mu)\Theta_2(\mu) \quad . \tag{2.29}$$

Thus the eigenvectors consist of the two continuum modes $\underline{\phi}_1(\eta,\mu)$ [Eq. (2.23)], $\eta\epsilon[-\frac{1}{\sigma},\frac{1}{\sigma}]$; $\underline{\phi}_2(\eta,\mu)$ [Eq. (2.25)], $\eta\epsilon[-1,1]$; and the discrete modes $\underline{F}_{i\pm}(\mu)$ [Eq. (2.20)].

III. TWO-GROUP FULL-RANGE COMPLETENESS[8]

The full-range theorem is stated as follows:

Any function $\underline{\psi}(\mu)$ of class G^1 can be expanded using the eigenvectors $\underline{\phi}_1(\eta,\mu)$, $\underline{\phi}_2(\eta,\mu)$, and $\underline{F}_{i\pm}(\mu)$.

We follow the standard procedure of attempting an expansion in terms of the continuum modes only; namely,

$$\underline{\psi}(\mu) = \begin{pmatrix} \psi_1(\mu) \\ \psi_2(\mu) \end{pmatrix} = \int_{-1/\sigma}^{1/\sigma} \alpha_1(\eta)\underline{\phi}_1(\eta,\mu)d\eta + \int_{-1}^{1} \alpha_2(\eta)\underline{\phi}_2(\eta,\mu)d\eta \ . \quad (3.1)$$

We substitute the explicit form of $\underline{\phi}_1(\eta,\mu)$ and $\underline{\phi}_2(\eta,\mu)$ as given by Eqs. (2.23) and (2.25) into Eq. (3.1), and perform the integrations where possible to arrive at

$$\psi_1(\mu) = \frac{\alpha_1(\mu/\sigma)}{\sigma C_{11}} + C_{12}P\int_{-1}^{1} \frac{\eta\alpha_2(\eta)d\eta}{\sigma\eta-\mu} \quad (3.2)$$

$$\psi_2(\mu) = -\frac{C}{C_{11}C_{12}} P\int_{-1/\sigma}^{1/\sigma} \frac{\eta\alpha_1(\eta)d\eta}{\eta-\mu} - \frac{\alpha_1(\mu)\theta_1(\mu)}{C_{12}C_{11}}\left[C_{11}-2C\mu\tau(\mu)\right]$$
$$+ P\int_{-1}^{1} \frac{\eta\alpha_2(\eta)g(\eta)d\eta}{\eta-\mu} + \alpha_2(\mu)\lambda(\mu) \ . \quad (3.3)$$

We solve Eq. (3.2) for $\alpha_1(\mu/\sigma)$ and then make the change of variable, $\mu/\sigma = \eta$ to obtain

$$\alpha_1(\eta) = \sigma C_{11}\psi_1(\sigma\eta) - C_{11}C_{12}\int_{-1}^{1} \frac{P\eta'\alpha_2(\eta')d\eta'}{\eta'-\eta} \ . \quad (3.4)$$

The insertion of Eq. (3.4) for $\alpha_1(\eta)$ into Eq. (3.3) yields

$$\psi_2(\mu) + \frac{C\sigma}{C_{12}} \int_{-1/\sigma}^{1/\sigma} \frac{P\eta\psi_1(\sigma\eta)d\eta}{\eta-\mu} + \frac{\sigma}{C_{12}} \psi_1(\sigma\mu)\theta_1(\mu)[C_{11}-2C\mu\tau(\mu)]$$

$$= C \int_{-1/\sigma}^{1/\sigma} \frac{P\eta d\eta}{\eta-\mu} \int_{-1}^{1} \frac{P\eta'\alpha_2(\eta')d\eta'}{\eta'-\eta} - \theta_1(\mu)(2C\mu\tau(\mu)-C_{11}) \int_{-1}^{1} \frac{P\eta'\alpha_2(\eta')d\eta'}{\eta'-\mu}$$

$$+ \int_{-1}^{1} \frac{P\eta\alpha_2(\eta)g(\eta)d\eta}{\eta-\mu} + \alpha_2(\mu)\lambda(\mu) \ . \qquad (3.5)$$

The integration over η in the first term on the right-hand side of Eq. (3.5) can now be performed by using the Poincaré-Bertrand formula[14] and the partial fraction decomposition

$$\frac{\eta}{(\eta-\mu)(\eta'-\eta)} = \frac{1}{\eta'-\mu}\left(\frac{\mu}{\eta-\mu} + \frac{\eta'}{\eta'-\eta}\right). \qquad (3.6)$$

The result is

$$C \int_{-1/\sigma}^{1/\sigma} \frac{P\eta d\eta}{\eta-\mu} \int_{-1}^{1} \frac{P\eta'\alpha_2(\eta')d\eta'}{\eta'-\eta} = -C\pi^2\mu^2\alpha_2(\mu)\theta_1(\mu) - 2C \int_{-1}^{1} \frac{P\eta'\alpha_2(\eta')}{\eta'-\mu}$$

$$\cdot\ [\theta_1(\mu)\tau(\sigma\mu)+\theta_2(\mu)\tau(1/\sigma\mu)-\theta_1(\eta')\tau(\sigma\eta')$$

$$-\ \theta_2(\eta')\tau(1/\sigma\eta')] \ . \qquad (3.7)$$

We define

$$\psi'(\mu) = \psi_2(\mu) + \frac{C\sigma}{C_{12}} P \int_{-1/\sigma}^{1/\sigma} \frac{\eta\psi_1(\sigma\eta)d\eta}{\eta-\mu} + \frac{\sigma}{C_{12}} \psi_1(\sigma\mu)\theta_1(\mu)[C_{11}-2C\mu\tau(\mu)]. \qquad (3.8)$$

By using Eq. (3.7) and Eq. (3.8) and recalling Eqs. (2.28) and (2.29), we write

$$\psi'(\mu) = \frac{\Omega^+(\mu)-\Omega^-(\mu)}{2\pi i\mu} P \int_{-1}^{1} \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} + \frac{[\Omega^+(\mu)+\Omega^-(\mu)]\alpha_2(\mu)}{2} \ . \qquad (3.9)$$

As usual we introduce an auxiliary function

$$N(z) = \frac{1}{2\pi i} \int_{-1}^{1} \frac{\eta\alpha_2(\eta)d\eta}{\eta - z} \tag{3.10}$$

with boundary values given by the Plemelj formulae[14]:

$$N^{\pm}(\mu) = \frac{1}{2\pi i} P \int_{-1}^{1} \frac{\eta\alpha_2(\eta)d\eta}{\eta - \mu} \pm \frac{1}{2}\mu\alpha_2(\mu) . \tag{3.11a}$$

Therefore,

$$\alpha_2(\mu) = \frac{N^+(\mu) - N^-(\mu)}{\mu} . \tag{3.11b}$$

We write Eq. (3.9) in terms of these boundary values to obtain the factored form

$$\mu\psi'(\mu) = N^+(\mu)\Omega^+(\mu) - N^-(\mu)\Omega^-(\mu) . \tag{3.12}$$

This has the immediate solution

$$N(z) = \frac{1}{2\pi i\ \Omega(z)} \int_{-1}^{1} \frac{\mu\psi'(\mu)d\mu}{\mu - z} . \tag{3.13}$$

From Eq. (3.10) we note that N(z) must be analytic in the complex plane cut from -1 to 1. In order that N(z) have this property for $z = \pm\eta_i$ we require

$$\int_{-1}^{1} \frac{\mu\psi'(\mu)d\mu}{\mu \mp \eta_i} = 0 \tag{3.14}$$

where we recall the $\pm\eta_i$ are the discrete eigenvalues.

Our original expansion of $\underline{\psi}(\mu)$ was only in terms of the continuum modes. We have the discrete modes available to satisfy Eq. (3.14). Thus we make the replacement of $\underline{\psi}(\mu)$ by

$$\underline{\psi}(\mu) - \sum_i A_{i+} \underline{F}_{i+}(\mu) - \sum_i A_{i-} \underline{F}_{i-}(\mu) \ . \qquad (3.15)$$

We recall that $\underline{\psi}(\mu)$ contains components $\psi_1(\mu)$ and $\psi_2(\mu)$, and $\psi'(\mu)$ is a function of these components as given by Eq. (3.8). Thus $\psi'(\mu)$ in Eq. (3.14) is adjusted according to (3.15) and with two pairs of roots we would have four equations with four unknowns from which the discrete coefficients, $A_{i\pm}$, could be found. With the discrete coefficient known we would then determine $\alpha_2(\mu)$ from Eq. (3.11b) where the boundary value of N(z) are determined from Eq. (3.13). Also in Eq. (3.13) we must modify $\psi'(\mu)$ according to (3.15). With $\alpha_2(\mu)$ known, $\alpha_1(\mu)$ is calculated from Eq. (3.4). A better procedure for the full-range case is to prove an orthogonality theorem as Siewert and Shieh[8] have done. This procedure makes possible the calculation of various normalization integrals from which the expansion coefficient can be derived directly for any particular full-range problem by taking scalar products.

IV. TWO-GROUP HALF-RANGE CASE

From the completeness proof of Zelazny and Kuszell,[6] we know that the normal modes of the transport equation provide us with sufficient eigenfunctions to solve half-space problems. By a procedure which is in many respects similar to the completeness theorem proof described in the previous chapter, we develop equations for the expansion coefficients in a form convenient for numerical calculations.

The expansion for the half-range case, which we assume is valid from the work of Żelazny and Kuszell, is

$$\underline{\psi}(\mu) = \begin{pmatrix} \psi_1(\mu) \\ \psi_2(\mu) \end{pmatrix} = \int_0^{1/\sigma} \alpha_1(\eta)\underline{\phi}_1(\eta,\mu)d\eta + \int_0^1 \alpha_2(\eta)\underline{\phi}_2(\eta,\mu)d\eta \ . \tag{4.1}$$

We note that we are using the continuum modes only, the discrete mode will be introduced later. Using the explicit form of $\underline{\phi}_1(\eta,\mu)$ and $\underline{\phi}_2(\eta,\mu)$ [Eqs. (2.3) and (2.25)] in Eq. (4.1) and performing the integration over the delta functions yields

$$\psi_1(\mu) = \frac{\alpha_1(\mu/\sigma)}{\sigma C_{11}} + C_{12}P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\sigma\eta-\mu} \tag{4.2a}$$

and

$$\psi_2(\mu) = -\frac{C}{C_{11}C_{12}}P\int_0^{1/\sigma}\frac{\eta\alpha_1(\eta)d\eta}{\eta-\mu} - \frac{1}{C_{11}C_{12}}[C_{11}-2C\mu\tau(\mu)]\alpha_1(\mu)\theta_1(\mu)$$
$$+ P\int_0^1 \frac{\eta\alpha_2(\eta)g(\eta)d\eta}{\eta-\mu} + \lambda(\mu)\alpha_2(\mu) \ . \tag{4.2b}$$

Making the change of variable $\mu \to \mu\sigma$ in Eq. (4.2a) and solving for $\alpha_1(\mu)$, we obtain

$$\alpha_1(\mu) = \sigma C_{11}\psi_1(\mu\sigma) - C_{11}C_{12} + \int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} \quad . \tag{4.3}$$

The insertion of Eq. (4.3) into Eq. (4.2b) gives

$$\psi_2(\mu) + \frac{C\sigma}{C_{12}} P\int_0^1 \frac{\eta\psi_1(\sigma\eta)d\eta}{\eta-\mu} + \frac{\sigma}{C_{12}}[C_{11}-2C\mu\tau(\mu)]\psi_1(\sigma\mu)\theta_1(\mu)$$

$$= C\,P\int_0^{1/\sigma} \frac{\eta' d\eta'}{\eta'-\mu} P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\eta'} + [C_{11}-2C\mu\tau(\mu)]\theta_1(\mu)\,P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu}$$

$$+ P\int_0^1 \frac{\eta\alpha_2(\eta)g(\eta)d\eta}{\eta-\mu} + \lambda(\mu)\alpha_2(\mu) \ . \tag{4.4}$$

The Poincaré-Bertrand formula[14] and the partial fraction decomposition

$$\frac{\eta'}{(\eta'-\mu)(\eta-\eta')} = \frac{1}{\eta-\mu}\left(\frac{\mu}{\eta'-\mu} + \frac{\eta}{\eta-\eta'}\right) \tag{4.5}$$

enable us to perform an integration over $d\eta'$ in the first term on the right-hand side of Eq. (4.4). The result is

$$CP\int_0^{1/\sigma} \frac{\eta' d\eta' P}{\eta'-\mu} \int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\eta'} = P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu}\Big[\theta_1(\mu)C\mu\ell n\left(\frac{1}{\sigma\mu} - 1\right)$$

$$+ \theta_2(\mu)C\mu\ell n\left(1 - \frac{1}{\sigma\mu}\right) - \theta_1(\eta)C\eta\,\ell n\left(\frac{1}{\sigma\eta} - 1\right)$$

$$- \theta_2(\eta)C\eta\,\ell n\left(1 - \frac{1}{\sigma\eta}\right)\Big] - C\pi^2\mu^2\alpha_2(\mu)\theta_1(\mu) \ . \tag{4.6}$$

We can write Eq. (2.26) as

$$g(\eta) = C_{22} - C\eta\,\ell n\left(1 + \frac{1}{\sigma\eta}\right) + C\theta_1(\eta)\eta\,\ell n\left(\frac{1}{\sigma\eta} - 1\right) + C\theta_2(\eta)\eta\,\ell n\left(1 - \frac{1}{\sigma\eta}\right) \tag{4.7}$$

where we have used Eq. (2.7c).

The insertion of Eqs. (4.6) and (4.7) into Eq. (4.4) yields, after some cancellation and rearrangement, the compact form

$$\psi'(\mu) + C\int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu} = \frac{\Omega^+(\mu)-\Omega^-(\mu)}{2\pi i\mu} P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} + \frac{\Omega^+(\mu)+\Omega^-(\mu)}{2}\alpha_2(\mu). \tag{4.8}$$

Here we have defined

$$\psi'(\mu) = \psi_2(\mu) + \frac{C\sigma}{C_{12}} P\int_0^1 \frac{\eta\psi_1(\sigma\eta)d\eta}{\eta-\mu} + \frac{\sigma}{C_{12}}\psi_1(\sigma\mu)\Theta_1(\mu)[C_{11}-2C\mu\tau(\mu)] \tag{4.9}$$

and

$$k(\eta,\mu) = \eta\,\ell n\left(1+\frac{1}{\sigma\eta}\right) - \mu\,\ell n\left(1+\frac{1}{\sigma\mu}\right). \tag{4.10}$$

We note that the second term on the left-hand side of Eq. (4.8) is a nondegenerate Fredholm term. If this term were absent, Eq. (4.8) could be solved directly by standard procedures.[1] If it were degenerate, the method of Shure and Natelson[15] could be used. However, neither of these situations obtains, and no closed form solution of Eq. (4.8) has been found. Thus, we describe in Chapter VI an iterative procedure similiar to that used by Mitsis[1,16] to solve the critical slab problem and by McCormich and Mendelson[17] in treating the slab albedo problem.

We define

$$\psi''(\mu) \equiv \psi'(\mu) + C\int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu}. \tag{4.11}$$

Next we introduce a function N(z) defined by

$$N(z) = \frac{1}{2\pi i}\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-z}. \tag{4.12}$$

Following Case and Zweifel[1] if $\alpha_2(\eta)$ of class G exists then N(z) has the following properties:

1. N(z) is analytic in the complex plane cut along the real axis from 0 to 1;

2. $N(z) \sim \frac{1}{z}$ as $|z| \to \infty$;

3. $$N^{\pm}(\mu) = \frac{1}{2\pi i} P \int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} \pm \frac{1}{2}\mu\alpha_2(\mu). \quad (4.13)$$

We note from Property 3 that

$$\alpha_2(\mu) = \frac{N^+(\mu)-N^-(\mu)}{\mu} . \quad (4.14)$$

Inserting Eqs. (4.11) and (4.13) into Eq. (4.8), we find (after some rearrangement) that

$$\mu\psi''(\mu) = N^+(\mu)\Omega^+(\mu) - N^-(\mu)\Omega^-(\mu) . \quad (4.15)$$

We recall that $\Omega(z)$ is analytic in the complex plane cut from -1 to 1. We note from Property 1 that $N(z)$ is analytic in the complex plane cut from 0 to 1. This requires (as in one-speed theory[1]) the introduction of a function $X(z)$ such that

$$\frac{X^+(\mu)}{X^-(\mu)} = \frac{\Omega^+(\mu)}{\Omega^-(\mu)}, \quad \mu > 0 . \quad (4.16)$$

The $X(z)$ function satisfying the necessary restrictions[1] for the half-range and for one pair of discrete roots only is

$$X(z) = \frac{1}{1-z} \exp \frac{1}{\pi} \int_0^1 \frac{\mathrm{Arg}\Omega^+(\mu)d\mu}{\mu-z} . \quad (4.17)$$

The ratio condition, Eq. (4.16), is inserted into Eq. (4.15) to yield

$$\gamma(\mu)\psi''(\mu) = N^+(\mu)X^+(\mu) - N^-(\mu)X^-(\mu) \quad (4.18)$$

where

$$\gamma(\mu) \quad = \quad \mu\,\frac{X^+(\mu)}{\Omega^+(\mu)} \; . \tag{4.19}$$

Assuming that the left-hand side of Eq. (4.18) is known, we can write the solution to Eq. (4.18) as

$$N(z) \quad = \quad \frac{1}{2\pi i X(z)} \int_0^1 \frac{\gamma(\mu)\psi''(\mu)d\mu}{\mu - z} \; . \tag{4.20}$$

The Plemelj formulae give the boundary values of N(z) from Eq. (4.20). We insert these boundary values in Eq. (4.14) to obtain

$$\alpha_2(\mu) \quad = \quad \frac{1}{2\pi i\mu}\left(\frac{1}{X^+(\mu)} - \frac{1}{X^-(\mu)}\right) \; P\int_0^1 \frac{\gamma(\mu')\psi''(\mu')d\mu'}{\mu' - \mu} + \frac{1}{2\mu}\left(\frac{1}{X^+(\mu)} + \frac{1}{X^-(\mu)}\right)$$
$$\cdot \; \gamma(\mu)\psi''(\mu) \; . \tag{4.21}$$

(However, this is not a solution because we note from Eq. (4.11) that the unknown $\alpha_2(\mu)$ is still contained in $\psi''(\mu)$.) We next define

$$\ell_1(\mu) \quad = \quad -\frac{1}{2\pi i\mu}\left(\frac{1}{X^+(\mu)} - \frac{1}{X^-(\mu)}\right) \quad = \quad \frac{\Omega^+(\mu) - \Omega^-(\mu)}{2\pi i\gamma(\mu)\Omega^+(\mu)\Omega^-(\mu)} \tag{4.22a}$$

and

$$\ell_2(\mu) \quad = \quad \frac{1}{2\mu}\left(\frac{1}{X^+(\mu)} + \frac{1}{X^-(\mu)}\right)\gamma(\mu) \quad = \quad \frac{\Omega^+(\mu) + \Omega^-(\mu)}{2\Omega^+(\mu)\Omega^-(\mu)} \; . \tag{4.22b}$$

The last form of Eqs. (4.22) is derived from using Eqs. (4.16) and (4.19). By defining the singular integral operator

$$O(\mu) \quad \equiv \quad \ell_1(\mu) \; P\int_0^1 \frac{\gamma(\mu')d\mu'}{\mu - \mu'} + \ell_2(\mu) \; . \tag{4.23}$$

We can write Eq. (4.21) in the compact form

$$\alpha_2(\mu) = O(\mu)\psi''(\mu). \tag{4.24}$$

Property 2 requires that $N(z) \sim \frac{1}{z}$ as $|z| \to \infty$. We note from Eq. (4.17) that $X(z) \sim -\frac{1}{z}$ as $z \to \infty$. Thus from Eq. (4.20), we require

$$\int_0^1 \gamma(\mu)\left[\psi'(\mu) + C\int_0^1 \frac{d\eta\,\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}\right]d\mu = 0 \tag{4.25}$$

where we have used Eq. (4.11) for $\psi''(\mu)$. For the case of one pair of discrete roots we have the discrete eigenfunction available to satisfy Eq. (4.25). We make the replacement of $\underline{\psi}(\mu)$ in Eq. (4.25) by

$$\underline{\psi}(\mu) - A_+\underline{F}_{1+}(\mu) . \tag{4.26}$$

We recall that $\psi'(\mu)$ is defined by Eq. (4.9) and is a functional of the components of $\underline{\psi}(\mu)$, i.e., $\psi_1(\mu)$ and $\psi_2(\mu)$. We define $\phi_+(\mu)$ as the corresponding functional of the components of $\underline{F}_{1+}(\mu)$. Thus the replacement given by the expression (4.26) is equivalent to replacing $\psi'(\mu)$ in Eq. (4.25) by

$$\psi'(\mu) - A_+\phi_+(\mu) . \tag{4.27}$$

With this replacement made in Eq. (4.25), we then solve for A_+ to yield

$$A_+ = \frac{\int_0^1 \gamma(\mu)\psi'(\mu)d\mu + C\int_0^1 \gamma(\mu)d\mu \int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu}}{\int_0^1 \gamma(\mu)\phi_+(\mu)d\mu} . \tag{4.28}$$

Likewise with Eq. (4.27) inserted into Eq. (4.11) and subsequently into Eq. (4.24), we obtain

$$\alpha_2(\mu) = O(\mu)[\psi'(\mu) - A_+\phi_+(\mu)] + C\, O(\mu) \int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu} . \qquad (4.29)$$

Finally the replacement of $\psi_1(\mu\sigma)$ by $\psi_1(\mu\sigma)-A_+F_{1+,1}(\mu)$ in Eq. (4.3) yields

$$\alpha_1(\mu) = \sigma C_{11}\left[\psi_1(\sigma\mu) - A_+F_{1+,1}(\sigma\mu)\right] - C_{11}C_{12}\, P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} . \qquad (4.30)$$

An iteration procedure for solving Eqs. (4.28) and (4.29) for A_+ and $\alpha_2(\mu)$ is discussed in Chapter VI. Providing this procedure converges, we can then insert A_+ and $\alpha_2(\mu)$ into Eq. (4.30) and solve for $\alpha_1(\mu)$ competely determining all expansion coefficients.

A number of important simplifications are now made for the terms containing $\phi_+(\mu)$ in Eqs. (4.28) and (4.29). First, from Eq. (4.9) we can write the explicit form

$$\phi_+(\mu) = F_{1+,2}(\mu) + \frac{C\sigma}{C_{12}}\, P\int_0^1 \frac{\eta F_{1+,1}(\sigma\mu)d\eta}{\eta-\mu} + \frac{\sigma}{C_{12}} F_{1+,1}(\sigma\mu)\Theta_1(\mu)[C_{11} - 2C\mu\tau(\mu)]. \qquad (4.31)$$

Next we insert the discrete modes as given by Eq. (2.20) into Eq. (4.31) and perform the integration to obtain

$$\phi_+(\mu) = \frac{\eta_1}{\eta_1-\mu}\Bigg[C_{22} + C_{11}\Theta_1(\mu) + C\mu\Theta_1(\mu)\ln\left(\frac{1}{\sigma\mu} - 1\right) + C\mu\Theta_2(\mu)\ln\left(1 - \frac{1}{\sigma\mu}\right)$$
$$- 2C\Theta_1(\mu)\mu\tau(\mu) - C\eta_1\ln\left(1 + \frac{1}{\sigma\eta_1}\right)\Bigg] . \qquad (4.32)$$

It is easy to show that $f(\mu)$ from Eq. (2.29) can be written as

$$f(\mu) = C_{22} + C_{11}\Theta_1(\mu) - 2C\Theta_1(\mu)\mu\tau(\mu) - C\mu\Theta_1(\mu)\ln\left(1 + \frac{1}{\sigma\mu}\right) + C\mu\Theta_1(\mu)\ln\left(1 - \frac{1}{\sigma\mu}\right)$$
$$- C\mu\Theta_2(\mu)\ln\left(1 + \frac{1}{\sigma\mu}\right) + C\mu\Theta_2(\mu)\ln\left(1 - \frac{1}{\sigma\mu}\right) \qquad (4.33)$$

where we have used Eq. (2.7c). We insert Eq. (4.33) into Eq. (4.32) [recalling Eq. (4.10)] to write the compact form

$$\phi_+(\mu) = \frac{\eta_1}{\eta_1-\mu}\,[f(\mu)-Ck(\eta_1,\mu)]\ . \qquad (4.34)$$

The substitution of Eq. (4.34) into the integrand of the denominator of Eq. (4.28) yields

$$\int_0^1 \gamma(\mu)\phi_+(\mu)d\mu = -\eta_1 X(\eta_1) - C\int_0^1 \frac{\gamma(\mu)\eta_1 k(\eta_1,\mu)d\mu}{\eta_1-\mu} \qquad (4.35)$$

where we have used the X-function identity given by Eq. (A.1) to write

$$X(\eta_1) = \int_0^1 \frac{\gamma(\mu)f(\mu)d\mu}{\mu-\eta_1}\ . \qquad (4.36)$$

Next we consider the term $O(\mu)\phi_+(\mu)$ in Eq. (4.29). With $O(\mu)$ given by Eq. (4.23) and $\phi_+(\mu)$ by Eq. (4.34), we write

$$O(\mu)\phi_+(\mu) = \ell_1(\mu)\ P\int_0^1 \frac{\gamma(\mu')\eta_1 f(\mu')d\mu'}{(\mu-\mu')(\eta_1-\mu')} + \frac{\ell_2(\mu)\eta_1 f(\mu)}{\eta_1-\mu} - C\,O(\mu)\left[\frac{\eta_1 k(\eta_1,\mu)}{\eta_1-\mu}\right] \qquad (4.37)$$

The partial fraction decomposition

$$\frac{\eta_1}{(\mu-\mu')(\eta_1-\mu')} = \frac{\eta_1}{\eta_1-\mu}\left(\frac{1}{\mu-\mu'} - \frac{1}{\eta_1-\mu'}\right)$$

inserted into the first term on right-hand side of Eq. (4.37) yields

$$\ell_1(\mu)P\int_0^1 \frac{\gamma(\mu')\eta_1 f(\mu')d\mu'}{(\mu-\mu')(\eta_1-\mu')} = \ell_1(\mu)\,\frac{\eta_1}{\eta_1-\mu}\left[P\int_0^1\frac{\gamma(\mu')f(\mu')d\mu'}{\mu-\mu'} - \int_0^1 \frac{\gamma(\mu')f(\mu')d\mu'}{\eta_1-\mu'}\right] \qquad (4.38)$$

The last term in brackets in Eq. (4.38) is $-X(\eta_1)$ [see Eq. (4.36)] and the first term can be written in terms of the boundary values of $X(z)$ [see Eq. (A.1)]. Explicitly,

$$P\int_0^1 \frac{\gamma(\mu')f(\mu')d\mu'}{\mu-\mu'} = -\frac{X^+(\mu)+X^-(\mu)}{2} = -\frac{\gamma(\mu)}{2\mu}\left[\Omega^+(\mu)+\Omega^-(\mu)\right] . \quad (4.39)$$

The last form in Eq. (4.39) was derived by using Eqs. (4.16) and (4.19). We insert Eq. (4.39) into Eq. (4.38) to obtain

$$\ell_1(\mu)\, P\int_0^1 \frac{\gamma(\mu')\eta_1 f(\mu')d\mu'}{(\mu-\mu')(\eta_1-\mu')} = \ell_1(\mu)\,\frac{\eta_1}{\eta_1-\mu}\left[X(\eta_1) - \frac{\gamma(\mu)}{2\mu}\,(\Omega^+(\mu)+\Omega^-(\mu))\right] . \quad (4.40)$$

We recall from Eq. (2.29) that

$$f(\mu) = \frac{\Omega^+(\mu)-\Omega^-(\mu)}{2\pi i\mu} . \quad (4.41)$$

We insert Eqs. (4.22), (4.40) and (4.41) into Eq. (4.37) to obtain (after some cancellation)

$$O(\mu)\phi_+(\mu) = \frac{\ell_1(\mu)\eta_1 X(\eta_1)}{\eta_1-\mu} - C\,O(\mu)\left[\frac{\eta_1 k(\eta_1,\mu)}{\eta_1-\mu}\right] . \quad (4.42)$$

Now Eqs. (4.35) and (4.42) can be substituted into Eqs. (4.28) and (4.29) respectively to obtain a somewhat simpler form

$$A_+ = \frac{\int_0^1 \gamma(\mu)\psi'(\mu)d\mu + C\int_0^1 \gamma(\mu)d\mu \int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu}}{-\eta_1 X(\eta_1) - C\int_0^1 \frac{\gamma(\mu)\eta_1 k(\eta_1,\mu)d\mu}{\eta_1-\mu}} \quad (4.43a)$$

and

$$\alpha_2(\mu) = O(\mu)\psi'(\mu) + C\,O(\mu)\int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu}$$
$$- A_+\left\{\frac{\ell_1(\mu)\eta_1 X(\eta_1)}{\eta_1-\mu} - C\,O(\mu)\left[\frac{\eta_1 k(\eta_1,\mu)}{\eta_1-\mu}\right]\right\} . \quad (4.43b)$$

We recall that the kernel $k(\eta,\mu)$ is defined by Eq. (4.10). The operator $O(\mu)$ is given by Eq. (4.23) and $\ell_1(\mu)$ by (4.22a). Equations (4.43) are the set which will be treated numerically, as simultaneous equations for the expansion coefficients A_+ and $\alpha_2(\mu)$. After A^+ and $\alpha_2(\mu)$ are obtained, $\alpha_1(\mu)$ is computed from

$$\alpha_1(\mu) = \sigma C_{11}\left[\psi_1(\sigma\mu) - \frac{A_+ C_{12}\eta_1}{\sigma(\eta_1-\mu)}\right] - C_{11}C_{12}P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} \quad . \qquad (4.44)$$

This completes the reduction of the general two-group expansion. In the next chapter, we shall obtain some specific forms for $\psi'(\mu)$ in Eqs. (4.43) and for $\psi_1(\sigma\mu)$ in Eq. (4.44). In fact with these forms for $\psi'(\mu)$ and appropriate X-function identities, the integrals in Eq. (4.43) can be partially performed.

V. APPLICATIONS OF TWO-GROUP SINGULAR EIGENFUNCTION EXPANSIONS

A. INTRODUCTION

We have selected for detailed study the two-group Milne and constant source problems. These problems are representative of the type of two-group half-space problems that can be solved by our method. Two half-space problems appear also to be soluable. In fact one probably can solve any two group transport problem that is also soluable in the one-group case, although in the two-group case less analytical and more numerical analysis is required. Even in one-group theory the X-function must be generated by the computer or obtained from tables. Also in order to obtain the angular flux, total flux, and current in the medium, we must calculate principal value integrals on the computer. The point is that the computer is an essential tool to obtain complete results even in the one-group case.

We shall find some helpful simplifications similar to those obtained in Chapter IV before beginning the numerical work.

B. MILNE PROBLEM*

We define the two-group Milne problem for one pair of discrete roots in a manner similiar to the one-group case.[1] The solution must satisfy the conditions

$$\underline{\psi}(o;\mu) = 0, \quad \mu > 0 \tag{5.1a}$$

*This definition is correct only for two discrete eigenvalues.

and

$$\underline{\psi}(z,\mu) \underset{z\to\infty}{\sim} \underline{F}^{*}_{1-}(\mu)e^{z/\eta_1} . \tag{5.1b}$$

The solution which obeys Eq. (5.1b) is expanded in the two-group normal modes of the transport equation as

$$\underline{\psi}(z,\mu) = A_{-}\underline{F}_{1-}(\mu)e^{z/\eta_1} + A_{+}\underline{F}_{1+}(\mu)e^{-z/\eta_1} + \int_0^{1/\sigma}\alpha_1(\eta)\underline{\phi}_1(\eta,\mu)e^{-z/\eta}d\eta$$

$$+ \int_0^1 \alpha_2(\eta)\underline{\phi}_2(\eta,\mu)e^{-z/\eta}\, d\eta . \tag{5.2}$$

We use the boundary condition given by Eq. (5.1a) (normalize by setting $A_{-} = 1$) to obtain

$$-\underline{F}_{1-}(\mu) = A_{+}\underline{F}_{1+}(\mu) + \int_0^{1/\sigma}\alpha_1(\eta)\underline{\phi}_1(\eta,\mu)d\eta + \int_0^1 \alpha_2(\eta)\underline{\phi}_2(\eta,\mu)d\eta \tag{5.3}$$

Therefore the arbitrary expansion function, denoted by $\underline{\psi}_n(\mu)$, becomes for the Milne problem [see Eq. (2.20)],

$$\underline{\psi}_n(\mu) = \begin{pmatrix}\psi_1(\mu)\\ \psi_2(\mu)\end{pmatrix} = -\begin{pmatrix}C_{12}\eta_1/\sigma\eta_1+\mu\\ \eta_1 t(\eta_1)/\eta_1+\mu\end{pmatrix} . \tag{5.4}$$

The appropriate $\psi_n'(\mu)$ for the Milne problem (see Eq. (4.9)) is closely related to the $\phi_+(\mu)$ as defined by Eq. (4.31). In fact

$$\psi_n'(\mu) = -\phi_+(\mu,-\eta_1) . \tag{5.5}$$

This means that

$$\psi_n'(\mu) = -\frac{\eta_1}{\eta_1+\mu}\left[f(\mu)-Ck(-\eta_1,\mu)\right] \tag{5.6}$$

Thus we have from Eqs. (4.35) and (4.42) the result that

$$\int_0^1 \gamma(\mu)\psi_n'(n)d\mu = -\eta_1 X(-\eta_1) + C\int_0^1 \frac{\gamma(\mu')\eta_1 k(-\eta_1,\mu')d\mu'}{\eta_1+\mu} \tag{5.7}$$

and

$$O(\mu)\psi_n'(\mu) = -\frac{\ell_1(\mu)\eta_1 X(-\eta_1)}{\eta_1+\mu} + CO(\mu)\left[\frac{\eta_1 k(-\eta_1,\mu)}{\eta_1+\mu}\right]. \tag{5.8}$$

We insert Eqs. (5.7) and (5.8) into Eqs. (4.43a) and (4.43b) to obtain

$$A_+ = \frac{-\eta_1 X(-\eta_1)+C\int_0^1 \frac{\gamma(\mu')\eta_1 k(-\eta_1,\mu')d\mu'}{\eta_1+\mu} + C\int_0^1 \gamma(\mu)d\mu \int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu}}{-\eta_1 X(\eta_1) - C\int_0^1 \frac{\gamma(\mu)\eta_1 k(\eta_1,\mu)d\mu}{\eta_1-\mu}} \tag{5.9a}$$

$$\alpha_2(\mu) = -\frac{\ell_1(\mu)\eta_1 X(-\eta_1)}{\eta_1+\mu} + C\,O(\mu)\left[\frac{\eta_1 k(-\eta_1,\mu)}{\eta_1+\mu}\right] + C\,O(\mu)\int_0^1 \frac{\eta\alpha_2(\eta)k(\eta,\mu)d\eta}{\eta-\mu}$$

$$- A_+\left\{\frac{\ell_1(\mu)\eta_1 X(\eta_1)}{\eta_1-\mu} - C\,O(\mu)\left[\frac{\eta_1 k(\eta_1,\mu)}{\eta_1-\mu}\right]\right\}. \tag{5.9b}$$

Since

$$\psi_1(\sigma\mu) = -\frac{C_{12}\eta_1}{\sigma(\eta_1+\mu)}.$$

We have from Eq. (4.30) [considering Eq. (2.20)] that

$$\alpha_1(\mu) = -C_{11}C_{12}\eta_1\left(\frac{1}{\eta_1+\mu} + \frac{A_+}{\eta_1-\mu}\right) - C_{11}C_{12}P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} \tag{5.9c}$$

Equations (5.9) are the final reduced equations for the Milne problem. We note that Eqs. (5.9a) and (5.9b) are two coupled equations with unknowns $\alpha_2(\mu)$ and A_+. These equations are solved by an iteration process described in Chapter VI. The operator $O(\mu)$ is a singular integral operator which requires special treatment otherwise; the solution is straightforward. Finally with A_+ and $\alpha_2(\mu)$ known, we obtain $\alpha_1(\mu)$ from Eq. (5.9c).

The limiting case of C = 0 is of some interest. We note that the discrete mode expansion coefficient becomes (see Eq. (5.9a))

$$A_+ = \frac{X(-\eta_1)}{X(\eta_1)} \quad . \tag{5.10}$$

We recall that this is identical to the one-group Milne problem result.[1] This is apparently different from Siewert and Zweifel's result but we recall that they considered the case for C = 0 and the discrete eigenvalues were infinite. When the discrete eigenvalues are written in the form of Eq. (2.20) we are implicitly assuming that the eigenvalues are finite.

Also from Eq. (5.9b), we have

$$\alpha_2(\mu) = -\frac{2\ell_1(\mu)\eta_1^2 X(-\eta_1)}{\eta_1^2-\mu^2} \, . \tag{5.11}$$

In neutron transport theory, the physical problems for which C = 0 are quite specialized and we shall not consider this case further.

We can prove from the form of the operator $O(\mu)$ and Eq. (4.43b) that

$$\alpha_2(\mu) \to 0 \text{ for } \mu = \frac{1}{\sigma} \text{ and } 1. \tag{5.12}$$

This result is important because otherwise the angular flux would be singular at these values of μ. This follows from the fact that for any particular half-space problem the solution is written in terms of the expansion coefficients and the discrete and continuum mode eigenvectors with these eigenvectors containing terms with $\tau(\sigma\mu)$, $\tau(1/\sigma\mu)$ and $\tau(\mu)$. We note that $\tau(\sigma\mu)$ and $\tau(1/\sigma\mu)$ are singular at $\mu = 1/\sigma$ and $\tau(\mu)$ is singular for $\mu = 1$. To prove (5.12), we note from Eq. (4.22) that

$$\ell_1(\mu) \underset{\mu\to 1/\sigma-}{\sim} \frac{1}{\tau(\sigma\mu)} \to 0 \qquad (5.13a)$$

$$\ell_1(\mu) \underset{\mu\to 1/\sigma+}{\sim} \frac{1}{\tau(1/\sigma\mu)} \to 0 \qquad (5.13b)$$

$$\ell_1(\mu) \underset{\mu\to 1-}{\sim} \frac{1}{[\tau(\mu)]^2} \to 0 \quad . \qquad (5.13c)$$

Similar results follow for $\ell_2(\mu)$. The operator $O(\mu)$ as given by Eq. (4.23) contains in each term either $\ell_1(\mu)$ or $\ell_2(\mu)$ and we note from Eqs. (4.43) that these functions always appear multiplying principal value integrals or functions which are bounded at these values of μ. At least this statement is true for $\mu = 1/\sigma$ and we note from (5.13c) that things are still all right at $\mu = 1$ because of the squared function in the denominator.

With the expansion coefficients known from the computer solution of Eqs. (5.9), the two-group angular fluxes are calculated from Eq. (5.2). The eigenvectors given by Eqs. (2.20), (2.23) and (2.25) are substituted in Eq. (5.2) and the integration performed where possible to derive

$$\psi_1(z,\mu) = \frac{C_{12}\eta_1 e^{z/\eta_1}}{\sigma\eta_1+\mu} + \frac{C_{12}\eta_1 A_+ e^{-z/\eta_1}}{\sigma\eta_1-\mu} + \frac{1}{C_{11}\sigma}\alpha_1(\mu/\sigma)e^{-\sigma z/\mu}[\Theta_1(\mu)+\Theta_2(\mu)]$$
$$+ C_{12}P\int_0^1 \frac{\eta\alpha_2(\eta)e^{-z/\eta}d\eta}{\sigma\eta-\mu} \qquad (5.14a)$$

where

$$-1 \leq \mu \leq 1$$

and

$$\psi_2(z,\mu) = \frac{\eta_1 t(\eta_1)e^{z/\eta_1}}{\eta_1+\mu} + \frac{\eta_1 t(\eta_1)A_+e^{-z/\eta_1}}{\eta_1-\mu} - \frac{C}{C_{11}C_{12}} P\int_0^{1/\sigma} \frac{\eta\alpha_1(\eta)e^{-z/\eta}d\eta}{\eta-\mu}$$

$$- \frac{1}{C_{12}C_{11}} \alpha_1(\mu)[C_{11}-2C\mu\tau(\mu)]\theta_1(\mu)e^{-z/\mu} + P\int_0^1 \frac{\eta g(\eta)\alpha_2(\eta)e^{-z/\eta}d\eta}{\eta-\mu}$$

$$+ \lambda(\mu)\alpha_2(\mu)e^{-z/\mu}[\theta_1(\mu)+\theta_2(\mu)], \quad -1 \le \mu \le 1 . \qquad (5.14b)$$

For the angular distribution to the left we note that the integrals are not singular. A good criterion for the accuracy of the numerical methods is to see how closely condition (5.1a) is satisfied. For convenience in computer calculation, the replacement in Eq. (5.14a) of μ by $\mu\sigma$ is made to yield

$$\psi_1(z,\mu\sigma) = \frac{C_{12}\eta_1 e^{z/\eta_1}}{\sigma(\eta_1+\mu)} + \frac{C_{12}\eta_1 A_+e^{-z/\eta_1}}{\sigma(\eta_1-\mu)} + \frac{1}{C_{11}\sigma}\alpha_1(\mu)e^{-z/\mu}\theta_1(\mu)$$

$$+ \frac{C_{12}}{\sigma} P\int_0^1 \frac{\eta\alpha_2(\eta)e^{-z/\eta}d\eta}{\eta-\mu}, \quad -1/\sigma \le \mu \le 1/\sigma . \qquad (5.15)$$

The total flux and current for each group are derived by appropriate integrals over $d\mu$ and $\mu d\mu$, respectively. We shall use superscripts on the ρ's to indicate group number. Thus,

$$\rho_0^{(1)}(z) = \int_{-1}^1 \psi_1(z,\mu)d\mu = 2C_{12}\eta_1\tau\left(\frac{1}{\sigma\eta_1}\right)[e^{z/\eta_1}+A_+e^{-z/\eta_1}] + \frac{1}{C_{11}}$$

$$\times \int_0^{1/\sigma} \alpha_1(\mu')e^{-z/\mu'}d\mu' - C_{12}\int_0^1 \eta\alpha_2(\eta)e^{-z/n}(g(\eta)-C_{22})d\eta \qquad (5.16a)$$

$$\rho_1^{(1)}(z) = \int_{-1}^{1} \mu\psi_1(z,\mu)d\mu = 2C_{12}\eta_1 e^{z/\eta_1}[1-\sigma\eta_1\tau\left(\frac{1}{\sigma\eta_1}\right)] + 2C_{12}\eta_1 e^{-z/\eta_1}$$

$$\times\ A_+[\sigma\eta_1\tau\left(\frac{1}{\sigma\eta_1}\right)-1] + \frac{\sigma}{C_{11}} \int_0^{1/\sigma} \mu'\alpha_1(\mu')e^{-z/\mu'}d\mu'$$

$$-\ 2C_{12}\int_0^1 d\eta\eta\alpha_2(\eta)e^{-z/\eta} - \sigma C_{12}\int_0^1 \eta^2\alpha_2(\eta)e^{-z/\eta}(g(\eta)-C_{22})d\eta \qquad (5.16b)$$

$$\rho_0^{(2)}(z) = \int_{-1}^{1} \psi_2(\mu)d\mu = 2\eta_1 t(\eta_1)\tau\left(\frac{1}{\eta_1}\right)[e^{z/\eta_1}+A_+e^{-z/\eta_1}]$$

$$-\ \frac{2C}{C_{11}C_{12}}\int_0^{1/\sigma}\eta\alpha_1(\eta)\tau(\eta)e^{-z/\eta}d\eta - \frac{1}{C_{11}C_{12}}\int_0^{1/\sigma} d\mu[C_{11}-2C\mu\tau(\mu)]e^{-z/\mu}\alpha_1(\mu)$$

$$+\ 2\int_0^1 \eta g(\eta)\alpha_2(\eta)\tau(\eta)e^{-z/\eta}d\eta + \int_0^1 \lambda(\eta)\alpha_2(\eta)e^{-z/\eta}d\eta \qquad (5.16c)$$

$$\rho_1^{(2)}(z) = \int_{-1}^{1} \mu\psi_2(z,\mu)d\mu = 2\eta_1 t(\eta_1)e^{z/\eta_1}[1-\eta_1\tau\left(\frac{1}{\eta_1}\right)]+2\eta_1 t(\eta_1)e^{-z/\eta_1}$$

$$\times\ A_+[\eta_1\tau\left(\frac{1}{\eta_1}\right)-1] - \frac{2C}{C_{11}C_{12}}\int_0^{1/\sigma}\eta\ \alpha_1(\eta)e^{-z/\eta}[\eta\tau(\eta)-1]\ d\eta$$

$$-\ \frac{1}{C_{11}C_{12}}\int_0^{1/\sigma}\eta\alpha_2(\eta)[C_{11}-2C\eta\tau(\eta)]e^{-z/\eta}d\eta+2\int_0^1 d\eta g(\eta)\alpha_2(\eta)[\eta\tau(\eta)-1]\eta$$

$$\times\ e^{-z/\eta} + \int_0^1 \eta\lambda(\eta)\alpha_2(\eta)e^{-z/\eta}d\eta\ . \qquad (5.16d)$$

The extrapolation distance (the distance to the left of the interface at which the asymptotic component of the density vanishes) is given by either Eq. (5.16a) or Eq. (5.16c). Thus we wish to determine z_0 such that

$$e^{z_0/\eta_1} + A_+e^{-z_0/\eta_1} = 0\ . \qquad (5.17)$$

The solution for z_0 from this equation gives the same result as in the one-speed theory[1]; namely,

$$z_0 = -\frac{\eta_1}{2}\ \ell n\left(-\frac{1}{A_+}\right). \qquad (5.18)$$

Again we emphasize that for one pair of discrete roots the extrapolation distances are equal for each group. For four discrete roots, we would calculate a different extrapolation distance for each group. Baran[9] has studied this problem in detail.

C. CONSTANT ISOTROPIC SOURCE PROBLEM

Assume an isotropic source S_{O2} in group two (the associated problem with a source in group one is virtually identical). We now seek solutions to the inhomogeneous transport equation which vanish at $+\infty$ subject to the condition

$$\underline{\psi}(o,\mu) = 0 \text{ for } \mu > 0. \tag{5.19}$$

The solution consists of a particular integral, $\underline{\psi}_P(z,\mu)$, plus a solution of the homogeneous equations, $\underline{\psi}_c(z,\mu)$. The latter consists only of those modes which vanish at $+\infty$, i.e.,

$$\underline{\psi}_c(z,\mu) = A_+ e^{-z/\eta_1} \underline{F}_{1+}(\mu) + \int_0^{1/\sigma} \alpha_1(\eta)\underline{\phi}_1(\eta,\mu)e^{-z/\eta}d\eta + \int_0^1 \alpha_2(\eta)\underline{\phi}_2(\eta,\mu)e^{-z/\eta}d\eta \tag{5.20}$$

The particular integral can be found from the two-group transport equations (Eq. 2.2) in the limit as $z\to\infty$. In this case, $\underline{\psi}(z,\mu)$ approaches a constant value denoted for each group by ψ_{1S} and ψ_{2S}. With $\underline{\psi}(z,\mu)$ constant, Eq. (2.2) reduces to a pair of simultaneous equations which are easily solved to yield

$$\psi_{1S} = \frac{2SC_{12}}{(1-2C_{22})(\sigma-2C_{11})-4C_{12}C_{21}} = S_1 \tag{5.21a}$$

and

$$\psi_{2S} = \frac{S(\sigma-2C_{11})}{(1-2C_{22})(\sigma-2C_{11})-4C_{21}C_{12}} = S_2 \tag{5.21b}$$

where

$$S = S_{20}/\sigma_2 .$$

We normalize all constant source problems to a unit source neutron in group two, i.e., $S_{20} = 1$. The complete solution is written as

$$\underline{\psi}(z,\mu) = \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} + A_+ e^{-z/\eta_1} \underline{F}_{1+}(\mu) + \int_0^{1/\sigma} \alpha_1(\eta)\underline{\phi}_1(\eta,\mu)e^{-z/\eta}d\eta + \int_0^1 \alpha_2(\eta)\underline{\phi}_2(\eta,\mu) \times e^{-z/\eta}\, d\eta \quad . \tag{5.22}$$

By setting z = 0 in Eq. (5.22) and applying Eq. (5.19), we obtain

$$-\begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \int_0^{1/\sigma} \alpha_1(\eta)\underline{\phi}_1(\eta,\mu)d\eta + \int_0^1 \alpha_2(\eta)\underline{\phi}_2(\eta,\mu)d\eta + A_+\underline{F}_{1+}(\mu) \; . \tag{5.23}$$

We repeat here for convenience Eq. (4.8) of Chapter IV,

$$\psi'(\mu) = \psi_2(\mu) + \frac{C\sigma}{C_{12}} \int_0^{1/\sigma} \frac{P\eta\psi_1(\sigma\eta)d\eta}{\eta-\mu} + \frac{\sigma}{C_{12}} \psi_1(\sigma\mu)\Theta_1(\mu)[C_{11}-2C\mu\tau(\mu)] \; . \tag{4.8}$$

And we note from Eq. (5.23) that

$$\underline{\psi}(\mu) = \begin{pmatrix} \psi_1(\mu) \\ \psi_2(\mu) \end{pmatrix} = -\begin{pmatrix} S_1 \\ S_2 \end{pmatrix} . \tag{5.24}$$

By inserting Eqs. (5.24) into the appropriate terms of Eq. (4.8) and then performing the integration on the second term on the right-hand side, we find

$$\psi_S'(\mu) = -S_2 - \frac{\sigma S_1}{C_{12}}\left[\frac{C}{\sigma} + C\mu\theta_1(\mu)\ell n\left(\frac{1}{\sigma\mu} - 1\right) + C\mu\theta_2(\mu)\ell n\left(1 - \frac{1}{\sigma\mu}\right)\right.$$
$$\left. -2C\mu\tau(\mu)\theta_1(\mu)+C_{11}\theta_1(\mu)\right] . \tag{5.25}$$

The term in brackets in the second term in the right-hand side of Eq. (5.25) has terms similar to Eq. (4.33). In fact, we can write

$$\psi_S'(\mu) = -S_2 - \frac{\sigma S_1}{C_{12}}\left[\frac{C}{\sigma} + f(\mu)+C\mu\ell n\left(1 + \frac{1}{\sigma\mu}\right) - C_{22}\right] . \tag{5.26}$$

We recall from Chapter IV that we need

$$O(\mu)\psi_S'(\mu) \tag{5.27a}$$

and

$$\int_0^1 \gamma(\mu)\psi_S'(\mu)d\mu \tag{5.27b}$$

in order to calculate the expansion coefficients A_+ and $\alpha_2(\mu)$. By the same method that was used in Chapter IV to simplify $O(\mu)\phi_+(\mu)$, we can easily prove

$$O(\mu)f(\mu) = 0. \tag{5.28}$$

Also from Eq. (A.1) in Appendix A, we have that

$$\lim_{z\to\infty} zX(z) = -\int_0^1 \gamma(\mu)f(\mu)d\mu . \tag{5.29}$$

But from Eq. (4.17), we see that

$$X(z) \underset{z\to\infty}{\sim} -\frac{1}{z} \tag{5.30}$$

Therefore from Eq. (5.29), we obtain

$$\int_0^1 \gamma(\mu) f(\mu) d\mu \;=\; 1 \;. \tag{5.31}$$

Finally this gives the result that

$$O(\mu)\psi_S'(\mu) \;=\; O(\mu)\left[w - \frac{\sigma S_1 C}{C_{12}} \;\mu \ell n\left(1 + \frac{1}{\sigma\mu}\right)\right] \tag{5.32a}$$

and

$$\int_0^1 \gamma(\mu)\psi_S'(\mu) d\mu \;=\; -\frac{\sigma S_1}{C_{12}} + \int_0^1 \gamma(\mu)\left[w - \frac{\sigma S_1 C}{C_{12}} \mu \ell n\left(1 + \frac{1}{\sigma\mu}\right)\right] d\mu \tag{5.32b}$$

where

$$w \;=\; -S_2 - \frac{S_1 C}{C_{12}} + \frac{\sigma S_1 C_{22}}{C_{12}} \;. \tag{5.32c}$$

S_1 and S_2 are defined by Eqs. (5.21).

We insert Eqs. (5.32) into Eqs. (4.43) to obtain

$$A_+ = \frac{-\dfrac{\sigma S_1}{C_{12}} + \displaystyle\int_0^1 \gamma(\mu)\left[w - \frac{\sigma S_1 C}{C_{12}} \mu \ell n\left(1 + \frac{1}{\sigma\mu}\right)\right] d\mu + C\int_0^1 \gamma(\mu) d\mu \int_0^1 \frac{\eta\alpha_2(\eta) k(\eta,\mu) d\eta}{\eta - \mu}}{-\eta_1 X(\eta_1) - C\displaystyle\int_0^1 \frac{\gamma(\mu) k(\eta_1,\mu) d\mu}{\eta_1 - \mu}} \tag{5.33a}$$

and

$$\alpha_2(\mu) \;=\; O(\mu)\left[w - \frac{\sigma S_1 C}{C_{12}} \mu \ell n\left(1 + \frac{1}{\sigma\mu}\right)\right] + C\, O(\mu) \int_0^1 \frac{\eta\alpha_2(\eta) k(\eta,\mu) d\eta}{\eta - \mu}$$
$$- A_+ \left[\frac{\ell_1(\mu)\eta_1 X(\eta_1)}{\eta_1 - \mu} - CO(\mu)\left(\frac{\eta_1 k(\eta_1,\mu)}{\eta_1 - \mu}\right)\right]. \tag{5.33b}$$

The final equation for $\alpha_1(\mu)$ is obtained from Eq. (4.44) where

$$\psi_1(\sigma\mu) \;=\; -S_1 \;.$$

Explicitly,

$$\alpha_1(\mu) = -\sigma C_{11}S_1 - \frac{C_{11}C_{12}\eta_1 A_+}{\eta_1-\mu} - C_{11}C_{12}\, P\int_0^1 \frac{\eta\alpha_2(\eta)d\eta}{\eta-\mu} \quad . \qquad (5.33c)$$

Equations (5.33) are the final reduced equations for the constant source problem. We refer the reader to the paragraph following Eq. (5.9c) for comments concerning the solution to this set of equations.

The angular fluxes for the constant source problem are given by Eqs. (5.14) where we replace the first term in the right-hand side by S_1 and S_2, respectively. The neutron current in each group is given by Eqs. (5.16b) and (5.16d) if we delete the first term on the right-hand side. For the total flux we replace the first term (term with positive exponential) on the right-hand side of Eqs. (5.16a) and (5.16c) by $2S_1$ and $2S_2$, respectively.

VI. NUMERICAL METHODS AND COMPUTER SOLUTION TO HALF-SPACE PROBLEMS

A. PROGRAM FOR FINDING NUMBER, TYPE, AND VALUE OF THE DISCRETE EIGENVALUES

In solving Eqs. (5.9) and (5.33) for the expansion coefficients, the function $\gamma(\mu)$ must be calculated. But (as shown in Appendix A) the roots of the dispersion equation must first be found. A computer program was written which first finds the number and type of eigenvalues from Table 2.1 and then determines the magnitude of these eigenvalues. The method that was found quite effective was the false position method.[18] For the problems studied in this thesis we have only one pair of real discrete roots. We concentrate on finding only the positive eigenvalue η_1 because we know from Eq. (2.18) that the other eigenvalue is $-\eta_1$. The false position method require two starting values which we denote by $\eta_1^{(1)}$ and $\eta_2^{(1)}$. The subscript here means that these are two starting values while the superscript is the iteration index. To obtain good starting values we calculate $\Omega(\eta)$ for $\eta = 1.000001$. We then increase η by .1 until $\Omega(\eta)$ changes sign. We select $\eta_1^{(1)}$ and $\eta_2^{(1)}$ such that $\Omega(\eta_1^{(1)})$ is opposite in sign to $\Omega(\eta_2^{(1)})$. From these four values a value of η_3 is calculated according to

$$\eta_3 = \frac{\eta_1^{(1)}\Omega(\eta_2^{(1)})-\eta_2^{(1)}\Omega(\eta_1^{(1)})}{\Omega(\eta_2^{(1)})-\Omega(\eta_1^{(1)})} .$$

η_3 is the intersection on the η axis of a straight line which joins the points $(\eta_1^{(1)},\Omega(\eta_1^{(1)}))$ and $(\eta_2^{(1)},\Omega(\eta_2^{(1)}))$. For the next iteration the program selects

$\eta_1^{(2)}$ and $\eta_2^{(2)}$ from η_3, $\eta_1^{(1)}$, and $\eta_2^{(1)}$ such that the corresponding functional values for $\Omega(\eta)$ are smallest in absolute value. For the specific problems studied in this thesis only three iterations were required to find a root η_1 such that

$$\Omega(\eta_1) < 10^{-7} .$$

This program is listed in Appendix D.

B. DISCUSSION OF MESH SPACING

In two-group, half-space problem there are always two basic integration intervals. We see from previous chapters that we have ordinary integrals and principal value intervals for integration ranges of

$$0 < \mu < \frac{1}{\sigma}$$

and

$$\frac{1}{\sigma} < \mu < 1.$$

We shall see in the next section that in the evaluation of principal value integrals the singularity is subtracted. This procedure gives rise to a logarithm term which is singular at the end points of integration. Therefore we use the midpoint approximation in the evaluation of all integrals. In this approximation the interval from 0 to $1/\sigma$ is divided into P equal intervals and all functions are evaluated at the midpoint of each of the P intervals. A similar procedure is used for the mesh spacing in the interval from $1/\sigma$ to 1.

C. NUMERICAL EVALUATION OF SINGULAR INTEGRALS

In the solution of Eqs. (5.9) and (5.33) for A_+ and $\alpha_2(\mu)$ we must evaluate singular integrals of the type

$$P \int_0^1 \frac{F(\mu')d\mu'}{\mu'-\mu} \quad .$$

The function $F(\mu')$ in two-group, half-space problems studied in this thesis always contain factors of $\gamma(\mu)$ as well as logarithmic functions. For example, from Eq. (4.43) all half-space problems have singular integrals where $F(\mu)$ is of the form

$$F(\mu) = \frac{\eta_1\gamma(\mu)k(\eta_1,\mu)}{\eta_1-\mu} \tag{6.2}$$

where we recall that

$$k(\eta,\mu) = \eta \ell n \left(1 + \frac{1}{\sigma\eta}\right) - \mu \ell n \left(1 + \frac{1}{\sigma\mu}\right) \quad .$$

For the Milne problem we have in addition other integrals involving

$$F(\mu) = \frac{\eta_1\gamma(\mu)k(-\eta_1,\mu)}{\eta_1+\mu} \quad . \tag{6.3}$$

While the constant source problem has another integral where

$$F(\mu) = \left[w - \frac{\sigma S_1 C}{C_{12}} \mu \ell n \left(1 + \frac{1}{\sigma\mu}\right)\right] \gamma(\mu). \tag{6.4}$$

The details for evaluating $\gamma(\mu)$ are given in Appendix A. The presence of logarithm factors and $\gamma(\mu)$ in the function $F(\mu)$ requires special care in order that an inordinate amount of computer time is not taken.

By usual procedures[1] the singularity is subtracted to yield

$$\int_0^1 P \frac{F(\mu')d\mu'}{\mu'-\mu} = \int_0^1 \frac{[F(\mu')-F(\mu)]d\mu'}{\mu'-\mu} + F(\mu)\ln\left(\frac{1-\mu}{\mu}\right) . \qquad (6.5)$$

The functions $F(\mu)$ and $\ln(1-\mu)/\mu$ are now evaluated at the midpoint of all the intervals for μ between 0 and 1, and these values are stored in the fast access memory of the computer. Let us assume that the singularity is at some midpoint value μ_i. Then we approximate the principal value integral in Eq. (6.5) by

$$\int_0^1 P \frac{F(\mu')d\mu'}{\mu'-\mu} \simeq \sum_{j=1}^{D}{}' \frac{[F(\mu_j)-F(\mu_i)]h_j}{\mu_j-\mu_i} + h_i F'(\mu_i) + F(\mu_i)\ln\left(\frac{1-\mu_i}{\mu_i}\right) \qquad (6.6)$$

The prime on the summation indicates that in the sum the term $j = i$ is not included. This particular term is given by the second term on the right-hand side of Eq. (6.6). Also h_j is the width of interval j. We are using the trapezodial rule with the midpoint approximation in the evaluation of the integral term on the right-hand side of Eq. (6.5).

We note that the second term on the right-hand side of Eq. (6.6) has a derivative factor. When the singular point μ_i is not in the interval adjacent to the end points or adjacent to the intervals where an interval change is made, i.e., $\mu = 1/\sigma$, this second term on the right-hand side of Eq. (6.6) is approximated by

$$h_i F'(\mu_i) = \frac{1}{2}[F(\mu_{i+1})-F(\mu_{i-1})] \quad .$$

When the singularity is at the midpoint of one of the other four remaining intervals we use[19]

$$h_i F'(\mu_i) \simeq \begin{cases} \frac{1}{3}\,[F(\mu_2)+3F(\mu_1)-4F(0)], & i = 1 \quad (6.7a) \\ \frac{1}{3}\,[4F(1/\sigma)-3F(\mu_P)-F(\mu_{P-1})], & i = P \quad (6.7b) \\ \frac{1}{3}\,[F(\mu_{P+2})+3F(\mu_{P+1})-F(1/\sigma)], & i = P+1 \quad (6.7c) \\ \frac{1}{3}\,[4F(1)-3F(\mu_D)-F(\mu_{D-1})], & i = D. \quad (6.7d) \end{cases}$$

We have P intervals from 0 to $1/\sigma$ and a total of D intervals from 0 to 1.

Following to some extent Bareiss and Neumann,[19] we shall derive in detail Eq. (6.7a). Let us first calculate the contribution of the integral term on the right-hand side of Eq. (6.5) to one general interval of width h about μ', i.e.,

$$\mu - \frac{h}{2} \leq \mu' \leq \mu + \frac{h}{2} .$$

We have

$$\int_{\mu-\frac{h}{2}}^{\mu+\frac{h}{2}} \frac{[F(\mu')-F(\mu)]d\mu'}{\mu'-\mu} = \int_{-h/2}^{h/2} \frac{[F(y+\mu)-F(\mu)]dy}{y} \quad (6.8)$$

where we used the change of variable $y = \mu'-\mu$. We expand $F(y+\mu)$ in a Taylor series about μ to yield

$$F(y+\mu) = F(\mu) + yF'(\mu) + \frac{y^2}{2} F''(\mu) + \ldots \quad (6.9)$$

Inserting this expansion in Eq. (6.8) and integrating over dy yields

$$\int_{-h/2}^{h/2} [F'(\mu) + \frac{y}{2} F''(\mu) + \frac{y^2}{3!} F'''(\mu) + \ldots]dy = hF'(\mu) + \frac{h^3}{72} F'''(\mu) + \ldots \quad (6.10)$$

Thus by keeping only the first term on the right-hand side of Eq. (6.10) we are omitting terms of $\mathcal{O}(h^3)$ or higher.

For Eq. (6.7a) we need to find a good approximation for $h_1F(\mu_1)$ where $\mu_1 = \frac{1}{2}h_1$ and h_1 is the width of the first interval. To this end we write a Taylor series for $F(\mu+h)$; namely,

$$F(\mu+h) = F(\mu) + hF'(\mu) + \frac{h^2}{2!}F''(\mu) + \mathcal{O}(h^3) \quad . \tag{6.11}$$

We insert $\mu = \frac{1}{2}h_1$ in Eq. (6.11), and recalling from the midpoint values that $\mu_2 = \frac{3}{2}h_1$, we find

$$F(\mu_2) = F(\mu_1) + h_1F'(\mu_1) + \frac{h_1^2}{2}F''(\mu_1) + \mathcal{O}(h_1^3). \tag{6.12}$$

Next we replace h by $-h_1/2$ and μ by $h_1/2$ in Eq. (6.11) to arrive at

$$F(0) = F(\mu_1) - \frac{h_1}{2}F'(\mu_1) + \frac{h_1^2}{8}F''(\mu_1) + \mathcal{O}(h^3) \quad . \tag{6.13}$$

Solving Eq. (6.13) for $\frac{h_1^2}{2}F''(\mu_1)$ yields

$$\frac{h_1^2}{2}F''(\mu_1) = 4F(0) - 4F(\mu_1) + 2hF'(\mu_1) - 4\mathcal{O}(h^3) \quad . \tag{6.14}$$

This result is substituted into Eq. (6.12) to eliminate the second derivative term. We then solve for $h_1F'(\mu_1)$ to obtain Eq. (6.7a). Equations (6.7b), (6.7c) and (6.7d) are derived in a similar manner.

The nonsingular integrals are also evaluated by the midpoint approximation. For example the integral in Eq. (5.9a) is approximated as follows:

$$\int_0^1 \frac{\gamma(\mu)\eta_1 k(\eta_1,\mu)d\mu}{\eta_1-\mu} \simeq \sum_{j=1}^{D} \frac{\gamma(\mu_j)\eta_1 k(\eta_1,\mu_j)h_j}{\eta_1-\mu_j} \tag{6.15}$$

D. ITERATION PROCEDURE FOR THE EXPANSION COEFFICIENTS

To solve Eqs. (4.28) and (4.29) in the general case, we first approximate A_+ by

$$A_+^{(0)} = \frac{\int_0^1 \gamma(\mu)\psi'(\mu)d\mu}{\int_0^1 \gamma(\mu)\phi_+(\mu)d\mu} \quad . \tag{6.16}$$

The first iterate solution for $\alpha_2(\mu)$ is given by

$$\alpha_2^{(1)}(\mu) = O(\mu)[\psi'(\mu)-A_+^{(0)}\phi_+(\mu)] \quad . \tag{6.17}$$

The superscript on A_+ and $\alpha_2(\mu)$ specifies the iteration index. Equation (6.17) is then used in Eq. (4.28) to yield $A_+^{(1)}$ and then the second iterate on $\alpha_2(\mu)$ is found; namely,

$$\alpha_2^{(2)}(\mu) = O(\mu)[\psi'(\mu)-A_+^{(1)}\phi_+(\mu)] + C\, O(\mu) \int_0^1 \frac{\eta\alpha_2^{(1)}(\mu)k(\eta,\mu)d\eta}{\eta-\mu} \tag{6.18}$$

Continuing in this manner, we have for the n'th iterative solution

$$\alpha_2^{(n)}(\mu) = O(\mu)[\psi'(\mu)-A_+^{(n-1)}\phi_+(\mu)] + C\, O(\mu) \int_0^1 \frac{\eta\alpha_2^{(n-1)}(\mu)k(\eta,\mu)d\eta}{\eta-\mu} . \tag{6.19}$$

We assume that for most physically interesting problems, e.g., Milne and constant source, the above procedure converges in the sense that given an $\epsilon > 0$ we can find an integer M such that for all $m > M$ and $\mu\epsilon[0,1]$

$$|\alpha_2^m(\mu)-\alpha_2^{m-1}(\mu)| < \epsilon \; . \tag{6.20}$$

For the problems studied in this thesis, convergence was achieved in seven iterations where $\epsilon = 10^{-7}$. An alternate method of solution by matrix inversion is discussed in Appendix C.

VII. SPHERICAL HARMONIC SOLUTIONS TO THE CONSTANT SOURCE AND MILNE PROBLEM

In the present chapter some commonly used approximation methods are used to solve the Milne and constant source problems which have been treated exactly in the earlier chapters of this thesis. We restrict our attention to the P_1, P_3, and DP_1 cases,[1] and in the following chapter, compare results in order to derive a feeling for the validity of the various approximation schemes.

In the P_1 and P_3 cases the angular flux is expanded in a series of Legendre polynomials as

$$\underline{\psi}(z,\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu)\underline{\rho}_\ell(z) , \tag{7.1}$$

with

$$\underline{\rho}_\ell(z) = \begin{pmatrix} \rho_\ell^{(1)}(z) \\ \rho_\ell^{(2)}(z) \end{pmatrix} \quad \text{and } \underline{\psi}(z,\mu) = \begin{pmatrix} \psi_1(z,\mu) \\ \psi_2(z,\mu) \end{pmatrix} .$$

The superscript on the ρ's denotes the group number.

We follow the standard procedure[1] of substituting Eq. (7.1) into Eq. (2.2), multiplying by $P_k(\mu)$ and integrating over $d\mu$. By including a source term in group two (consistent with Chapter V) and using the identity

$$\mu P_\ell(\mu) = \frac{1}{2\ell+1} [(\ell+1)P_{\ell+1}(\mu)+\ell P_{\ell-1}(\mu)]$$

with the orthogonality relation

$$\int_{-1}^{1} P_{\ell}(\mu)P_k(\mu)d\mu = \frac{2}{2\ell+1}\,\delta_{\ell k} ,$$

the two group P_ℓ equations become

$$\frac{1}{2k+1}\left[k\,\frac{d\rho_{k-1}^{(1)}(z)}{dz} + (k+1)\,\frac{d\rho_{k+1}^{(1)}(z)}{dz}\right] + \sigma\rho_k^{(1)}(z)$$

$$= [2C_{11}\rho_o^{(1)}(z)+2C_{12}\rho_o^{(2)}(z)]\delta_{ko} \qquad (7.2a)$$

$$\frac{1}{2k+1}\left[k\,\frac{d\rho_{k-1}^{(2)}(z)}{dz} + (k+1)\,\frac{d\rho_{k+1}^{(2)}(z)}{dz}\right] + \rho_k^{(2)}(z)$$

$$= [2C_{21}\rho_o^{(1)}(z)+2C_{22}\rho_o^{(2)}(z)+2S]\delta_{ko} \qquad (7.2b)$$

where as before

$$S = \frac{S_{2o}}{\sigma_2} .$$

The P_ℓ approximation is made by truncating the expansion in Eq. (7.1) i.e.,

$$\rho_m(z) = 0 \quad \text{for} \quad m > \ell . \qquad (7.3)$$

In particular, the P_1 equations are

$$\frac{d\rho_1^{(1)}(z)}{dz} + \sigma\rho_o^{(1)}(z) = 2C_{11}\rho_o^{(1)}(z)+2C_{12}\rho_o^{(2)}(z), \qquad (7.4a)$$

$$\frac{d\rho_o^{(1)}(z)}{dz} + 3\sigma\rho_1^{(1)}(z) = 0 , \qquad (7.4b)$$

$$\frac{d\rho_1^{(2)}(z)}{dz} + \rho_o^{(2)}(z) = 2C_{21}\rho_o^{(1)}(z)+2C_{22}\rho_o^{(2)}(z)+2S , \qquad (7.4c)$$

and

$$\frac{d\rho_o^{(2)}(z)}{dz} + 3\rho_1^{(2)}(z) = 0 . \qquad (7.4d)$$

These equations are solved by first finding the eigenvalues of the homogeneous set. Assume solutions of the form

$$\rho_i^{(1)}(z) = \sum A_{ij} e^{k_j z} \qquad (7.5a)$$

and

$$\rho_i^{(2)}(z) = \sum B_{ij} e^{k_j z} . \qquad (7.5b)$$

The substitution of Eqs. (7.5) into Eqs. (7.4) and cancellation of the space dependence yields the following eigenvalue equations:

$$A_{1j}k_j + (\sigma-2C_{11})A_{oj} - 2C_{12}B_{oj} = 0 \qquad (7.6a)$$

$$A_{oj}k_j + 3\sigma A_{1j} = 0 \qquad (7.6b)$$

$$B_{1j}k_j + (1-2C_{22})B_{oj} - 2C_{21}A_{oj} = 0 \qquad (7.6c)$$

$$B_{oj}k_j + 3B_{1j} = 0 . \qquad (7.6d)$$

A nontrivial solution exists to Eqs. (7.6) if and only if the secular determinant vanishes:

$$\begin{vmatrix} k & \sigma-2C_{11} & 0 & -2C_{12} \\ 3\sigma & k & 0 & 0 \\ 0 & -2C_{21} & k & 1-2C_{22} \\ 0 & 0 & 3 & k \end{vmatrix} = 0 \qquad (7.7)$$

The expansion of Eq. (7.7) yields

$$k^4 + Bk^2 + D = 0 \tag{7.8a}$$

where

$$B = -3[1-2C_{22}+\sigma(\sigma-2C_{11})] \tag{7.8b}$$

and

$$D = 9\sigma[\sigma(1-2C_{22})-2C_{11}+4C] \ . \tag{7.8c}$$

For the problems studied in this thesis, we obtain four real roots to Eqs. (7.8). We denote these roots by $\pm k_1$ and $\pm k_2$ where $k_1 < k_2$.

The particular integral solution to Eqs. (7.4) is derived by realizing as $z\to\infty$ the total flux in each group becomes constant. From Eqs. (7.4b) and (7.4d), the current in each group is zero. Thus from Eqs. (7.4a) and (7.4c) we have a pair of simultaneous equations whose solution is

$$\rho_o^{(1)}(z) \underset{z\to\infty}{=} \frac{4SC_{12}}{(1-2C_{22})(\sigma-2C_{11})-4C_{12}C_{21}} = 2S_1 \tag{7.9a}$$

and

$$\rho_o^{(2)}(z) \underset{z\to\infty}{=} \frac{2(\sigma-2C_{11})S}{(1-2C_{22})(\sigma-2C_{11})-4C_{12}C_{21}} = 2S_2 \ . \tag{7.9b}$$

For the constant source problem the solutions as given by Eqs. (7.5) must be finite as $z\to\infty$. This requires that we consider only the negative real roots of Eq. (7.8a). Also from Eqs. (7.6), A_{1j} and B_{1j} can be found in terms of A_{oj} and B_{oj}. Thus we write solutions to Eqs. (7.4) as follows:

$$\rho_0^{(1)}(z) = A_{02}e^{-k_1 z} + A_{04}e^{-k_2 z} + 2S_1 \qquad (7.10a)$$

$$\rho_1^{(1)}(z) = A_{02}f_1(k_1)e^{-k_1 z} + A_{04}f_1(k_2)e^{-k_2 z} \qquad (7.10b)$$

$$\rho_0^{(2)}(z) = A_{02}f_2(k_1)e^{-k_1 z} + A_{04}f_2(k_2)e^{-k_2 z} + 2S_2 \qquad (7.10c)$$

$$\rho_1^{(2)}(z) = A_{02}f_3(k_1)e^{-k_1 z} + A_{04}f_3(k_2)e^{-k_2 z} . \qquad (7.10d)$$

The functions $f_n(k)$ are given by

$$f_1(k) = \frac{k}{3\sigma} \qquad (7.11a)$$

$$f_2(k) = \frac{3\sigma(\sigma-2C_{11})-k^2}{6\sigma C_{12}} \qquad (7.11b)$$

$$f_3(k) = \frac{k[3\sigma(\sigma-2C_{11})-k^2]}{18\sigma C_{12}} . \qquad (7.11c)$$

The corresponding Milne problem solutions to Eqs. (7.4) are

$$\rho_0^{(1)}(z) = e^{k_1 z} + A_{02}e^{-k_1 z} + A_{04}e^{-k_2 z} \qquad (7.12a)$$

$$\rho_1^{(1)}(z) = f_1(-k_1)e^{k_1 z} + A_{02}f_1(k_1)e^{-k_1 z} + A_{04}f_1(k_2)e^{-k_2 z} \qquad (7.12b)$$

$$\rho_0^{(2)}(z) = f_2(k_1)e^{k_1 z} + A_{02}f_2(k_1)e^{-k_1 z} + A_{04}f_2(k_2)e^{-k_2 z} \qquad (7.12c)$$

$$\rho_1^{(2)}(z) = f_3(-k_1)e^{k_1 z} + A_{02}f_3(k_1)e^{-k_1 z} + A_{04}f_3(k_2)e^{-k_2 z}. \qquad (7.12d)$$

Here we have used the same normalization as in Chapter V. We note that there are two arbitrary constants in Eqs. (7.10) and Eqs. (7.12) which are determined by the boundary conditions at $z = 0$. We approximate the rigorous boundary condition

$$\underline{\psi}(o,\mu) = 0 \text{ for } \mu > 0 \qquad (7.13)$$

by the lowest order Marshak boundary condition,[1]

$$\int_o^1 \mu\underline{\psi}(o,\mu)d\mu = 0 . \qquad (7.14)$$

For the P_1 approximation the angular flux is given by Eq. (7.1) where $\underline{\rho}_\ell(z) = 0$ for $\ell > 1$. Thus we have in this approximation that

$$\underline{\psi}(z,\mu) = \frac{1}{2}\,\underline{\rho}_o(z) + \frac{3}{2}\,\mu\underline{\rho}_1(z) . \qquad (7.15)$$

The substitution of Eq. (7.15) into Eq. (7.14) and subsequent integration yields

$$\frac{1}{2}\,\underline{\rho}_o(o) + \underline{\rho}_1(o) = 0 . \qquad (7.16)$$

For the constant source problem, the boundary condition given by Eq. (7.16) [when related back to Eqs. (7.10)] yields

$$A_{o2}g(k_1) + A_{o4}g(k_2) = -S_1 \qquad (7.17a)$$

and

$$A_{o2}h(k_1) + A_{o4}h(k_2) = -S_2 \qquad (7.17b)$$

where

$$g(k) = \frac{1}{2} + f_1(k)$$

and

$$h(k) = \frac{1}{2}\,f_2(k) + f_3(k) .$$

Likewise, from Eqs. (7.12)

$$A_{O2}g(k_1) + A_{O4}g(k_2) = -g(-k_1) \qquad (7.18a)$$

and

$$A_{O2}h(k_1) + A_{O4}h(k_2) = -h(-k_1) \ . \qquad (7.18b)$$

With the coefficients determined, the complete solution in this approximation is given by Eq. (7.15) where the ρ's are given by Eqs. (7.10) and (7.12) for the constant source and Milne problem respectively. In the problems considered here the eigenvalues are real. One of these roots is less than unity (in absolute value) while the other is greater. Thus in two-group theory we obtain one of the continuum eigenvalues even in the P_1 approximation. In the one-speed case[1] the P_1 approximation yields only the asymptotic solution, i.e., the eigenvalues are all greater than unity in absolute value. (At least the above statements were found to be true for the two-group problems considered in this thesis.)

The two-group extrapolation distance is found from either Eq. (7.12a) or (7.12c). We set $A_{O4} = 0$ and solve for the extrapolation distance Z_O. This gives

$$Z_O = -\frac{1}{2k_1}\,\ell n\left(-\frac{1}{A_{O2}}\right) \ . \qquad (7.19)$$

We note that the extrapolation distance is the same for each group and is given by Eq. (7.19). This result can be contrasted with the usual[3] procedure of using an extrapolation distance for each group given in the isotropic scattering case by $.7104\lambda_1$ and $.7104\lambda_2$ where λ_1 and λ_2 are the total mean free paths for Group 1 and Group 2, respectively.

In the P_3 approximation, we truncate Eq. (7.1) by

$$\underline{\rho}_\ell(z) = 0 \text{ for } \ell > 3 . \tag{7.20}$$

This condition along with Eqs. (7.2) and setting k = 0,1,2 and 3 yields the following set:

$$\frac{d\rho_1^{(1)}(z)}{dz} + (\sigma - 2C_{11})\rho_0^{(1)}(z) - 2C_{12}\rho_0^{(2)}(z) = 0 \tag{7.21a}$$

$$\frac{2d\rho_2^{(1)}(z)}{dz} + \frac{d\rho_0^{(1)}(z)}{dz} + 3\sigma\rho_1^{(1)}(z) = 0 \tag{7.21b}$$

$$\frac{3d\rho_3^{(1)}(z)}{dz} + \frac{2d\rho_1^{(1)}(z)}{dz} + 5\sigma\rho_2^{(1)}(z) = 0 \tag{7.21c}$$

$$\frac{3d\rho_2^{(1)}(z)}{dz} + 7\sigma\rho_3^{(1)}(z) = 0 \tag{7.21d}$$

$$\frac{d\rho_1^{(2)}(z)}{dz} + (1 - 2C_{22})\rho_0^{(2)}(z) - 2C_{21}\rho_0^{(1)}(z) = 2S \tag{7.21e}$$

$$\frac{2d\rho_2^{(2)}(z)}{dz} + \frac{d\rho_0^{(2)}(z)}{dz} + 3\rho_1^{(2)}(z) = 0 \tag{7.21f}$$

$$\frac{3d\rho_3^{(2)}(z)}{dz} + \frac{2d\rho_1^{(2)}(z)}{dz} + 5\rho_2^{(2)}(z) = 0 \tag{7.21g}$$

$$\frac{3d\rho_2^{(2)}(z)}{dz} + 7\rho_3^{(2)}(z) = 0 . \tag{7.21h}$$

By a procedure analogous to the previous P_1 solution we obtain from Eqs. (7.21) a secular determinant of order eight which, upon expansion, yields

$$Ck^8 + Dk^6 + Ek^4 + Fk^2 + G = 0 . \tag{7.22}$$

The coefficients in this equation are given by

$$C = 81 \tag{7.23a}$$

$$D = 990(C_{22}+C_{11}\sigma) - 810(1+\sigma^2) \tag{7.23b}$$

$$E = 100\sigma(11C_{11}-9\sigma)(11C_{22}-9) + 945[1-2C_{22}+\sigma^2(\sigma-2C_{11})] - 110^2\sigma C_{21}C_{12} \tag{7.23c}$$

$$F = 1050\sigma(1-2C_{22})(11C_{11}-9\sigma) + 1050\sigma^3(\sigma-2C_{11})(11C_{22}-9) + 210\cdot 110\sigma C_{21}C_{12}(1+\sigma^2) \tag{7.23d}$$

$$G = (105)^2\sigma^3(\sigma-2C_{11})(1-2C_{22}) - (210)^2\sigma^3C_{21}C_{12} . \tag{7.23e}$$

In analogy with the P_1 solutions, we can write immediately the solutions for both the constant source and Milne problem. The constant source problem solutions are

$$\rho_n^{(1)}(z) = \sum_{j=1}^{4} A_{oj}f_n(k_j)e^{-k_jz} + 2S_1\delta_{no} \tag{7.24a}$$

$$n = 0,1,2,3$$

$$\rho_n^{(2)}(z) = \sum_{j=1}^{4} A_{oj}f_{n+4}(k_j)e^{-k_jz} + 2S_2\delta_{no} . \tag{7.24b}$$

And the Milne problem solutions are given by

$$\rho_n^{(1)}(z) = \sum_{j=1}^{4} A_{oj}f_n(k_j)e^{-k_jz} + f_n(-k_1)e^{k_1z} \tag{7.25a}$$

$$n = 0,1,2,3$$

$$\rho_n^{(2)}(z) = \sum_{j=1}^{4} A_{oj}f_{n+4}(k_j)e^{-k_jz} + f_{n+4}(-k_1)e^{k_1z} . \tag{7.25b}$$

In Eqs. (7.24) and (7.25) we define

$$f_o(k) = 1 \quad (7.26a)$$

$$f_1(k) = \frac{k(35\sigma^2-9k^2)}{5\sigma(21\sigma^2-11k^2)} \quad (7.26b)$$

$$f_2(k) = \frac{14k\sigma f_1(k)}{35\sigma^2-9k^2} \quad (7.26c)$$

$$f_3(k) = \frac{3k}{7\sigma} f_2(k) \quad (7.26d)$$

$$f_4(k) = \frac{10C_{21}(21-11k^2)}{k^2(9k^2-35)+5(1-2C_{22})(21-11k^2)} \quad (7.26e)$$

$$f_5(k) = \frac{k(35-9k^2)}{5(21-11k^2)} f_4(k) \quad (7.26f)$$

$$f_6(k) = \frac{14k}{35-9k^2} f_5(k) \quad (7.26g)$$

$$f_7(k) = \frac{3k}{7} f_6(k) \quad . \quad (7.26h)$$

The Milne problem is normalized as before and we identify the four possible positive roots of Eq. (7.22) as k_1, k_2, k_3, and k_4 where k_1 is the root of smallest magnitude.

The unknown coefficients in Eqs. (7.24) or Eqs. (7.25) are now determined by two Marshak[1] boundary conditions; namely,

$$\int_0^1 P_1(\mu)\underline{\psi}(o,\mu)d\mu = 0 \quad , \quad (7.27a)$$

$$\int_0^1 P_3(\mu)\underline{\psi}(o,\mu)d\mu = 0 . \qquad (7.27b)$$

In this approximation the angular density at z = 0 is

$$\underline{\psi}(o,\mu) = \frac{1}{2}\underline{\rho}_0(o) + \frac{3}{2}P_1(\mu)\underline{\rho}_1(o) + \frac{5}{2}P_2(\mu)\underline{\rho}_2(o) + \frac{7}{2}P_3(\mu)\underline{\rho}_3(o) . \qquad (7.28)$$

We substitute Eq. (7.28) into Eqs. (7.27) and perform the integration over dμ to derive

$$\frac{1}{2}\underline{\rho}_0(o) + \underline{\rho}_1(o) + \frac{5}{8}\underline{\rho}_2(o) = 0 \qquad (7.29a)$$

and

$$\frac{1}{4}\underline{\rho}_0(o) + \frac{3}{5}\underline{\rho}_1(o) + \frac{5}{8}\underline{\rho}_2(o) + \frac{2}{5}\underline{\rho}_3(o) = 0 . \qquad (7.29b)$$

Thus for the constant source or the Milne problem, Eqs. (7.29) give us the four equations needed to determine the unknown coefficients. Specifically, we have for the constant source problem the following set of equations:

$$\sum_{j=1}^{4} g(k_j)A_{oj} = -S_1 \qquad (7.30a)$$

$$\sum_{j=1}^{4} h(k_j)A_{oj} = -\frac{S_1}{2} \qquad (7.30b)$$

$$\sum_{j=1}^{4} t(k_j)A_{oj} = -S_2 \qquad (7.30c)$$

$$\sum_{j=1}^{4} s(k_j)A_{oj} = -\frac{S_2}{2} . \qquad (7.30d)$$

And for the Milne problem,

$$\sum_{j=1}^{4} g(k_j)A_{oj} = -g(-k_1) \qquad (7.31a)$$

$$\sum_{j=1}^{4} h(k_j)A_{oj} = -h(-k_1) \qquad (7.31b)$$

$$\sum_{j=1}^{4} t(k_j)A_{oj} = -t(-k_1) \qquad (7.31c)$$

$$\sum_{j=1}^{4} s(k_j)A_{oj} = -s(-k_1). \qquad (7.31d)$$

Here we have

$$g(k) = \frac{1}{2} + f_1(k) + \frac{5}{8} f_2(k) \qquad (7.32a)$$

$$h(k) = \frac{1}{4} + \frac{3}{5} f_1(k) + \frac{5}{8} f_2(k) + \frac{2}{5} f_3(k) \qquad (7.32b)$$

$$t(k) = \frac{1}{2} f_4(k) + f_5(k) + \frac{5}{8} f_6(k) \qquad (7.32c)$$

$$s(k) = \frac{1}{4} f_4(k) + \frac{3}{5} f_5(k) + \frac{5}{8} f_6(k) + \frac{2}{5} f_7(k) \qquad (7.32d)$$

With the coefficients, i.e., A's, known from solving either Eqs. (7.31) or (7.32), we can obtain the total flux and current from Eqs. (7.24) or (7.25) or the angular flux from Eq. (7.1). Also the extrapolation distance is given by Eq. (7.19) with A_{o2} derived, in this approximation, from Eqs. (7.31).

An approximation method which permits the exact specification of the boundary condition at a free surface is the so-called double $P_1(DP_1)$. This is in contrast to the ordinary P_ℓ method in which the boundary condition can be fulfilled only approximately (for example, in the previous section we used the Marshak condition). The angular flux is expanded as

$$\underline{\psi}(z,\mu) = \sum_{\ell=0}^{\infty} (2\ell+1)P_\ell(2\mu-1)\underline{\rho}_\ell^+(z), \quad 0 \leq \mu \leq 1$$

$$= \sum_{\ell=0}^{\infty} (2\ell+1)P_\ell(2\mu+1)\underline{\rho}_\ell^-(z), \quad -1 \leq \mu \leq 0 \quad . \tag{7.33}$$

In the DP_1 approximation, we set

$$\underline{\rho}_\ell^+(z) = \underline{\rho}_\ell^-(z) = 0 \quad \text{for} \quad \ell > 1 \quad . \tag{7.34}$$

The boundary condition at the vacuum-medium interface is

$$\underline{\rho}_0^+(o) = \underline{\rho}_1^+(o) = 0 \ . \tag{7.35}$$

We shall see that this approximation is of the same computational difficulty as the P_3 approximation, but apparently gives better accuracy.

For the solution of Eq. (2.2) in this approximation we substitute the expansion given by Eq. (7.33) into Eqs. (2.2) and multiply successively by $P_0(2\mu-1)$, $P_1(2\mu-1)$, $P_0(2\mu+1)$, $P_1(2\mu+1)$ and integrate over $d\mu$. The range of integration for the first two cases is from 0 to 1 while the latter two is from -1 to 0. We easily derive the following equations:

$$\frac{d\rho_0^{(1)+}(z)}{dz} + \frac{d\rho_1^{(1)+}(z)}{dz} + 2\sigma\rho_0^{(1)+}(z) = 2C_{11}\rho_0^{(1)}(z) + 2C_{12}\rho_0^{(2)}(z) \tag{7.36a}$$

$$\frac{d\rho_0^{(1)+}(z)}{dz} + 3\frac{d\rho_1^{(1)+}(z)}{dz} + 6\sigma\rho_1^{(1)+}(z) = 0 \tag{7.36b}$$

$$\frac{d\rho_1^{(1)-}(z)}{dz} - \frac{d\rho_0^{(1)-}(z)}{dz} + 2\sigma\rho_0^{(1)-}(z) = 2C_{11}\rho_0^{(1)}(z) + 2C_{12}\rho_0^{(2)}(z) \tag{7.36c}$$

$$\frac{d\rho_0^{(1)-}(z)}{dz} - 3\,\frac{d\rho_1^{(1)-}(z)}{dz} + 6\sigma\rho_1^{(1)-}(z) = 0 \qquad (7.36d)$$

$$\frac{d\rho_0^{(2)+}(z)}{dz} + \frac{d\rho_1^{(2)+}(z)}{dz} + 2\rho_0^{(2)+}(z) = 2C_{21}\rho_0^{(1)}(z) + 2C_{22}\rho_0^{(2)}(z) + 2S \qquad (7.36e)$$

$$\frac{d\rho_0^{(2)+}(z)}{dz} + 3\,\frac{d\rho_1^{(2)+}(z)}{dz} + 6\rho_1^{(2)+}(z) = 0 \qquad (7.36f)$$

$$\frac{d\rho_1^{(2)-}(z)}{dz} - \frac{d\rho_0^{(2)-}(z)}{dz} + 2\rho_0^{(2)-}(z) = 2C_{21}\rho_0^{(1)}(z) + 2C_{22}\rho_0^{(2)}(z) + 2S \qquad (7.36g)$$

$$\frac{d\rho_0^{(2)-}(z)}{dz} - 3\,\frac{d\rho_1^{(2)-}(z)}{dz} + 6\rho_1^{(2)-}(z) = 0\ . \qquad (7.36h)$$

Here the total flux in each group is

$$\rho_0^{(1)}(z) = \int_{-1}^{1} \psi_1(z,\mu)d\mu = \rho_0^{(1)+}(z) + \rho_0^{(1)-}(z) \qquad (7.37a)$$

$$\rho_0^{(2)}(z) = \int_{-1}^{1} \psi_2(z,\mu)d\mu = \rho_0^{(2)+}(z) + \rho_0^{(2)-}(z)\ . \qquad (7.37b)$$

We could now obtain a secular determinant from Eqs. (7.36) in a manner quite similar to the P_3 approximation. It has been found convenient[21] to derive an equivalent set of equations which are in form very similar to Eqs. (7.21). First we write the following identities

$$P_1(\mu) = \frac{1}{2}\,[P_1(2\mu-1)+P_0(2\mu-1)] \qquad (7.38a)$$

$$P_1(\mu) = \frac{1}{2}\,[P_1(2\mu+1)-P_0(2\mu+1)] \qquad (7.38b)$$

$$P_2(\mu) = \frac{1}{4}\,[P_2(2\mu-1)+3P_1(2\mu-1)] \qquad (7.38c)$$

$$P_2(\mu) = \frac{1}{4}\,[P_2(2\mu+1)-3P_1(2\mu+1)] \qquad (7.38d)$$

$$P_3(\mu) = \frac{1}{8}\,[P_3(2\mu-1)+5P_2(2\mu-1)+3P_1(2\mu-1)-P_o(2\mu-1)] \qquad (7.38e)$$

$$P_3(\mu) = \frac{1}{8}\,[P_3(2\mu+1)-5P_2(2\mu+1)+3P_1(2\mu+1)+P_o(2\mu+1)]\ . \qquad (7.38f)$$

We use identities given by Eqs. (7.38a) and (7.38b) to obtain the net current for each group, i.e.,

$$\rho_1^{(1)}(z) = \int_{-1}^{1} P_1(\mu)\psi_1(z,\mu)d\mu = \frac{1}{2}\,[\rho_o^{(1)+}(z)-\rho_o^{(1)-}(z)] + \frac{1}{2}\,[\rho_1^{(1)+}(z)+\rho_1^{(1)-}(z)] \qquad (7.39a)$$

$$\rho_1^{(2)}(z) = \int_{-1}^{1} P_1(\mu)\psi_2(z,\mu)d\mu = \frac{1}{2}\,[\rho_o^{(2)+}(z)-\rho_o^{(2)-}(z)] + \frac{1}{2}\,[\rho_1^{(2)+}(z)+\rho_1^{(2)-}(z)] \qquad (7.39b)$$

Similiarly by using the appropriate identities above and considering the truncation given by Eq. (7.34), we obtain

$$\underline{\rho}_2(z) = \frac{3}{4}\,[\underline{\rho}_1^+(z)-\underline{\rho}_1^-(z)] \qquad (7.40)$$

and

$$\underline{\rho}_3(z) = \frac{1}{8}\,[\underline{\rho}_o^-(z)-\underline{\rho}_o^+(z)] + \frac{3}{8}\,[\underline{\rho}_1^+(z)+\underline{\rho}_1^-(z)]\ . \qquad (7.41)$$

$\underline{\rho}_2(z)$ and $\underline{\rho}_3(z)$ are approximate full-range moments because we omit terms of $\underline{\rho}_\ell^+$ and $\underline{\rho}_\ell^-$ for $\ell > 1$.

From Eqs. (7.37), (7.39), (7.40), and (7.41), we can easily solve for the half-range moments to yield

$$\underline{\rho}_o^+(z) = \frac{3}{4}\,\underline{\rho}_1(z) - \underline{\rho}_3(z) + \frac{1}{2}\,\underline{\rho}_o(z) \qquad (7.42a)$$

$$\underline{\rho}_o^-(z) = \frac{1}{2}\,\underline{\rho}_o(z) - \frac{3}{4}\,\underline{\rho}_1(z) + \underline{\rho}_3(z) \qquad (7.42b)$$

$$\underline{\rho}_1^+(z) = \frac{2}{3}\,\underline{\rho}_2(z) + \frac{1}{4}\,\underline{\rho}_1(z) + \underline{\rho}_3(z) \tag{7.42c}$$

$$\underline{\rho}_1^-(z) = \frac{1}{4}\,\underline{\rho}_1(z) + \underline{\rho}_3(z) - \frac{2}{3}\,\underline{\rho}_2(z) \quad . \tag{7.42d}$$

By appropriate linear combinations of Eqs. (7.36), we derive an equivalent set of equations in terms of the full-range approximate moments; namely,

$$\frac{d\rho_1^{(1)}(z)}{dz} + (\sigma - 2C_{11})\rho_0^{(1)}(z) = 2C_{12}\rho_0^{(2)}(z) \tag{7.43a}$$

$$\frac{d\rho_0^{(1)}(z)}{dz} + 2\,\frac{d\rho_2^{(1)}(z)}{dz} + 3\sigma\rho_1^{(1)}(z) = 0 \tag{7.43b}$$

$$3\,\frac{d\rho_1^{(1)}(z)}{dz} + 4\,\frac{d\rho_3^{(1)}(z)}{dz} + 8\sigma\rho_2^{(1)}(z) = 0 \tag{7.43c}$$

$$\frac{d\rho_2^{(1)}(z)}{dz} + 6\sigma\rho_3^{(1)}(z) = 0 \tag{7.43d}$$

$$\frac{d\rho_1^{(2)}(z)}{dz} + (1 - 2C_{22})\rho_0^{(2)}(z) = 2C_{21}\rho_0^{(1)}(z) + 2S \tag{7.43e}$$

$$\frac{d\rho_0^{(2)}(z)}{dz} + 2\,\frac{d\rho_2^{(2)}(z)}{dz} + 3\rho_1^{(2)}(z) = 0 \tag{7.43f}$$

$$3\,\frac{d\rho_1^{(2)}(z)}{dz} + 4\,\frac{d\rho_3^{(2)}(z)}{dz} + 8\rho_2^{(2)}(z) = 0 \tag{7.43g}$$

$$\frac{d\rho_2^{(2)}(z)}{dz} + 6\rho_3^{(2)}(z) = 0 \ . \tag{7.43h}$$

For example, to obtain Eq. (7.43a), Eq. (7.36a) is added to Eq. (7.36c) where the derivative term is simplified by Eq. (7.39a). The other equations are derived in a similar manner.

We now solve Eqs. (7.43) in a manner analogous to the P_3 approximation. The characteristic equation obtained (on expansion of the secular determinant) is

$$Ck^8 + Dk^6 + Ek^4 + Fk^2 + G = 0 \qquad (7.44)$$

where the coefficients are now given by

$$C = -1 \qquad (7.45a)$$

$$D = 24[\sigma(\sigma-C_{11})+1-C_{22}] \qquad (7.45b)$$

$$E = 576\sigma[C_{21}C_{12}+(1-C_{22})(C_{11}-\sigma)] - 36[\sigma^3(\sigma-2C_{11}) + 1-2C_{22}] \qquad (7.45c)$$

$$F = -864\sigma[(C_{11}-\sigma)(1-2C_{22}) - \sigma^2(1-C_{22})(\sigma-2C_{11})] - 1728C_{21}C_{12}\sigma(\sigma^2+1) \qquad (7.45d)$$

$$G = -1296\sigma^3(\sigma-2C_{11})(1-2C_{22}) + 5184C_{21}C_{12}\sigma^3. \qquad (7.45e)$$

The solutions to Eqs. (7.43) is exactly the same as the P_3 solutions. For the constant source problem the solution is given by Eqs. (7.24) and for the Milne problem by Eqs. (7.25) where Eqs. (7.26) are replaced by

$$f_0(k) = 1 \qquad (7.46a)$$

$$f_1(k) = \frac{k(12\sigma^2-k^2)}{12\sigma(3\sigma^2-k^2)} \qquad (7.46b)$$

$$f_2(k) = \frac{9\sigma k f_1(k)}{2(12\sigma^2-k^2)} \qquad (7.46c)$$

$$f_3(k) = \frac{k f_2(k)}{6\sigma} \qquad (7.46d)$$

$$f_4(k) = \frac{24C_{21}(k^2-3)}{k^2(12-k^2)+12(1-2C_{22})(k^2-3)} \qquad (7.46e)$$

$$f_5(k) = \frac{k(k^2-12)f_4(k)}{12(k^2-3)} \qquad (7.46f)$$

$$f_6(k) = \frac{9kf_5(k)}{2(12-k^2)} \tag{7.46g}$$

$$f_7(k) = \frac{kf_6(k)}{6} . \tag{7.46g}$$

The boundary conditions in terms of the half-range moments are given by Eq. (7.35). From Eqs. (7.42a) and (7.42c) we write the equivalent boundary conditions in terms of the full-range moments as

$$\frac{1}{2}\,\underline{\rho_0}(o) + \frac{3}{4}\,\underline{\rho_1}(o) - \underline{\rho_3}(o) = 0 \tag{7.47a}$$

and

$$\frac{1}{4}\,\underline{\rho_1}(o) + \frac{2}{3}\,\underline{\rho_2}(o) + \underline{\rho_3}(o) = 0 . \tag{7.47b}$$

For the DP_1 approximation, we define

$$g(k) = \frac{1}{2} + \frac{3}{4} f_1(k) - f_3(k) \tag{7.48a}$$

$$h(k) = \frac{1}{4} f_1(k) + \frac{2}{3} f_2(k) + f_3(k) \tag{7.48b}$$

$$t(k) = \frac{1}{2} f_4(k) + \frac{3}{4} f_5(k) - f_7(k) \tag{7.48c}$$

$$s(k) = \frac{1}{4} f_5(k) + \frac{2}{3} f_6(k) + f_7(k) . \tag{7.48d}$$

The equations for determination of the unknown coefficients is identical [except we use Eqs. (7.48)] to either Eqs. (7.30) or (7.31) depending on whether we are solving the constant source problem or the Milne problem. The total flux and current is given by Eqs. (7.24) or (7.25), respectively, the extrapolation distance by Eq. (7.19), and the angular distribution by Eq. (7.33) with the truncation indicated by Eq. (7.34). In terms of the full-range moments the angular distribution from Eqs. (7.33) and (7.42) is

$$\underline{\psi}(z,\mu) = \frac{1}{2}\,\underline{\rho}_0(z)-2\underline{\rho}_2(z) - 4\underline{\rho}_3(z) + \mu[4\rho_2(z) + \frac{3}{2}\,\rho_1(z) + 6\rho_3(z)], \quad 0 \leq \mu \leq 1 \tag{7.49a}$$

and

$$\underline{\psi}(z,\mu) = \frac{1}{2}\,\underline{\rho}_0(z)-2\underline{\rho}_2(z)+4\underline{\rho}_3(z)+\mu[-4\rho_2(z) + \frac{3}{2}\,\rho_1(z)+6\rho_3(z)], \quad -1 \leq \mu \leq 0. \tag{7.49b}$$

We note the discontinuity in the angular distribution at $\mu = 0$. In the next chapter, these solutions are evaluated numerically for some specific cases.

VIII. NUMERICAL RESULTS AND COMPARISONS

We have selected four problems for detailed study. These are all light water systems. The first problem which we label Set I is for ordinary light water. Set II, III, and IV consist of boarted light water at concentrations of 1.025, 2.99, and 6.35 barns/hydrogen atom respectively. The ranges of the energy groups are chosen as

Group 1: 0. eV < E < .0253 eV

and

Group 2: .0253 eV < E < .532 eV

The thermal spectra and cross section averaging procedures were performed by using the INCITE[22] code. The McMurry-Russell[23] H_2O kernel was used at room temperature (293°K). The results of these cross section calculations are listed in Table 8.1.

TABLE 8.1

TWO-GROUP MACROSCOPIC CROSS SECTIONS

Set No.	σ_1	σ_2	σ_{1a}	σ_{2a}	σ_{11}	σ_{22}	σ_{12}	σ_{21}
I	4.8822	3.2343	.03166	.01498	3.8180	2.8669	.3524	1.0326
II	4.9270	3.1686	.09725	.04424	3.7953	2.8005	.3239	1.0345
III	5.0914	3.0707	.28011	.11738	3.7659	2.6828	.2705	1.0454
IV	5.3220	2.9738	.58336	.22326	3.6906	2.5341	.2164	1.0481

Recall that these cross sections must be modified to

$$\sigma = \sigma_1/\sigma_2$$

and

$$C_{ij} = \sigma_{ij}/2\sigma_2 .$$

A computer program as described in Chapter VI is then used to find the eigenvalues of Eq. (2.17) i.e., the dispersion equation. For the four problem sets listed in Table 8.1, two real roots are obtained.

In the process of solving the problems by approximate methods as detailed in Chapter VII, we also must obtain the roots of the characteristic equations i.e., Eqs. (7.8a), (7.22), and (7.44). The eigenvalues for the exact calculation and the approximate methods are given in Table 8.2 where from Eq. (2.3) and Eqs. (7.5), we see that $k_j = 1/\eta_j$.

The eigenvalues for $\eta > 1$ provide the asymptotic solution to the one-group transport equation. This is also true in two-speed transport theory and we note in Table 8.2 that the P_1 discrete eigenvalues are closer to the exact values for Set I and Set II than are the P_3 or DP_1 values. But we observe that as more absorption is added to the medium the P_3 discrete eigenvalues become almost identical to the exact eigenvalues (see Set III and Set IV in Table 8.2).

With the discrete exact eigenvalues determined for each case, four Milne problem were solved by using the computer program listed in Appendix D. The behavior of the expansion coefficients for Set I and Set IV is shown in Fig. 8.1 and Fig. 8.2 respectively. For all problem sets, i.e., Milne and constant source, we always obtained the sharp resonance-like behavior in $\alpha_2(\mu)$. The "resonance" always appeared for μ between $1/\sigma$ and 1. In comparing Fig.

TABLE 8.2

EIGENVALUES OF THE TWO-GROUP TRANSPORT EQUATION

Set No.	Exact		P_1		P_3		DP_1	
	Discrete	Continuum	Discrete	Continuum	Discrete	Continuum	Discrete	Continuum
I	7.1869	$0 < \eta < 1$	7.2482	.7435	7.2647	.8599 .4835 .3040	7.2636	.8359 .2786 .1760
II	4.1793	$0 < \eta < 1$	4.1746	.7158	4.2040	.8293 .4823 .2941	4.2019	.8054 .2780 .1703
III	2.5958	$0 < \eta < 1$	2.5456	.6494	2.5961	.7569 .4788 .2725	2.5918	.7333 .2765 .1581
IV	1.9361	$0 < \eta < 1$	1.8638	.5683	1.9363	.6704 .4730 .2479	1.9287	.6466 .2740 .1444

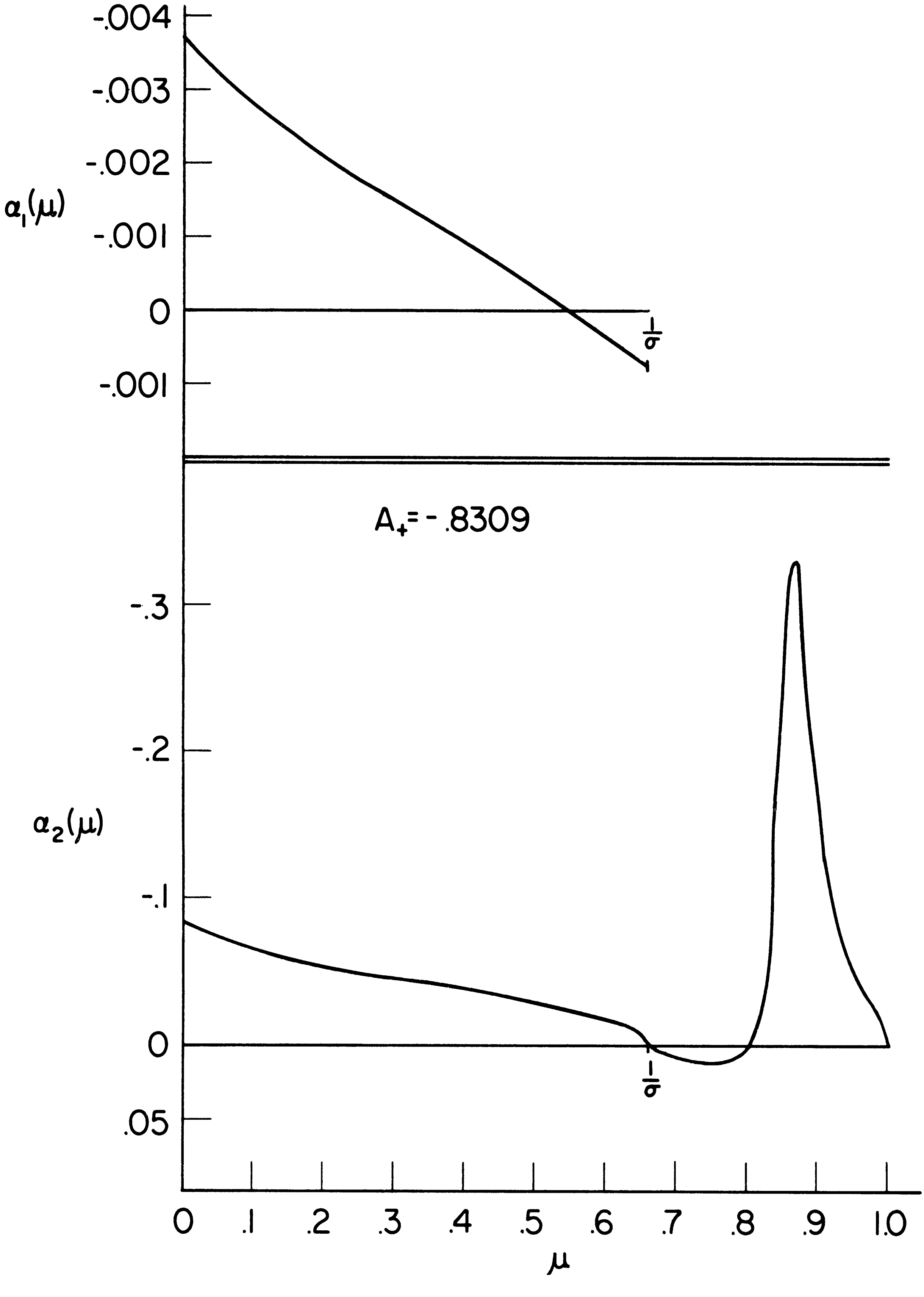

Fig. 8.1. Expansion coefficients for Milne problem, Set I.

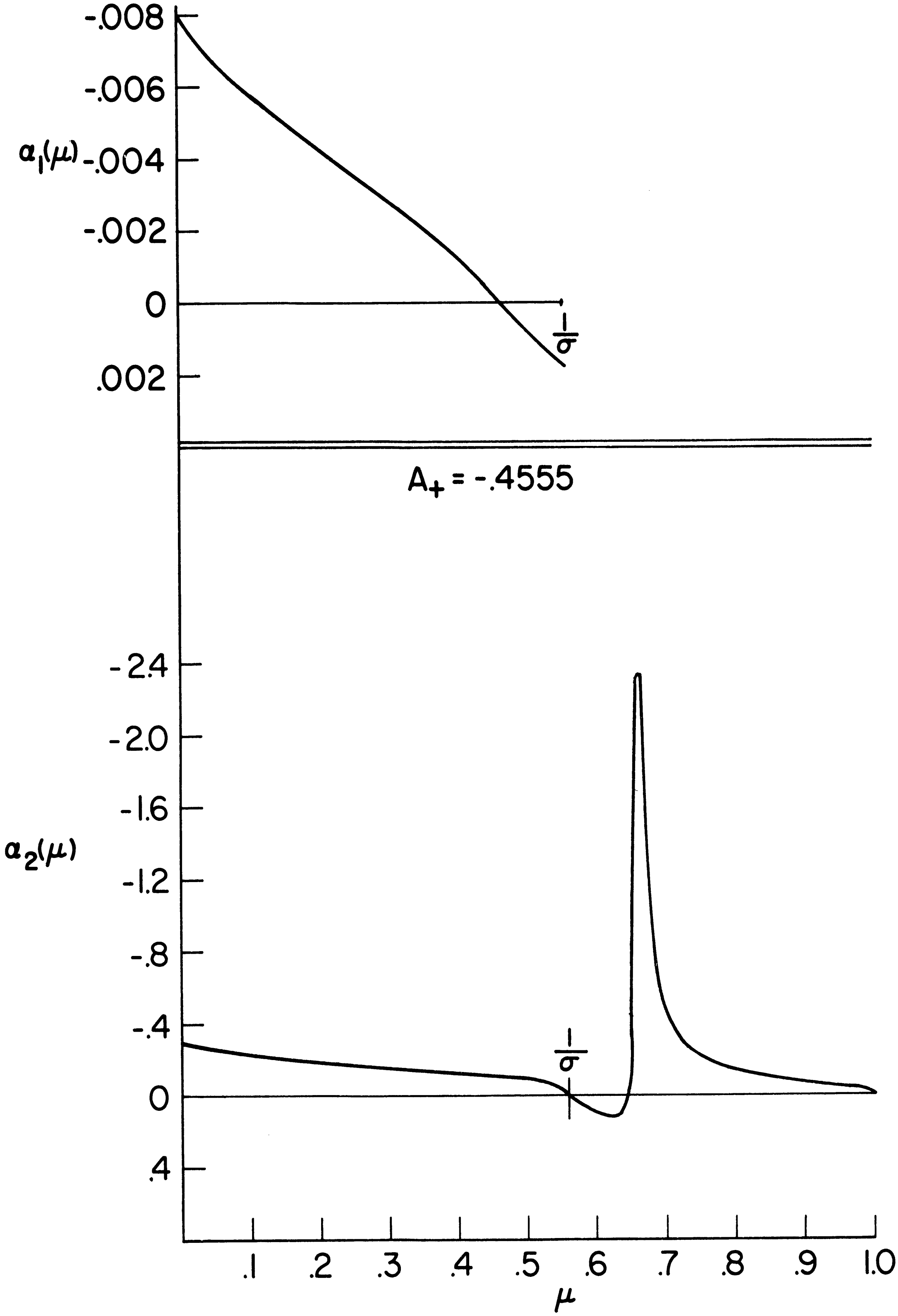

Fig. 8.2. Expansion coefficients for Milne problem, Set IV.

8.1 with Fig. 8.2 we see that the added absorption causes the resonance to shift closer to $1/\sigma$ and to become much narrower and higher (note the change of scale for $\alpha_2(\mu)$ in Fig. 8.1 and Fig. 8.2).

In solving the Milne problem we obtain the extrapolation distances by using Eq. (5.18). The extrapolation distances were also caculated from the approximate methods using Eq. (7.19). The results are shown in Table 8.3.

TABLE 8.3

EXTRAPOLATION DISTANCES FOR MILNE PROBLEMS

Set No.	Exact	P_1	P_3	DP_1
I	.6658	.6217	.6736	.6944
II	.6783	.6286	.7111	.7320
III	.7121	.6476	.7976	.8177
IV	.7613	.6735	.9279	.9432

We see from Table 8.3 that the P_1 results are consistently too low while the P_3 results are two high and with increased absorption the P_1 and P_3 results become progressively less accurate. The DP_1 extrapolation distances are about 3% higher than the P_3.

Angular distributions, total flux, and current are compared only for the constant source problems since the general conclusions should be valid for either problem. Also the constant source problem is of more interest for reactor applications. All distances into the medium are given in units of mean free path (m.f.p.) where we use the larger m.f.p. of the two energy groups, i.e., $1/\sigma_2$.

In Fig. 8.3 the exact angular distribution of Group 1 at the interface is compared to that obtained by the three approximation methods. The P_1 exit distribution fits the exact fairly well. As expected the P_1 approximation gives both positive and negative inward components. The P_3 calculation also gives a negative inward contribution which is difficult to show on the scale that we use in Fig. 8.3. We have indicated the DP_1 results by points at $\pm 90°$ and at $\pm 101.5°$. For $\theta > 101.5°$ the points for the DP_1 calculation were very close to the exact results. We note the discontinuity in the angular distribution at $\theta = \pm 90°$ for the exact and DP_1 calculations.

In Fig. 8.4 we make a similar comparison of exit angular distribution for group 2. We observe the change of scale; otherwise the distributions are quite similar.

The angular distribution at a distance of 1 m.f.p. in the medium is shown in Fig. 8.5. As can be seen from the figure the P_3 and DP_1 results are very close to the exact results. The DP_1 results are slightly closer to the exact results than are the P_3.

We show in Fig. 8.6 the change in the exact angular distribution as a function of distance into the medium for group 2. We observe how the angular distribution becomes progressively more isotropic and increases in magnitude with distance into the medium.

The effect of added adsorption on the exit angular distribution for group 2 is shown in Fig. 8.7.

As a measure of the peaking of the exit angular distribution, we compute the ratio of the angular flux at $\mu = -1$ to that at $\mu = 0$. In the constant

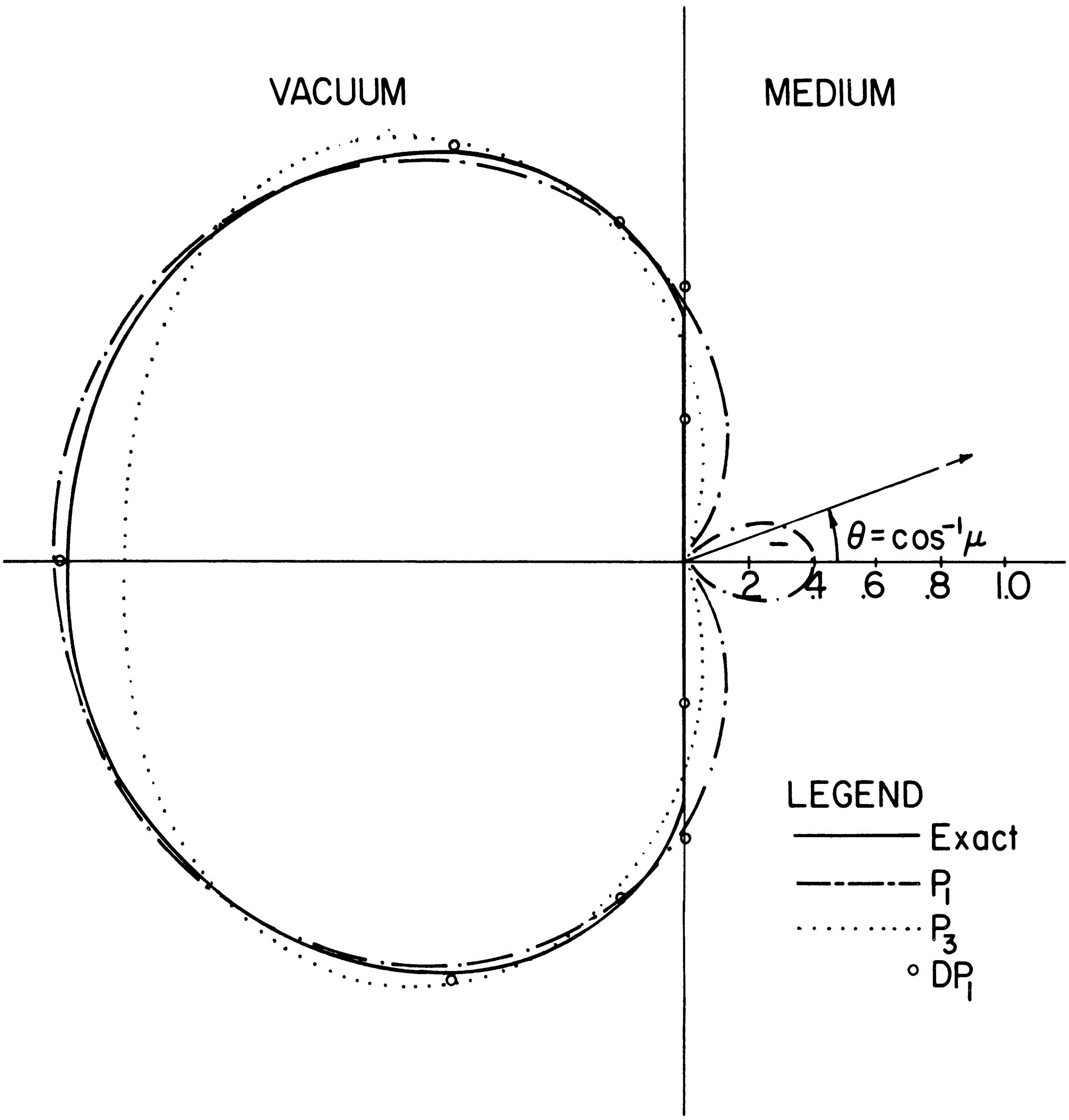

Fig. 8.3. Constant source angular distribution for Group 1, $\psi_1(0,\theta)$, Set I.

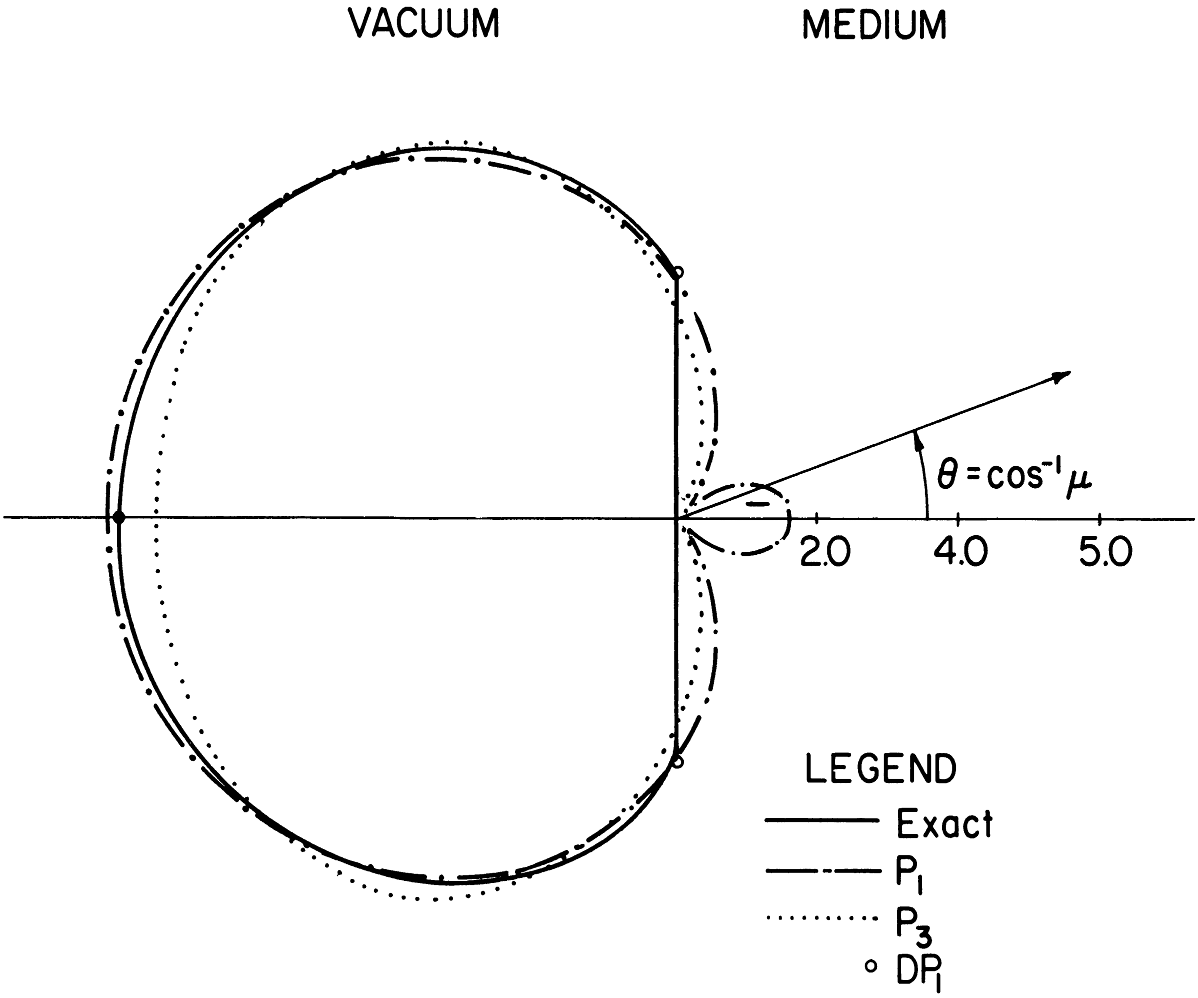

Fig. 8.4. Constant source angular distribution for Group 2, $\psi_2(0,\theta)$, Set I.

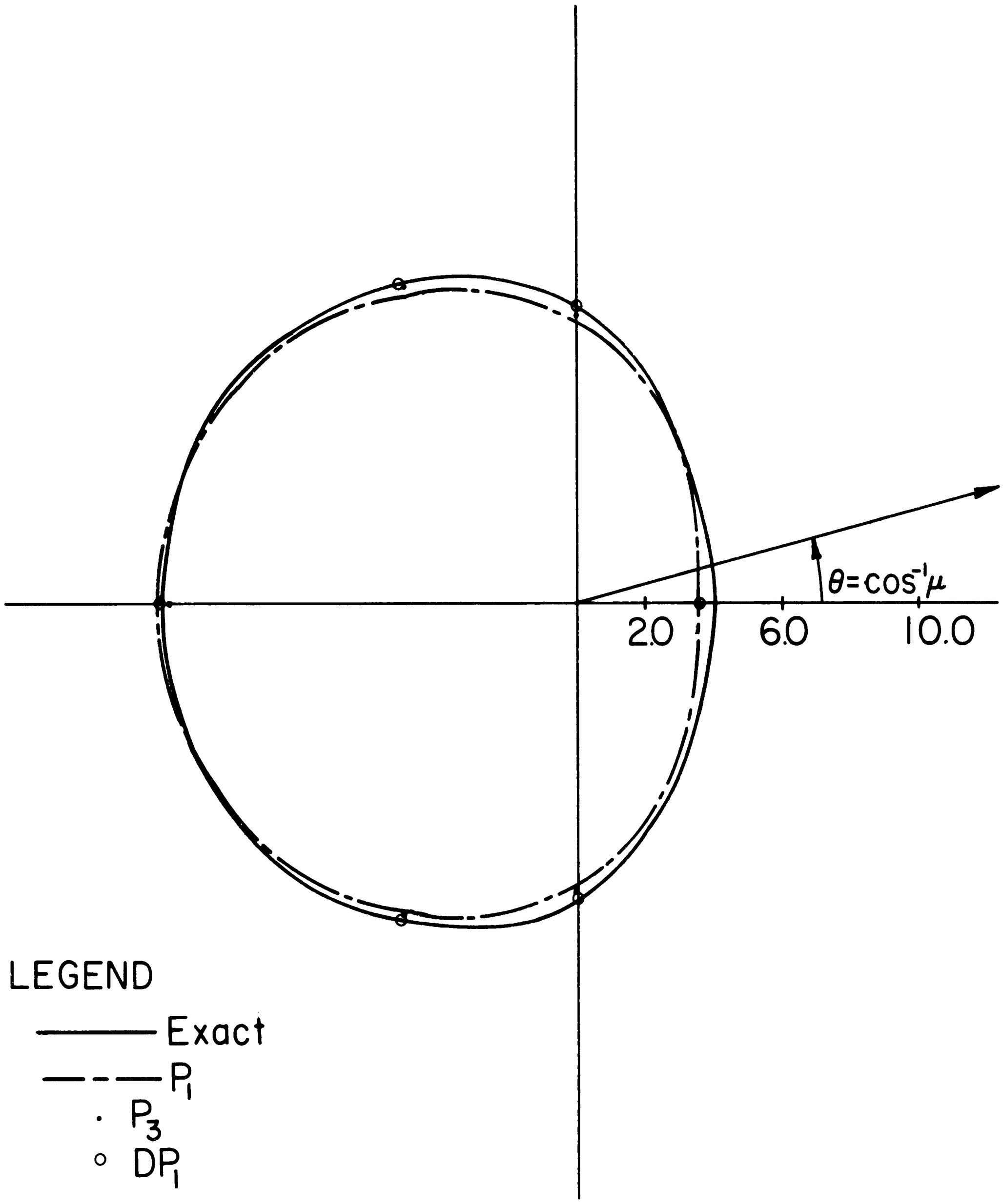

Fig. 8.5. Constant source angular distribution for Group 2, $\psi_2(1,\theta)$, Set I.

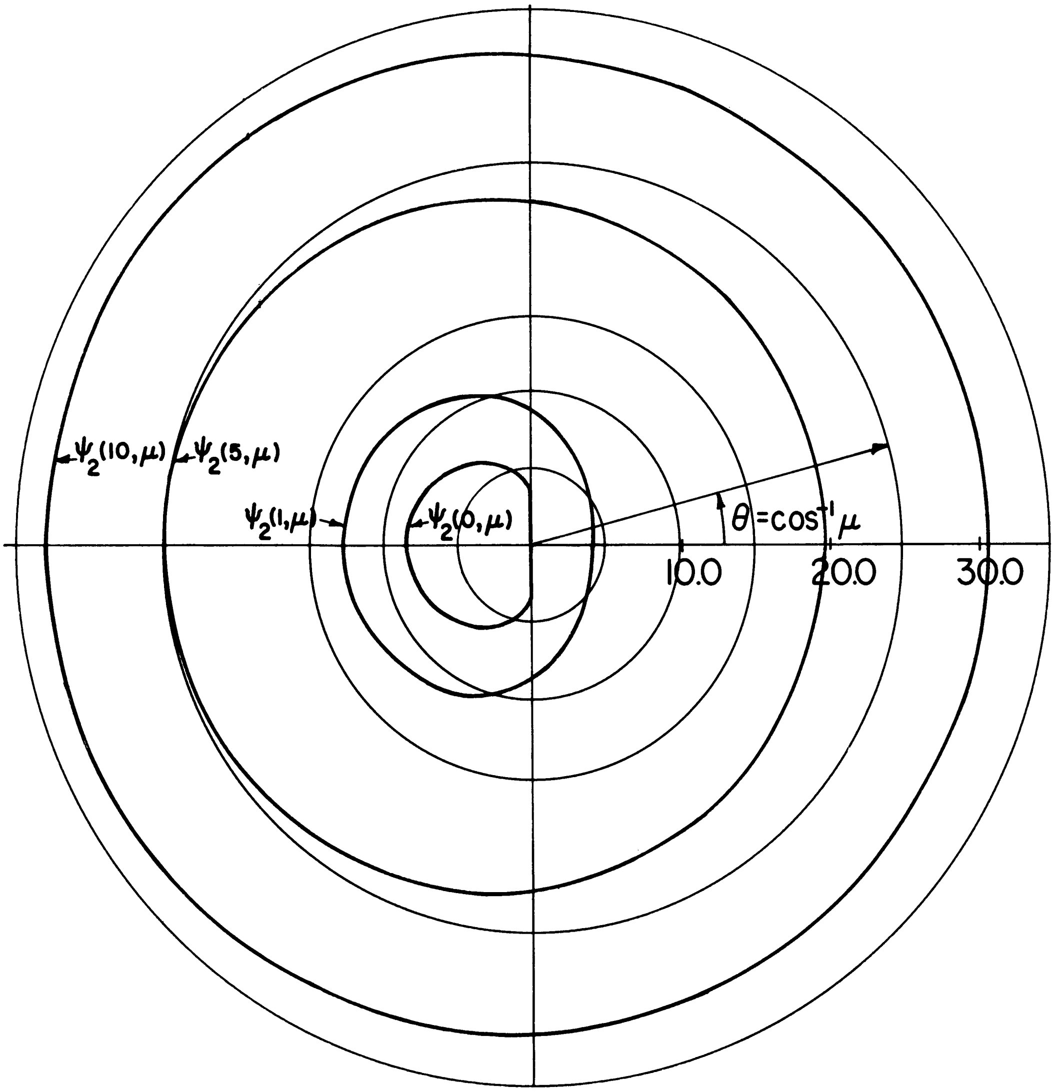

Fig. 8.6. Modifications in exact angular distribution with distance into the medium, Set I.

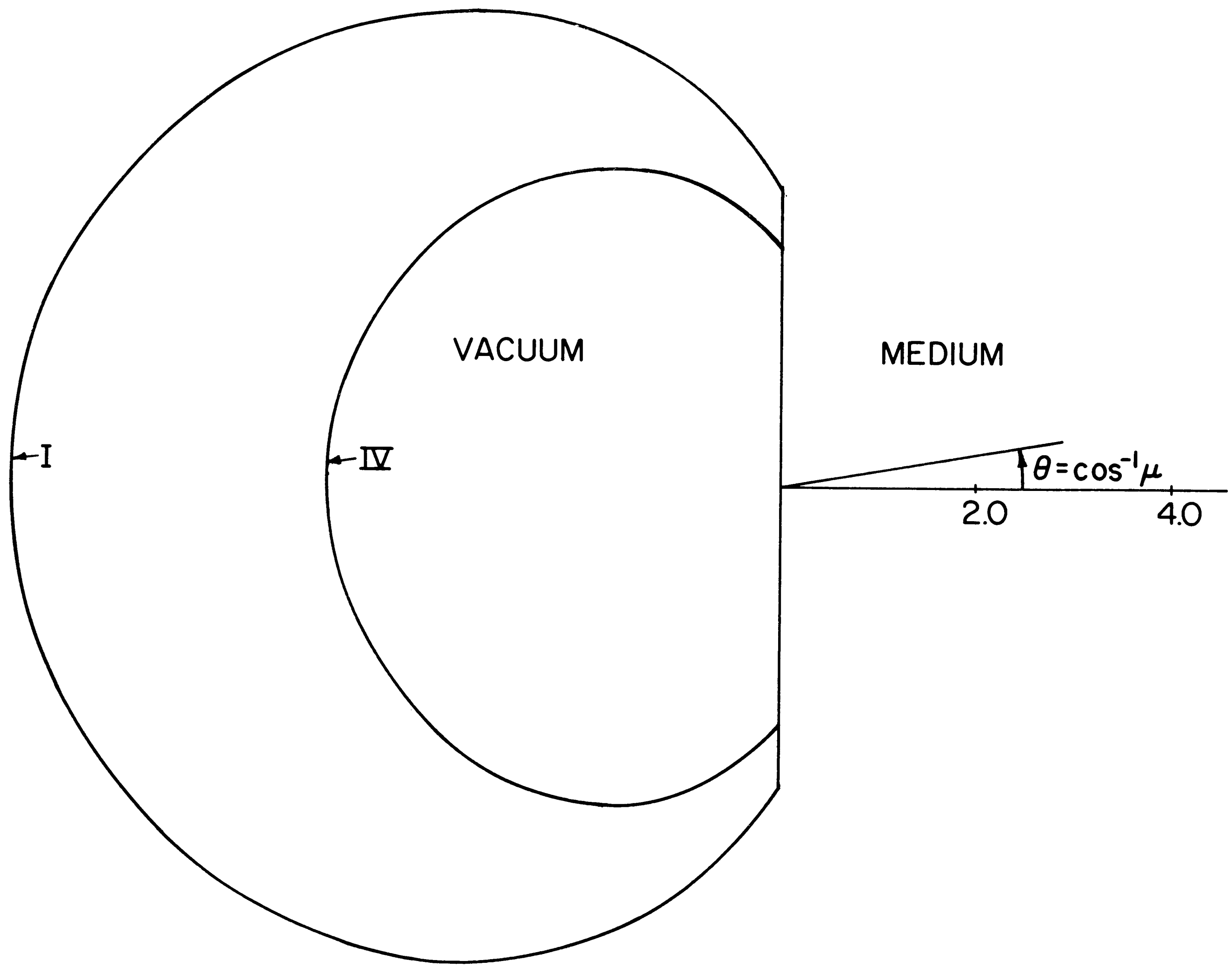

Fig. 8.7. Absorption effect on exact exit angular distribution for constant source problem, Group 2, Sets I and IV.

source problem, this ratio is 2.48 for Set I (pure water) while for Set IV (most poisoned case) it is 2.10. Thus with increased absorption the peaking in the forward direction becomes less pronounced. We observe the opposite effect for the Milne problem which is in agreement with the one-speed theory.[1] Specifically, the ratios for the Milne problem are 2.91 and 3.77 for Set I and IV respectively.

In reactor physics analysis the total flux and current are of most interest and utility. In Figs. 8.8 and 8.9 we show the exact total flux for Group 2 using Set I and Set IV, respectively. The approximate methods give a total flux quite close to the exact results, thus making a compariton of results difficult on the scale that we are using in these figures. Nevertheless we attempt to show in Fig. 8.9 the exact total flux and the approximate total flus. The DP_1 calculation gives a total flux so close to the exact value that a separate line could not be drawn. We indicate in each figure with a horizontal line the asymptotic total flux.

Numerical results for Set I and Set IV and Group 1 and Group 2 are given in Tables 8.4 to 8.6. Also the error is given in percent where we define

$$\text{error} = \frac{[\underline{\rho}_o\,(\text{approx}) - \underline{\rho}_o(\text{exact})]\cdot 100}{\underline{\rho}_o\,(\text{exact})} \quad .$$

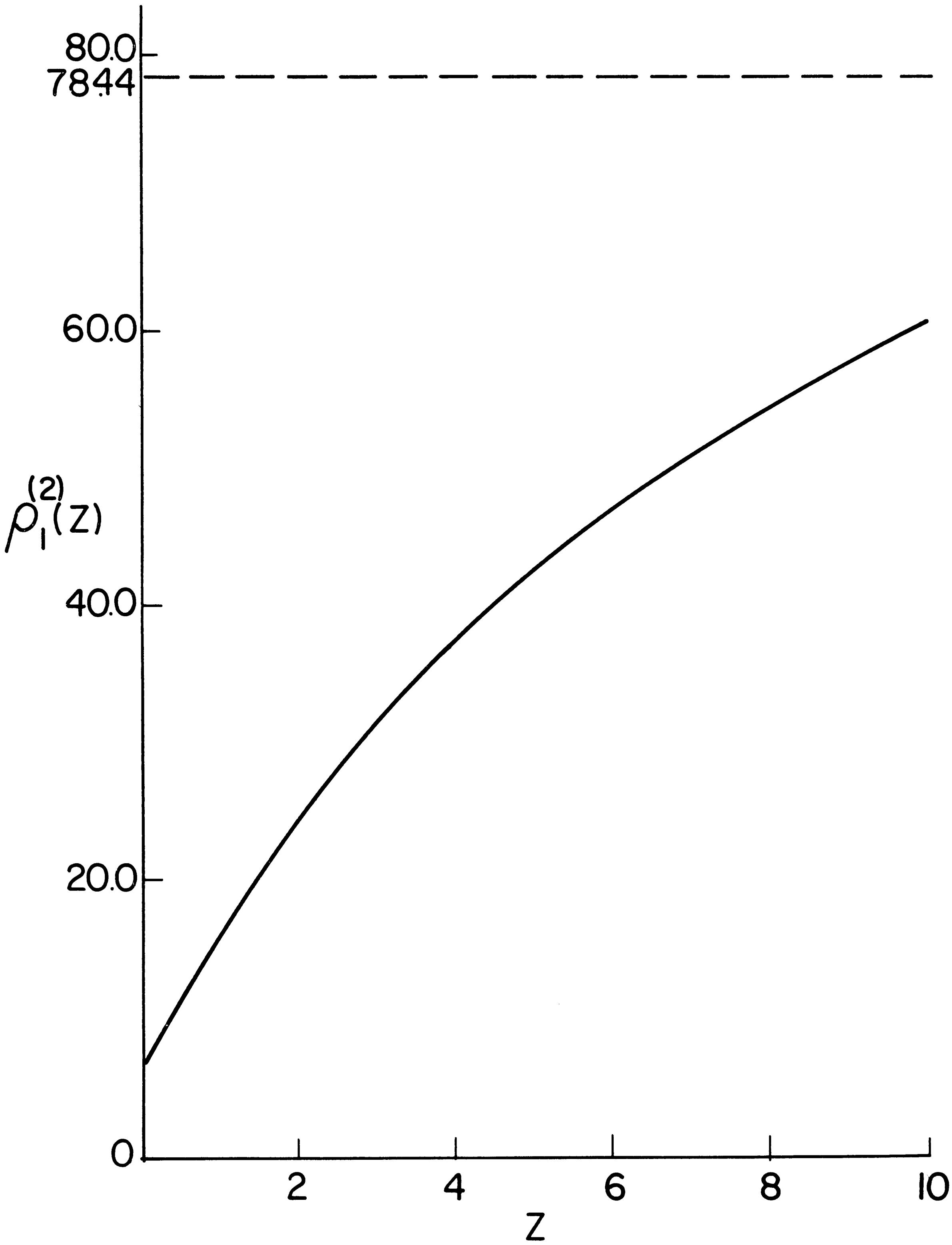

Fig. 8.8. Exact total flux for the constant source vs. distance into the medium, Group 2, Set I.

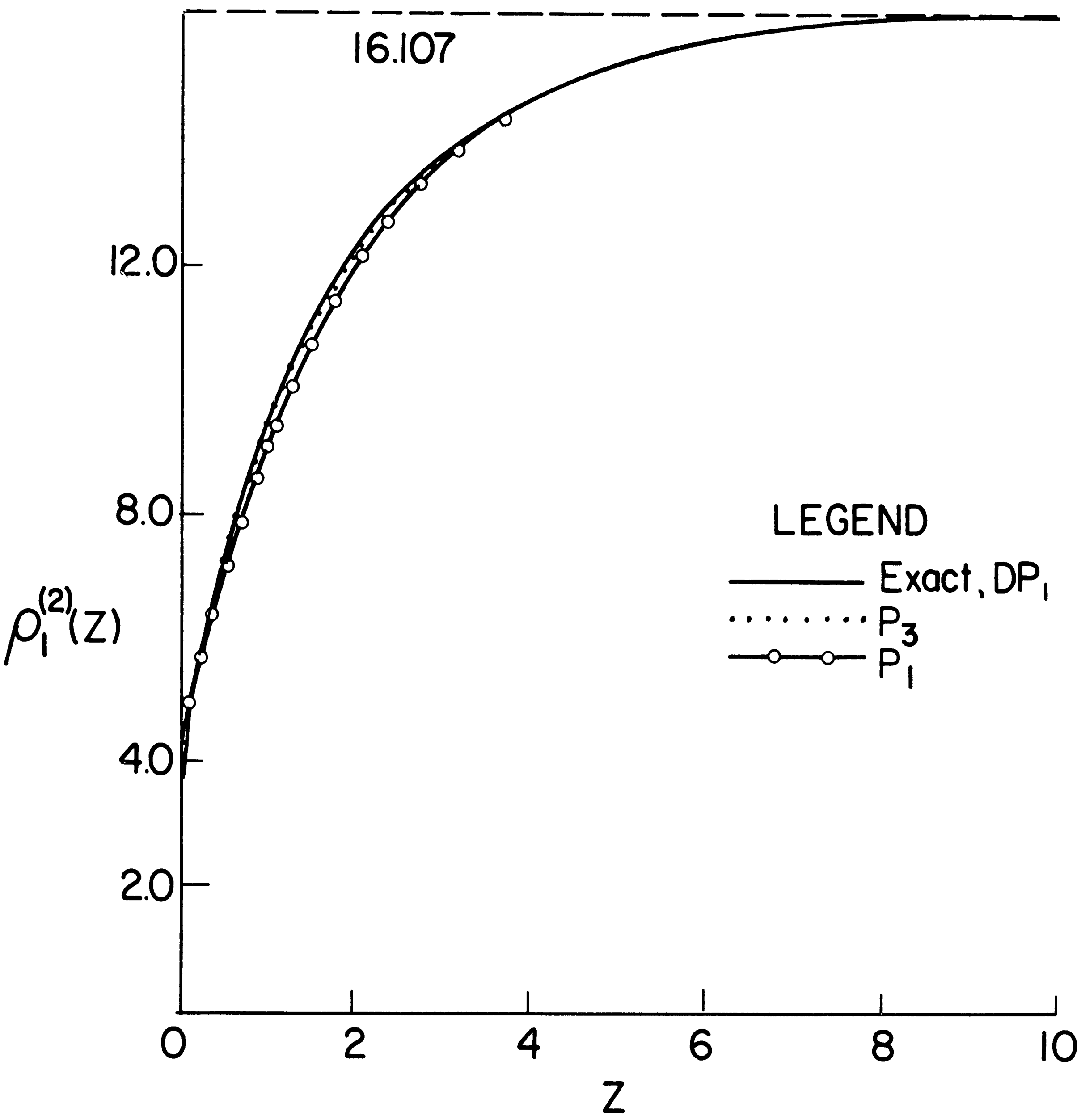

Fig. 8.9. Total flux for the constant source vs. distance into the medium, Group 2, Set IV.

TABLE 8.4

TOTAL FLUXES FOR GROUP 1, SET I

Distance (m.f.p.)	Exact	P_1	Error	P_3	Error	DP_1	Error
0	1.4106	1.5966	+13.1	1.4630	+3.7	1.3975	-.9
.5	3.4424	3.3089	- 3.9	3.3768	-1.9	3.4364	-.2
1.0	5.0450	4.8649	- 3.6	4.9675	-1.5	5.0164	-.6
1.5	6.4926	6.2946	- 3.0	6.4008	-1.4	6.4449	-.7
2.0	7.8245	7.6194	- 2.6	7.7207	-1.3	7.7613	-.8
3.0	10.2009	9.9946	- 2.0	10.0829	-1.2	10.1198	-.8
5.0	14.0417	13.8530	- 1.3	13.9153	- .8	13.9427	-.7
10.0	20.0287	19.8987	- .6	19.9202	- .5	19.9362	-.5

TABLE 8.5

TOTAL FLUXES FOR GROUP 2, SET I

Distance (m.f.p.)	Exact	P_1	Error	P_3	Error	DP_1	Error
0	5.7604	6.5009	+12.9	6.2100	+7.8	5.6877	-1.2
.5	11.6354	11.2336	- 3.5	11.3838	-2.2	11.5746	- .5
1.0	16.2810	15.6776	- 3.7	15.9721	-2.0	16.1772	- .6
1.5	20.5104	19.8403	- 3.3	20.1670	-1.7	20.3304	- .9
2.0	24.4239	23.7335	- 2.8	24.0507	-1.5	24.1878	-1.0
3.0	31.4543	30.7663	- 2.2	31.0381	-1.4	31.1478	-1.0
5.0	42.8775	42.2395	- 1.5	42.4243	-1.1	42.5066	- .9
10.0	60.7205	60.2340	- .8	60.2984	- .7	60.3425	- .6

TABLE 8.6

TOTAL FLUXES FOR GROUP 1, SET IV

Distance (m.f.p.)	Exact	P_1	Error	P_3	Error	DP_1	Error
0	3.2683	3.6563	+11.8	3.4226	+4.6	3.2625	-.2
.5	8.3076	7.9137	- 4.7	8.2312	- .9	8.3723	+.8
1.0	11.5025	11.1189	- 3.3	11.4584	- .4	11.5392	+.3
1.5	13.8524	13.5487	- 2.2	13.8201	- .2	13.8656	+.1
2.0	15.6174	15.3999	- 1.4	15.5924	- .2	15.6174	0
3.0	17.9790	17.8879	- .5	17.9585	- .1	17.9702	0
5.0	20.1820	20.1908	+ 0	20.1717	- .1	20.1776	0
10.0	21.2945	21.3033	+ 0	21.2945	+ 0	21.2959	0

We note the accuracy of the P_3 calculation which is always within one or two percent of the exact value except at the interface. Even at the interface the error is always less than 8%. The error is always negative for the P_1 and P_3 approximations except at the boundary where the error is several percent positive. We observe that the DP_1 calculation gives a significant improvement in accuracy over the P_3 especially at the interface.

Finally, we compare in Fig. 8.10 the current for the exact calculation with that obtained by the approximation methods. The P_3 and DP_1 currents were very close to the exact. Nevertheless, the DP_1 calculation gave the best results in every case studied.

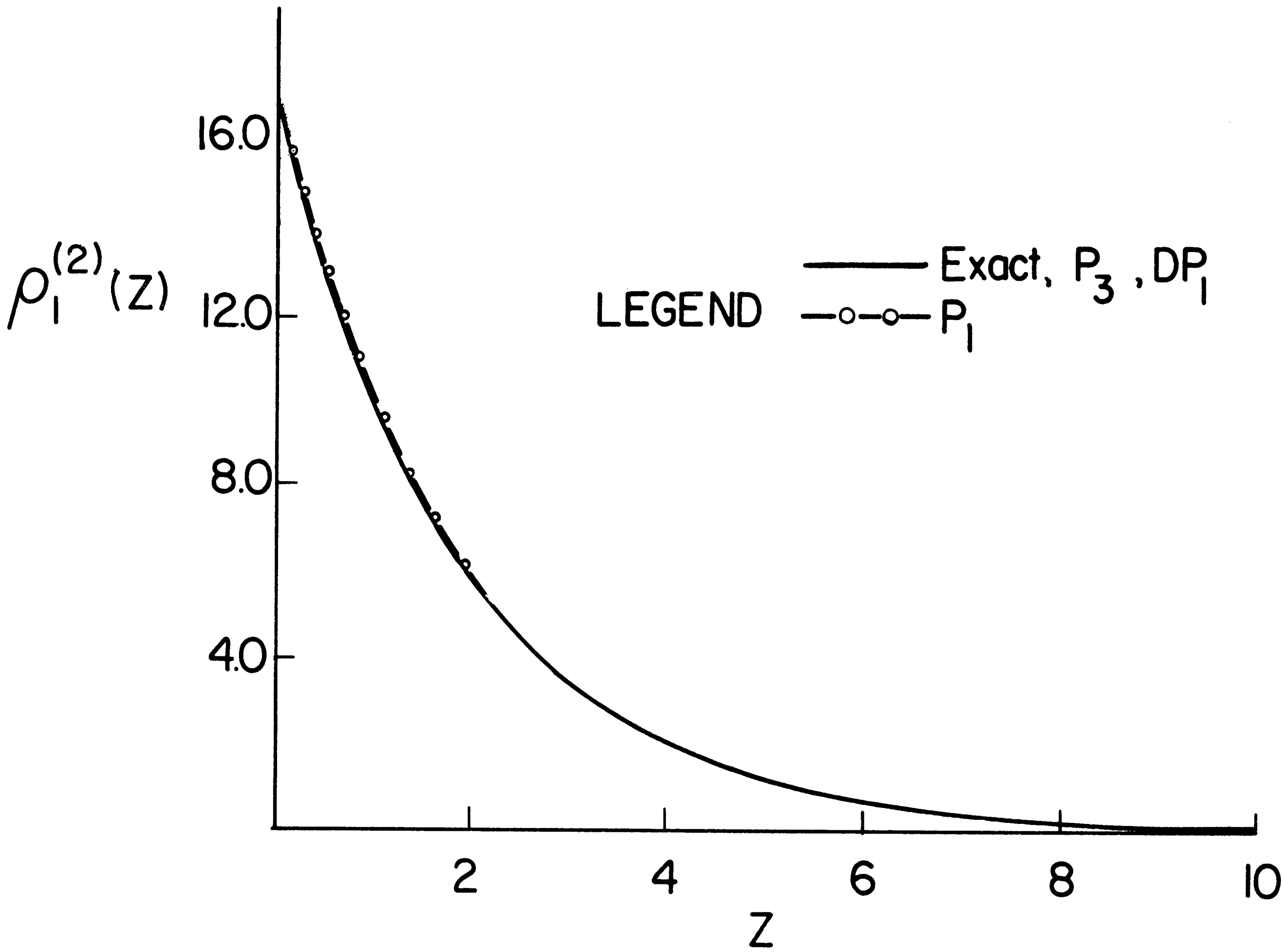

Fig. 8.10. Constant source current vs. distance for Group 2, Set IV.

IX. CONCLUSIONS

In the general two-group transport problem an exact analytical solution has not been found. Nevertheless by the Case[11] approach we have succeeded in deriving a pair of coupled equations (one is a singular integral equation) which are conveniently solved by numerical methods. Singular integral equations are often easier to solve than Fredholm equations. This is true in this thesis and may be generally valid.[25]

We develop in this work computer codes in the Michigan Algorithm Decoder Language (MAD) from which anyone can (with different cross section sets) test the accuracy of conventional approximation methods.

The numerical calculations show that although the P_1 approximation yields fairly good results for the total flux and current, the angular distribution is not so well represented especially at the interface. The P_3 approximation improves on the P_1 but we continue (as in the P_1) to obtain negative inward angular fluxes at the interface. The DP_1 method improves significantly on the P_3 angular fluxes as well as on the total flux and current. The DP_1 method has the important property that the boundary condition at a vacuum-medium interface can be specified exactly even in the lowest order approximation. Thus the exit angular distribution at the boundary is well-represented.

An interesting observation from this work is that in the constant source case the exit angular distribution becomes less pronounced in the forward direction with increased absorption in the medium. This is in contrast to the Milne problem where the opposite effect is noted.

We recall that the P_3 and DP_1 approximation present the same computational difficulty. From this study we conclude that in two-group reactor physics design analysis (with reactor parameter similar to those studied here) the DP_1 approximation is to be preferred over the P_3 approximation. This conclusion has also been stated by Weinberg and Wigner[24] in the one group case but never (to our knowledge) has it been tested against exact calculations in two-group problems. Of course, we realize that for complete core design calculations on complicated power or research reactors multigroup diffusion theory may still be the only feasible approach.

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APPENDIX A

THE EVALUATION OF $\gamma(\mu)$

Half-space identities quite similar to those in the one group case[1] exist for the two group case. As the method of proving these identities parallels closely that for the one group case as given in Case and Zweifel,[1] we shall omit the details in this work. The X-function identities that we use in this work are

$$X(z) = \int_0^1 \frac{\gamma(\mu)f(\mu)d\mu}{\mu-z} \tag{A.1}$$

$$X(z)X(-z) = \frac{\Omega(z)}{\Omega(\infty)(\eta_1^2-z^2)} \tag{A.2}$$

$$X(z) = \int_0^1 \frac{\mu f(\mu)d\mu}{\Omega(\infty)(\eta_1^2-\mu^2)X(-\mu)(\mu-z)} \tag{A.3}$$

We are considering only the case of one pair of discrete eigenvalues. Actually the only modification needed for the four eigenvalue cases is that we must make the replacement in identity (A.2) and (A.3) of $\eta_1^2-z^2$ by $(\eta_1^2-z^2)\cdot(\eta_2^2-z^2)$ where η_1 and η_2 are the two positive eigenvalues. Also in the above identities from Eq. (2.29),

$$f(\mu) = \frac{\Omega^+(\mu)-\Omega^-(\mu)}{2\pi i\mu} = C_{22} + [C_{11}-2C\mu\tau(\mu)-2C\mu\tau(\sigma\mu)]\theta_1(\mu)-2C\mu\tau(1/\sigma\mu)\theta_2(\mu) \tag{A.4}$$

and from the dispersion equation we have

$$\Omega(\infty) = 1 - \frac{2C_{11}}{\sigma} - 2C_{22} + \frac{4C}{\sigma}. \tag{A.5}$$

The method developed by Shure and Natelson[15] is now used to obtain a rapidly convergent integral equation which is then used to calculate the X-function and $\gamma(\mu)$. We write from Eq. (A.2),

$$\frac{\Omega(z)}{X(z)X(-z)} = \frac{1 - \frac{z^2}{\eta_1^2}}{X^2(o)} . \tag{A.6}$$

We then define a new function $\kappa(z)$ such that

$$\kappa(z) = \left(\frac{1}{X(o)} - z\right) X(z) \tag{A.7}$$

and note that $\kappa(o) = \kappa(\infty) = 1$.

We solve Eq. (A.7) for X(z) and substitute in Eq. (A.6) to arrive at

$$\frac{\Omega(z)}{\kappa(z)\kappa(-z)} = \frac{1 - \frac{z^2}{\eta_1^2}}{1-z^2X^2(o)} . \tag{A.8}$$

Boundary values are now taken of Eq. (A.8) to

$$\kappa^+(\mu) - \kappa^-(\mu) = \frac{1-\mu^2X^2(o)}{1 - \frac{\mu^2}{\eta_1^2}} \left[\frac{\Omega^+(\mu)-\Omega^-(\mu)}{\kappa(\mu)}\right] \tag{A.9}$$

We observe that the function $(\kappa(z)-1)/z$ is analytic in the complex plane with a cut from 0 to 1 along the real axis. A direct application of Cauchy's theorem around this cut gives

$$\frac{\kappa(z)-1}{z} = \frac{1}{2\pi i} \int_o^1 \frac{\kappa^+(\mu)-\kappa^-(\mu)d\mu}{\mu(\mu-z)} . \tag{A.10}$$

We substitute into Eq. (A.9) the boundary value of $\Omega(z)$ as given in Eq. (A.4) and then insert this result into Eq. (A.10) to obtain an integral equation for $\kappa(-z)$. This integral equation is

$$\kappa(-z) = 1 - z \int_0^1 \frac{[1-\mu^2 X^2(o)]f(\mu)d\mu}{\left(1 - \frac{\mu^2}{\eta_1^2}\right)(\mu+z)\kappa(-\mu)} \quad . \tag{A.11}$$

In the monoenergetic case this integral can be carried out explicitly in the first approximation,[15] i.e., for $\kappa(-z) = 1$, but in Eq. (A.11) above the function $f(\mu)$ occurs and thus numerical procedures must be resorted to immediately. Actually Eq. (A.11) is a nonlinear singular integral equation because from Eq. (A.4) and for $C \neq 0$ $f(\mu) \to \pm\infty$ as $\mu \to \frac{1}{\sigma}$.

To simplify the notation, we define

$$g(\mu,z) = \frac{[1-\mu^2 X^2(o)]\mu}{\left(1 - \frac{\mu^2}{\eta_1^2}\right)(\mu+z)\kappa(-\mu)} \quad . \tag{A.12}$$

By using Eq. (A.4) for $f(\mu)$ in Eq. (A.11) and by standard techniques of subtracting the singularity, we easily obtain

$$\begin{aligned} \kappa(-z) = {} & 1 - z \int_0^1 \frac{g(\mu,z)}{\mu} [C_{22}+(C_{11}-2C\mu\tau(\mu))\Theta_1(\mu)]d\mu \\ & + 2Cz \int_0^1 [g(\mu,z)-g(\tfrac{1}{\sigma},z)][\tau(\sigma\mu)\Theta_1(\mu)+\tau(1/\sigma\mu)\Theta_2(\mu)]d\mu \\ & + 2Cz\, g(\tfrac{1}{\sigma},z) \int_0^1 [\tau(\sigma\mu)\Theta_1(\mu)+\tau(1/\sigma\mu)\Theta_2(\mu)]d\mu \quad . \end{aligned} \tag{A.13}$$

This last integral in Eq. (A.13) can be performed to yield

$$\int_0^1 [\tau(\sigma\mu)\Theta_1(\mu)+\tau(1/\sigma\mu)\Theta_2(\mu)]d\mu = \frac{1}{\sigma}[\sigma\tau(1/\sigma) + \frac{1}{2}\ell n(\sigma^2-1)] \quad . \tag{A.14}$$

Because of the form of the integrands in Eq. (A.13) the integration is performed separately for $0 \leq \mu \leq 1/\sigma$ and $1/\sigma \leq \mu \leq 1$. Eight point Gauss quadrature is now used to evaluate the integrals and we iterate on $\kappa(-z) = 1$

for the first iteration. In a sample problem after five iterations the maximum difference in any of the 32 values of κ was less than 10^{-6}.

From Eq. (A.7) we see that

$$X(-\mu) = \frac{\kappa(-\mu)}{\frac{1}{X(o)} + \mu} \tag{A.15}$$

and if we recall that

$$\gamma(\mu = \frac{\mu X^{+}(\mu)}{\Omega^{+}(\mu)} \tag{A.16}$$

then from Eq. (A.2),

$$\gamma(\mu) = \frac{\mu\eta_1^2 \left(\frac{1}{X(o)} + \mu\right) X^2(o)}{(\eta_1^2-\mu^2)\kappa(-\mu)} . \tag{A.17}$$

Once $\kappa(-z)$ is found then Eq. (A.17) gives $\gamma(\mu)$. The κ-function for one-speed theory and isotropic scattering can be obtained from Eq. (A.11) by defining

$$f(\mu) = \frac{C}{2}$$

and

$$X^2(o) = \frac{1}{\eta_1^2(1-C)}$$

where C has its usual one-speed definition.

The computer code for calculating $\gamma(\mu)$ is an integral part of the computer code which solves the exact Milne and constant source problems. This code is listed in Appendix D.

APPENDIX B

NECESSARY MODIFICATIONS FOR TWO PAIRS OF DISCRETE ROOTS

We have briefly noted in Appendix A the slight modification in the procedure to obtain $\gamma(\mu)$ if there exists two pair of discrete, finite roots. If the modification is carried through we can easily derive for $\gamma(\mu)$,

$$\gamma(\mu) = \frac{\mu\eta_1^2\eta_2^2\left(\frac{1}{X(o)} + \mu\right)X^2(o)}{(\eta_1^2-\mu^2)(\eta_2^2-\mu^2)\kappa(-\mu)} \tag{B.1}$$

where

$$X^2(o) = \frac{1}{\Omega(\infty)\eta_1^2\eta_2^2} \tag{B.2}$$

and the integral equation for $\kappa(-z)$ has the form

$$\kappa(-z) = 1 - z\int_0^1 \frac{[1-\mu^2X^2(o)]f(\mu)d\mu}{\left(1 - \frac{\mu^2}{\eta_1^2}\right)\left(1 - \frac{\mu^2}{\eta_2^2}\right)(\mu+z)\kappa(-\mu)} . \tag{B.3}$$

Her η_1, and η_2 are the two positive discrete eigenvalues.

The appropriate X(z) function for two pair of discrete roots is

$$X(z) = \frac{1}{(1-z)^2}\exp\frac{1}{\pi}\int_0^1 \frac{\text{Arg }\Omega^+(\mu)d\mu}{\mu-z} . \tag{B.4}$$

And in order that $N(z) \sim \frac{1}{z}$ as $z \to \infty$ we require from Eq. (4.20) that

$$\int_0^1 \gamma(\mu)\left[\psi'(\mu) + C\int_0^1 \frac{d\eta\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}\right]d\mu = 0 \tag{B.5}$$

and

$$\int_0^1 \mu\gamma(\mu)\left[\psi'(\mu) + C\int_0^1 \frac{d\eta\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}\right]d\mu = 0 . \tag{B.6}$$

We have two discrete modes available to satisfy Eqs. (B.5) and (B.6) and thus we make the replacement of $\psi'(\mu)$ by $\psi'(\mu)-A_{1+}\phi_{1+}(\mu)-A_{2+}\phi_{2+}(\mu)$. This gives two equations with two unknowns assuming $\alpha_2(\mu)$ has been determined. The equations are

$$\int_0^1 \gamma(\mu)\psi'(\mu)d\mu - A_{1+}\int_0^1 \gamma(\mu)\phi_{1+}(\mu)d\mu - A_{2+}\int_0^1 \gamma(\mu)\phi_{2+}(\mu)d\mu + C\int_0^1 \gamma(\mu)d\mu$$

$$(x)\int_0^1 \frac{d\eta\,\eta\,\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu} = 0 \qquad \text{(B.7)}$$

and

$$\int_0^1 \mu\gamma(\mu)\psi'(\mu)d\mu - A_{1+}\int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu - A_{2+}\int_0^1 \mu\gamma(\mu)\phi_{2+}(\mu)d\mu$$

$$+ C\int_0^1 \mu\gamma(\mu)d\mu \int_0^1 \frac{d\eta\,\eta\,\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu} = 0 \ . \qquad \text{(B.8)}$$

We solve these two equations for A_{1+} and A_{2+} to obtain

$$A_{1+} = \Bigg[\int_0^1 \gamma(\mu)\phi_{2+}(\mu)d\mu \int_0^1 \mu\gamma(\mu)\psi'(\mu)d\mu - \int_0^1 \mu\gamma(\mu)\phi_{2+}(\mu)d\mu \int_0^1 \gamma(\mu)\psi'(\mu)d\mu$$

$$+ \int_0^1 \gamma(\mu')\phi_{2+}(\mu')d\mu' \int_0^1 d\mu\,\mu\gamma(\mu) \int_0^1 \frac{d\eta\,\eta\,\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}$$

$$- \int_0^1 \mu'\gamma(\mu')\phi_{2+}(\mu')d\mu' \int_0^1 d\mu\gamma(\mu) \int_0^1 \frac{d\eta\,\eta\,\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}\Bigg] \Bigg/ \Bigg[\int_0^1 \gamma(\mu)\phi_{2+}(\mu)d\mu$$

$$(x)\int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu - \int_0^1 \mu\gamma(\mu)\phi_{2+}(\mu)d\mu \int_0^1 \gamma(\mu)\phi_{1+}(\mu)d\mu\Bigg] \qquad \text{(B.9)}$$

$$A_{2+} = \Bigg[\int_0^1 \gamma(\mu)\phi_{1+}(\mu)d\mu \int_0^1 \mu\gamma(\mu)\psi'(\mu)d\mu - \int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu \int_0^1 \gamma(\mu)\psi'(\mu)d\mu$$

$$+ \int_0^1 \gamma(\mu')\phi_{1+}(\mu')d\mu' \int_0^1 d\mu\,\mu\gamma(\mu) \int_0^1 \frac{d\eta\,\eta\,\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu} - \int_0^1 \mu'\gamma(\mu')\phi_{1+}(\mu')d\mu'$$

$$(x)\int_0^1 d\mu\gamma(\mu) \int_0^1 \frac{d\eta\,\eta\,\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}\Bigg] \Bigg/ \Bigg[\int_0^1 \gamma(\mu)\phi_{1+}(\mu)d\mu \int_0^1 \mu\gamma(\mu)\phi_{2+}(\mu)d\mu$$

$$- \int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu \int_0^1 \gamma(\mu)\phi_{2+}(\mu)d\mu\Bigg] \ . \qquad \text{(B.10)}$$

The only fundamental difference, other than more terms in this result, from the case treated in the text is the presence of terms of the type

$$\int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu \quad . \tag{B.11}$$

We recall that

$$\phi_{1+}(\mu) = \frac{\eta_1}{\eta_1-\mu}\,[f(\mu)-Ck(\eta_1,\mu)] \quad . \tag{B.12}$$

Inserting this into the above integral we find

$$\int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu = \int_0^1 \mu\gamma(\mu)\,\frac{\eta_1}{\eta_1-\mu}\,f(\mu)d\mu - C\int_0^1 \mu\gamma(\mu)\,\frac{\eta_1}{\eta_1-\mu}\,k(\eta_1,\mu)d\mu . \tag{B.13}$$

The first integral can be written as

$$\int_0^1 \mu\gamma(\mu)\,\frac{\eta_1}{\eta_1-\mu}\,f(\mu)d\mu = -\eta_1\int_0^1 \gamma(\mu)f(\mu)d\mu + \int_0^1 \gamma(\mu)\,\frac{\eta_1^2}{\eta_1-\mu}\,f(\mu)d\mu \quad . \tag{B.14}$$

We recall the X-function defined by Eq. (A.1) is also valid for the two pair case, i.e.,

$$X(z) = \int_0^1 \frac{\gamma(\mu)f(\mu)d\mu}{\mu-z} \quad . \tag{A.1}$$

We note that

$$\lim_{z\to\infty} zX(z) = -\int_0^1 \gamma(\mu)f(\mu)d\mu \quad . \tag{B.15}$$

But from Eq. (B.4)

$$X(z) \underset{z\to\infty}{\to} \frac{1}{z^2} \tag{B.16}$$

thus

$$-\int_0^1 \gamma(\mu)f(\mu)d\mu = 0 \quad .$$

And we find for the integral expression (B.11) that

$$\int_0^1 \mu\gamma(\mu)\phi_{1+}(\mu)d\mu \;=\; -\eta_1 X(\eta_1) - C\int_0^1 \mu\gamma(\mu)\frac{\eta_1^2}{\eta_1-\mu}k(\eta_1,\mu)d\mu \;. \qquad (B.17)$$

Similar results can easily be derived for the other integrals of this type in Eqs. (B.9) and (B.10).

The basic equations for finding $\alpha_2(\mu)$ would be the same as before except $\psi'(\mu)$ is replaced by $\psi'(\mu)-A_{1+}\phi_{1+}(\mu)-A_{2+}\phi_{2+}(\mu)$. Of course quite basic to the solution of $\alpha_2(\mu)$ is the shape of the function $\gamma(\mu)$ which would certainly have a different functional form.

Lastly the equation for $\alpha_1(\mu)$ is modified as follows:

$$\alpha_1(\mu) \;=\; \sigma C_{11}[\psi_1(\sigma\mu) - A_{1+}F_{1+}^{(1)}(\sigma\mu) - A_{2+}F_{2+}^{(1)}(\sigma\mu)] - C_{11}C_{12}\int_0^1 \frac{P\eta\alpha_2(\eta)d\eta}{\eta-\mu} \qquad (B.18)$$

Here the functions $F_{1+}^{(1)}(\sigma\mu)$ and $F_{2+}^{(1)}(\sigma\mu)$ are given by

$$F_{1+}^{(1)}(\sigma\mu) \;=\; \frac{C_{12}\eta_1}{\sigma(\eta_1-\mu)} \qquad (B.19a)$$

$$F_{2+}^{(1)}(\sigma\mu) \;=\; \frac{C_{12}\eta_2}{\sigma(\eta_2-\mu)} \;. \qquad (B.19b)$$

The simplification of $O(\mu)\phi_{1+}(\mu)$ and $O(\mu)\phi_{2+}(\mu)$ would proceed in exactly the same manner as for $O(\mu)\phi_{+}(\mu)$ in Chapter IV.

APPENDIX C

AN ALTERNATE SOLUTION METHOD TO EQ. (4.29)

It is possible that there are values of C for problems of interest where the iteration technique described in Chapter VI will not converge at all or will converge very slowly. The method of solution outlined in this appendix will give a solution for these cases.

For convenience we repeat Eqs. (4.28) and (4.29) of Chapter IV:

$$A_+ = \frac{\int_0^1 \gamma(\mu)\psi'(\mu)d\mu + C\int_0^1 \gamma(\mu)d\mu \int_0^1 \frac{d\eta\,\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}}{\int_0^1 \gamma(\mu)\phi_+(\mu)d\mu} \tag{4.28}$$

and

$$\alpha_2(\mu) = O(\mu)[\psi'(\mu) - A_+\phi_+(\mu)] + C\;O(\mu)\int_0^1 \frac{d\eta\,\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu} . \tag{4.29}$$

We define

$$M_{O+} = \int_0^1 \gamma(\mu)\phi_+(\mu)d\mu \tag{C.1}$$

$$A_+^{(o)} = \frac{\int_0^1 \gamma(\mu)\psi'(\mu)d\mu}{M_{O+}} . \tag{C.2}$$

We substitute Eq. (4.28) into Eq. (4.29) to arrive at

$$\alpha_2(\mu) = O(\mu)\psi'(\mu) - A_+^{(o)}O(\mu)\phi_+(\mu) - C\,\frac{O(\mu)\phi_+(\mu)\int_0^1 \gamma(\mu)d\mu\int_0^1 \frac{d\eta\,\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu}}{M_{O+}}$$

$$+ \; C\;O(\mu)\int_0^1 \frac{d\eta\,\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu} . \tag{C.3}$$

Equation (C.3) is now reduced to a set of linear equations. We again use the midpoint approximation to evaluate the integrals. For example the last integral in Eq. (C.3) is

$$\int_0^1 \frac{d\eta\eta\alpha_2(\eta)k(\eta,\mu)}{\eta-\mu} \simeq \sum_{i=1}^{D} \frac{\eta_i\alpha_2(\eta_i)k(\eta_i,\mu)h_i}{\eta_i-\mu}. \qquad (C.4)$$

h_i is the width of the ith interval.

For the integral in the third term on the right-hand side of Eq. (C.3), we write

$$\int_0^1 \gamma(\mu)d\mu \sum_{i=1}^{D} \frac{\eta_i\alpha_2(\eta_i)k(\eta_i,\mu)h_i}{\eta_i-\mu} \simeq \sum_{i=1}^{D} \alpha_2(\eta_i)h_i \sum_{j=1}^{D} \frac{\gamma(\mu_j)\eta_i k(\eta_i,\mu_j)h_j}{\eta_i-\mu_j} \qquad (C.5)$$

When j=i in the sum over j, we use L'Hospital's rule to write

$$\frac{\eta_i k(\eta_i,\mu_j)}{\eta_i-\mu_j} = \eta_i \log(1 + \frac{1}{\sigma\eta_i}) - \frac{\eta_i}{1+\sigma\eta_i} . \qquad (C.6)$$

Thus we have for Eq. (C.3) the set of equations

$$\alpha_2(\mu_k) = O(\mu_k)\psi'(\mu) - A_+^{(o)}O(\mu_k)\phi_+(\mu) - \frac{CO(\mu_k)\phi_+(\mu)}{M_{o+}} \sum_{i=1}^{D} \alpha_2(\eta_i)h_i \sum_{j=1}^{D}$$

$$(x) \frac{\gamma(\mu_j)\eta_i k(\eta_i,\mu_j)h_j}{\eta_i-\mu_j} + CO(\mu_k) \sum_{i=1}^{D} \frac{\alpha_2(\eta_i)\eta_i k(\eta_i,\mu)h_i}{\eta_i-\mu} \qquad (C.7)$$

For clarity, we write the explicit form for $O(\mu_k)\psi'(\mu)$,

$$O(\mu_k)\psi'(\mu) = \ell_1(\mu_k) \int_0^1 \frac{\mathbf{P}\gamma(\mu')\psi'(\mu')d\mu'}{\mu_k-\mu'} + \ell_2(\mu_k)\psi'(\mu_k) . \qquad (C.8)$$

Equation (C.7) in matrix-vector form is

$$\underline{\underline{A}}\,\underline{\alpha_2} = \underline{g} \tag{C.9}$$

where

$$A_{\ell m} = C\,\frac{O(\mu_\ell)\phi_+(\mu)}{M_{O+}}\,h_m \sum_{j=1}^{D} \frac{\gamma(\mu_j)\eta_m k(\eta_m,\mu_j)h_j}{\eta_m-\mu_j} - C\,O(\mu_\ell)\left[\frac{\eta_m k(\eta_m,\mu)h_m}{\eta_m-\mu}\right] \tag{C.10}$$

$$A_{\ell\ell} = 1 + \frac{C\,O(\mu_\ell)\phi_+(\mu)}{M_{O+}}\,h_\ell \sum_{j=1}^{D} \frac{\gamma(\mu_j)\eta_\ell k(\eta_\ell,\mu_j)h_j}{\eta_\ell-\mu_j} - CO(\mu_\ell)\left[\frac{\eta_\ell k(\eta_\ell,\mu)h_\ell}{\eta_\ell-\mu}\right] \tag{C.11}$$

$$\underline{\alpha_2} = \begin{bmatrix} \alpha_2(\mu_1) \\ \alpha_2(\mu_2) \\ \cdot \\ \cdot \\ \cdot \\ \alpha_2(\mu_D) \end{bmatrix} \qquad \underline{g} = \begin{bmatrix} O(\mu_1)\psi'(\mu)-A_+^{(o)}O(\mu_1)\phi_+(\mu) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ O(\mu_D)\psi'(\mu)-A_+^{(o)}\ (\mu_D)\phi_+(\mu) \end{bmatrix} \tag{C.12}$$

Equation (C.9) is now solved by standard matrix inversion. It was found that the iteration method (discussed in Chapter VI) was much faster with the same number of points. Nevertheless this matrix inversion method can always be applied for any value of C. One obvious requirement for a solution to Eq. (C.9) is

$$\det|\underline{\underline{A}}| \neq 0 .$$

APPENDIX D

COMPUTER CODE LISTING

Five computer programs are listed in this appendix. We denote these programs by Program 1, 2, 3, 4, and 5. For Program 1 we tabulate a list of principal variables and refer the reader to Table 2.1 for information on the number and type of eigenvalues. The false position method for finding the roots of a transcendental equation is discussed in Ref. 18. We have inserted remark cards into the other programs to give details of the solution procedure. In many cases these cards refer to the appropriate equations in the text.

We have listed the replacement cards at the end of Program 2, 3, and 4 which, when inserted into the previous program, will give a program for the solutions to the constant source problem. In Program 5 the changes for the DP_1 are almost analogous to the P_3, therefore, we have not listed these cards i.e., we have listed only the solution to the constant source problem in the DP_1 approximation. At the end of each program is a list of sample input data. All programming was done in the Michigan Algorithm Decoder (MAD) language.[26]

Program Number 1: List of Principal Variables

Program Symbol	Definition
D1	det $\lvert \underline{\underline{C}} \rvert$
C1	C_{11} (See Eq. (2.2))
C2	C_{12}
C3	C_{21}
C4	C_{22}
SIG	σ
OMEGAX.	Subroutine for calculating $\Omega(z)$ for z real (see Eq. (2.17))
OMEGAY.	Subroutine for calculating $\Omega(z)$ for z pure imaginary
ITMAX	Maximum number of iterations permitted for converging on the roots of $\Omega(z)$.[18]
EPS1	Convergence criterion for $\Omega(z)$.
EPS2	Criterion for terminating program when denominator is too small in false position method.[18]
ITX	Number of iterations, k.
FX(1)	$\Omega(x_1^k)$
FX(2)	$\Omega(x_2^k)$
FX(3)	$\Omega(x_3^k)$

PROGRAM 1

```
        R PROGRAM FOR FINDING THE REAL AND/OR IMAGINARY ROOTS OF THE
        R DISPERSION EQUATION FOR TWO GROUP TRANSPORT THEORY BY THE
        R FALSE POSITION METHOD
         DIMENSION X(3), FX(3), Y(3), FY(3)
         INTEGER ITMAX, ITX, ITY, I, J, R
START    READ AND PRINT DATA ITMAX, EPS1, EPS2,
        1C1, C2, C3, C4, SIG
           D1=C1*C4-C2*C3
           D2=C1+SIG*C4
         D3=C1+SIG*C4-2.*D1
           D4=D1*ELOG.((SIG+1.)/(SIG-1.))
         WHENEVER D1.E.0.
             WHENEVER D2.L.SIG/2.
             R=1
         PRINT COMMENT $ TWO REAL ROOTS$
             OR WHENEVER D2.G.SIG/2.
             R=2
             PRINT COMMENT $ TWO IMAGINARY ROOTS$
             OR WHENEVER D2.E.SIG/2.
             R=3
             PRINT COMMENT $ TWO INFINITE ROOTS$
             END OF CONDITIONAL
         OR WHENEVER D1.L.0.
             WHENEVER D3.L.SIG/2.
             R=1
             PRINT COMMENT $ TWO REAL ROOTS$
             OR WHENEVER D3.G.SIG/2.
             R=2
             PRINT COMMENT $ TWO IMAGINARY ROOTS$
             OR WHENEVER D3.E.SIG/2.
             R=3
             PRINT COMMENT $ TWO INFINITE ROOTS$
             END OF CONDITIONAL
         OR WHENEVER D1.G.0..AND.C4.G.D4
             WHENEVER D3.L.SIG/2.
             R=1
             PRINT COMMENT $ TWO REAL ROOTS$
             OR WHENEVER D3.G.SIG/2.
             R=2
             PRINT COMMENT $ TWO IMAGINARY ROOTS$
             OR WHENEVER D3.E.SIG/2.
             R=3
             PRINT COMMENT $ TWO INFINITE ROOTS$
             END OF CONDITIONAL
           OR WHENEVER D1.G.0..AND.C4.LE.D4
             WHENEVER C1.LE.SIG/2.AND.C4.GE.(1./2.).OR.
        1    C1.GE.SIG/2..AND.C4.LE.(1./2.)
             R=4
             PRINT COMMENT $ FOUR ROOTS TWO REAL AND TWO IMAGINARY$
```

PROGRAM 1 (Continued)

```
          OR WHENEVER C1.L.SIG/2..AND.C4.L.(1./2.)
          WHENEVER D3.L.SIG/2.
          R=5
          PRINT COMMENT $ FOUR REAL ROOTS$
          OR WHENEVER D3.G.SIG/2.
          R=4
          PRINT COMMENT $ FOUR ROOTS TWO REAL AND TWO IMAGINARY$
          OR WHENEVER D3.E.SIG/2.
          R=1
          PRINT COMMENT $ TWO REAL AND TWO INFINITE ROOTS$
          END OF CONDITIONAL
        OR WHENEVER C1.G.SIG/2..AND.C4.G.(1./2.)
          WHENEVER D3.L.SIG/2.
          R=6
          PRINT COMMENT $ FOUR IMAGINARY ROOTS$
          OR WHENEVER D3.G.SIG/2.
          R=4
          PRINT COMMENT $ TWO REAL AND TWO IMAGINARY ROOTS$
          OR WHENEVER D3.E.SIG/2.
          R=2
          PRINT COMMENT $ TWO IMAGINARY AND TWO INFINITE ROOTS$
          END OF CONDITIONAL
      END OF CONDITIONAL
      END OF CONDITIONAL
        WHENEVER R.E.1
      X=1.000001
      OMEGAR=OMEGAX.(X,C1,C4,D1,SIG)
      WHENEVER OMEGAR.L.0.
      THROUGH SERCH1, FOR X=1.100001,.1, OMEGAR.G.0..OR.X.G.20.
      WHENEVER X.G.19.75
      PRINT COMMENT $ NO SIGN CHANGE FROM NEG TO POS$
      THROUGH PRINT1, FOR Z=1.000001,.1, Z.G.20.
PRINT1  PRINT RESULTS Z, OMEGAX.(Z,C1,C4,D1,SIG)
      TRANSFER TO START
      END OF CONDITIONAL
SERCH1  OMEGAR=OMEGAX.(X,C1,C4,D1,SIG)
      OR WHENEVER OMEGAR.G.0.
      THROUGH SERCH2, FOR X=1.200001,.2, OMEGAR.L.0..OR.X.G.20.
      WHENEVER X.G.19.75
      PRINT COMMENT $ NO SIGH CHANGE FROM POS TO NEG$
      THROUGH PRINT2, FOR Z=1.000001,.2, Z.G.20.
PRINT2  PRINT RESULTS Z, OMEGAX.(Z,C1,C4,D1,SIG)
      TRANSFER TO START
      END OF CONDITIONAL
SERCH2  OMEGAR=OMEGAX.(X,C1,C4,D1,SIG)
      OTHERWISE
      PRINT COMMENT $ X=1.000001 IS A ROOT$
      TRANSFER TO START
      END OF CONDITIONAL
      X(1)=X-.2
```

PROGRAM 1 (Continued)

```
          X(2)=X-.1
          PRINT RESULTS X(1), OMEGAX.(X(1),C1,C4,D1,SIG),
         1X(2), OMEGAX.(X(2),C1,C4,D1,SIG)
            FX(1)=OMEGAX.(X(1),C1,C4,D1,SIG)
            FX(2)=OMEGAX.(X(2),C1,C4,D1,SIG)
            THROUGH LOOPXA, FOR ITX=1,1,ITX.G.ITMAX
          NUMER=X(2)*FX(1)-X(1)*FX(2)
            DENOM=FX(1)-FX(2)
            WHENEVER .ABS. DENOM.L..ABS.NUMER*EPS2
              PRINT COMMENT $ DENOMINATOR TOO SMALL$
            TRANSFER TO START
            END OF CONDITIONAL
            X(3)=NUMER/DENOM
            FX(3)=OMEGAX.(X(3),C1,C4,D1,SIG)
            WHENEVER.ABS.FX(3).LE.EPS1
            PRINT COMMENT $ PROCEDURE CONVERGED$
            PRINT RESULTS ITX,X(3),FX(3),R
          TRANSFER TO START
          END OF CONDITIONAL
          THROUGH LOOPXA, FOR I=1,1,I.G.2
          THROUGH LOOPXA, FOR J=I+1,1,J.G.3
          WHENEVER .ABS.FX(I).G..ABS.FX(J)
              TEMP=FX(I)
              FX(I)=FX(J)
              FX(J)=TEMP
              TEMP=X(I)
              X(I)=X(J)
              X(J)=TEMP
LOOPXA    END OF CONDITIONAL
          PRINT COMMENT $ NO CONVERGENCE$
            TRANSFER TO START
          OR WHENEVER R.E.2
          THROUGH SERCH3, FOR Y=.0001,.2, OMEGAI.L.0..OR.Y.G.40.
          WHENEVER Y.G.37.5
          PRINT COMMENT $ NO SIGN CHANGE FROM POS TO NEG$
          THROUGH PRINT3, FOR M=.0001,.2, M.G.40.
PRINT3    PRINT RESULTS M, OMEGAY.(M,C1,C4,D1,SIG)
          TRANSFER TO START
          END OF CONDITIONAL
SERCH3    OMEGAI=OMEGAY.(Y,C1,C4,D1,SIG)
          WHENEVER OMEGAY.(.0001,C1,C4,D1,SIG).L.0.
          Y(1)=.0001
          Y(2)=.2001
          OTHERWISE
          Y(1)=Y-.4
          Y(2)=Y-.2
          END OF CONDITIONAL
          PRINT RESULTS Y(1), OMEGAY.(Y(1),C1,C4,D1,SIG),
         1Y(2), OMEGAY.(Y(2),C1,C4,D1,SIG)
          FY(1)=OMEGAY.(Y(1),C1,C4,D1,SIG)
```

PROGRAM 1 (Continued)

```
        FY(2)=OMEGAY.(Y(2),C1,C4,D1,SIG)
        THROUGH LOOPYB,FOR ITY=1,1,ITY.G.ITMAX
        NUMER=Y(2)*FY(1)-Y(1)*FY(2)
        DENOM=FY(1)-FY(2)
          WHENEVER .ABS.DENOM.L..ABS.NUMER*EPS2
          PRINT COMMENT $ DENOMINATOR TOO SMALL$
          TRANSFER TO START
          END OF CONDITIONAL
          Y(3)=NUMER/DENOM
        FY(3)=OMEGAY.(Y(3),C1,C4,D1,SIG)
          WHENEVER .ABS.FY(3).LE.EPS1
          PRINT COMMENT $ PROCEDURE CONVERGED$
          PRINT RESULTS ITY, Y(3),FY(3),R
          TRANSFER TO START
          END OF CONDITIONAL
          THROUGH LOOPYB, FOR I=1,1,I.G.2
        THROUGH LOOPYB, FOR J=I+1,1,J.G.3
        WHENEVER .ABS. FY(I).G..ABS.FY(J)
          TEMP=FY(I)
          FY(I)=FY(J)
          FY(J)=TEMP
          TEMP=Y(I)
          Y(I)=Y(J)
          Y(J)=TEMP
 LOOPYB END OF CONDITIONAL
        PRINT COMMENT $ NO CONVERGENCE$
        OR WHENEVER R.E.4
        THROUGH SERCH4, FOR X=1.000001,.05,OMEGAR.L.0..OR.X.G.20.
        WHENEVER X.G.19.75
        PRINT COMMENT $ NO SIGN CHANGE FOR REAL ROOTS$
        THROUGH PRINT4, FOR N=1.000001,.2, N.G.20.
PRINT4  PRINT RESULTS N, OMEGAX.(N,C1,C4,D1,SIG)
        TRANSFER TO IMAGR
        END OF CONDITIONAL
SERCH4  OMEGAR=OMEGAX.(X,C1,C4,D1,SIG)
        WHENEVER OMEGAX.(1.000001,C1,C4,D1,SIG).L.0.
        X(1)=1.000001
        X(2)=1.100001
        OTHERWISE
        X(1)=X-.1
        X(2)=X-.05
        END OF CONDITIONAL
        PRINT RESULTS X(1), OMEGAX.(X(1),C1,C4,D1,SIG),
       1X(2), OMEGAX.(X(2),C1,C4,D1,SIG)
          FX(1)=OMEGAX.(X(1),C1,C4,D1,SIG)
          FX(2)=OMEGAX.(X(2),C1,C4,D1,SIG)
          THROUGH LOOPXC, FOR ITX=1,1,ITX.G.ITMAX
          NUMER=X(2)*FX(1)-X(1)*FX(2)
        DENOM=FX(1)-FX(2)
        WHENEVER .ABS. DENOM.L..ABS.NUMER*EPS2
```

PROGRAM 1 (Continued)

```
         PRINT COMMENT $ DENOMINATOR FOR REAL ROOTS TOO SMALL$
         TRANSFER TO IMAGR
         END OF CONDITIONAL
         X(3)=NUMER/DENOM
         FX(3)=OMEGAX.(X(3),C1,C4,D1,SIG)
         PRINT RESULTS X(3), FX(3)
         WHENEVER .ABS.FX(3).LE.EPS1
         PRINT COMMENT $ PROCEDURE FOR REAL ROOTS CONVERGED$
         PRINT RESULTS ITX, X(3), FX(3), R
         TRANSFER TO IMAGR
         END OF CONDITIONAL
         THROUGH LOOPXC, FOR I=1,1,I.G.2
         THROUGH LOOPXC, FOR J=I+1,1,J.G.3
         WHENEVER .ABS.FX(I).G..ABS.FX(J)
         TEMP=FX(I)
         FX(I)=FX(J)
         FX(J)=TEMP
         TEMP=X(I)
         X(I)=X(J)
         X(J)=TEMP
         PRINT RESULTS X(1), FX(1), X(2), FX(2)
 LOOPXC  END OF CONDITIONAL
         PRINT COMMENT $ NO CONVERGENCE FOR REAL ROOTS$
IMAGR    THROUGH SERCH5, FOR Y=.0001,.05,OMEGAI.L.0..OR.Y.G.40.
         WHENEVER Y.G.40.
         PRINT COMMENT $ NO SIGN CHANGE FOR IMAG ROOTS$
         THROUGH PRINT5, FOR T=.0001,.2, T.G.40.
PRINT5   PRINT RESULTS T, OMEGAY.(T,C1,C4,D1,SIG)
         TRANSFER TO START
         END OF CONDITIONAL
SERCH5   OMEGAI=OMEGAY.(Y,C1,C4,D1,SIG)
         Y(1)=Y-.10
         Y(2)=Y-.05
         PRINT RESULTS Y(1), OMEGAY.(Y(1),C1,C4,D1,SIG),
        1Y(2), OMEGAY.(Y(2),C1,C4,D1,SIG)
         FY(1)=OMEGAY.(Y(1),C1,C4,D1,SIG)
         FY(2)=OMEGAY.(Y(2),C1,C4,D1,SIG)
         THROUGH LOOPYD, FOR ITY=1,1,ITY.G.ITMAX
         NUMER=Y(2)*FY(1)-Y(1)*FY(2)
         DENOM=FY(1)-FY(2)
         WHENEVER .ABS. DENOM.L..ABS.NUMER*EPS2
         PRINT COMMENT $ DENOMINATOR FOR IMAG. ROOTS TOO SMALL$
         TRANSFER TO START
         END OF CONDITIONAL
         Y(3)=NUMER/DENOM
         FY(3)=OMEGAY.(Y(3),C1,C4,D1,SIG)
         PRINT RESULTS Y(3), FY(3)
         WHENEVER .ABS. FY(3).LE.EPS1
         PRINT COMMENT $ PROCEDURE FOR IMAG. ROOTS CONVERGED$
         PRINT RESULTS ITY,Y(3),FY(3),R
```

PROGRAM 1 (Concluded)

```
          TRANSFER TO START
          END OF CONDITIONAL
          THROUGH LOOPYD, FORJ=I+1,1,J.G.3
          WHENEVER .ABS. FY(I).G..ABS.FY(J)
          THROUGH LOOPYD,FORI=1,1,I.G.2
          THROUGH LOOPYD, FOR J=I+1,1,J.G.3
          TEMP=FY(I)
          FY(I)=FY(J)
          FY(J)=TEMP
          TEMP=Y(I)
          Y(I)=Y(J)
          Y(J)=TEMP
          PRINT RESULTS Y(1), FY(1), Y(2), FY(2)
 LOOPYD   END OF CONDITIONAL
          PRINT COMMENT $ NO CONVERGENCE FOR IMAG ROOTS$
          OTHERWISE
          PRINT COMMENT $ ROOTS ARE INFINITE OR WE HAVE
         1 FOUR REAL OR FOUR IMAGINARY ROOTS$
          END OF CONDITIONAL
          TRANSFER TO START
          END OF PROGRAM
$ COMPILE MAD, EXECUTE
          EXTERNAL FUNCTION (X,C1,C4,D1,SIG)
          INTERNAL FUNCTION T1.(X)=X*ELOG.((SIG*X+1.)/(SIG*X-1.))
          INTERNAL FUNCTION T2.(X)=X*ELOG.((X+1.)/(X-1.))
          ENTRY TO OMEGAX.
          OMEGAX=1.-C1*T1.(X)-C4*T2.(X)+D1*T1.(X)*T2.(X)
          FUNCTION RETURN OMEGAX
          END OF FUNCTION
$ COMPILE MAD, EXECUTE
          EXTERNAL FUNCTION(Y,C1,C4,D1,SIG)
          INTERNAL FUNCTION S1.(Y)=2.*Y*ATAN.(1./(SIG*Y))
          INTERNAL FUNCTION S2.(Y)=2.*Y*ATAN.(1./Y)
          ENTRY TO OMEGAY.
          OMEGAY=1.-C1*S1.(Y)-C4*S2.(Y)+D1*S1.(Y)*S2.(Y)
          FUNCTION RETURN OMEGAY
          END OF FUNCTION
$ DATA
$ DATA
 ITMAX=50, EPS1=1.E-7, EPS2=1.E-20, C1=.59023, C2=.05448, C3=.15963,
 C4=.44320, SIG=1.50951      *
```

PROGRAM 2

```
$ COMPILE MAD, EXECUTE
          R THIS IS THE SOLUTION FOR THE EXACT MILNE PROBLEM                  OM
           DIMENSION Y(16), S(16), W1(16), W2(16), T(16), T1(16), R(16),
          1 R1(16), KY(16), KS(16), KY1(16), KS1(16), DIFF(32),
          1 Z1(92), KAPP(92), GU(96), ELG(92), ELG1(92), FK(8648,DIN),
          1 FU(846,VIM), FUL(10), FUU(10), FUM(10), XFMI(92), OMAG1(92),
          1 OMAG2(92), ALPHA2(828,VIN), SU(96), DIF(92), FKK(92),
          1 FKU(92), FTK(92), ALPHA1(92), ANGR1(184), FUMM(10),
          1 FUMP(10), ANG(92), ANG0(92), ANG1(92), AGDIP2(92),
          1 AGDIM2(92), AGDIP1(92), AGDIM1(92), Z2(92),XFPI(92),
          1 OPHI(92), OPSI(92), FBK(92), EXPO(92), Z3(20), ANGR(184)
           INTEGER P1, K, P, J, I, L, ITMAX, ITMAXX, L1, P3, D, ZEE
           VECTOR VALUES VIM=2,0,0
           VECTOR VALUES VIN=2,0,0
           VECTOR VALUES DIN=2,0,0
           PROGRAM COMMON FU, FUL, FUM, FUU, N, ELG, Z1, H1, H2, P3, D,
          1  SG
          R VECTOR VALUES FOR GAUSS QUADRATURE
           VECTOR VALUES X(1)=.0950125098, .2816035508, .4580167777,
          1 .6178762444, .7554044084,.8656312024, .9445750231,
          2 .9894009350
           VECTOR VALUES W(1)=.1894506105, .1826034150, .1691565194,
          1 .1495959888, .1246289713, .0951585117, .0622535239,
          2 .0271524594
           FTRAP.
          R INTERNAL FUNCTIONS FOR KAPPA FUNCTION CALCULATION
           INTERNAL FUNCTION F.(V1,Y1,KAP)=(1.-V1*V1*X02)*V1/((1.-V1*V1/
          1 (ETA*ETA))*(V1+Y1)*KAP)
           INTERNAL FUNCTION FG.(V1,Y1,KAP)=1./((V1+Y1)*KAP)
 START     READ AND PRINT DATA
          R NOTE THAT P, P3 AND D ARE DECLARED TO BE INTEGERS
           P=N
           P3=N3
           D=P+P3
           VIM(2)=D+2
           VIN(2)=D
           DIN(2)=D+2
          R THIS PART OF PROGRAM OBTAINS A KAPPA FUNCTION WITHIN A
          R SPECIFIED ACCURACY EPS
          R PARAMETERS FOR GAUSS QUADRATURE INTERVAL FROM 1./SIG TO 1.
           A=(SIG-1.)/(2.*SIG)
           B=(SIG+1.)/(2.*SIG)
          RCALCULATION OF DETERMINANT OF C MATRIX SEE EQ.(2.2)
           D1=C1*C4-C2*C3
          R R.H.S. OF EQ.(A.14) MULTIPLIED BY C
           Q=D1/SIG*(SIG*(ELOG.((SIG+1.)/(SIG-1.)))+ELOG.(SIG*SIG-1.))
          R SEE EQ.(A.2) AND EQ.(A.5),(X(0) SQUARED)
           X02=1./((1.-2.*C1/SIG-2.*C4+4.*D1/SIG)*(ETA*ETA))
           THROUGH EVAL, FOR K=1,1, K.G.8
```

PROGRAM 2 (Continued)

```
      R NEW VARIABLES CALCULATED FOR GAUSS QUADRATURE, REGION 1
      R SEE REF. (18)
       Y(K)=X(K)/(2.*SIG)+1./(2.*SIG)
       Y(K+8)=-X(K)/(2.*SIG)+1./(2.*SIG)
       W1(K)=W(K)/(2.*SIG)
       W1(K+8)=W(K)/(2.*SIG)
      R NEW VARIABLES CALCULATED FOR GAUSS QUADRATURE, REGION 2
       S(K)=X(K)*A+B
       S(K+8)=-X(K)*A+B
       W2(K)=W(K)*A
EVAL   W2(K+8)=W(K)*A
       THROUGH EVAL2, FOR J=1,1, J.G.16
      R FUNCTIONS IN EQ.(A.13) THAT ARE DEPENDENT ON INTEGRATION IN-
      R TERVAL (MU) ONLY  (NOTE GAUSS WEIGHTS ARE INCLUDED)
       T(J)=(C4+C1-D1*Y(J)*ELOG.((1.+Y(J))/(1.-Y(J))))*(1.-Y(J)*Y(J)
      1 *X02)*W1(J)/(1.-Y(J)*Y(J)/(ETA*ETA))
       T1(J)=W1(J)*D1*ELOG.((1.+SIG*Y(J))/(1.-SIG*Y(J)))
       R(J)=W2(J)*C4*(1.-S(J)*S(J)*X02)/ (1.-S(J)*S(J)/(ETA*ETA))
EVAL2  R1(J)=W2(J)*D1*ELOG.((SIG*S(J)+1.)/(SIG*S(J)-1.))
       INTERNAL FUNCTION (Z)
       ENTRY TO G.
      R THIS INTERNAL FUNCTION CALCULATES KAPPA FOR A SPECIFIED Z
       SUM=0
       THROUGH EVAL3, FOR L=1,1, L.G.16
EVAL3  SUM=SUM+T(L)*FG.(Y(L),Z,KY(L))-T1(L)*(F.(Y(L),Z,KY(L))-F.(1./
      1 SIG,Z,KSG))+R(L)*FG.(S(L),Z,KS(L))-R1(L)*(F.(S(L),Z,KS(L))-
      2 F.(1./SIG,Z,KSG))
       FUNCTION RETURN 1.-Z*SUM+Q*Z*F.(1./SIG,Z,KSG)
       END OF FUNCTION
      R AN ITERATION PROCESS COMMENCES AT THIS POINT WHERE FOR
      R INITIAL VALUS OF KAPPA WE SET KAPPA=1. THE ITERATION
      R CONTINUES UNTIL THE MAXIMUM DIFFERENCE BETWEEN ANY TWO
      R VALUES OF KAPPA IS LESS THAN EPS
       MAX=1.
       KSG=1.
       THROUGH EVAL4, FOR L=1,1, L.G.16
       KY(L)=1.
EVAL4  KS(L)=1.
       THROUGH EVAL5, FOR J=1,1, J.G.ITMAX.OR.MAX.L.EPS
       THROUGH EVAL6, FOR K=1,1, K.G.16
       KY1(K)=G.(Y(K))
       KS1(K)=G.(S(K))
       DIFF(K)=.ABS.(KY(K)-KY1(K))
EVAL6  DIFF(K+16)=.ABS.(KS(K)-KS1(K))
       KSG1=G.(1./SIG)
       MAX=DIFF(1)
       THROUGH ALPHA, FOR L=2,1, L.G.32
ALPHA  WHENEVER DIFF(L).G.MAX, MAX=DIFF(L)
       WHENEVER J.G.ITMAX
       PRINT COMMENT $ MAXIMUM NUMBER OF ITERATIONS FOR KAP EXCEED$
```

PROGRAM 2 (Continued)

```
          PRINT RESULTS MAX, J
          TRANSFER TO START
          OR WHENEVER MAX.L.EPS
          PRINT COMMENT $ PROCEDURE FOR KAPPA FUNCTION CONVERGED$
          PRINT RESULTS MAX, J, KY(1)...KY(16), KS(1)...KS(16)
          TRANSFER TO GO
          OTHERWISE
          KSG=KSG1
          THROUGH SWITCH, FOR L1=1,1, L1.G.16
          KY(L1)=KY1(L1)
SWITCH    KS(L1)=KS1(L1)
EVAL5     END OF CONDITIONAL
         R THIS CONCLUDES THE CALCULATION OF KAPPA
 GO       CONTINUE
         R NUMBER NEEDED FOR X-FUNCTION AND GAMMA FUNCTION
          SR=1./SQRT.(X02)
         R SET-UP MESH SPACING MIDPOINT VALUES
          SG=1./SIG
         R INTERVAL SPACING FOR REGION 1
          H1=SG/N
         R INTERVAL SPACING FOR REGION 2
          H2=(1.-SG)/N3
          K=1
         R MIDPOINT VALUES OF MU VARIABLE DETERMINED
          THROUGH COMP1, FOR U=1.,1., K.G.D
          WHENEVER K.LE.P
          Z1(K)=(U-.5)*H1
          OTHERWISE
          Z1(K)=Z1(P)+.5*H1+(U-N-.5)*H2
          END OF CONDITIONAL
   COMP1  K=K+1
          PRINT RESULTS SG, H1, H2, Z1(1)...Z1(D)
         R VARIOUS CONSTANTS NEEDED LATER
         R IF WE WANT TO SOLVE THE EXACT CONSTANT SOURCE PROBLEM WE
         R INSERT CARDS NO. 1S, 2S, 3S AND 4S
          PI=3.14159265
         R HERE WE CALCULATE KAPPA FIRST AT 1./SIG AND 1. AND THEN
         R GAMMA AT THESE SAME VALUES
          KAPSG=G.(SG)
          GU(D+1)=SG*ETA*ETA*(SR+SG)*X02/((ETA*ETA-SG*SG)*KAPSG)
          KAONE=G.(1.)
          GU(D+2)=ETA*ETA*(SR+1.)*X02/((ETA*ETA-1.)*KAONE)
         R KAPPA AT TWO DISCRETE ROOTS
          KAPM=G.(ETA)
          KAPP=G.(-ETA)
         R FIRST TERM IN EQ.(4.10) FOR DISCRETE ROOTS ONLY
          ELGETP=ETA*ELOG.(1.+SG/ETA)
         R MILNE CARD ONLY
          ELGETM=-ETA*ELOG.(1.-SG/ETA)
         R SEE EQUATION FOLLOWING EQ.(2.20)
```

PROGRAM 2 (Continued)

```
 ANGC=C4-D1*(ELGETP+ELGETM)
R THE LAST TERM IN EQ.(4.10) CALCULATED FOR 1. AND 1./SIG
 ELGONE=ELOG.(1.+SG)
 ELGSG=SG*ELOG.(2.)
R EQS.(6.2) AND (6.3) EVALUATED AT 0., 1./SIG AND 1.
 FUL(1)=0.
 FUL(2)=0.
 FUM(1)=GU(D+1)*ETA/(ETA+SG)*(ELGETM-ELGSG)                    5M
 FUM(2)=GU(D+1)*ETA/(ETA-SG)*(ELGETP-ELGSG)
 FUU(1)=GU(D+2)*ETA/(ETA+1.)*(ELGETM-ELGONE)                   6M
 FUU(2)=GU(D+2)*ETA/(ETA-1.)*(ELGETP-ELGONE)
R X-FUNCTION EVALUATED AT DISCRETE ROOTS (SEE EQ.(A.15)
R MILNE CARD ONLY
 XFM=KAPM/(SR+ETA)
 XFP=KAPP/(SR-ETA)
 PRINT RESULTS KAPSG, GU(D+1), KAONE, GU(D+2), KAPM, ELGETM,
1 ELGONE, ELGSG, XFM, XFP
R INTERNAL FUNCTION FOR THE BOUNDARY VALUES OF OMEGA EQ.(2.21)
 INTERNAL FUNCTION OM4.(Z)=Z
 INTERNAL FUNCTION O1.(Z)=Z*ELOG.((1.+Z)/(1.-Z))
 INTERNAL FUNCTION O2.(Z)=Z*ELOG.((1.+SIG*Z)/(1.-SIG*Z))
 INTERNAL FUNCTION O3.(Z)=Z*ELOG.((SIG*Z+1.)/(SIG*Z-1.))
 THROUGH COMP2, FOR K=1,1, K.G.D
R COMPUTATION TO CHANGE MU VARIABLE TO ANGLE IN DEGREES FOR
R EASIER PLOTTING
 ANRP=ARCCOS.(Z1(K))
 ANRM=ARCCOS.(-Z1(K))
 ANGR(K)=ANRP*360./(2.*PI)
 ANGR(K+D) =ANRM*360./(2.*PI)
 WHENEVER Z1(K).L.SG
 Z11=Z1(K)*SIG
 ANRP1=ARCCOS.(Z11)
 ANRM1=ARCCOS.(-Z11)
 ANGR1(K)=ANRP1*360./(2.*PI)
 ANGR1(K+P) =ANRM1*360./(2.*PI)
 END OF CONDITIONAL
R CALCULATION OF KAPPA THEN GAMMA FUNCTION FOR ALL MIDPOINT
R VALUES (SEE EQ.(A.17))
 KAPP(K)=G.(Z1(K))
 GU(K)=Z1(K)*ETA*ETA*(SR+Z1(K))*X02/((ETA*ETA-Z1(K)*Z1(K))*
1 KAPP(K))
R CALCULATION OF LOGARITHM TERM IN EQ.(6.6)
 ELG(K)=ELOG.((1.-Z1(K))/Z1(K))
R LAST TERM OF EQ.(4.10) EVALUATED AT ALL MIDPOINT VALUES
 ELG1(K)=Z1(K)*ELOG.(1.+SG/Z1(K))
R CALCULATION OF EQ.(6.2) AND EQ.(6.3) AT ALL MIDPOINT VALUES
 FKU(K)=ETA/(ETA-Z1(K))*(ELGETP-ELG1(K))
 FU(2,K)=GU(K)*FKU(K)
  FKK(K)=ETA/(ETA+Z1(K))*(ELGETM-ELG1(K))                      7M
 FU(1,K)=GU(K)*FKK(K)
```

PROGRAM 2 (Continued)

```
       R EQS.(4.22) EVALUATED FOR EACH REGION
        WHENEVER Z1(K).L.SG
        S1=O1.(Z1(K))
        S2=O2.(Z1(K))
        S3=OM4.(Z1(K))
        S4=S3*S3
        DENOM1=(1.-C4*S1-C1*S2+D1*S1*S2-PI*PI*D1*S4).P.2+PI*PI*S4*
       1 (C4+C1-D1*(S2+S1)).P.2
        NUMN1=S3*(C4+C1-D1*(S1+S2))
        NUMP1=1.-C4*S1-C1*S2+D1*S1*S2-PI*PI*D1*S4
        OMAG1(K) = NUMN1/(DENOM1*GU(K))
          OMAG2(K)      =NUMP1/DENOM1
       R FIRST TERM OF EQS.(4.42) AND (5.8) EVALUATED
       R MILNE CARD ONLY
        XFMI(K)=ETA*XFM/(ETA+Z1(K))*OMAG1(K)
        XFPI(K)=OMAG1(K)*ETA*XFP/(ETA-Z1(K))
       R FUNCTIONS NEEDED LATER FOR ANGULAR DISTRIBUTIONS
        ANG(K)=C4-D1*S2
        ANG1(K)=C1-D1*S1
        ANGO(K)=NUMP1+PI*PI*D1*S4
       R SAME REMARKS AS ABOVE BUT FOR REGION 2
        OTHERWISE
        T1=O1.(Z1(K))
        T2=O3.(Z1(K))
        T3=OM4.(Z1(K))
        T4=T3*T3
        DENOM2=(1.-C4*T1-C1*T2+D1*T1*T2).P.2+PI*PI*T4*(C4-D1*T2).P.2
        NUMN2=T3*(C4-D1*T2)
        NUMP2=1.-C4*T1-C1*T2+D1*T1*T2
        OMAG1(K) =NUMN2/(DENOM2*GU(K))
          OMAG2(K)      =NUMP2/DENOM2
       R MILNE CARD ONLY
        XFMI(K)=ETA*XFM/(ETA+Z1(K))*OMAG1(K)
        XFPI(K)=OMAG1(K)*ETA*XFP/(ETA-Z1(K))
        ANG(K)=C4-D1*T2
        ANGO(K)=NUMP2
        ANG1(K)=0.
COMP2   END OF CONDITIONAL
       R INTEGRALS IN EQ.(5.9A) EVALUATED EXCEPT INTEGRAL WITH ALPHA2
       R A SUBROUTINE IS USED WHICH IS FOUND AT END OF PROGRAM
        INTEGM=INT.(1)
        INTEGP=INT.(2)
       R EQ.(4.35) EVALUATED
        APLDEN=-ETA*XFP-D1*INTEGP
       R EQ.(6.16) EVALUATED
        APLUS1=(-ETA*XFM+D1*INTEGM)/APLDEN                              8M
        PRINT RESULTS KAPP(1)...KAPP(D), GU(1)...GU(D),
       1 ELG(1)...ELG(D), ANGO(1)...ANGO(D), FKK(1)...FKK(D),
       1 FU(1,1)...FU(1,D), XFMI(1)...XFMI(D), FUM(1), FUU(1),
       1OMAG1(1)...OMAG1(D), OMAG2(1)...OMAG2(D),
```

PROGRAM 2 (Continued)

```
        1 XFPI(1),..XFPI(D), APLUS1, APLDEN,     INTEGP, INTEGM
         THROUGH COMP3, FOR K=1,1, K.G.D
        R EQS.(4.42) AND (5.8) EVALUATED, PVI. IS A SUBROUTINE LISTED
        R AT THE END  WHICH CALCULATES PRINCIPAL VALUE INTEGRALS
         OPHI(K)=D1*(OMAG1(K)*PVI.(1,2,K)-OMAG2(K)*FKU(K))+XFPI(K)
         OPSI(K)=-D1*(OMAG1(K)*PVI.(1,1,K)-OMAG2(K)*FKK(K))-XFMI(K)       9M
        R INITIAL VALUE OF ALPHA2 CALCULATED SEE EQ.(6.17)
         ALPHA2(1,K)=OPSI(K)-APLUS1*OPHI(K)
COMP3    PRINT RESULTS Z1(K), ALPHA2(1,K), OPHI(K), OPSI(K)
        R INTEGRAND IN SECOND TERM OF NUMERATOR OF EQ.(4.43A)
        R CALCULATED EXCLUDING ALPHA2
         THROUGH COMP4, FOR J=1,1, J.G.D
         THROUGH COMP4, FOR K=1,1, K.G.D+2
         WHENEVER K.E.D+1
         FK(J,K)=Z1(J)/(Z1(J)-SG)*(ELG1(J)-ELGSG)
         OR WHENEVER K.E.D+2
         FK(J,K)=Z1(J)/(Z1(J)-1.)*(ELG1(J)-ELGONE)
         OR WHENEVER J.E.K
         FK(J,K)=ELG1(K)-Z1(K)/(1.+SIG*Z1(K))
         OTHERWISE
         FK(J,K)=Z1(J)/(Z1(J)-Z1(K))*(ELG1(J)-ELG1(K))
COMP4    END OF CONDITIONAL
        R HERE WE START THE ITERATION PROCEDURE FOR APLUS AND ALPHA2
         MAXX=1.
         THROUGH COMP5, FOR J=2,1, J.G.ITMAXX.OR.MAXX.L.EPSI
         THROUGH COMP6, FOR K=1,1, K.G.D+2
        R FIRST INTEGRATION PERFORMED IN EQ.(4.43A)
         SUM1=0.
         SUM2=0.
         THROUGH COMP7, FOR I=1,1, I.G.D
         WHENEVER I.LE.P
         SUM1=SUM1+FK(I,K)*ALPHA2(J-1,I)
         OTHERWISE
         SUM2=SUM2+FK(I,K)*ALPHA2(J-1,I)
COMP7    END OF CONDITIONAL
         SU(K)=SUM1*H1+SUM2*H2
COMP6    FU(J,K)=SU(K)*GU(K)
        R SECOND INTEGRATION PERFORMED IN EQ.(4.43A)
         INTG=INT.(J)
        R NEW VALUE OF A+ CALCULATED
         APLUS=APLUS1+INTG/APLDEN*D1
         PRINT RESULTS FU(J,1)...FU(J,D+2), SU(1)...SU(D+2) , INTG
         FUL(J)=0.
        R FUNCTIONS NEEDED FOR NEXT PRINCIPAL VALUE INTEGRAL
         FUM(J)=FU(J,D+1)
         FUU(J)=FU(J,D+2)
         PRINT RESULTS FUL(J), FUM(J), FUU(J), APLUS
         THROUGH COMP8, FOR K=1,1, K.G.D
        R NEW VALUES OF ALPHA2
         ALPHA2(J,K)=OPSI(K)-APLUS*OPHI(K)+D1*(-OMAG1(K)*PVI.(1,J,K)+
```

PROGRAM 2 (Continued)

```
         1 OMAG2(K)*SU(K))
         R DIFFERENCE BETWEEN PREVIOUS AND NEW VALUES OF ALPHA2
COMP8     DIF(K)=ALPHA2(J,K)-ALPHA2(J-1,K)
          PRINT RESULTS DIF(1)...DIF(D)
         R LOCATE MAXIMUM DIFFERENCE
          MAXX=.ABS.(DIF(1))
          THROUGH COM1, FOR L=2,1, L.G.D
COM1      WHENEVER .ABS.(DIF(L)).G.MAXX, MAXX=.ABS.(DIF(L))
          WHENEVER J.E.ITMAXX
          PRINT COMMENT $ MAXIMUM NUMBER OF ITERATIONS FOR ALPHA2 EXD$
          PRINT RESULTS MAXX, J
          TRANSFER TO START
         R EPSI IS CRITERION FOR TERMINATION OF ITERATION PROCEDURE
          OR WHENEVER MAXX.L.EPSI
          PRINT COMMENT $ PROCEDURE FOR ALPHA2 CONVERGED$
          TRANSFER TO GOO
          OTHERWISE
          PRINT RESULTS MAXX, J, ALPHA2(J,1)...ALPHA2(J,D)
COMP5     END OF CONDITIONAL
GOO       PRINT RESULTS ALPHA2(J,1)...ALPHA2(J,D), Z1(1)...Z1(D), MAXX
         R FINAL CONVERGED CALCULATION OF A+ (SEE EQ.(5.9C))
          THROUGH  COM5, FOR K=1,1, K.G.D
          SUM1=0.
          SUM2=0.
          THROUGH  COM6, FUR I=1,1, I.G.D
          WHENEVER I.LE.P
          SUM1=SUM1+FK(I,K)*ALPHA2(J,I)
          OTHERWISE
          SUM2=SUM2+FK(I,K)*ALPHA2(J,I)
COM6      END OF CONDITIONAL
          SU(K)=SUM1*H1+SUM2*H2
COM5      FU(J,K)=SU(K)*GU(K)
          ALPAI=INT.(J)
          PRINT RESULTS SU(1)...SU(D), FU(J,1)...FU(J,D)
          THROUGH COM4, FOR K=1,1, K.G.D
COM4      FU(J+1,K)=Z1(K)*ALPHA2(J,K)
          APLUS=APLUS1+ALPAI/APLDEN*D1
          FUL(J+1)=0.
          FUM(J+1)=0.
          FUU(J+1)=0.
          THROUGH COM3, FOR K=1,1, K.G.D
          ALPHA1(K)=-ETA*C2*C1*(1./(ETA+Z1(K))+APLUS/(ETA-Z1(K)))-C2*C1    10M
         1*PVI.(1,J+1,K)
COM3      PRINT RESULTS Z1(K), ALPHA1(K)
         R INTERNAL FUNCTION FOR QUADRATIC INTERPOLATION
          INTERNAL FUNCTION QUAD.(Z,X0,F0,X1,F1,X2,F2)=F0+(Z-X0)*(F1-
         1 F0)/(X1-X0)+(Z-X0)*(Z-X1)/(X2-X0)*((F2-F1)/(X2-X1)-(F1-F0)
         1 /(X1-X0))
         R MILNE CARD ONLY
          EXTRAP=-ETA/2.*ELOG.(-1./APLUS)
```

PROGRAM 2 (Continued)

```
          PRINT RESULTS APLUS, EXTRAP,      ALPAI
         R CALCULATION OF ANGULAR DISTRIBUTION FOLLOWS(SEE EQS.(5,14)
         R AND (5.15))
          THROUGH C04, FOR L=1,1, L.G.ZEE
          THROUGH C06, FOR K=1,1, K.G.D
C06       EXPO(K)=EXP.(-Z3(L)/Z1(K))
          THROUGH C01, FOR K=1,1, K.G.D
          SUM1=0.
          SUM2=0.
          SUM3=0.
          SUM4=0.
          SUM5=0.
          SUM6=0.
          FU(1,K)=Z1(K)*ALPHA1(K)*EXPO(K)
          FU(2,K)=Z1(K)*ANG(K)*ALPHA2(J,K)*EXPO(K)
           FU(3,K)=Z1(K)*ALPHA2(J,K)*EXPO(K)
          THROUGH C03, FOR I=1,1, I.G.D
          WHENEVER I.LE.P
          SUM1=SUM1+Z1(I)*ALPHA1(I)/(Z1(I)+Z1(K))*EXPO(I)
          SUM2=SUM2+Z1(I)*ANG(I)*ALPHA2(J,I)/(Z1(I)+Z1(K))*EXPO(I)
          SUM3=SUM3+Z1(I)*ALPHA2(J,I)/(Z1(I)+Z1(K))*EXPO(I)
          WHENEVER Z1(K).G.SG,SUM6 =SUM6 +Z1(I)*ALPHA1(I)/(Z1(I)-Z1(K))
         1 *EXPO(I)
          OTHERWISE
          SUM4=SUM4+Z1(I)*ANG(I)*ALPHA2(J,I)/(Z1(I)+Z1(K))*EXPO(I)
          SUM5 =SUM5 +Z1(I)*ALPHA2(J,I)/(Z1(I)+Z1(K))*EXPO(I)
C03       END OF CONDITIONAL
          FKK(K)=SUM1*H1
          FKU(K)=SUM2*H1+SUM4*H2
          FTK(K)=SUM3*H1+SUM5*H2
C01       FBK(K)=H1*SUM6
          FUL(1)=0.
          FUM(1)=SG*QUAD.(SG,Z1(P-1),ALPHA1(P-1),Z1(P),ALPHA1(P),Z1(P+1
         1),ALPHA1(P+1))*EXP.(-Z3(L)/SG)
          FUL(2)=0.
          SG1=ALPHA2(J,P-1)*ANG(P-1)
          SG2=ALPHA2(J,P)*ANG(P)
          SG3=ALPHA2(J,P+1)*ANG(P+1)
          FUM(2)=SG*QUAD.(SG,Z1(P-1),SG1,Z1(P),SG2,Z1(P+1),SG3)*EXP.(
         1 -Z3(L)/SG)
          PRINT RESULTS SG1, SG2, SG3, FUM(2)
          FUU(2)=0.
          FUL(3)=0.
          FUM(3)=0.
          FUU(3)=0.
         R MILNE CARD ONLY
          EXPETM=EXP.(Z3(L)/ETA)
          EXPETP=EXP.(-Z3(L)/ETA)
          THROUGH C02, FOR K=1,1, K.G.D
          AGDIM2(K)=ETA*ANGC/(ETA-Z1(K))*EXPETM+ETA*ANGC*APLUS/(ETA+Z1(    11M
```

```
        1 K))*EXPETP-D1/(C1*C2)*FKK(K)+FKU(K)
         WHENEVER Z1(K).L.SG
         AGDIP2(K)=ETA*ANGC/(ETA+Z1(K))*EXPETM+ETA*ANGC*APLUS/(ETA-Z1(      12M
        1 K))*EXPETP-D1/(C1*C2)*PVI.(2,1,K)-ALPHA1(K)/(C2*C1)*ANG1(K)*
        1 EXPO(K)+PVI.(1,2,K)+ANGO(K)*ALPHA2(J,K)*EXPO(K)
         AGDIP1(K)=C2*ETA/(SIG*(ETA+Z1(K)))*EXPETM+C2*ETA*APLUS/(SIG*       13M
        1 (ETA-Z1(K)))*EXPETP+ALPHA1(K)/(C1*SIG)*EXPO(K)+C2/SIG*PVI.(1
        1 ,3,K)
         AGDIM1(K)=C2*ETA/(SIG*(ETA-Z1(K)))*EXPETM+C2*ETA*APLUS/(SIG*       14M
        1 (ETA+Z1(K)))*EXPETP+C2/SIG*FTK(K)
         PRINT RESULTS ANGR1(K), AGDIP1(K), ANGR1(K+P), AGDIM1(K)
         OTHERWISE
         AGDIP2(K)=ETA*ANGC/(ETA+Z1(K))*EXPETM+ETA*ANGC/(ETA-Z1(K))*       15M
        1 APLUS*EXPETP-D1/(C1*C2)*FBK(K)+PVI.(1,2,K)+ANGO(K)*ALPHA2(J,
        1 K)*EXPO(K)
         END OF CONDITIONAL
C02      PRINT RESULTS ANGR(K), AGDIP2(K), ANGR(K+D), AGDIM2(K)
         AGDIP2(P)=QUAD.(Z1(P), Z1(P-2), AGDIP2(P-2),Z1(P-1),AGDIP2(P
        1 -1),Z1(P+2),AGDIP2(P+2))
         AGDIP2(P+1)=QUAD.(Z1(P+1), Z1(P-1),AGDIP2(P-1),Z1(P+2),AGDIP2
        1 (P+2),Z1(P+3),AGDIP2(P+3))
         PRINT RESULTS AGDIP2(P), AGDIP2(P+1)
        R APPROPRIATE INTEGRALS TO OBTAIN THE TOTAL FLUX AND CURRENT
        R FOLLOWED BY A CALCULATION OF THE ASYMPTOTIC FLUX AND CURRENT
        R SEE EQS.(5.16)
         SUM1=0.
         SUM2=0.
         SUM3=0.
         SUM4=0.
         SUM5=0.
         SUM6=0.
         SUM7=0.
         SUM8=0.
         SUM9=0.
         SUM10=0.
         SUM11=0.
         SUM12=0.
         THROUGH C05, FOR K=1,1, K.G.D
         WHENEVER K.L.P+1
         Z2(K)=Z1(K)*SIG
         SUM1=SUM1+AGDIM1(K)
         SUM2=SUM2+AGDIP1(K)
         SUM3=SUM3+AGDIM2(K)
         SUM4=SUM4+AGDIP2(K)
         SUM5=SUM5-Z2(K)*AGDIM1(K)
         SUM6=SUM6+Z2(K)*AGDIP1(K)
         SUM7=SUM7-Z1(K)*AGDIM2(K)
         SUM8=SUM8+Z1(K)*AGDIP2(K)
         OTHERWISE
         SUM9=SUM9+AGDIM2(K)
```

PROGRAM 2 (Continued)

```
            SUM10=SUM10+AGDIP2(K)
            SUM11=SUM11-Z1(K)*AGDIM2(K)
            SUM12=SUM12+Z1(K)*AGDIP2(K)
  C05       END OF CONDITIONAL
            FLNEG1=SUM1*H1*SIG
            FLPOS1=SUM2*H1*SIG
            TOTFL1=FLNEG1+FLPOS1
            CUNEG1=SUM5*H1*SIG
            CUPOS1=SUM6*H1*SIG
            TOTCU1=CUNEG1+CUPOS1
            FLNEG2=SUM3*H1+SUM9*H2
            FLPOS2=SUM4*H1+SUM10*H2
            TOTFL2=FLNEG2+FLPOS2
            CUNEG2=SUM7*H1+SUM11*H2
            CUPOS2=SUM8*H1+SUM12*H2
            TOTCU2=CUNEG2+CUPOS2
            PRINT RESULTS FLNEG1, FLPOS1, TOTFL1, CUNEG1, CUPOS1, TOTCU1,
           1                FLNEG2, FLPOS2, TOTFL2, CUNEG2, CUPOS2, TOTCU2
            ARCSIG=ELGETP+ELGETM
            ASYFL1=C2*ARCSIG*(EXPETM+APLUS*EXPETP)                          16M
            ASYCU1=C2*ETA*EXPETM*(2.-SIG*ARCSIG)+C2*ETA*EXPETP*APLUS*(      17M
           1 SIG*ARCSIG-2.)
            ARCETA=ETA*ELOG.((ETA+1.)/(ETA-1.))
            ASYFL2=ANGC*ARCETA*(EXPETM+APLUS*EXPETP)                        18M
            ASYCU2=ETA*ANGC*EXPETM*(2.-ARCETA)+ETA*ANGC*APLUS*EXPETP*(      19M
           1 ARCETA-2.)
 C04        PRINT RESULTS ASYFL1, ASYCU1, ASYFL2, ASYCU2
            TRANSFER TO START
            END OF PROGRAM
$ COMPILE MAD, EXECUTE
           R SUBROUTINE FOR THE CALCULATION OF INTEGRALS BY MIDPOINT
           R APPROXIMATION- TRAPEZOIDAL RULE
            EXTERNAL FUNCTION INT.(J)
            INTEGER K, I, Q4, P, P1, P3, D, J
            DIMENSION FU(846,VIM), FUL(10), FUM(10), FUU(10), ELG(92),
           1 Z1(92)
            VECTOR VALUES VIM=2,0,0
            PROGRAM COMMON FU, FUL, FUM, FUU, N, ELG, Z1, H1, H2, P3, D,
           1  SG
            VIM(2)=D+2
            P=N
            SUM1=0.
            SUM2=0.
            THROUGH EVAL, FOR K=1,1, K.G.D
            WHENEVER K.LE.P
            SUM1=SUM1+FU(J,K)
            OTHERWISE
            SUM2=SUM2+FU(J,K)
  EVAL      END OF CONDITIONAL
            FUNCTION RETURN SUM1*H1+ SUM2*H2
```

PROGRAM 2 (Continued)

```
           END OF FUNCTION
$ COMPILE MAD, EXECUTE
          R SUBROUTINE FOR CALCULATING SINGULAR INTEGRALS SEE CHAPTER 6
           EXTERNAL FUNCTION PVI.(J,I,Q4)
           DIMENSION FU(846,VIM), FUL(10), FUM(10), FUU(10), ELG(92),
          1 Z1(92)
           VECTOR VALUES VIM=2,0,0
           INTEGER K, I, Q4, P, P1, P3, D, J
           PROGRAM COMMON FU, FUL, FUM, FUU, N, ELG, Z1, H1, H2, P3, D,
          1  SG
           P=N
           VIM(2)=D+2
           SUM=0.
           SUM1=0.
           SUM2=0.
           THROUGH COMP1, FOR K=1,1, K.G.D
           WHENEVER K.E.Q4
           WHENEVER Q4.E.1
           SUM=SUM+1./3.*(FU(I,2)+3.*FU(I,1)-4.*FUL(I))
           OR WHENEVER Q4.E.P
           SUM=SUM+1./3.*(4.*FUM(I)-3.*FU(I,P)-FU(I,P-1))
           OR WHENEVER Q4.E.P+1
           SUM=SUM+1./3.*(FU(I,P+2)+3.*FU(I,P+1)-4.*FUM(I))
           OR WHENEVER Q4.E.D
           SUM=SUM+1./3.*(4.*FUU(I) -3.*FU(I,D)-FU(I,D-1))
           OTHERWISE
           SUM=SUM+1./2.*(FU(I,Q4+1)-FU(I,Q4-1))
           END OF CONDITIONAL
           OTHERWISE
           WHENEVER K.LE.P
           SUM1=SUM1+(FU(I,K)-FU(I,Q4))/(Z1(K)-Z1(Q4))
           OTHERWISE
           SUM2=SUM2+(FU(I,K)-FU(I,Q4))/(Z1(K)-Z1(Q4))
           END OF CONDITIONAL
 COMP1     END OF CONDITIONAL
           WHENEVER J.E.1
           FUNCTION RETURN SUM+FU(I,Q4)*ELG(Q4)+H1*SUM1+H2*SUM2
           OTHERWISE
          R SINGULAR INTEGRAL FOR REGION 1 ONLY
           FUNCTION RETURN SUM+FU(I,Q4)*ELOG.(SG/Z1(Q4)-1.)+H1*SUM1
           END OF CONDITIONAL
           END OF FUNCTION
$ DATA
 C1=.61320, C2=.04404, C3=.17023, C4=.43685, SIG=1.65809, ETA=2.595825,
 EPS=.000001, N=22., ITMAXX=10, EPSI=.000001, N3=70.,
 Z3(1)=0.,.5,1.,1.5,2.,3.,5.,8.,10.,20., ZEE=10, ITMAX=10       *
          R THE SOLUTION TO THE CONSTANT PROBLEM IS OBTAINED BY
          R REPLACING IN THE PREVIOUS PROGRAM THE CARDS WITH M IN
          R COLUMN 77 BY THE FOLLOWING CARDS WITH S IN COLUMN 77. THE
          R NUMBERS MUST ALSO MATCH, FOR EXAMPLE 5M IS REPLACED BY 5S,
```

PROGRAM 2 (Concluded)

```
R ETC. ALSO WE MAY REMOVE FROM THE PREVIOUS DECK ALL CARDS
R PRECEDED  BY THE REMARK $MILNE PROBLEM ONLY$.  NOTE THAT
R THE FIRST FOUR CARDS AFTER THE FIRST ARE PLACED IN THE
R PREVIOUS DECK AT ONE DESIGNATED LOCATION.
R THIS IS THE SOLUTION FOR THE EXACT CONSTANT SOURCE PROBLEM
 CS1=2.*C2/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)
 CS2=(SIG-2.*C1)/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)
 CSW=-CS2-CS1*D1/C2+SIG*CS1*C4/C2
 CS3=SIG*CS1*D1/C2
 FUM(1)=GU(D+1)*(CSW-CS3*ELGSG)
 FUU(1)=GU(D+2)*(CSW-CS3*ELGONE)
 FKK(K)=CSW-CS3*ELG1(K)
 APLUS1=(-SIG*CS1/C2+INTEGM)/APLDEN
 OPSI(K)=-OMAG1(K)*PVI.(1,1,K)+OMAG2(K)*FKK(K)
 ALPHA1(K)=-CS1*SIG*C1-ETA*C2*C1*APLUS/(ETA-Z1(K))-C2*C1
 AGDIM2(K)=CS2                          +ETA*ANGC*APLUS/(ETA+Z1(K
 AGDIP2(K)=CS2                           +ETA*ANGC*APLUS/(ETA-Z1(
 AGDIP1(K)=CS1                             +C2*ETA*APLUS/(SIG*
 AGDIM1(K)=CS1                              +C2*ETA*APLUS/(SIG*
 AGDIP2(K)=CS2                           +ETA*ANGC/(ETA-Z1(K))*
 ASYFL1=2.*CS1+C2*ARCSIG*APLUS*EXPETP
 ASYCU1=                                +C2*ETA*EXPETP*APLUS*(
 ASYFL2=2.*CS2+ANGC*ARCETA*APLUS*EXPETP
 ASYCU2=                              +ETA*ANGC*APLUS*EXPETP*(
```

PROGRAM 3

```
$ COMPILE MAD, EXECUTE, DUMP, PRINT OBJECT
          R PROGRAM FOR SOLUTION OF THE MILNE PROBLEM                      OM
          R SPHERICAL HARMONICS-P1 APPROXIMATION                           OM
           DIMENSION X(3), FX(3),  RO(4),          COP1(2), COP2(2),
          1 F1(2), F2(2), EXP01(50), EXP02(50), RH01(50), RH11(50),
          1 RH02(50), RH12(50), Z3(50), PSI1(1050,VIM), PSI2(1050,DIM),
          1 COP3(2), ANGLE(21), EXP03(50),
          1 ASY01(50), ASY11(50), ASY02(50), ASY12(50)
           INTEGER I,J, Q, ZEE, ITMAX, ITX, ITY
           VECTOR VALUES VIM=2,0,21
           VECTOR VALUES DIM=2,0,21
 START     READ AND PRINT DATA
           PI=3.14159265
          R THE ROOTS OF EQ.(7.8A) ARE OBTAINED BY THE FALSE POSITION
          R METHOD (SEE REF. (28))
           D1=C1*C4-C2*C3
             B =-3.*(1.-2.*C4+SIG*SIG-2.*SIG*C1)
             D =9.*SIG*(SIG-2.*C1-2.*C4*SIG+4.*D1)
           PRINT RESULTS B, D, D1
           INTERNAL FUNCTION CHAR.(Z)=Z.P.4+B*Z.P.2+D
           T=.00000001
           Q=1
  ITER     CHAR0=CHAR.(T)
           WHENEVER CHAR0.L.0.
           THROUGH SERCH1, FOR Y=T,.02,CHAR1.G.0..OR.Y.G.40.
           WHENEVER Y.G.40.
           PRINT COMMENT $ NO SIGN CHANGE$
           TRANSFER TO START
           END OF CONDITIONAL
 SERCH1    CHAR1=CHAR.(Y)
           OTHERWISE
           THROUGH SERCH2, FOR Y=T,.02,CHAR1.L.0..OR.Y.G.40.
           WHENEVER Y.G.40.
           PRINT COMMENT $ NO SIGN CHANGE$
           TRANSFER TO START
           END OF CONDITIONAL
 SERCH2    CHAR1=CHAR.(Y)
           END OF CONDITIONAL
           X(1)=Y-.04
           X(2)=Y-.02
           FX(1)=CHAR.(X(1))
           FX(2)=CHAR.(X(2))
           PRINT RESULTS X(1), FX(1), X(2), FX(2)
           THROUGH LOOPXA, FOR ITX=1,1, ITX.G.ITMAX
           NUMER=X(2)*FX(1)-X(1)*FX(2)
           DENOM=FX(1)-FX(2)
           WHENEVER .ABS. DENOM.L..ABS.NUMER*EPS2
           PRINT COMMENT $ DENOMINATOR TOO SMALL$
           TRANSFER TO START
```

PROGRAM 3 (Continued)

```
        END OF CONDITIONAL
        X(3)=NUMER/DENOM
        FX(3)=CHAR.(X(3))
        WHENEVER .ABS.FX(3).LE.EPS1
        PRINT COMMENT $ PROCEDURE CONVERGED$
        TRANSFER TO ITER1
        END OF CONDITIONAL
        THROUGH LOOPXA, FOR I=1,1, I.G.2
        THROUGH LOOPXA, FOR J=I+1,1, J.G.3
        WHENEVER .ABS.FX(I).G..ABS.FX(J)
        TEMP=FX(I)
        FX(I)=FX(J)
        FX(J)=TEMP
        TEMP=X(I)
        X(I)=X(J)
        X(J)=TEMP
LOOPXA  END OF CONDITIONAL
        PRINT COMMENT $ NO CONVERGENCE$
        THROUGH EVAL6, FOR Y1=1.E-8, .02, Y1.G.30.
        CHAR3=CHAR.(Y1)
EVAL6   PRINT RESULTS Y1, CHAR3
        TRANSFER TO START
 ITER1  RO(Q)=X(3)
        PRINT RESULTS ITX, X(3), FX(3), Q
        T=Y-.02
        Q=Q+1
        WHENEVER Q.E.3, TRANSFER TO GO
        TRANSFER TO ITER
GO      PRINT RESULTS RO(1), RO(2)
       R END OF PROGRAM FOR OBTAINING THE ROOTS
        THROUGH EVAL1, FOR I=1,1, I.G.2
       R EQS.(7.11) EVALUATED
        COP1(I)=RO(I)/(3.*SIG)
        COP2(I)=(3.*SIG*(SIG-2.*C1)-RO(I)*RO(I))/(6.*SIG*C2)
        COP3(I)=COP2(I)*RO(I)/3.
       R SEE EQS. FOLLOWING EQS.(7.17)
        F1(I)=.50+COP1(I)
        F2(I)=COP2(I)/2.+COP3(I)
EVAL1   PRINT RESULTS COP1(I), COP2(I), COP3(I), F1(I), F2(I)
       R NEXT THREE CARDS FOR MILNE CASE ONLY (SEE EQS.(7.18A)
        COP4=-RO(1)/(3.*SIG)
        COP5=COP2(1)
        COP6=-RO(1)*COP5/3.
        F3=.5+COP4                                                    1M
        F4=.5*COP5+ COP6                                              2M
       R SEE EQS.(7.18A)
        BO2=(F4*F1(2)-F3*F2(2))/(F1(1)*F2(2)-F1(2)*F2(1))             3M
        BO4=(F3*F2(1)-F4*F1(1))/(F1(1)*F2(2)-F1(2)*F2(1))             4M
        PRINT RESULTS F3, F4, BO2, BO4
        THROUGH EVAL2, FOR I=1,1, I.G.ZEE
```

PROGRAM 3 (Continued)

```
         EXPO1(I)=EXP.(-RO(1)*Z3(I))
         EXPO2(I)=EXP.(-RO(2)*Z3(I))
        R MILNE CARD ONLY
         EXPO3(I)=EXP.(RO(1)*Z3(I))
        R SEE EQS.(7.12)
         RHO1(I)=EXPO3(I)+BO2*EXPO1(I)+BO4*EXPO2(I)                    5M
         ASYO1(I)=EXPO3(I)+BO2*EXPO1(I)                                6M
         RH11(I)=COP4*EXPO3(I)+BO2*COP1(1)*EXPO1(I)+BO4*COP1(2)*EXPO   7M
        R MILNE CARD ONLY
        1 2(I)
         ASY11(I)=COP4*EXPO3(I)+BO2*COP1(1)*EXPO1(I)                   8M
         RHO2(I)=COP5*EXPO3(I)+BO2*COP2(1)*EXPO1(I)+BO4*COP2(2)*       9M
        R MILNE CARD ONLY
        1 EXPO2(I)
         ASYO2(I)=COP5*EXPO3(I)+BO2*COP2(1)*EXPO1(I)                   10M
         RH12(I)=COP6*EXPO3(I)+BO2*COP3(1)*EXPO1(I)+ BO4*COP3(2)*      11M
        R MILNE CARD ONLY
        1 EXPO2(I)
         ASY12(I)=COP6*EXPO3(I)+BO2*COP3(1)*EXPO1(I)                   12M
EVAL2    PRINT RESULTS Z3(I), EXPO1(I), EXPO2(I), RHO1(I), RH11(I),
        1 RHO2(I), RH12(I), ASYO1(I), ASY11(I), ASYO2(I), ASY12(I)
        R ANGULAR DISTRIBUTION FOLLOWS
         Q=1
         THROUGH EVAL4, FOR L=1.,-.1, L.L.-1.
         ANGLE(Q)=360./(2.*PI)*ARCCOS.(L)
EVAL4    Q=Q+1
         ANGP=360./(2.*PI)*ARCCOS.(.975)
         ANGM=360./(2.*PI)*ARCCOS.(-.975)
         THROUGH EVAL7, FOR J=1,1, J.G.ZEE
         PSP1=.5*RHO1(J)+1.5*.975*RH11(J)
         PSM1=.5*RHO1(J)-1.5*.975*RH11(J)
         PSP2=.5*RHO2(J)+1.5*.975*RH12(J)
         PSM2=.5*RHO2(J)-1.5*.975*RH12(J)
         Q=1
         THROUGH EVAL3, FOR L=1.,-.1, L.L.-1.
         PSI1(J,Q)=.5*RHO1(J)+1.5*L*RH11(J)
         PSI2(J,Q)=.5*RHO2(J)+1.5*L*RH12(J)
         PRINT RESULTS ANGLE(Q), Z3(J), PSI1(J,Q), PSI2(J,Q)
EVAL3    Q=Q+1
 EVAL7   PRINT RESULTS ANGP, PSP1, PSP2, ANGM, PSM1, PSM2
        R NEXT TWO CARDS ARE MILNE CARDS ONLY
        R SEE EQ.(7.19)
         EXTRAP=-1./(2.*RO(1))*ELOG.(-1./BO2)
         PRINT RESULTS EXTRAP
         TRANSFER TO START
         END OF PROGRAM
$ DATA
 C1=.59023, C2=.05448, C3=.15963, C4=.44320,    Z3(1)=0.,.5,1.,1.5,2.,
  2.5,3.,3.5,4.,4.5,5.,8., 10., 20., EPS1=1.E-6, EPS2=1.E-20, SIG=1.50951,
  ZEE=14, ITMAX=50     *
```

PROGRAM 3 (Concluded)

```
R FOR THE CONSTANT SOURCE PROBLEM WE MAKE THE REPLACEMENT OF
R THE FOLLOWING CARDS EXACTLY AS WE DID IN THE PREVIOUS CASE
R PROGRAM FOR THE SOLUTION OF THE CONSTANT SOURCE PROBLEM           0S
R BY SPHERICAL HARMONICS-P1 APPROXIMATION                           0S
  S1=2.*C2/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)                        1S
  S2=(SIG-2.*C1)/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)                  2S
 A02=(S2*F1(2)-S1*F2(2))/(F1(1)*F2(2)-F1(2)*F2(1))                  3S
 A04=(S1*F2(1)-S2*F1(1))/(F1(1)*F2(2)-F1(2)*F2(1))                  4S
 RH01(I)=A02*EXP01(I)+A04*EXP02(I)+2.*S1                            5S
 ASY01(I)=A02*EXP01(I)+2.*S1                                        6S
 RH11(I)=COP1(1)*A02*EXP01(I)+COP1(2)*A04*EXP02(I)                  7S
 ASY11(I)=COP1(1)*A02*EXP01(I)                                      8S
 RH02(I)=COP2(1)*A02*EXP01(I)+COP2(2)*A04*EXP02(I)+2.*S2            9S
 ASY02(I)=COP2(1)*A02*EXP01(I)+2.*S2                                10S
 RH12(I)=COP3(1)*A02*EXP01(I)+COP3(2)*A04*EXP02(I)                  11S
 ASY12(I)=COP2(1)*A02*EXP01(I)                                      12S
```

PROGRAM 4

```
$ COMPILE MAD, EXECUTE, DUMP, PRINT OBJECT
          R PROGRAM FOR THE SOLUTION OF THE MILNE PROBLEM BY
          R SPHERICAL HARMONICS-P3 APPROXIMATION
           DIMENSION X(3), FX(3), RO(4), COP1(4), COP2(4), COP3(4),
          1 COP4(4), COP5(4), COP6(4), COP7(4), F1(4), F2(4), F3(4),
          1 F4(4), EXPO1(50), EXPO2(50), EXPO3(50), EXPO4(50), RHO1(50),
          1 RH11(50), RH21(50), RH31(50), RHO2(50), RH12(50), RH22(50),
          1 RH32(50), Z3(50), PSI1(1050,VIM), PSI2(1050,DIM), ANGLE(21),
          1 Y(4), A(20,VIN), ASYO1(50), ASYO2(50), EXPO5(50)
           INTEGER I,J, Q, ZEE, ITMAX, ITX, ITY
           VECTOR VALUES VIM=2,0,21
           VECTOR VALUES DIM=2,0,21
           VECTOR VALUES VIN=2,0,5
 START     READ AND PRINT DATA
           D1=C1*C4-C2*C3
           PI=3.14159265
           C=81.
           D=990.*(C4+C1*SIG)-810.*(1.+SIG*SIG)
           E=(110.*SIG*C1-90. *SIG*SIG)*(110.*C4-90.)+945.*(1.-2.*C4+SIG.
          1 P.3*(SIG-2.*C1))-110.*110.*SIG*C2*C3
           F=105.*(1.-2.*C4)*(110.*SIG*C1-90.*SIG*SIG)+105.*SIG.P.3*(
          1 SIG-2.*C1)*(110.*C4-90.)+210.*110.*SIG*C2*C3*(1.+SIG*SIG)
           G=105.*105.*SIG.P.3*(SIG-2.*C1)*(1.-2.*C4)-210.*210.*SIG.P.3
          1 *C2*C3
           PRINT RESULTS C, D, E, F, G
           INTERNAL FUNCTION CHAR.(Z)=C*Z.P.8+D*Z.P.6+E*Z.P.4+F*Z.P.2+G
           T=.00000001
           Q=1
  ITER     CHARO=CHAR.(T)
           CHAR1=0.
           WHENEVER CHARO.L.0.
           THROUGH SERCH1,FOR Y1=T,.01,CHAR1.G.0..OR.Y1.G.40.
           WHENEVER Y1.G.40.
           PRINT COMMENT $ NO SIGN CHANGE$
           TRANSFER TO START
           END OF CONDITIONAL
 SERCH1    CHAR1=CHAR.(Y1)
           OTHERWISE
           THROUGH SERCH2,FOR Y1=T,.01,CHAR1.L.0..OR.Y1.G.40.
           WHENEVER Y1.G.40.
           PRINT COMMENT $ NO SIGN CHANGE$
           TRANSFER TO START
           END OF CONDITIONAL
 SERCH2    CHAR1=CHAR.(Y1)
           END OF CONDITIONAL
           X(1)=Y1-.02
           X(2)=Y1-.01
           FX(1)=CHAR.(X(1))
           FX(2)=CHAR.(X(2))
```

PROGRAM 4 (Continued)

```
        THROUGH LOOPXA, FOR ITX=1,1, ITX.G.ITMAX
        NUMER=X(2)*FX(1)-X(1)*FX(2)
        DENOM=FX(1)-FX(2)
        WHENEVER .ABS. DENOM.L..ABS.NUMER*EPS2
        PRINT COMMENT $ DENOMINATOR TOO SMALL$
        TRANSFER TO START
        END OF CONDITIONAL
        X(3)=NUMER/DENOM
        FX(3)=CHAR.(X(3))
        WHENEVER .ABS.FX(3).LE.EPS1
        PRINT COMMENT $ PROCEDURE CONVERGED$
        TRANSFER TO ITER1
        OR WHENEVER Q.E.2.AND..ABS.FX(3).L..0003
        TRANSFER TO ITER1
        OR WHENEVER Q.E.3.AND..ABS.FX(3).L..003
        TRANSFER TO ITER1
        OR WHENEVER Q.E.4.AND..ABS.FX(3).L..1
        TRANSFER TO ITER1
        END OF CONDITIONAL
        THROUGH LOOPXA, FOR I=1,1, I.G.2
        THROUGH LOOPXA, FOR J=I+1,1, J.G.3
        WHENEVER .ABS.FX(I).G..ABS.FX(J)
        TEMP=FX(I)
        FX(I)=FX(J)
        FX(J)=TEMP
        TEMP=X(I)
        X(I)=X(J)
        X(J)=TEMP
        PRINT RESULTS X(1), FX(1), X(2), FX(2)
LOOPXA  END OF CONDITIONAL
        PRINT COMMENT $ NO CONVERGENCE$
        THROUGH EVAL6, FOR Y1=0.,.1, Y1.G.30.
        CHAR3=CHAR.(Y1)
EVAL6   PRINT RESULTS Y1, CHAR3
        TRANSFER TO START
ITER1   RO(Q)=X(3)
        PRINT RESULTS ITX, X(3), FX(3), Q
        T=Y1-.01
        Q=Q+1
        WHENEVER Q.E.5, TRANSFER TO GO
        TRANSFER TO ITER
GO      PRINT RESULTS RO(1)...RO(4)
       R END OF PROGRAM FOR CALCULATING THE ROOTS SEE CHAPTER 7 FOR
       R APPROPRIATE EQUATIONS FOR THE FOLLOWING PROGRAM
        THROUGH EVAL1, FOR I=1,1, I.G.4
        SQR=RO(I)*RO(I)
        SQSG=SIG*SIG
        COP1(I)=RO(I)*(35.*SQSG-9.*SQR)/(5.*SIG*(21.*SQSG-11.*SQR))
        COP2(I)=14.*RO(I)*SIG*COP1(I)/(35.*SQSG-9.*SQR)
        COP3(I)=3.*RO(I)*COP2(I)/(7.*SIG)
```

PROGRAM 4 (Continued)

```
         COP4(I)=10.*C3*(21.-11.*SQR)/(SQR*(9.*SQR-35.)+5.*(1.-2.*C4)
        1 *(21.-11.*SQR))
         COP5(I)=RO(I)*(35.-9.*SQR)*COP4(I)/(5.*(21.-11.*SQR))
         COP6(I)=14.*RO(I)*COP5(I)/(35.-9.*SQR)
         COP7(I)=3.*RO(I)*COP6(I)/7.
         F1(I)=.5+COP1(I)+5.*COP2(I)/8.
         F2(I)=.25+3.*COP1(I)/5.+5.*COP2(I)/8.+2.*COP3(I)/5.
         F3(I)=.5*COP4(I)+COP5(I)+5.*COP6(I)/8.
         F4(I)=.25*COP4(I)+3.*COP5(I)/5.+5.*COP6(I)/4.+2.*COP7(I)/5.
EVAL1    PRINT RESULTS RO(I), COP1(I), COP2(I), COP3(I), COP4(I),
        1 COP5(I), COP6(I), COP7(I), F1(I), F2(I), F3(I), F4(I)
        R FOR THE CONSTANT SOURCE PROBLEM WE INSERT CARDS 1S AND 2S
         A(1,5)=-.5+COP1(1)+5./8.*COP2(1)                                 3M
         A(2,5)=-.25+3./5.*COP1(1)+5./8.*COP2(1)+2./5.*COP3(1)            4M
         A(3,5)=-.5*COP4(1)+COP5(1)+5./8.*COP6(1)                         5M
         A(4,5)=-.25*COP4(1)+3./5.*COP5(1)+5./8.*COP6(1)+2./5.*COP7(1)    6M
         THROUGH EVAL5, FOR I=1,1, I.G.4
         A(1,I)=F1(I)
         A(2,I)=F2(I)
         A(3,I)=F3(I)
EVAL5    A(4,I)=F4(I)
         PRINT RESULTS A(1,1)...A(4,5)
         EPSS=1.E-20
         DETER=SIMUL.(4,A,Y,EPSS)
         PRINT RESULTS A(1,1)...A(4,5), Y(1)...Y(4), DETER
         THROUGH EVAL2, FOR I=1,1, I.G.ZEE
         EXPO1(I)=EXP.(-RO(1)*Z3(I))
         EXPO2(I)=EXP.(-RO(2)*Z3(I))
         EXPO3(I)=EXP.(-RO(3)*Z3(I))
         EXPO4(I)=EXP.(-RO(4)*Z3(I))
        R MILNE CARD ONLY
         EXPO5(I)=EXP.(RO(1)*Z3(I))
         ASYO1(I)=Y(1)*EXPO1(I)+EXPO5(I)                                  7M
         RHO1(I)=Y(1)*EXPO1(I)+Y(2)*EXPO2(I)+Y(3)*EXPO3(I)+Y(4)*          8M
        1 EXPO4(I)+EXPO5(I)                                               9M
         RH11(I)=Y(1)*COP1(1)*EXPO1(I)+Y(2)*COP1(2)*EXPO2(I)+Y(3)*        10M
        1 COP1(3)*EXPO3(I)+Y(4)*COP1(4)*EXPO4(I)-EXPO5(I)*COP1(1)         11M
         RH21(I)=Y(1)*COP2(1)*EXPO1(I)+Y(2)*COP2(2)*EXPO2(I)+Y(3)*        12M
        1 COP2(3)*EXPO3(I)+Y(4)*COP2(4)*EXPO4(I)-EXPO5(I)*COP2(1)         13M
         RH31(I)=Y(1)*COP3(1)*EXPO1(I)+Y(2)*COP3(2)*EXPO2(I)+Y(3)*        14M
        1 COP3(3)*EXPO3(I)+Y(4)*COP3(4)*EXPO4(I)-EXPO5(I)*COP3(1)         15M
         ASYO2(I)=Y(1)*COP4(1)*EXPO1(I)+EXPO5(I)*COP4(1)                  16M
         RHO2(I)=Y(1)*COP4(1)*EXPO1(I)+Y(2)*COP4(2)*EXPO2(I)+Y(3)*        17M
        1 COP4(3)*EXPO3(I)+Y(4)*COP4(4)*EXPO4(I)+EXPO5(I)*COP4(1)         18M
         RH12(I)=Y(1)*COP5(1)*EXPO1(I)+Y(2)*COP5(2)*EXPO2(I)+Y(3)*        19M
        1 COP5(3)*EXPO3(I)+Y(4)*COP5(4)*EXPO4(I)-EXPO5(I)*COP5(1)         20M
         RH22(I)=Y(1)*COP6(1)*EXPO1(I)+Y(2)*COP6(2)*EXPO2(I)+Y(3)*        21M
        1 COP6(3)*EXPO3(I)+Y(4)*COP6(4)*EXPO4(I)-EXPO5(I)*COP6(1)         22M
         RH32(I)=Y(1)*COP7(1)*EXPO1(I)+Y(2)*COP7(2)*EXPO2(I)+Y(3)*        23M
        1 COP7(3)*EXPO3(I)+Y(4)*COP7(4)*EXPO4(I)-EXPO5(I)*COP7(1)         24M
```

PROGRAM 4 (Continued)

```
 EVAL2    PRINT RESULTS Z3(I), RHO1(I), RH11(I), RHO2(I), RH12(I),
         1 ASYO1(I), ASYO2(I)
         R NEXT TWO CARDS ARE MILNE CARDS ONLY
          EXTRAP=-.5/RO(1)*ELOG.(-1./Y(1))
          PRINT RESULTS EXTRAP
         R ANGULAR DISTRIBUTION FOLLOWS
          Q=1
          THROUGH EVAL4, FOR L=1.,-.1, L.L.-1.
          ANGLE(Q)=360./(2.*PI)*ARCCOS.(L)
 EVAL4    Q=Q+1
          THROUGH EVAL3, FOR J=1,1, J.G.ZEE
          Q=1
          THROUGH EVAL3, FOR L=1.,-.1, L.L.-1.
          PSI1(J,Q)=.5*RHO1(J)+1.5*L*RH11(J)+1.25*(3.*L*L-1.)*RH21(J)
         1 +7./4.*(5.*L.P.3-3.*L)*RH31(J)
          PSI2(J,Q)=.5*RHO2(J)+1.5*L*RH12(J)+1.25*(3.*L*L-1.)*RH22(J)
         1 +7./4.*(5.*L.P.3-3.*L)*RH32(J)
          PRINT RESULTS ANGLE(Q), Z3(J), PSI1(J,Q), PSI2(J,Q)
 EVAL3    Q=Q+1
          TRANSFER TO START
          END OF PROGRAM
$ COMPILE MAD, EXECUTE, DUMP, PRINT OBJECT
         R THIS SUBROUTINE SOLVES THE SET OF SIMULTANEOUS EQUATIONS
         R SEE EQS.(7.30) AND (7.31) FOR DETAILS SEE REF. (18)
          EXTERNAL FUNCTION SIMUL.(N,A,X,EPS)
          DIMENSION IR(50), JC(50), CJ(50)
          NORMAL MODE IS INTEGER
          FLOATING POINT A, BIGA, X, DETER, EPS, AJCK
          NP1=N+1
          DETER=1.
          THROUGH L1, FOR K=1,1, K.G.N
          BIGA=0.
          THROUGH L2, FOR I=1,1, I.G.N
          THROUGH L2, FOR J=1,1, J.G.N
          THROUGH L3, FOR I1=1,1, I1.E.K
          THROUGH L3, FOR J1=1,1, J1.E.K
 L3       WHENEVER I.E.IR(I1).OR.J.E.JC(J1), TRANSFER TO L2
          WHENEVER .ABS.A(I,J).G.BIGA
          BIGA=.ABS.A(I,J)
          IR(K)=I
          JC(K)=J
 L2       END OF CONDITIONAL
          WHENEVER BIGA.L.EPS, FUNCTION RETURN 0
          BIGA=A(IR(K),JC(K))
          DETER = DETER*BIGA
          THROUGH L4, FOR J=1,1, J.G.NP1
 L4       A(IR(K),J)=A(IR(K),J)/BIGA
          THROUGH L1, FOR I=1,1, I.G.N
          WHENEVER I.NE.IR(K)
          AJCK=A(I,JC(K))
```

PROGRAM 4 (Concluded)

```
           THROUGH L6, FOR J=1,1, J.G.NP1
L6         A(I,J)=A(I,J)-AJCK*A(IR(K),J)
L1         END OF CONDITIONAL
           THROUGH L7, FOR I=1,1, I.G.N
           CJ(IR(I))=JC(I)
L7         X(JC(I))=A(IR(I),NP1)
           COUNT=0
           THROUGH L9, FOR I=1,1, I.E.N
           THROUGH L9, FOR J=I+1,1, J.G.N
           WHENEVER CJ(J).L.CJ(I)
           TEMP=CJ(J)
           CJ(J)=CJ(I)
           CJ(I)=TEMP
           COUNT = COUNT+1
L9         END OF CONDITIONAL
           WHENEVER COUNT/2*2.NE.COUNT, DETER=-DETER
           FUNCTION RETURN DETER
           END OF FUNCTION
$ DATA
 C1=.59023, C2=.05448, C3=.15963, C4=.44320,     Z3(1)=0.,.5,1.,1.5,2.,
  2.5,3.,3.5,4.,4.5,5.,8.,10.,20.,     EPS1=1.E-6, EPS2=1.E-20, SIG=1.50951,
  RO(1)=.1376522, 1.162925, 2.068132, 3.289316,
  ZEE=14, ITMAX=50    *
          R FOR THE CONSTANT SOURCE PROBLEM WE REFER THE READER TO THE
          R PREVIOUS INSTRUCTIONS FOR THE P1 CASE
          R PROGRAM FOR THE SOLUTION OF THE CONSTANT SOURCE PROBLEM          0S
          R BY SPHERICAL HARMONICS-P3 APPROXIMATION                          0S
            S1=2.*C2/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)                       1S
            S2=(SIG-2.*C1)/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)                 2S
           A(1,5)=-S1                                                        3S
           A(2,5)=-S1/2.                                                     4S
           ASY01(I)=Y(1)*EXP01(I)+2.*S1                                      7S
           RH01(I)=Y(1)*EXP01(I)+Y(2)*EXP02(I)+Y(3)*EXP03(I)+Y(4)*           8S
          1 EXP04(I)+2.*S1                                                   9S
           RH11(I)=Y(1)*COP1(1)*EXP01(I)+Y(2)*COP1(2)*EXP02(I)+Y(3)*         10S
          1 COP1(3)*EXP03(I)+Y(4)*COP1(4)*EXP04(I)                           11S
           RH21(I)=Y(1)*COP2(1)*EXP01(I)+Y(2)*COP2(2)*EXP02(I)+Y(3)*         12S
          1 COP2(3)*EXP03(I)+Y(4)*COP2(4)*EXP04(I)                           13S
           RH31(I)=Y(1)*COP3(1)*EXP01(I)+Y(2)*COP3(2)*EXP02(I)+Y(3)*         14S
          1 COP3(3)*EXP03(I)+Y(4)*COP3(4)*EXP04(I)                           15S
           ASY02(I)=Y(1)*COP4(1)*EXP01(I)+2.*S2                              16S
           RH02(I)=Y(1)*COP4(1)*EXP01(I)+Y(2)*COP4(2)*EXP02(I)+Y(3)*         17S
          1 COP4(3)*EXP03(I)+Y(4)*COP4(4)*EXP04(I)+2.*S2                     18S
           RH12(I)=Y(1)*COP5(1)*EXP01(I)+Y(2)*COP5(2)*EXP02(I)+Y(3)*         19S
          1 COP5(3)*EXP03(I)+Y(4)*COP5(4)*EXP04(I)                           20S
           RH22(I)=Y(1)*COP6(1)*EXP01(I)+Y(2)*COP6(2)*EXP02(I)+Y(3)*         21S
          1 COP6(3)*EXP03(I)+Y(4)*COP6(4)*EXP04(I)                           22S
           RH32(I)=Y(1)*COP7(1)*EXP01(I)+Y(2)*COP7(2)*EXP02(I)+Y(3)*         23S
          1 COP7(3)*EXP03(I)+Y(4)*COP7(4)*EXP04(I)                           24S
```

PROGRAM 5

```
$ COMPILE MAD. EXECUTE, DUMP, PRINT OBJECT
          R PROGRAM FOR THE SOLUTION OF THE CONSTANT SOURCE PROBLEM BY
          R SPHERICAL HARMONICS-DP1 APPROXIMATION
           DIMENSION X(3), FX(3), RO(4), COP1(4), COP2(4), COP3(4),
          1 COP4(4), COP5(4), COP6(4), COP7(4), F1(4), F2(4), F3(4),
          1 F4(4), EXP01(50), EXP02(50), EXP03(50), EXP04(50), RH01(50),
          1 RH11(50), RH21(50), RH31(50), RH02(50), RH12(50), RH22(50),
          1 RH32(50), Z3(50), PSI1(1050,VIM), PSI2(1050,DIM), ANGLE(21),
          1 Y(4), A(20,VIN), EXP05(50), ASY01(50), ASY02(50)
           INTEGER I,J, Q, ZEE, ITMAX, ITX, ITY
           VECTOR VALUES VIM=2,0,21
           VECTOR VALUES DIM=2,0,21
           VECTOR VALUES VIN=2,0,5
 START     READ AND PRINT DATA
           PI=3.14159265
           D1=C1*C4-C2*C3
           C=-1.
           D=24*(SIG*SIG-C1*SIG+1.-C4)
           E=576.*SIG*(C2*C3+(1.-C4)*(C1-SIG))-36.*(SIG.P.3*(SIG-2.*C1)+
          1 1.-2.*C4)
           F=-864.*SIG*((C1-SIG)*(1.-2.*C4)-(1.-C4)*SIG*SIG*(SIG-2.*C1))
          1 -1728.*C2*C3*SIG*(SIG*SIG+1.)
           G=-1296.*SIG.P.3*(SIG-2.*C1)*(1.-2.*C4)+5184.*C2*C3*SIG.P.3
           PRINT RESULTS C, D, E, F, G
           INTERNAL FUNCTION CHAR.(Z)=C*Z.P.8+D*Z.P.6+E*Z.P.4+F*Z.P.2+G
           T=.00000001
           Q=1
  ITER     CHAR0=CHAR.(T)
           CHAR1=0.
           WHENEVER CHAR0.L.0.
           THROUGH SERCH1,FOR Y1=T,.01,CHAR1.G.0..OR.Y1.G.40.
           WHENEVER Y1.G.40.
           PRINT COMMENT $ NO SIGN CHANGE$
           TRANSFER TO START
           END OF CONDITIONAL
 SERCH1    CHAR1=CHAR.(Y1)
           OTHERWISE
           THROUGH SERCH2,FOR Y1=T,.01,CHAR1.L.0..OR.Y1.G.40.
           WHENEVER Y1.G.40.
           PRINT COMMENT $ NO SIGN CHANGE$
           TRANSFER TO START
           END OF CONDITIONAL
 SERCH2    CHAR1=CHAR.(Y1)
           END OF CONDITIONAL
           X(1)=Y1-.02
           X(2)=Y1-.01
           FX(1)=CHAR.(X(1))
           FX(2)=CHAR.(X(2))
           THROUGH LOOPXA, FOR ITX=1,1, ITX.G.ITMAX
```

PROGRAM 5 (Continued)

```
          NUMER=X(2)*FX(1)-X(1)*FX(2)
          DENOM=FX(1)-FX(2)
          WHENEVER .ABS. DENOM.L..ABS.NUMER*EPS2
          PRINT COMMENT $ DENOMINATOR TOO SMALL$
          TRANSFER TO START
          END OF CONDITIONAL
          X(3)=NUMER/DENOM
          FX(3)=CHAR.(X(3))
          WHENEVER .ABS.FX(3).LE.EPS1
          PRINT COMMENT $ PROCEDURE CONVERGED$
          TRANSFER TO ITER1
          OR WHENEVER Q.E.3.AND..ABS.FX(3).L..005
          TRANSFER TO ITER1
          OR WHENEVER Q.E.4.AND..ABS.FX(3).L..01
          TRANSFER TO ITER1
          END OF CONDITIONAL
          THROUGH LOOPXA, FOR I=1,1, I.G.2
          THROUGH LOOPXA, FOR J=I+1,1, J.G.3
          WHENEVER .ABS.FX(I).G..ABS.FX(J)
          TEMP=FX(I)
          FX(I)=FX(J)
          FX(J)=TEMP
          TEMP=X(I)
          X(I)=X(J)
          X(J)=TEMP
          PRINT RESULTS X(1), FX(1), X(2), FX(2)
          WHENEVER FX(1).E.FX(2)
          FX(3)=FX(1)
          X(3)=X(1)
          TRANSFER TO ITER1
          END OF CONDITIONAL
 LOOPXA   END OF CONDITIONAL
          PRINT COMMENT $ NO CONVERGENCE$
          THROUGH EVAL6, FOR Y1=0.,.1, Y1.G.30.
          CHAR3=CHAR.(Y1)
EVAL6     PRINT RESULTS Y1, CHAR3
          TRANSFER TO START
  ITER1   RO(Q)=X(3)
          PRINT RESULTS ITX, X(3), FX(3), Q
          T=Y1-.01
          Q=Q+1
          WHENEVER Q.E.5, TRANSFER TO GO
          TRANSFER TO ITER
 GO       PRINT RESULTS RO(1)...RO(4)
           S1=2.*C2/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)
           S2=(SIG-2.*C1)/((1.-2.*C4)*(SIG-2.*C1)-4.*C2*C3)
          THROUGH EVAL1, FOR I=1,1, I.G.4
          SQR=RO(I)*RO(I)
          SQSG=SIG*SIG
          COP1(I)=RO(I)*(12.*SQSG-SQR)/(12.*SIG*(3.*SQSG-SQR))
```

PROGRAM 5 (Continued)

```
         COP2(I)=9.*SIG*RO(I)*COP1(I)/(2.*(12.*SQSG-SQR))
         COP3(I)=RO(I)*COP2(I)/(6.*SIG)
         COP4(I)=24.*C3*(SQR-3.)/(SQR*(12.-SQR)+12.*(1.-2.*C4)*(SQR-
        1 3.))
         COP5(I)=RO(I)*(SQR-12.)*COP4(I)/(12.*(SQR-3.))
         COP6(I)=9.*RO(I)*COP5(I)/(2.*(12.-SQR))
         COP7(I)=RO(I)*COP6(I)/6.
         F1(I)=.5+.75*COP1(I)-COP3(I)
         F2(I)=.25*COP1(I)+2./3.*COP2(I)+COP3(I)
         F3(I)=.5*COP4(I)+.75*COP5(I)-COP7(I)
         F4(I)=.25*COP5(I)+2./3.*COP6(I)+COP7(I)
EVAL1    PRINT RESULTS RO(I), COP1(I), COP2(I), COP3(I), COP4(I),
        1 COP5(I), COP6(I), COP7(I), F1(I), F2(I), F3(I), F4(I)
         A(1,5)=-S1
         A(2,5)=0.
         A(3,5)=-S2
         A(4,5)=0.
         THROUGH EVAL5, FOR I=1,1, I.G.4
         A(1,I)=F1(I)
         A(2,I)=F2(I)
         A(3,I)=F3(I)
EVAL5    A(4,I)=F4(I)
         PRINT RESULTS A(1,1)...A(4,5)
         EPSS=1.E-20
         DETER=SIMUL.(4,A,Y,EPSS)
         PRINT RESULTS A(1,1)...A(4,5), Y(1)...Y(4), DETER
         THROUGH EVAL2, FOR I=1,1, I.G.ZEE
         EXPO1(I)=EXP.(-RO(1)*Z3(I))
         EXPO2(I)=EXP.(-RO(2)*Z3(I))
         EXPO3(I)=EXP.(-RO(3)*Z3(I))
         EXPO4(I)=EXP.(-RO(4)*Z3(I))
         RHO1(I)=Y(1)*EXPO1(I)+Y(2)*EXPO2(I)+Y(3)*EXPO3(I)+Y(4)*
        1 EXPO4(I)+2.*S1
         ASYO1(I)=Y(1)*EXPO1(I)+2.*S1
         RH11(I)=Y(1)*COP1(1)*EXPO1(I)+Y(2)*COP1(2)*EXPO2(I)+Y(3)*
        1 COP1(3)*EXPO3(I)+Y(4)*COP1(4)*EXPO4(I)
         RH21(I)=Y(1)*COP2(1)*EXPO1(I)+Y(2)*COP2(2)*EXPO2(I)+Y(3)*
        1 COP2(3)*EXPO3(I)+Y(4)*COP2(4)*EXPO4(I)
         RH31(I)=Y(1)*COP3(1)*EXPO1(I)+Y(2)*COP3(2)*EXPO2(I)+Y(3)*
        1 COP3(3)*EXPO3(I)+Y(4)*COP3(4)*EXPO4(I)
         RHO2(I)=Y(1)*COP4(1)*EXPO1(I)+Y(2)*COP4(2)*EXPO2(I)+Y(3)*
        1 COP4(3)*EXPO3(I)+Y(4)*COP4(4)*EXPO4(I)+2.*S2
         ASYO2(I)=Y(1)*COP4(1)*EXPO1(I)+2.*S2
         RH12(I)=Y(1)*COP5(1)*EXPO1(I)+Y(2)*COP5(2)*EXPO2(I)+Y(3)*
        1 COP5(3)*EXPO3(I)+Y(4)*COP5(4)*EXPO4(I)
         RH22(I)=Y(1)*COP6(1)*EXPO1(I)+Y(2)*COP6(2)*EXPO2(I)+Y(3)*
        1 COP6(3)*EXPO3(I)+Y(4)*COP6(4)*EXPO4(I)
         RH32(I)=Y(1)*COP7(1)*EXPO1(I)+Y(2)*COP7(2)*EXPO2(I)+Y(3)*
        1 COP7(3)*EXPO3(I)+Y(4)*COP7(4)*EXPO4(I)
EVAL2    PRINT RESULTS Z3(I), RHO1(I), RH11(I), RHO2(I), RH12(I),
```

PROGRAM 5 (Continued)

```
           1 ASY01(I), ASY02(I)
           R ANGULAR DISTRIBUTION FOLLOWS
            Q=1
            THROUGH EVAL4, FOR L=1.,-.1, L.L.-1.
            ANGLE(Q)=360./(2.*PI)*ARCCOS.(L)
 EVAL4      Q=Q+1
            THROUGH EVAL3, FOR J=1,1, J.G.ZEE
            Q=1
            THROUGH EVAL3, FOR L=1.,-.1, L.L.-1.
            WHENEVER L.G..001
            PSI1(J,Q)=.5*RH01(J)-2.*RH21(J)-4.*RH31(J)+L*(4.*RH21(J)+
           1 3./2.*RH11(J)+6.*RH31(J))
            PSI2(J,Q)=.5*RH02(J)-2.*RH22(J)-4.*RH32(J)+L*(4.*RH22(J)+
           1 3./2.*RH12(J)+6.*RH32(J))
            OR WHENEVER L.L.-.001
            PSI1(J,Q)=.5*RH01(J)-2.*RH21(J)+4.*RH31(J)+L*(-4.*RH21(J)+
           1 3./2.*RH11(J)+6.*RH31(J))
            PSI2(J,Q)=.5*RH02(J)-2.*RH22(J)+4.*RH32(J)+L*(-4.*RH22(J)+
           1 3./2.*RH12(J)+6.*RH32(J))
           R HERE WE CALCULATE THE DISCONTINUITY IN THE ANGULAR
           R DISTRIBUTION AT MU=0.
            OR WHENEVER Q.E.11
            DISP1    =.5*RH01(J)-2.*RH21(J)-4.*RH31(J)+L*(4.*RH21(J)+
           1 3./2.*RH11(J)+6.*RH31(J))
            DISP2    =.5*RH02(J)-2.*RH22(J)-4.*RH32(J)+L*(4.*RH22(J)+
           1 3./2.*RH12(J)+6.*RH32(J))
            DISM1    =.5*RH01(J)-2.*RH21(J)+4.*RH31(J)+L*(-4.*RH21(J)+
           1 3./2.*RH11(J)+6.*RH31(J))
            DISM2    =.5*RH02(J)-2.*RH22(J)+4.*RH32(J)+L*(-4.*RH22(J)+
           1 3./2.*RH12(J)+6.*RH32(J))
            PRINT RESULTS DISP1, DISP2, DISM1, DISM2, ANGLE(Q)
            END OF CONDITIONAL
            PRINT RESULTS ANGLE(Q), Z3(J), PSI1(J,Q), PSI2(J,Q)
 EVAL3      Q=Q+1
            TRANSFER TO START
            END OF PROGRAM
$ COMPILE MAD, EXECUTE, DUMP, PRINT OBJECT
            EXTERNAL FUNCTION SIMUL.(N,A,X,EPS)
            DIMENSION IR(50), JC(50), CJ(50)
            NORMAL MODE IS INTEGER
            FLOATING POINT A, BIGA, X, DETER, EPS, AJCK
            NP1=N+1
            DETER=1.
            THROUGH L1, FOR K=1,1, K.G.N
            BIGA=0.
            THROUGH L2, FOR I=1,1, I.G.N
            THROUGH L2, FOR J=1,1, J.G.N
            THROUGH L3, FOR I1=1,1, I1.E.K
            THROUGH L3, FOR J1=1,1, J1.E.K
 L3         WHENEVER I.E.IR(I1).OR.J.E.JC(J1), TRANSFER TO L2
```

```
            WHENEVER .ABS.A(I,J).G.BIGA
            BIGA=.ABS.A(I,J)
            IR(K)=I
            JC(K)=J
L2          END OF CONDITIONAL
            WHENEVER BIGA.L.EPS, FUNCTION RETURN 0
            BIGA=A(IR(K),JC(K))
            DETER = DETER*BIGA
            THROUGH L4, FOR J=1,1, J.G.NP1
L4          A(IR(K),J)=A(IR(K),J)/BIGA
            THROUGH L1, FOR I=1,1, I.G.N
            WHENEVER I.NE.IR(K)
            AJCK=A(I,JC(K))
            THROUGH L6, FOR J=1,1, J.G.NP1
L6          A(I,J)=A(I,J)-AJCK*A(IR(K),J)
L1          END OF CONDITIONAL
            THROUGH L7, FOR I=1,1, I.G.N
            CJ(IR(I))=JC(I)
L7          X(JC(I))=A(IR(I),NP1)
            COUNT=0
            THROUGH L9, FOR I=1,1, I.E.N
            THROUGH L9, FOR J=I+1,1, J.G.N
            WHENEVER CJ(J).L.CJ(I)
            TEMP=CJ(J)
            CJ(J)=CJ(I)
            CJ(I)=TEMP
            COUNT = COUNT+1
L9          END OF CONDITIONAL
            WHENEVER COUNT/2*2.NE.COUNT, DETER=-DETER
            FUNCTION RETURN DETER
            END OF FUNCTION
$ DATA
 C1=.59023, C2=.05448, C3=.15963, C4=.44320,    Z3(1)=0.,.5,1.,1.5,2.,
  2.5,3.,3.5,4.,4.5,5.,8.,10.,20.,    EPS1=1.E-6, EPS2=1.E-20, SIG=1.50951,
  ZEE=14, ITMAX=50    *
           R FOR THE SOLUTION TO THE MILNE PROBLEM IN THIS
           R APPROXIMATION WE REFER THE READER TO THE PREVIOUS P3 PROGRAM
           R FOR THE APPROPRIATE CHANGES. ALSO SEE CHAPTER 7
```