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SOME TECHNIQUES TO EVALUATE THE SCATTERING SOURCE IN THE DISCRETE ORDINATE TRANSPORT EQUATION WITH HIGHLY ANISOTROPIC SCATTERING

by

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A MASTER'S THESIS

submitted in partial fulfillment of the
requirements for the degree

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1980

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1.0 INTRODUCTION

1.1 Statement of the Problem

In many practical problems it is often necessary to solve the transport equation with a highly anisotropic scattering cross section. The multigroup approximation of the transport equation introduces highly anisotropic group-to-group transfer cross sections in the scattering source term for the elastic scattering of neutrons [1] and the Compton scattering of photons [2]. The anisotropy arises as a result of the limitations on the allowed scattering angles for a given group-to-group transfer, imposed by the conservation of momentum and energy constraints [1]. In neutron shielding problems, some materials such as iron and oxygen exhibit "antiresonances" or "windows" in their total cross sections [3,4]. To analyze accurately the angular transmitted flux or leakage from these shielding materials, a very fine energy group structure is necessary in the antiresonance region. Such fine energy group structure invariably introduces a high degree of anisotropy in the scattering transfer cross sections. Highly anisotropic scattering cross sections are also encountered in one-speed radiative transfer problems [5]. In this case, the anisotropy results not from the calculational procedure, i.e., multigroup approximation, but from the fact that the scattering itself is highly anisotropic. The forward scattering function in this case can become so highly peaked in the forward direction that a several hundred term Legendre function expansion may be necessary for an adequate representation.

The purpose of this study is to develop techniques to evaluate the scattering source term in the transport equation involving highly anisotropic scattering cross sections. Instead of using a traditional truncated Legendre polynomial expansion [6] for the scattering cross section, which often produces negative fluxes or flux oscillations, several techniques are discussed that are based on the exact kernel method developed by Odom [7], which uses non-expanded form of the scattering function.

In Chapter 2, two coordinate transformations of the scattering source terms in the transport equation are reviewed. These transformations are chosen to facilitate accurate evaluation of the scattering source term involving scattering functions with narrow angular support such as those occur in fine multigroup shielding calculations. The properties of the transformations as well as their advantages and disadvantages are discussed.

In Chapter 3, several methods, based on the two coordinate transformations, are presented for the numerical evaluation of the scattering source term in the discrete ordinate transport equation. The accuracy of a low-order polynomial approximation for the angular flux in the evaluation of the scattering source term is assessed on a simple test problem. A method is also discussed for the analytical evaluation of the scattering source term using piecewise polynomial approximations for the angular flux and cross sections.

To understand better the purpose and the method of calculation given here, it is important to review the previous work which has been carried out by other authors. This is done in the next section.

1.2 Review of Previous Work

The traditional approach to treat the anisotropic scattering functions (differential cross section in one-speed problems, and group-to-group cross sections in multigroup problems) in the scattering source term is to use a global (full-range) Legendre polynomial expansion [6]. For highly anisotropic scattering functions, such a Legendre polynomial expansion requires a very large number of expansion terms [8]. A high order expansion often renders the solution of the discrete ordinate transport equation impractical as a result of excessive computational effort, or if a lower order truncated expansion is used, severe oscillations or spurious negative flux values may result.

Attia and Harms [9] have used partial-range Legendre function expansions to represent the angular dependence of the neutron group transfer cross sections. It is shown by them that this representation can avoid negative cross sections, and is superior to global Legendre function expansion. No prescription, however, is given as to how to evaluate the scattering source term in the transport equation using this representation of the cross sections.

Odom and Shultis [1] have developed a method (exact kernel method) to calculate the elastic group-to-group neutron cross sections without recourse to the traditional Legendre polynomial expansions. These cross sections can be readily used in a discrete ordinate formulation of the transport equation to obtain accurate numerical results for those situations in which the group-to-group transfer is highly anisotropic (as in transport problems involving fine group structure with light element scattering), and which ordinarily require a very high order Legendre expansions. The method however requires relatively large computer storage compared to the traditional Legendre expansion method.

In order to obviate the need for large computer storage in the exact kernel method, Mikols and Shultis [10] have developed a low-order piecewise linear approximation to the group-to-group elastic scattering transfer cross sections. It has been shown that the low-order approximation resembles quite closely the exact transfer distribution while the Legendre expansion technique yields oscillatory and even negative fluxes.

Ryman [2] has applied the exact kernel method to the solution of gamma photon transport problems and has obtained accurate solutions of problems which are characterized by a highly anisotropic source and by highly peaked, group-to-group, transfer cross sections which have narrow ranges of angular support. He also developed a new semi-analytic technique for computing exact kernel transfer cross sections. This method allows rapid computations of exact kernel cross sections with an accuracy satisfactory for most transport calculations. He has also developed a least squares approximation to exact kernel cross sections, which, when used with a standard discrete ordinates code based on Legendre expansions, gives improved accuracy for the computed scalar flux densities in highly anisotropic transport problems.

Hong [11] has applied the exact kernel method to the calculation of the anisotropic group-to-group cross sections for neutron inelastic scattering. It was shown that a low-order piecewise linear approximation for the group transfer cross sections is also a good approximation when inelastic scattering is present. Hong also developed a method to evaluate the scattering source term in the transport equation using piecewise polynomial approximations for angular flux and the transfer cross sections.

In-depth studies have been made for the accurate angular representation of highly anisotropic group-to-group cross sections, but little work has been done to date on the use of variable transformation in the scattering source term involving the highly anisotropic cross sections, which facilitates its accurate evaluation.

2.0 TRANSFORMATION OF VARIABLES IN THE SCATTERING SOURCE TERM OF THE MULTIGROUP NEUTRON TRANSPORT EQUATION

The scattering source term for transfer from energy group g' to energy group g in the multigroup neutron transport equation can be written as [6,12]

$$S_{g'\to g}(\underline{r},\underline{\Omega}) = \int_{\underline{\Omega}'} d\underline{\Omega}' \; \sigma_{g'\to g}(\underline{\Omega}\cdot\underline{\Omega}') \; \Psi_{g'}(\underline{r},\underline{\Omega}), \tag{2.1}$$

or more explicitly, for slab geometry, as

$$S_{g'\to g}(x,\mu,\phi) = \int_{-1}^{+1} d\mu' \int_{0}^{2\pi} d\phi' \; \sigma_{g'\to g}(\mu_o) \; \Psi_{g'}(x,\mu',\phi'), \tag{2.2}$$

where x is the distance into the slab, $\underline{\Omega} = (\mu',\phi')$ is the neutron direction before scattering, $\underline{\Omega}' = (\mu',\phi')$ is the neutron direction after scattering, $\Psi_{g'}(x,\Omega')$ is the neutron angular flux in group g' in direction $\underline{\Omega}'$ at point x and $\sigma_{g'\to g}(\underline{\Omega}\cdot\underline{\Omega}')$ is the macroscopic cross section for transfer from group g' to group g through a scattering angle, $\cos^{-1}(\underline{\Omega}\cdot\underline{\Omega}')$. Here μ is the polar angle, ϕ is the azimuthal angle and $\mu_o = \underline{\Omega}\cdot\underline{\Omega}'$ is the cosine of the scattering angle given by

$$\mu_o = \mu\mu' + (1-\mu^2)^{1/2} \; (1-\mu'^2)^{1/2} \cos(\phi'-\phi). \tag{2.3}$$

The slab is assumed homogeneous and isotropic so that the cross sections depend only on the scattering angle.

In fine multigroup neutron transport calculations, the group-to group cross sections, $\sigma_{g'\to g}(\mu_o)$ often have a narrow angular support, i.e., $\sigma_{g'\to g}(\mu_o)$ is non-zero over a small portion of the domain of μ_o, as a result of the restrictions imposed by the conservation of momentum and energy (1). A typical example of the group-to-group cross sections having narrow angular support is shown in Fig. 2.1 (7). Such transfer cross sections make the accurate numerical evaluation of the angular integration in the source term very difficult. In order to faciliate integration over the angular support of the cross sections in Eq. (2.2), it is profitable to seek a transformation of variables in the scattering source term such that μ_o itself is an integration variable. In this chapter two transformations of the scattering source term are studied which permit its accurate evaluation.

In Section 2.1 the limits of the scattering source integral when the group-to-group cross sections have narrow angular support are discussed for the untransformed case, i.e., when the integration variables left as μ' and ϕ'. Section 2.2 is devoted to the study of the transformation of integration variables from (μ',ϕ') to (μ',μ_o). Finally, in Section 2.3, the transformation of integration variables from (μ',ϕ') to (μ_o,ξ) where ξ is an angle discussed in that section is studied.

2.1 Limits of the Scattering Source Integral

Let $[\mu_{o,min},\mu_{o,max}]$ define the angular support of the group-to-group cross section, $\sigma_{g'\to g}(\mu_o)$, i.e., $\sigma_{g'\to g}(\mu_o)$ has a non-zero value only when $\mu_{o,min} < \mu_o < \mu_{o,max}$. Then in order to carry out accurately the integration in Eq. (2.2) using a low order numerical quadrature, it is necessary to find the limits of the μ' and ϕ' integral

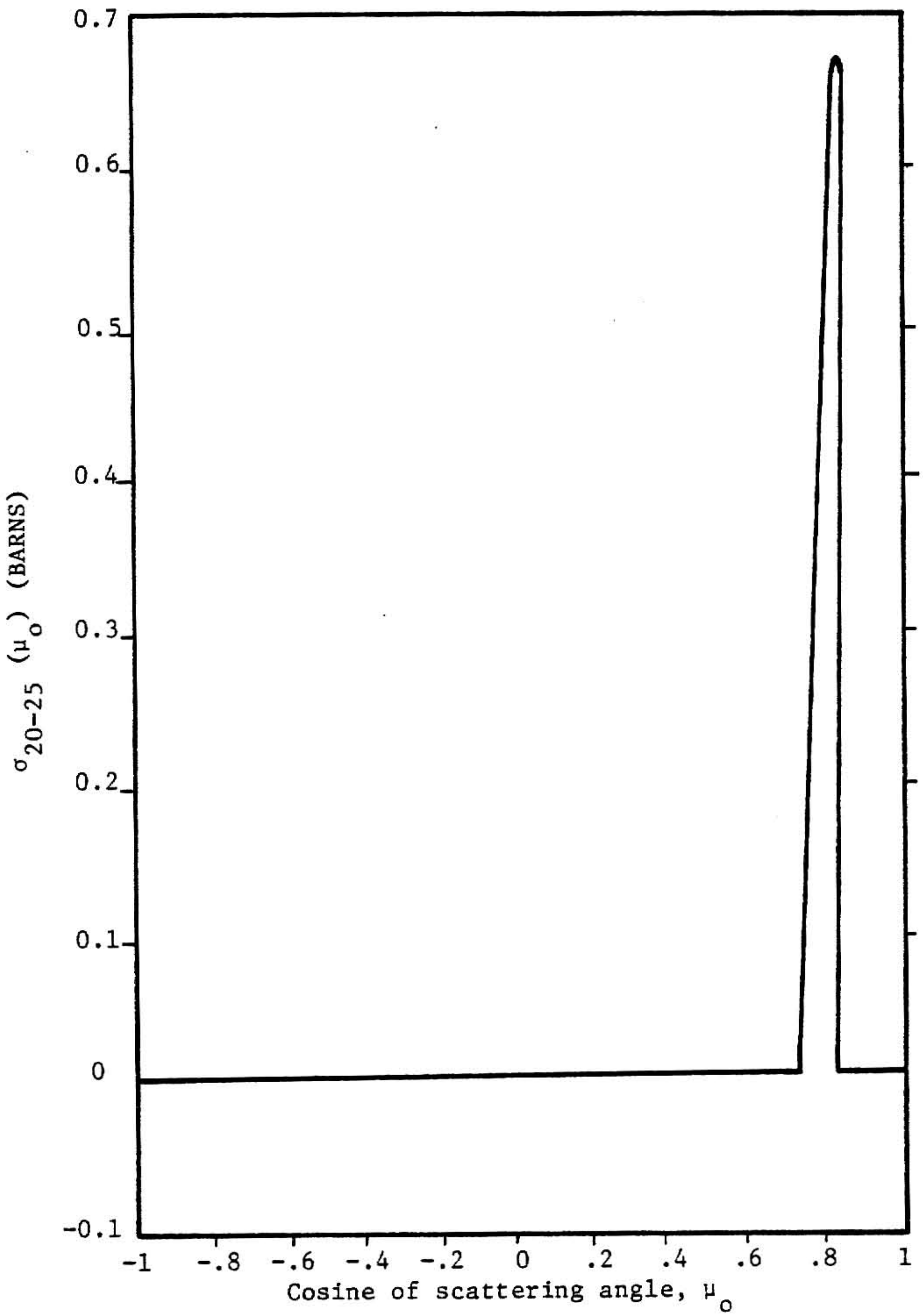

Fig. 2.1. Hydrogen multigroup cross section for group 20 (2.0190 - 2.2313 MeV) to group 25 (1.2246 - 1.3534 MeV) transfer.

such that the numerical integration is only over the cross section support $[\mu_{o,min},\mu_{o,max}]$.

The desired limits of integration for Eq. (2.2) can be found from the "iso-μ_o" curves in the (μ',ϕ') integration plane as shown in Figs. 2.2-2.5. These curves are obtained by plotting $(\phi'-\phi)$ as a function of μ' for fixed μ_o and μ, using Eq. (2.3). It is noted from these figures that to find the limits of the ϕ'-integral such that the integration is carried out over the region between two iso-μ_o curves, it is generally necessary to break the range of integration over μ' into several sub-ranges, since the limits of integration over ϕ' are different in each subrange. For example, it is also noted that for $\mu_o > |\mu|$ or $\mu_o < -|\mu|$, the iso-μ_o curves begin from $\phi'=\phi$ or $(\phi+\pi)$ or $(\phi+2\pi)$ and terminate at the same line, whereas for $-|\mu| < \mu_o < |\mu|$, the iso-μ_o curves begin from $\phi'=\phi$ and terminate at the line $\phi'=\phi+2\pi$. Thus, the limits of the ϕ'-integral depend on the location of $\mu_{o,min}$ and $\mu_{o,max}$ relative to $\pm|\mu|$. The procedure to find these limits for the case $-|\mu| < \mu_{o,min}, \mu_{o,max} < |\mu|$ is considered in detail below. Other cases can be handled in an analogous manner. A more general discussion is given in Section 2.1.1 where the azimuthally symmetric problem is considered.

Suppose $\mu_{o,min}$ and $\mu_{o,max}$ are such that $-|\mu| < \mu_{o,min}, \mu_{o,max} < |\mu|$. The desired region of integration for such a case is shown in Fig. 2.6. To find the limits of μ' and ϕ' integrals which correspond to this region of integration, it is necessary to break the range of integration over μ' in three parts as follows: [see Fig. 2.6]

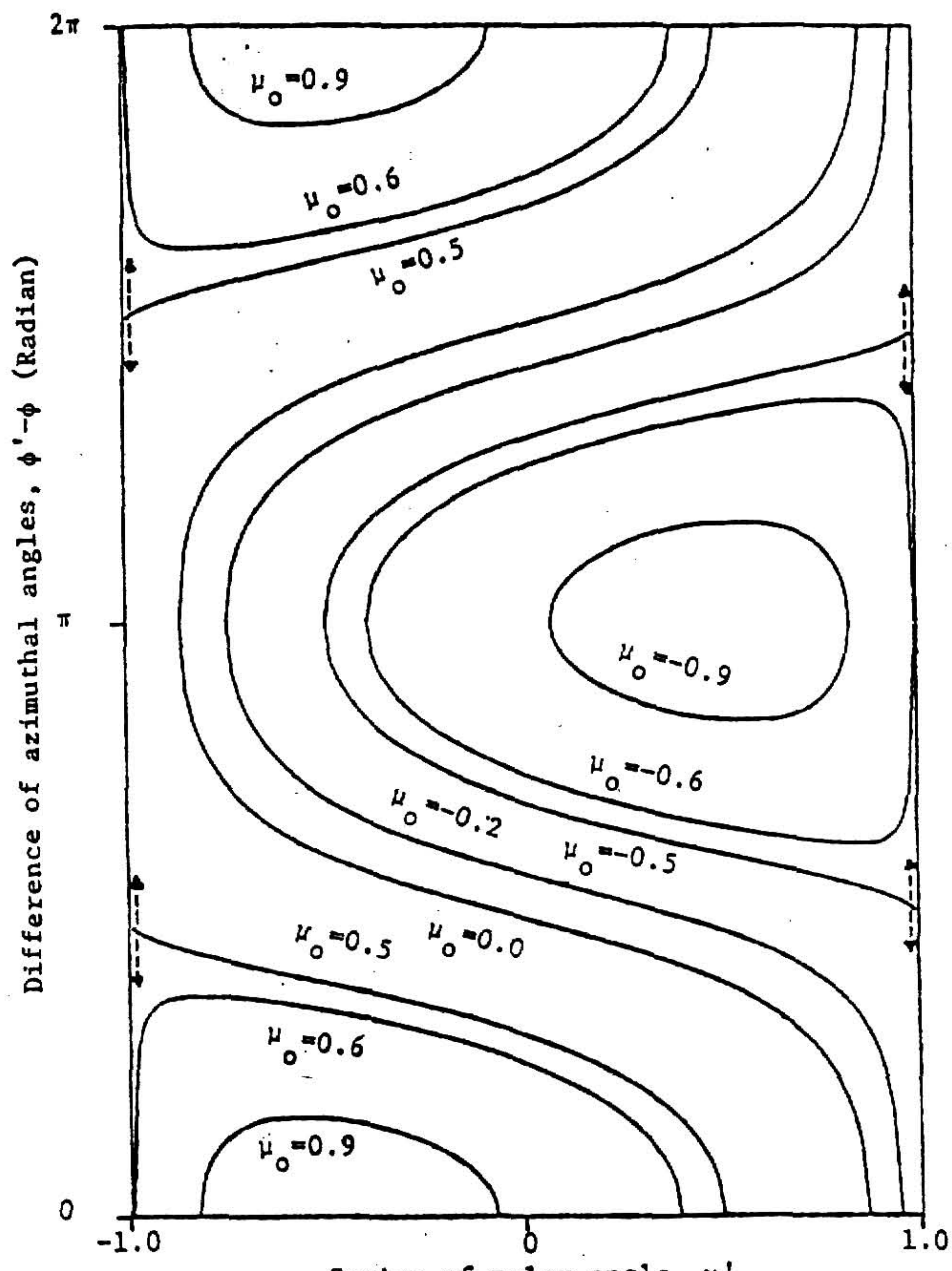

Fig. 2.2. Iso-μ_o curves in the (μ', ϕ') plane (μ=0.5).

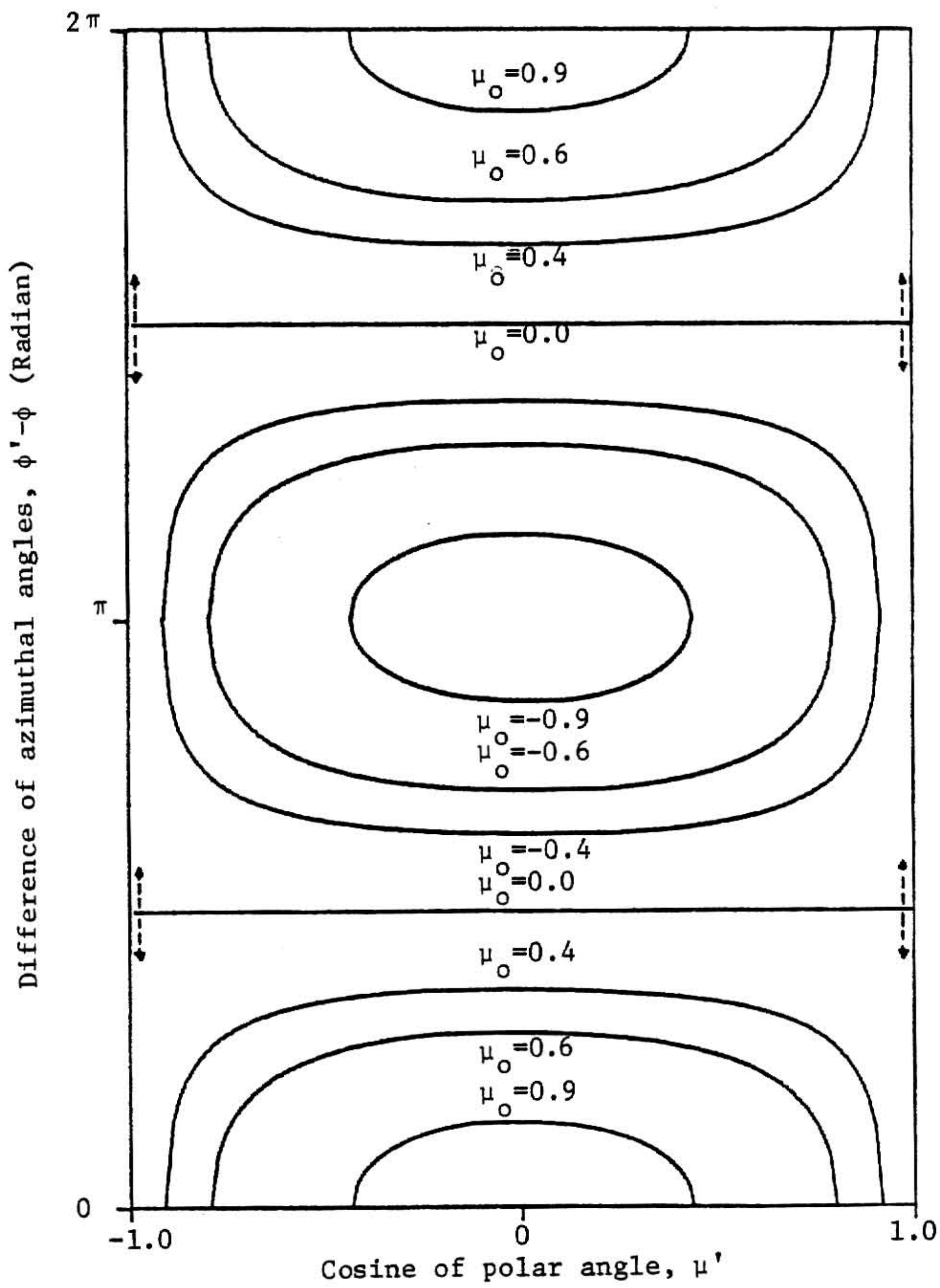

Fig. 2.3. Iso-μ_o curves in the (μ',ϕ') plane $(\mu=0)$.

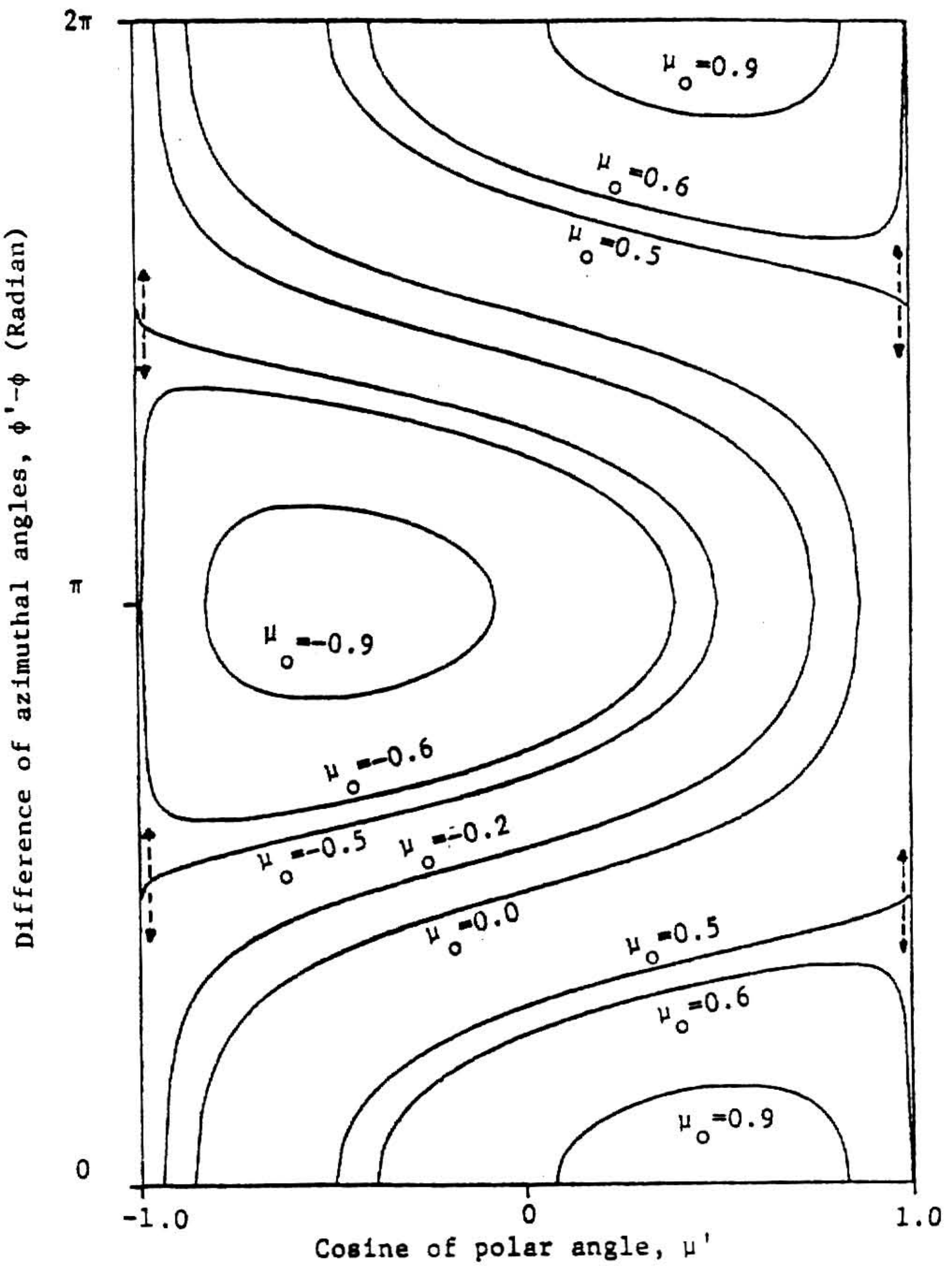

Fig. 2.4. Iso-μ_o curves in the (μ',ϕ') plane $(\mu=-0.5)$.

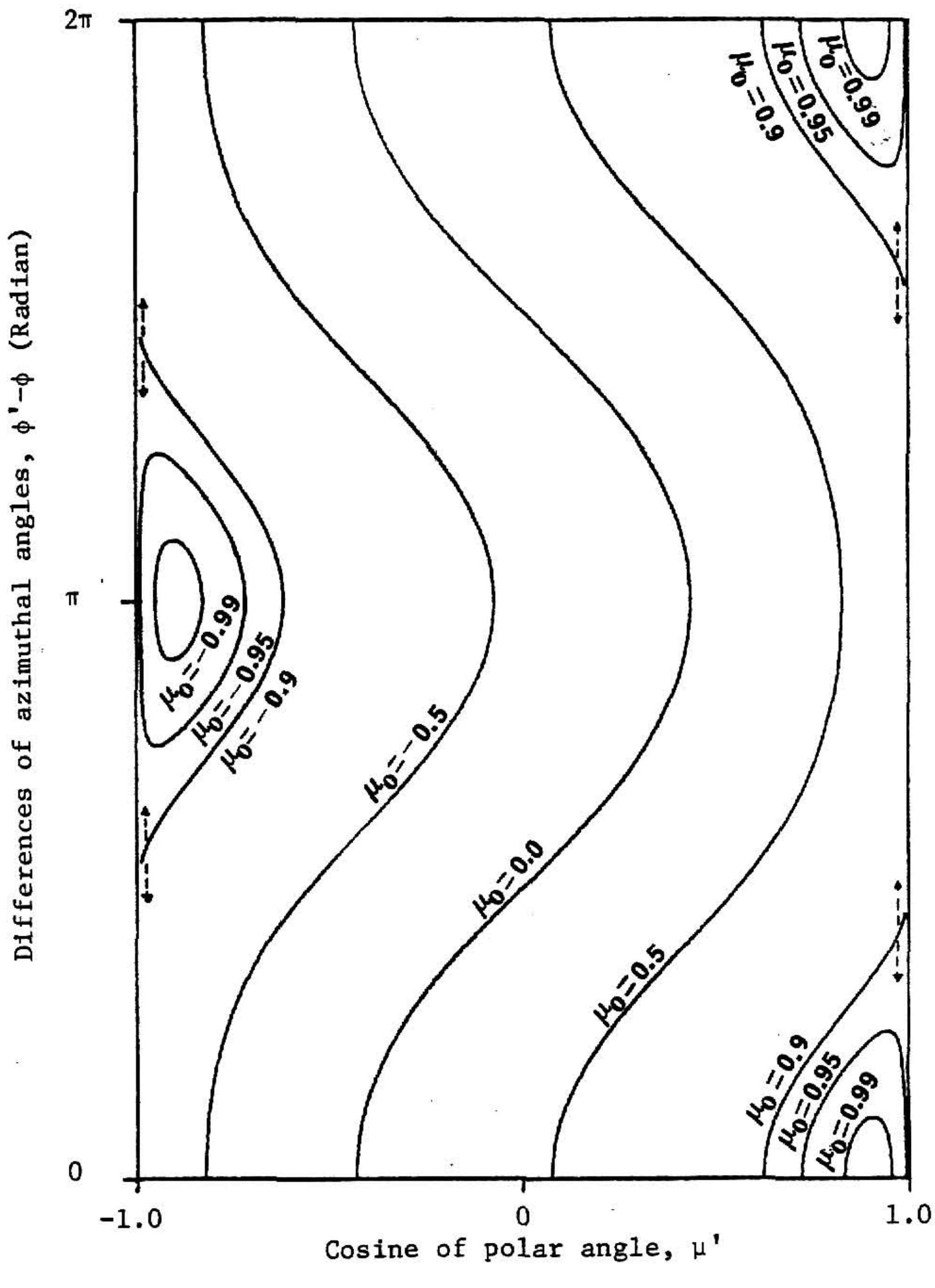

Fig. 2.5. Iso-μ_o curves in the (μ',ϕ') plane ($\bar{\mu}$=0.9).

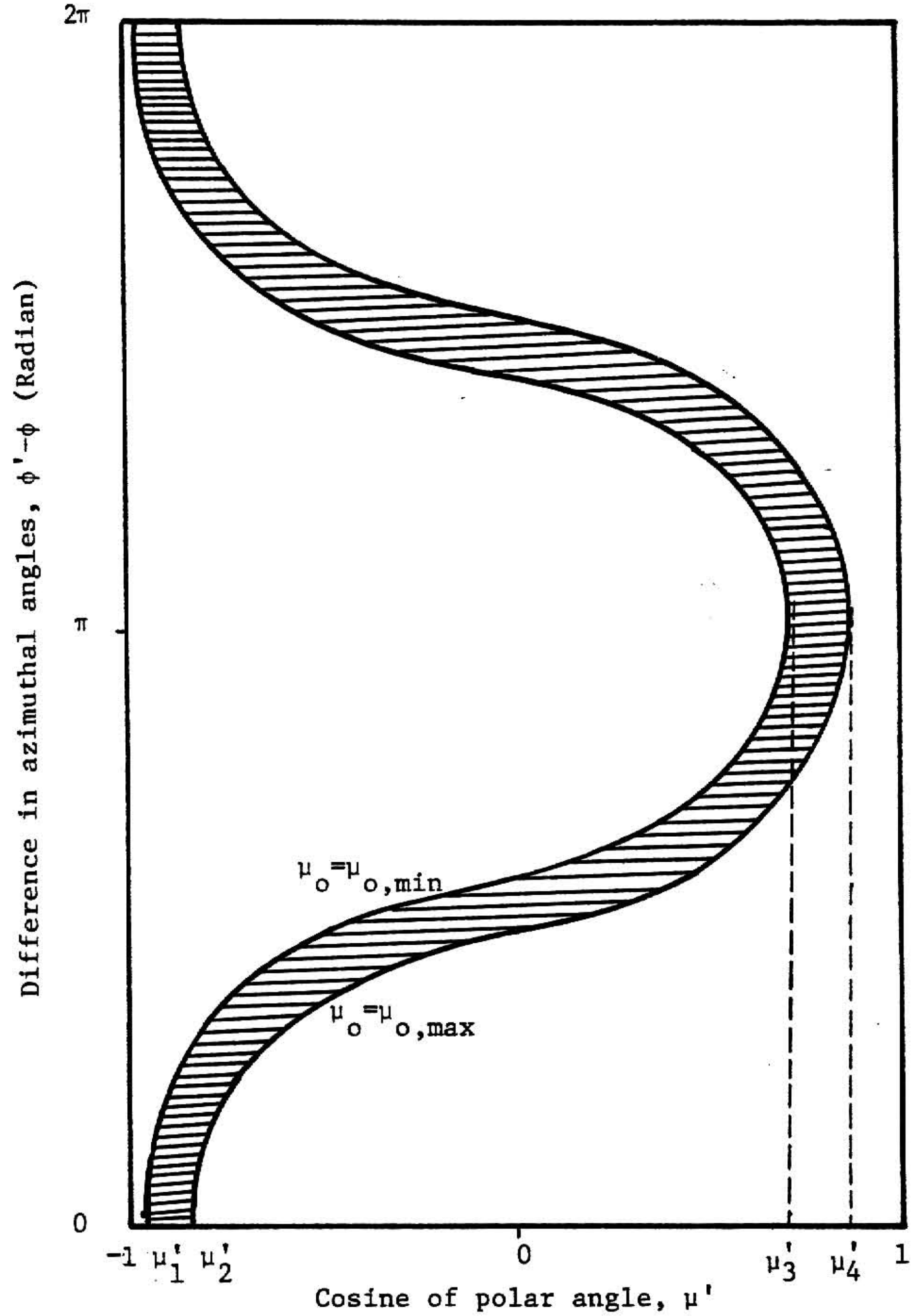

Fig. 2.6. Domain of integration when group-to-group cross section has non-zero value for $\mu_{o,min} < \mu_o < \mu_{o,max}$ (indicated by shaded region).

i) $\mu'_1 \leq \mu' \leq \mu'_2$ for which $\phi \leq \phi' \leq \phi'_{min}$ and $2\pi-\phi'_{min} \leq \phi' \leq \phi + 2\pi$

ii) $\mu'_2 \leq \mu' \leq \mu'_3$ for which $\phi'_{max} \leq \phi' \leq \phi'_{min}$ and $2\pi-\phi'_{min} \leq \phi' \leq 2\pi-\phi'_{max}$

iii) $\mu'_3 \leq \mu' \leq \mu'_4$ for which $\phi'_{max} \leq \phi' \leq \phi+\pi$ and $\phi+\pi \leq \phi' \leq 2\pi-\phi'_{max}$

Here ϕ'_{min} and ϕ'_{max} denote the values of ϕ' corresponding to $\mu_{o,min}$ and $\mu_{o,max}$, respectively for given μ and μ'. Expressions for ϕ'_{min} and ϕ'_{max} follow directly from Eq. (2.3) and are given by

$$\phi'_{min} = \phi + \cos^{-1} \{(\mu_{o,min}-\mu\mu')/(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}\}, \qquad (2.4)$$

and

$$\phi'_{max} = \phi + \cos^{-1} \{(\mu_{o,max}-\mu\mu')/(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}\}. \qquad (2.5)$$

The quantities μ'_1, μ'_2, μ'_3 and μ'_4 are given by the roots of the equations

$$\mu_{o,min} = \mu\mu' \pm (1-\mu^2)^{1/2} (1-\mu'^2)^{1/2}, \qquad (2.6a)$$

and

$$\mu_{o,max} = \mu\mu' \pm (1-\mu^2)^{1/2} (1-\mu'^2)^{1/2}, \qquad (2.6b)$$

i.e.,

$$\{\mu'_1,\mu'_2,\mu'_3,\mu'_4\} = \text{ordered } \{\overline{\mu'_1},\overline{\mu'_2},\overline{\mu'_3},\overline{\mu'_4}\} \qquad (2.7)$$

where

$$\overline{\mu'_1} = \mu\mu_{o,min} - (1-\mu^2)^{1/2} (1-\mu^2_{o,min})^{1/2}, \qquad (2.8)$$

$$\overline{\mu'_2} = \mu\mu_{o,max} - (1-\mu^2)^{1/2} (1-\mu^2_{o,max})^{1/2}, \qquad (2.9)$$

$$\overline{\mu'_3} = \mu\mu_{o,min} + (1-\mu^2)^{1/2} (1-\mu^2_{o-min})^{1/2}, \qquad (2.10)$$

and

$$\overline{\mu'_4} = \mu\mu_{o,max} + (1-\mu^2)^{1/2} (1-\mu^2_{o,max})^{1/2}. \qquad (2.11)$$

The scattering source term can therefore be written as

$$S_{g'\to g}(x,\mu,\phi) = \int_{\mu_1'}^{\mu_2'} d\mu' \left(\int_{\phi}^{\phi'_{min}} d\phi'\ \sigma\Psi + \int_{2\pi-\phi'_{min}}^{\phi+2\pi} d\phi'\ \sigma\Psi\right)$$

$$+ \int_{\mu_2'}^{\mu_3'} d\mu' \left(\int_{\phi'_{max}}^{\phi'_{min}} d\phi'\ \sigma\Psi + \int_{2\pi-\phi'_{min}}^{2\pi-\phi'_{max}} d\phi'\ \sigma\Psi\right)$$

$$+ \int_{\mu_3'}^{\mu_4'} d\mu' \left(\int_{\phi'_{max}}^{\phi+\pi} d\phi'\ \sigma\Psi + \int_{\phi+\pi}^{2\pi-\phi'_{max}} d\phi'\ \sigma\Psi\right). \tag{2.12}$$

For convenience, the subscripts and arguments of σ and Ψ in the above equation have been omitted.

2.1.1 Azimuthally Symmetric Case

For the azimuthally symmetric case, the angular flux distribution is independent of the azimuthal angle, ϕ. This case arises when the external source incident on the slab is azimuthally symmetric such as the normally incident source. In this case the scattering source given by Eq. (2.2) reduces to

$$S_{g'\to g}(x,\mu) = \int_{-1}^{+1} d\mu'\ \Psi_{g'}(x,\mu') \int_0^{2\pi} d\phi'\ \sigma_{g'\to g}(\mu_o), \tag{2.13}$$

where $s_{g'\to g}(x,\mu)$ and $\Psi_{g'}(x,\mu')$ are the azimuthally averaged values defined by

$$S_{g'\to g}(x,\mu) = \frac{1}{2\pi}\int_0^{2\pi} d\phi\ S_{g'\to g}(x,\mu,\phi), \tag{2.14}$$

and

$$\Psi_{g'}(x,\mu') = \frac{1}{2\pi}\int_0^{2\pi} d\mu'\ \Psi_{g'}(x,\mu',\phi'). \tag{2.15}$$

Equation (2.13) is obtained from Eq. (2.2) by integrating over the azimuthal angle and using the fact that the ϕ'-integral in Eq. (2.13) is independent of ϕ.

From Eq. (2.3) it is clear that μ_o is symmetric about $\phi'=\pi$. Hence, Eq. (2.13) becomes

$$S_{g'\to g}(x,\mu) = 2\int_{-1}^{+1} d\mu'\ \Psi_g\ (x,\mu')\int_0^{\pi} d\phi'\ \sigma_{g'\to g}(\mu_o). \qquad (2.16)$$

Thus only half the ϕ' integration range need be considered in the evaluation of the scattering source term when the angular flux is azimuthally symmetric.

The appropriate limits of the μ' and ϕ' integrals in Eq. (2.16) when $\sigma_{g'\to g}(\mu_o)$ has angular support between $\mu_{o,min}$ and $\mu_{o,max}$ can be found from Figs. 2.2-2.6. It is necessary to decompose the domain of integration into several subdomains as

$$\int_{-1}^{+1} d\mu' \int_0^{\pi} d\phi' = \int_{-1}^{\mu_1'} d\mu' \int_{\phi_1'}^{\phi_2'} d\phi' + \int_{\mu_1'}^{\mu_2'} d\mu' \int_{\phi_3'}^{\phi_4'} d\phi'$$

$$+ \int_{\mu_2'}^{\mu_3'} d\mu' \int_{\phi_5'}^{\phi_6'} d\phi' + \int_{\mu_3'}^{\mu_4'} d\mu' \int_{\phi_7'}^{\phi_8'} d\phi' + \int_{\mu_4'}^{1} d\mu' \int_{\phi_9'}^{\phi_{10}'} d\phi' \qquad (2.17)$$

where μ_i', i=1,2,...4 are given by Eqs. (2.7)-(2.11), and values of ϕ_i',i=1,2,...10 are listed in Table 2.1.

Reversing the order of integration in Eq. (2.17) does not result in any simplication of the scattering source term. Although for the case $-|\mu| < \mu_{o,min},\mu_{o,max} < |\mu|$, such a change eliminates the need for μ' break points, the limits of the μ'-integral becomes very complicated.

Table 2.1. Limits of ϕ' Integrals in Eq. (2.17).

Case	ϕ'_1	ϕ'_2	ϕ'_3	ϕ'_4	ϕ'_5	ϕ'_6	ϕ'_7	ϕ'_8	ϕ'_9	ϕ'_{10}
	Limits of ϕ'-Integrals									
1. $\mu_{o,min}, \mu_{o,max} < -\lvert\mu\rvert$	–	–	c[+]	π	c	d[++]	c	π	–	–
2. $-\lvert\mu\rvert < \mu_{o,min}, \mu_{o,max} < \lvert\mu\rvert$	–	–	0	d	c	d	c	π	–	–
3. $\mu_{o,min}, \mu_{o,max} > \lvert\mu\rvert$	–	–	0	d	c	d	0	d	–	–
4. $\mu_{o,min} < -\lvert\mu\rvert, -\lvert\mu\rvert < \mu_{o,max} < \lvert\mu\rvert$										
a. $\mu>0, \overline{\mu}'_1 < \overline{\mu}'_2$[+++]	0	π	0	d	c	d	c	π	–	–
b. $\mu>0, \overline{\mu}'_1 > \overline{\mu}'_2$	0	π	c	π	c	d	c	π	–	–
c. $\mu<0, \overline{\mu}'_3 > \overline{\mu}'_4$	–	–	c	π	c	d	0	d	0	π
d. $\mu<0, \overline{\mu}'_3 < \overline{\mu}'_4$	–	–	c	π	c	d	c	π	0	π
5. $-\lvert\mu\rvert < \mu_{o,min} < \lvert\mu\rvert, \mu_{o,max} > \lvert\mu\rvert$										
a. $\mu>0, \overline{\mu}'_1 < \overline{\mu}'_2$	–	–	0	d	c	d	c	π	0	π
b. $\mu>0, \overline{\mu}'_1 > \overline{\mu}'_2$	–	–	0	d	c	d	0	d	0	π
c. $\mu<0, \overline{\mu}'_3 > \overline{\mu}'_4$	0	π	0	d	c	d	0	d	–	–
d. $\mu<0, \overline{\mu}'_2 < \overline{\mu}'_4$	0	π	c	π	c	d	0	d	–	–
6. $\mu_{o,min} < -\lvert\mu\rvert, \mu_{o,max} > \lvert\mu\rvert$										
a. $\mu>0$, max $[\overline{\mu}'_1, \overline{\mu}'_3] <$ min $[\overline{\mu}'_2, \overline{\mu}'_4]$	0	π	0	d	c	d	c	π	0	π
b. $\mu>0$, max $[\overline{\mu}'_1, \overline{\mu}'_3] >$ min $[\overline{\mu}'_2, \overline{\mu}'_4]$	0	π	0	d	0	π	c	π	0	π
c. $\mu<0$, min $[\overline{\mu}'_1, \overline{\mu}'_3] >$ max $[\overline{\mu}'_2, \overline{\mu}'_4]$	0	π	c	π	c	d	0	d	0	π
d. $\mu<0$, min $[\overline{\mu}'_1, \overline{\mu}'_3] <$ max $[\overline{\mu}'_2, \overline{\mu}'_4]$	0	π	c	π	0	π	0	d	0	π

[+] $c = \phi'_{max} = \cos^{-1} [(\mu_{o,max} - \mu\mu')/(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}]$

[++] $d = \phi'_{min} = \cos^{-1} [(\mu_{o,min} - \mu\mu')/(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}]$

[+++] For definitions of $\overline{\mu}'_i$, i=1,2,...4, see Eqs. (2.8)-(2.11).

2.2 Transformation of Integration Variables From (μ',ϕ') to (μ',μ_o)

2.2.1 Transformation Equations

For simplicity, the azimuthally symmetric case is first considered. In this case, the scattering source term for transfer from energy group g' to energy group g is given by Eq. (2.16) with

$$\mu_o = \mu\mu' + (1-\mu^2)^{1/2} (1-\mu'^2)^{1/2} \cos\phi'. \qquad (2.18)$$

A transformation of the above source integral is sought such that the integration variables are μ' and μ_o. Upon changing the variable integration from ϕ' to μ_o in Eq. (2.16) one obtains

$$S_{g'\to g}(x,\mu) = \int_{-1}^{+1} d\mu' \ \Psi_{g'}(x,\mu') \int_{D*} d\mu_o \ |J| \ \sigma_{g'\to g}(\mu_o), \qquad (2.19)$$

where $J = \partial\phi'/\partial\mu_o$ is the Jacobian of transformation, and D* is image of the limits of the ϕ'-integral under the transformation.

To evaluate the Jacobian, one obtains from Eq. (2.18)

$$\frac{\partial\mu_o}{\partial\phi'} = -(1-\mu^2)^{1/2} (1-\mu'^2)^{1/2} \sin\phi'. \qquad (2.20)$$

The variable ϕ' can be eliminated from Eq. (2.20) using Eq. (2.18). After some algebra one obtains

$$\frac{\partial\mu_o}{\partial\phi'} = -(1 - \mu^2 - \mu'^2 - \mu_o^2 + 2\mu\mu'\mu_o)^{1/2},$$

and hence,

$$J \equiv \partial\phi'/\partial\mu_o = -(1 - \mu^2 - \mu'^2 - \mu_o^2 + 2\mu\mu'\mu_o)^{-1/2}. \qquad (2.21)$$

Thus, with this transformation of the azimuthal angle to the cosine of the scattering angle, the group-to-group scattering source becomes

$$S_{g'\to g}(x,\mu) = \int_{-1}^{+1} d\mu' \ \Psi_{g'}(x,\mu') \int_{D*} d\mu_o \ \frac{\sigma_{g'\to g}(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o+2\mu\mu'\mu_o)^{1/2}} \qquad (2.22)$$

The limits of integration in the μ_o-integral can be readily found. One then obtains

$$S_{g'\to g}(x,\mu) = 2\int_{-1}^{+1} d\mu'\ \Psi_{g'}(x,\mu) \int_{f_1}^{f_2} d\mu_o \frac{\sigma_{g'\to g}(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}}, \qquad (2.23)$$

where

$$f_1(\mu,\mu') = \mu\mu' - (1-\mu^2)^{1/2}\ (1-\mu'^2)^{1/2}, \qquad (2.24)$$

and

$$f_2(\mu,\mu') = \mu\mu' + (1-\mu^2)^{1/2}\ (1-\mu'^2)^{1/2}. \qquad (2.25)$$

It is readily verified that the integrand in Eq. (2.23) is unbounded at the limits of the μ_o-integral. Despite these singularities, the μ_o-integral exists if $\sigma_{g'\to g}(\mu_o)$ is a well-behaved function (e.g. bounded), and μ^2, $\mu'^2 \neq 1$. The singularities in the μ_o-integral can be removed for numerical evaluation as is shown in Chapter 3.

2.2.2 <u>Transformation Mappings</u>

The mappings of the boundary of the (μ',ϕ') plane onto the (μ',μ_o) plane, as shown in Figs. 2.7a-2.7c, are next examined. These mappings are obtained using Eq. (2.18). It is clear from these figures that a one-to-one correspondence exists for all points except for $\mu,\mu' = \pm 1$.

In Figs. 2.8a and 2.8b, the inverse Jacobian (see Eq. 2.21) has been plotted as a function of μ_o, $f_1 \leq \mu_o \leq f_2$, for various values of μ and μ'. Here f_1 and f_2 denote the lower and the upper limits of the μ_o-integral in Eq. (2.23), and are given by Eqs. (2.24) and (2.25), respectively. From these figures, the following trends about the limits of integration in the μ_o-integral are observed.

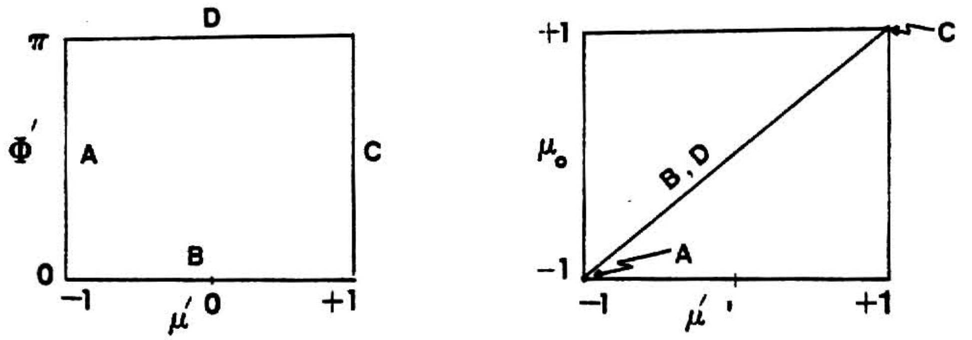

Fig. 2.7a. Transformation mappings, $\mu = +1$.

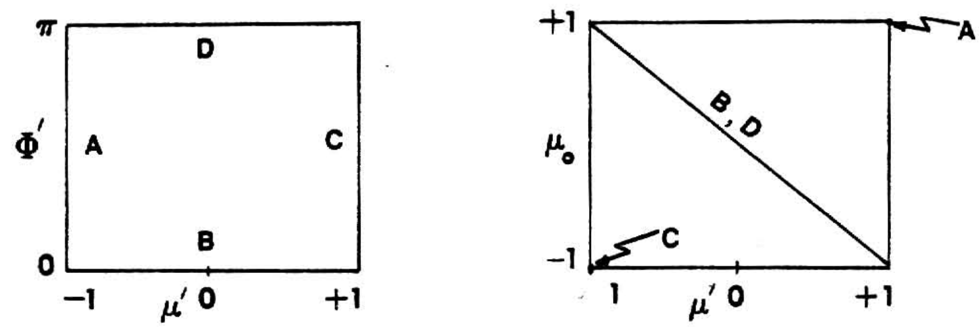

Fig. 2.7b. Transformation mappings, $\mu = -1$.

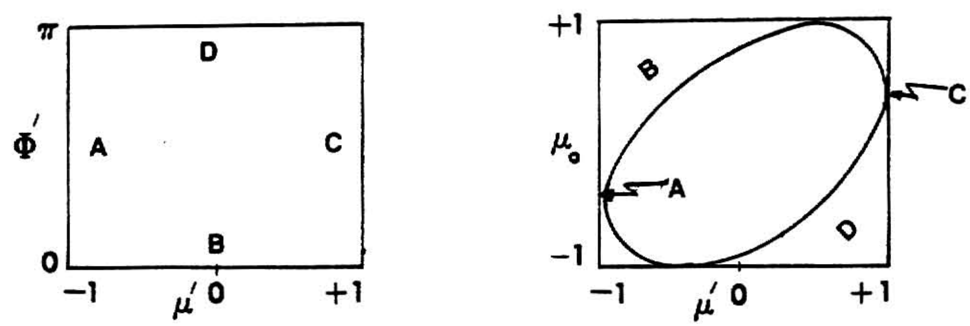

Fig. 2.7c. Transformation mappings, $\mu^2 \neq 1$ (μ=0.5).

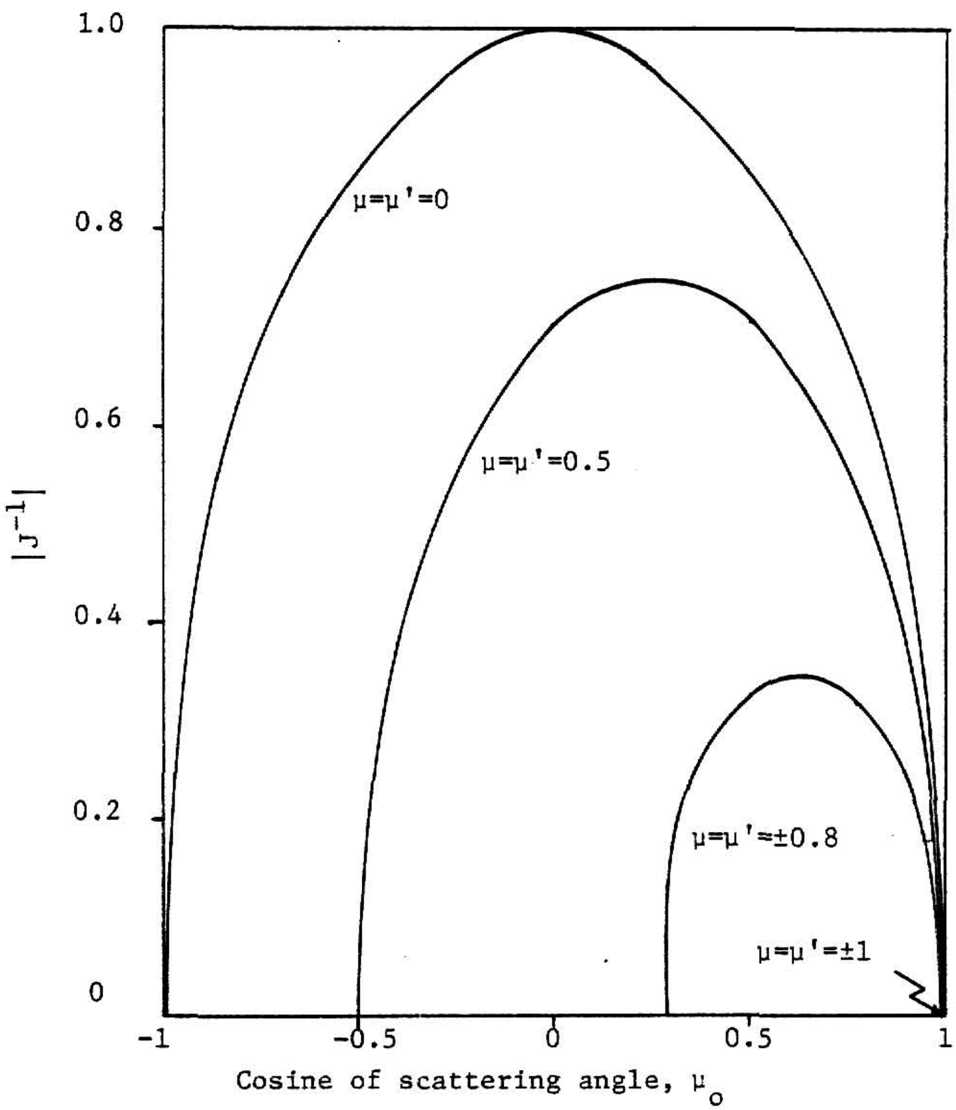

Fig. 2.8a. Inverse Jacobian as a function of μ_o; $\mu=\mu'$.

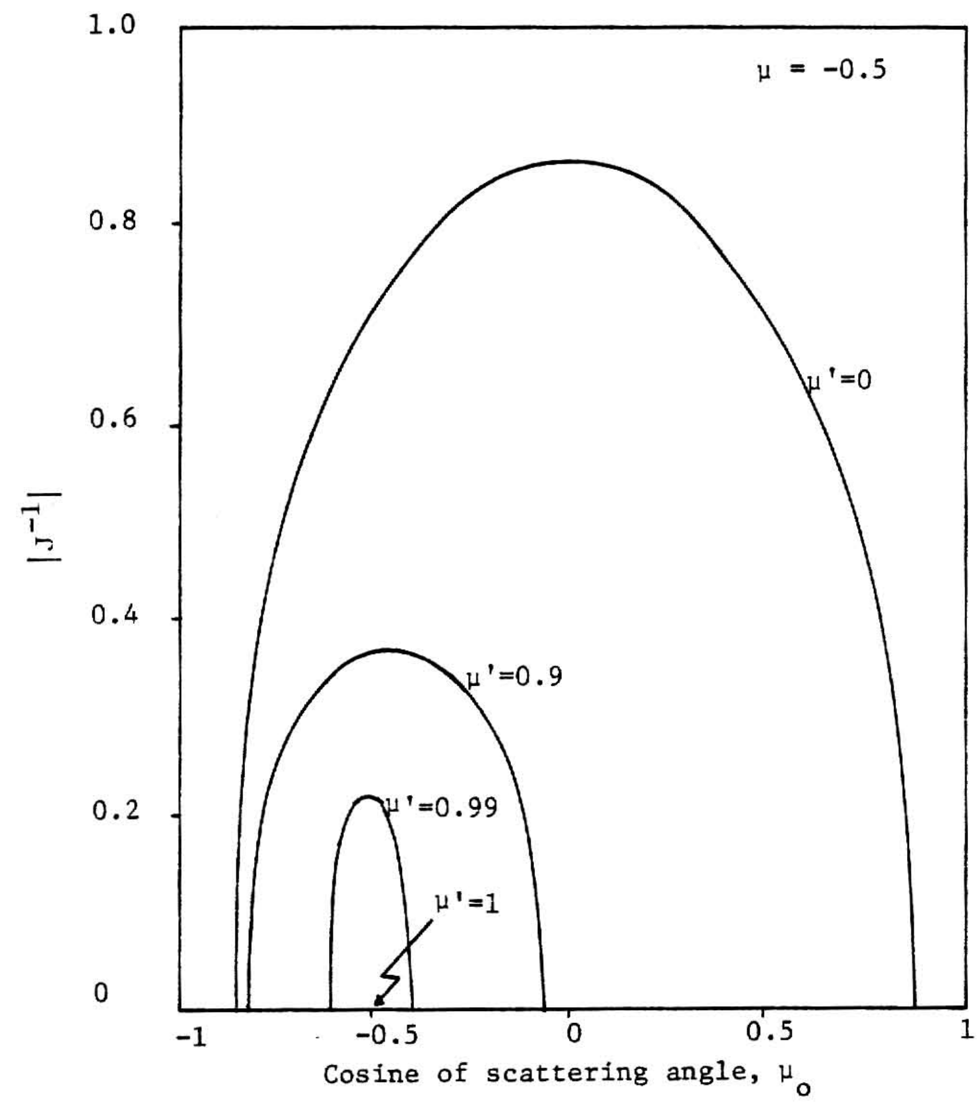

Fig. 2.8b. Inverse Jacobian as a 'function of μ_o; $\mu \neq \mu'$.

For $\mu = \mu'$, the upper limit of integration is equal to unity for all μ', and the lower limit of integration monotonically shifts from -1 to +1 as μ' varies from 0 to 1. For $\mu \neq \mu'$, both the upper and the lower limits monotonically shifts from -1 and +1 as μ' varies from 0 to 1 and collapses at $\mu_o = \mu$. The common feature is that as $\mu' \to 1$, the domain of integration shrinks to zero. The same is true for $\mu' \to -1$ or $\mu \to \pm 1$.

2.2.3 Limits of the Scattering Source Integral When the Group-to-Group Cross Sections Have Narrow Angular Support

When the group-to-group cross section, $\sigma_{g'\to g}(\mu_o)$ has a narrow angular support between $\mu_{o,min}$ and $\mu_{o,max}$, the form of the group-to-group scattering source term is given by

$$S_{g'\to g}(x,\mu) = 2 \int_{-1}^{+1} d\mu' \, \Psi_{g'}(x,\mu') \, A_{g'\to g}(\mu,\mu'), \tag{2.26}$$

where

$$A_{g'\to g}(\mu,\mu') = \begin{cases} \displaystyle\int_{\alpha}^{\beta} d\mu_o \frac{\sigma_{g'\to g}(\mu_o)}{(1-\mu^2-\mu_o'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}}, & \alpha<\beta \\ 0 & \alpha>\beta \end{cases} \tag{2.27}$$

$$\alpha = \max \quad \{f_1(\mu,\mu'), \mu_{o,min}\}, \tag{2.28}$$

and

$$\beta = \min \{f_2(\mu,\mu'), \mu_{o,max}\}. \tag{2.29}$$

It may be noted that α is greater than β only if $f_1(\mu,\mu') > \mu_{o,max}$, or $\mu_{o,min} > f_2(\mu,\mu')$. For both of these cases $\sigma_{g'\to g} \equiv 0$, and hence $A_{g'\to g}(\mu,\mu')$ also vanishes, as seen from Eq. (2.27).

Since $A_{g'\to g}(\mu,\mu')$ vanishes for some values of μ' in Eq. (2.27), μ'-subranges are sought such that $A_{g'\to g}(\mu,\mu')$ is non-zero over these sub-ranges. These subranges may be found the the μ_o-μ' diagram as shown in Fig. 2.9. The μ_o-μ' diagram is obtained by plotting μ_o as a function of μ' for fixed μ and $\phi' = 0$ or π, using Eq. 2.18. From Fig. 2.9 it is clear that if the cross section $\sigma_{g'\to g}(\mu_o)$ has support over the whole range of μ_o, the scattering source term is given by

$$S_{g'\to g}(x,\mu) = 2\int_{-1}^{+1} d\mu'\ \Psi_{g'}(x,\mu') \int_{f_1}^{f_2} d\mu_o\ \frac{\sigma_{g'\to g}(\mu_o)}{D}, \qquad (2.30)$$

where

$$D = (1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}. \qquad (2.31)$$

If, on the other hand, the cross section has angular support between $\mu_{o,min}$ and $\mu_{o,max}$, the domain of integration is as shown in Fig. 2.9. In order to carry out integration over this domain, it is necessary to break the range of μ' in three parts as follows:

i) $\mu_1' \leq \mu' \leq \mu_2'$ for which $\mu_{o,min} \leq \mu_o \leq f_2$

ii) $\mu_2' \leq \mu' \leq \mu_3'$ for which $\mu_{o,min} \leq \mu_o \leq \mu_{o,max}$

iii) $\mu_3' \leq \mu' \leq \mu_4'$ for which $f_1 \leq \mu_o \leq \mu_{o,max}$

where μ_1', μ_2', μ_3' and μ_4' are same as those defined in Section 2.1, and are given by Eqs. (2.7-2.11). The scattering source term, is, therefore given by

$$S_{g'\to g}(x,\mu) = 2\left(\int_{\mu_1'}^{\mu_2'} d\mu'\ \Psi\int_{\mu_{o,min}}^{f_2} d\mu_o\ \frac{\sigma}{D} + \int_{\mu_2'}^{\mu_3'} d\mu'\Psi \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o\,\frac{\sigma}{D}\right.$$
$$\left. + \int_{\mu_3'}^{\mu_4'} d\mu'\ \Psi \int_{f_1}^{\mu_{o,max}} d\mu_o\ \frac{\sigma}{D}\right). \qquad (2.32)$$

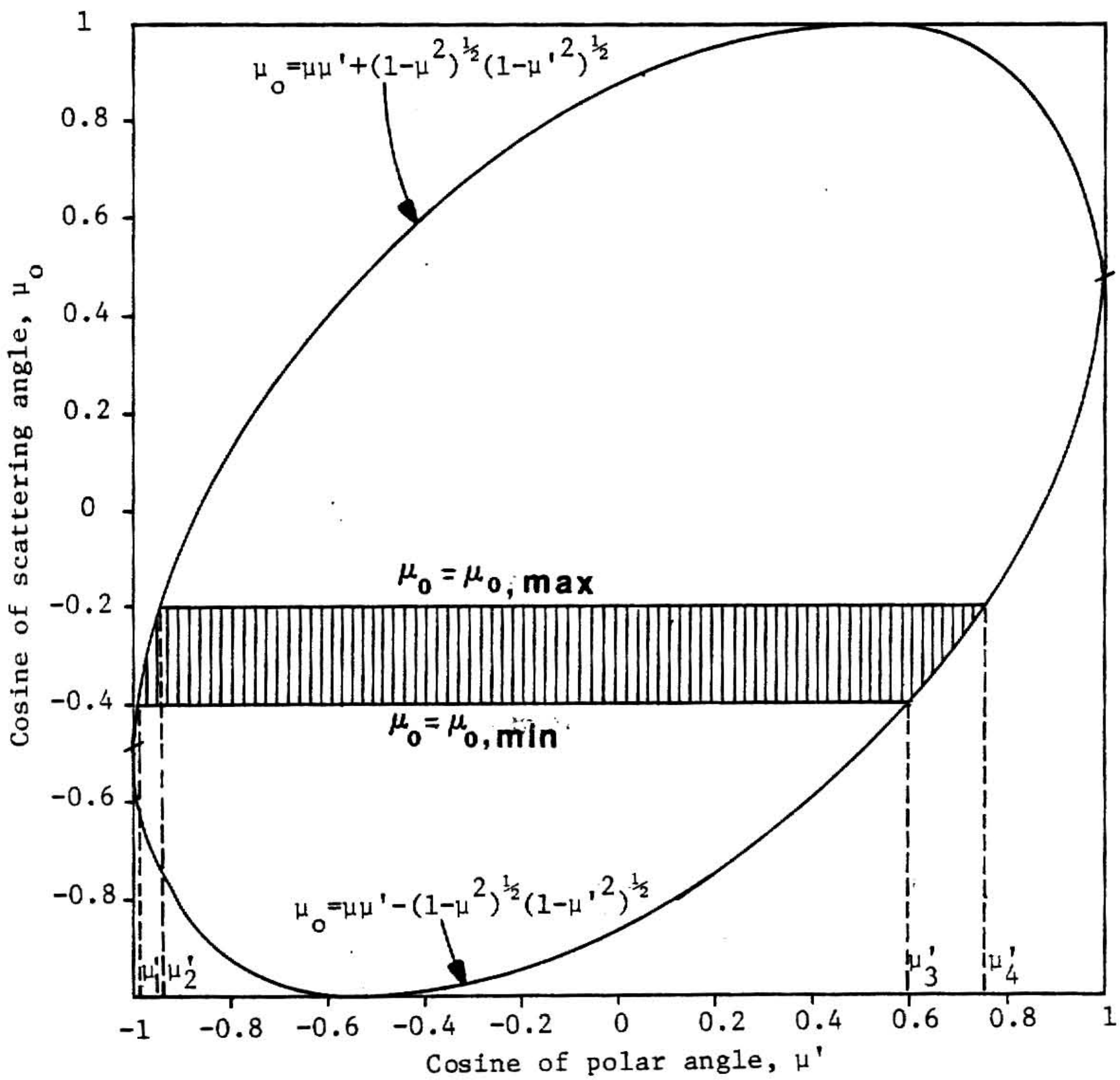

Fig. 2.9. μ_o-μ' diagram (μ=0.5, ϕ'=0 and π). Shaded region shows the domain of integration when group-to-group cross section has non-zero value for $\mu_{o,min}<\mu_o<\mu_{o,max}$.

For convenience, the subscripts and arguments of Ψ and σ in the above equation have been omitted.

An alternative approach for the evaluation of the group-to-group scattering source term is to reverse the order of integration in Eq. (2.30). From Fig. 2.10 it is seen that

$$S_{g'\to g}(x,\mu) = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o \ \sigma_{g'\to g}(\mu_o) \int_{\bar{f}_1}^{\bar{f}_2} d\mu' \frac{\Psi_{g'}(x,\mu')}{(1-\mu^2-\mu'^2\mu_o^2+2\mu\mu'\mu_o)^{1/2}} , \quad (2.33)$$

where

$$\bar{f}_1(\mu,\mu_o) = \mu\mu_o - (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2}, \quad (2.34)$$

and

$$\bar{f}_2(\mu,\mu_o) = \mu\mu_o + (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2}. \quad (2.35)$$

It is interesting to note that reversing the order of integration in Eq. (2.30) simplifies the form of the group-to-group scattering source term since it is no longer necessary to split the range of integration of the outer integral into several subranges and find the limits of the inner integral for each of these subranges which is quite cumbersome.

2.2.4 Azimuthally Dependent Case

The azimuthally-dependent case will now be considered. In this case, the scattering source term is given by

$$S_{g'\to g}(x,\mu,\phi) = \int_{-1}^{+1} d\mu' \int_{0}^{2\pi} d\phi' \ \sigma_{g'\to g}(\mu_o) \ \Psi_{g'}(x,\mu',\phi'), \quad (2.36)$$

where

$$\mu_o = \mu\mu' + (1-\mu^2)^{1/2} (1-\mu'^2)^{1/2} \cos(\phi'-\phi). \quad (2.37)$$

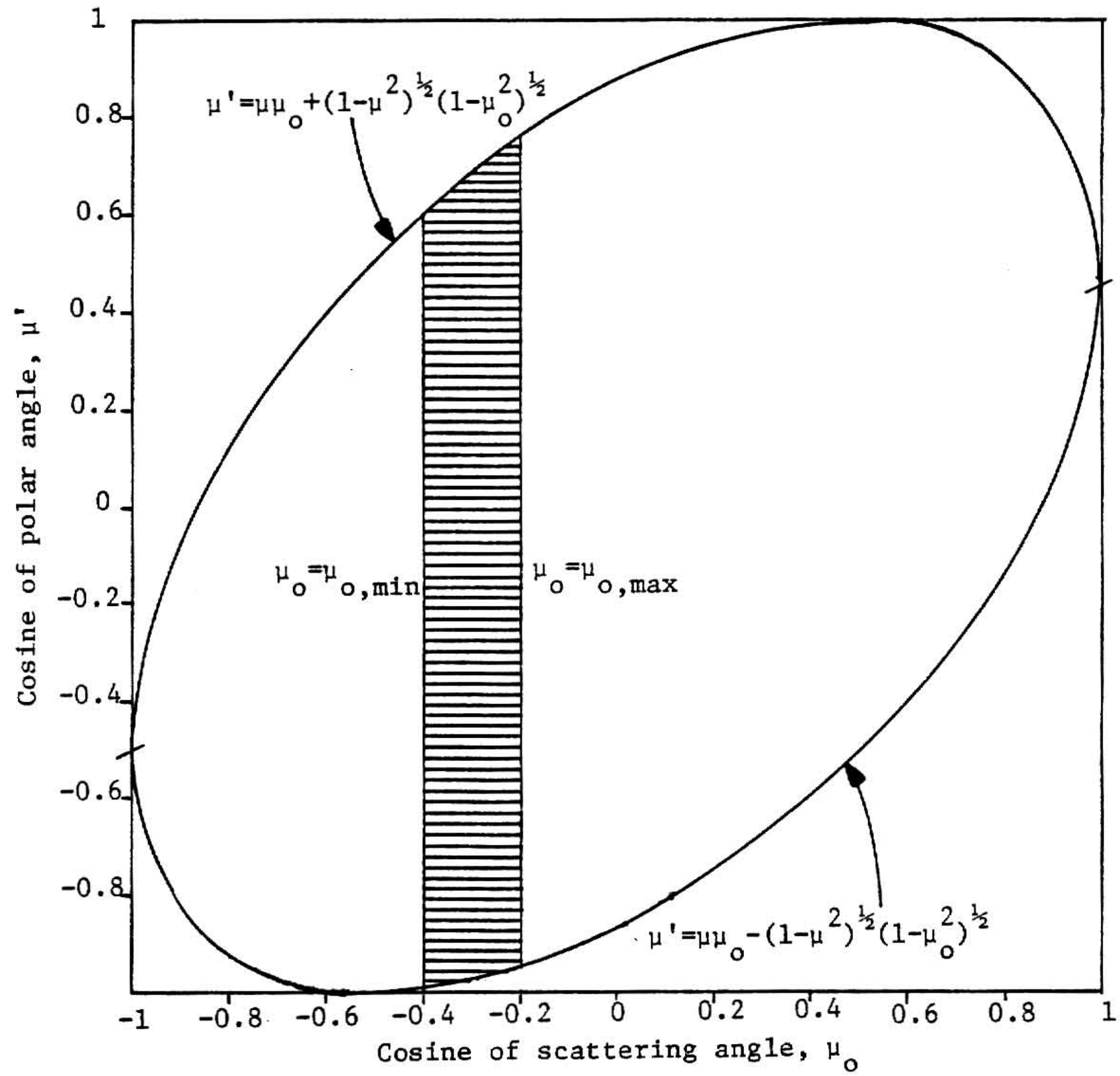

Fig. 2.10. μ'-μ_o diagram (μ=0.5, ϕ'=0 and π). Shaded region shows the domain of integration when group-to-group cross section has non-zero value for $\mu_{o,min}<\mu_o<\mu_{o,max}$.

Upon changing of variable of integration from ϕ' to μ' in Eq. (2.36) one obtains

$$S_{g'\to g}(x,\mu,\phi) = \int_{-1}^{+1} d\mu' \int_{c_1}^{c_2} d\mu_o \frac{\sigma_{g'\to g}(\mu_o)\ \Psi_{g'}[x,\mu',f^*(\mu',\mu_o,\mu,\phi)]}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}}, \tag{2.38}$$

where

$$c_1 = \mu\mu' + (1-\mu^2)^{1/2}\ (1-\mu'^2)^{1/2}\ \cos(2\pi-\phi), \tag{2.39}$$

$$c_2 = \mu\mu' + (1-\mu^2)^{1/2}\ (1-\mu'^2)^{1/2}\ \cos\phi, \tag{2.40}$$

and

$$f^*(\mu',\mu_o,\mu,\phi) = \phi + \cos^{-1}\{(\mu_o-\mu\mu')/(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}\}. \tag{2.41}$$

Clearly, the form of the scattering source term becomes very complicated, and it appears that the change of variable of integration from ϕ' to μ_o is not useful for the azimuthally dependent case.

2.3 Transformation of Integration Variables From (μ',ϕ') to (μ_o,ξ)

2.3.1 Transformation Equations

A transformation of the scattering source integral of Eq. (2.2) is sought such that the integration variables are μ_o and ξ where ξ is the angle of revolution about the $\underline{\Omega}$ direction as shown in Fig. 2.11. This transformation was first suggested, although not fully developed, by Odom [7]. In Fig. 2.11, $\hat{e}_1$, $\hat{e}_2$ and $\hat{e}_3$ represent unit vectors in the direction of x, y and z axis, respectively.

To find μ' as a function of μ_o and ξ, consider the orientation of the coordinate system as shown in Fig. 2.12. In terms of the coordinate axes of this figure,

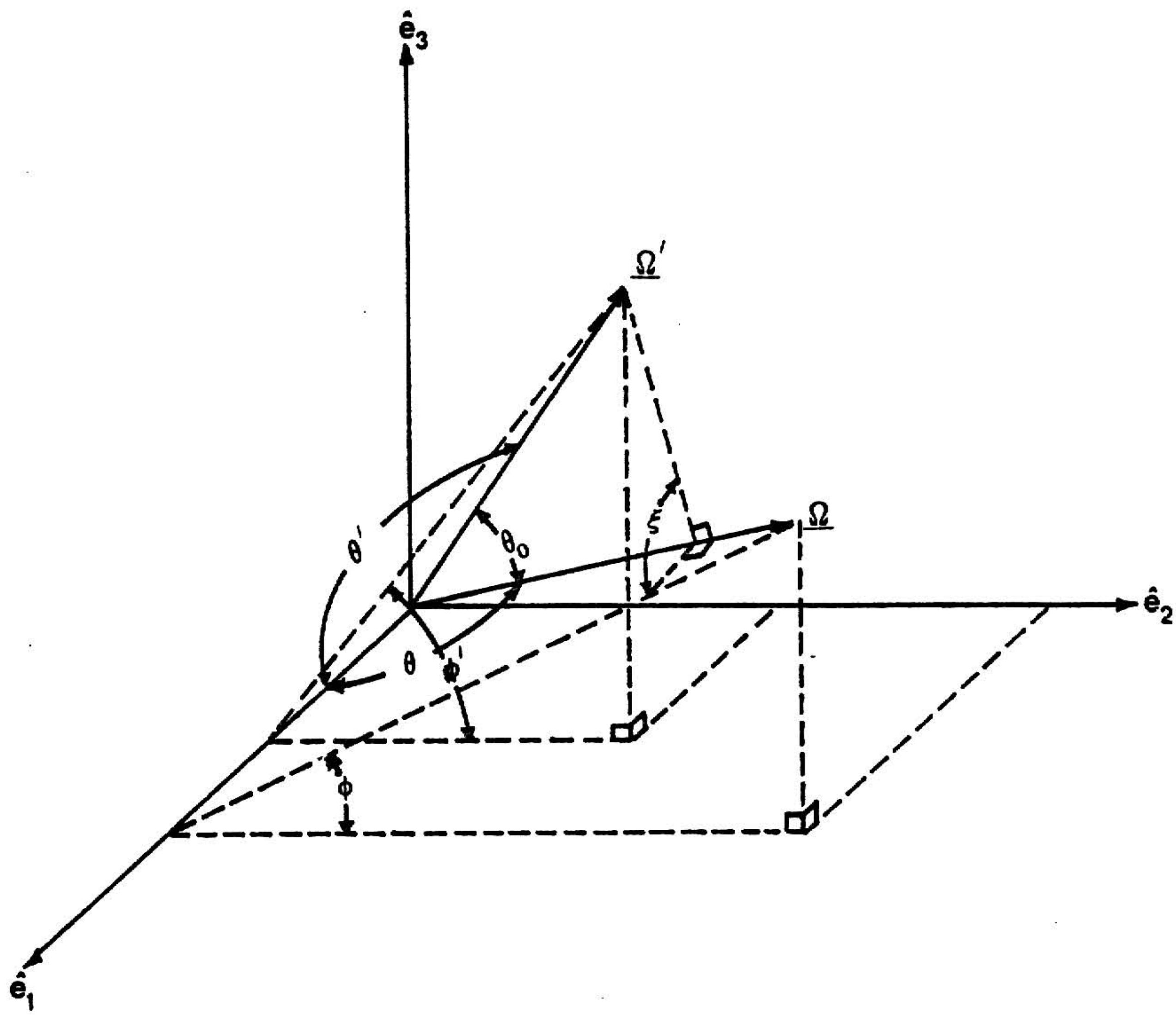

Fig. 2.11. Coordinate system.

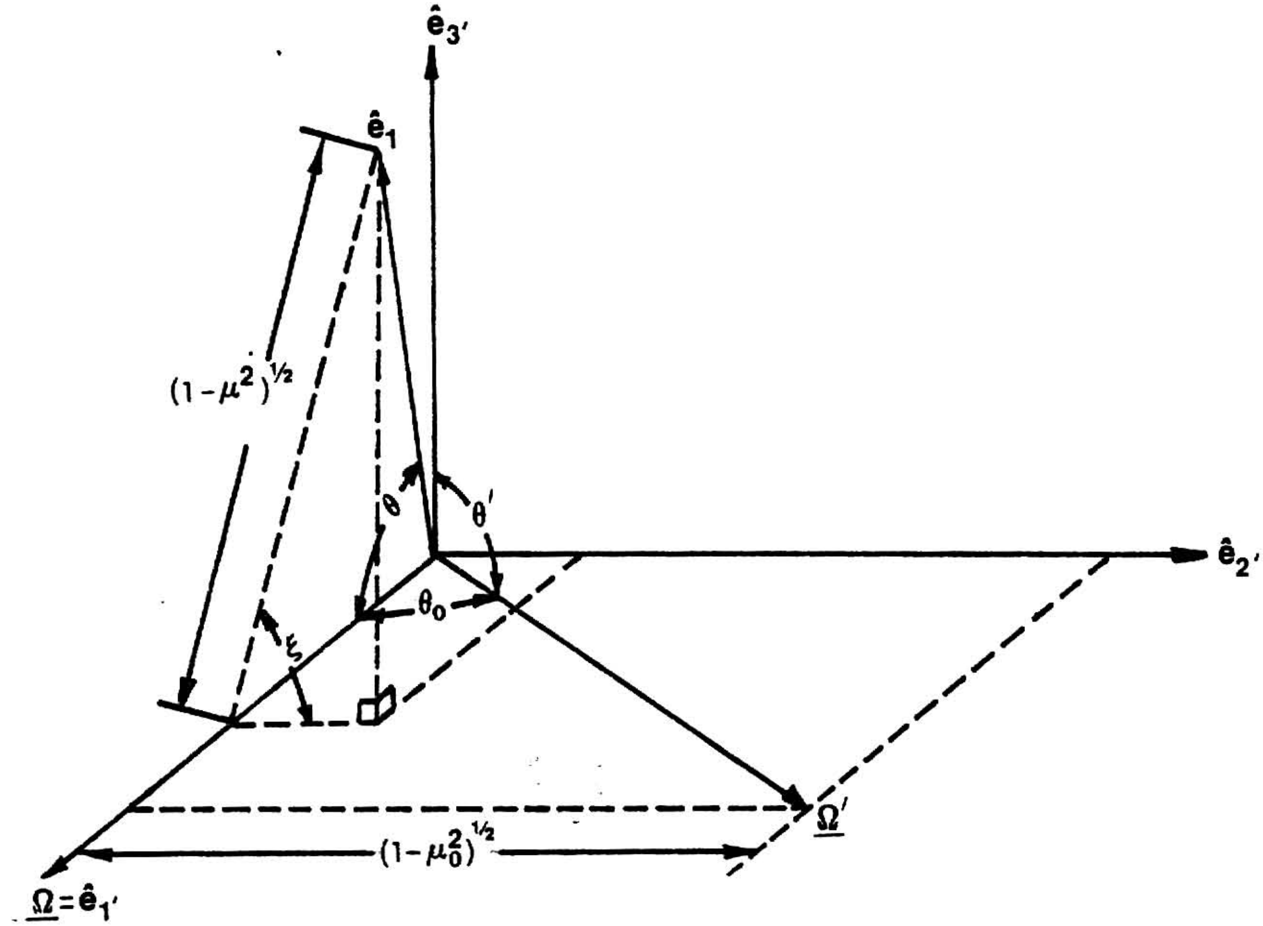

Fig. 2.12. Reorientation of coordinate system.

$$\hat{e}_1 = \mu\hat{e}_1' + (1-\mu^2)^{1/2} \cos\xi \; \hat{e}_2' + (1-\mu^2)^{1/2} \; \hat{e}_3' ,$$

and

$$\underline{\Omega}' = \mu_o \; \hat{e}_1' + (1-\mu_o^2)^{1/2} \; \hat{e}_2' + 0 \; \hat{e}_3'.$$

Therefore,

$$\mu' = \hat{e}_1 \cdot \underline{\Omega}' = \mu\mu_o + (1-\mu^2)^{1/2} \; (1-\mu_o^2)^{1/2} \cos\xi. \tag{2.42}$$

To find ϕ' as a function of μ_o and ξ, consider the orientation of the coordinate system as shown in Fig. 2.13. From this figure it is seen that (with r and t defined in the figure),

$$(1-\mu'^2)^{1/2} \sin(\phi'-\phi) = r = (1-\mu_o^2)^{1/2} \sin(\pi-\xi),$$

or

$$(1-\mu'^2)^{1/2} \sin(\phi'-\phi) = (1-\mu_o^2)^{1/2} \sin\xi. \tag{2.43}$$

Also,

$$(1-\mu'^2)^{1/2} \cos(\phi'-\phi) = t = \mu_o \sin\theta + (1-\mu_o^2)^{1/2} \cos(\pi-\xi) \cos\theta,$$

or,

$$(1-\mu'^2)^{1/2} \cos(\phi'-\phi) = \mu_o \; (1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2} \cos\xi. \tag{2.44}$$

From Eqs. (2.43) and (2.44) one then obtains

$$\phi' = \phi + \tan^{-1} \left[\frac{(1-\mu_o^2)^{1/2} \sin\xi}{\mu_o(1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2} \cos\xi} \right]. \tag{2.45}$$

Equations (2.42) and (2.45) define the transformation equations. The derivation of the transformation equations given above is based on the work of Ryman [13].

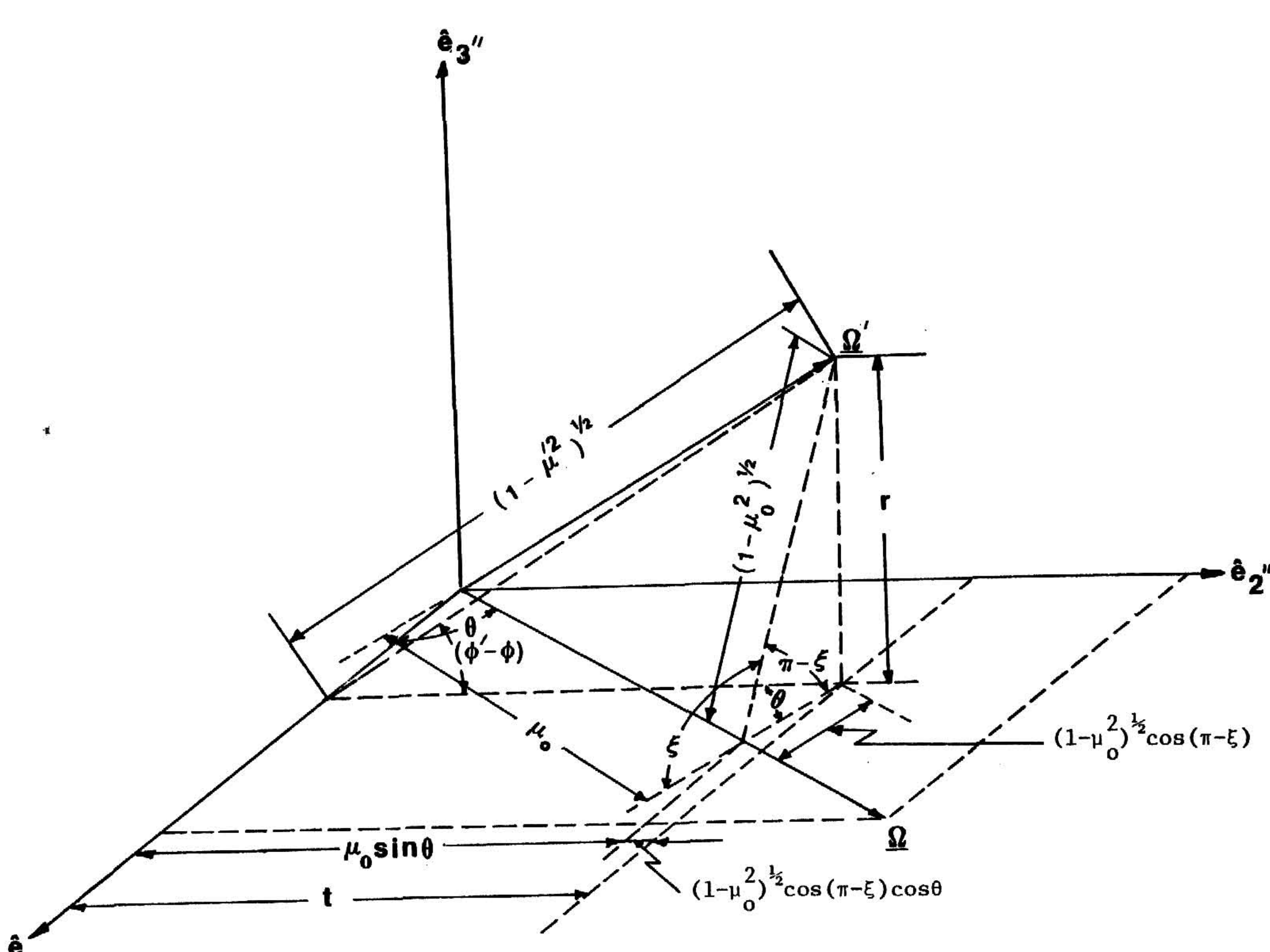

Fig. 2.13. Second reorientation of coordinate system.

Applying these transformations, and using the standard formula for the change of variables in a double integral [14], the scattering source term can be written as

$$S_{g'\to g}(x,\mu,\phi) = \int_{-1}^{+1} d\mu' \int_0^{2\pi} d\phi' \, \sigma_{g'\to g}(\mu_o) \, \Psi_{g'}(x,\mu',\phi')$$

$$= \int_{-1}^{+1} d\mu_o \, \sigma_{g'\to g}(\mu_o) \int_0^{2\pi} d\xi \, |J| \, \Psi_{g'}(x,g_1,g_2). \tag{2.46}$$

where J is the Jacobian of transformation, and is given by

$$J = \begin{vmatrix} \frac{\partial\mu'}{\partial\mu_o} & \frac{\partial\mu'}{\partial\xi} \\ \frac{\partial\phi'}{\partial\mu_o} & \frac{\partial\phi'}{\partial\xi} \end{vmatrix} = \frac{\partial\mu'}{\partial\mu_o}\frac{\partial\phi'}{\partial\xi} - \frac{\partial\mu'}{\partial\xi}\frac{\partial\phi'}{\partial\mu_o}, \tag{2.47}$$

and

$$g_1(\mu,\mu_o,\xi) = \mu\mu_o + (1-\mu^2)^{1/2} \, (1-\mu_o^2)^{1/2} \cos\xi, \tag{2.48}$$

$$g_2(\mu,\phi,\mu_o,\xi) = \phi + \tan^{-1} \frac{(1-\mu_o^2)^{1/2}\cos\xi}{\mu_o(1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2}\cos\xi}. \tag{2.49}$$

In order to find the Jacobian it is necessary to evaluate the partial derivatives in Eq. (2.47).

From Eq. (2.42) one obtains

$$\frac{\partial\mu'}{\partial\mu_o} = \mu - \mu_o(1-\mu_o^2)^{-1/2} \, (1-\mu^2)^{1/2} \cos\xi, \tag{2.50}$$

and

$$\frac{\partial\mu'}{\partial\xi} = -\,(1-\mu^2)^{1/2} \, (1-\mu_o^2)^{1/2} \sin\xi. \tag{2.51}$$

Also, from Eqs. (2.43) and (2.44), after some algebra, one finds (see Appendix A)

$$\frac{\partial\phi'}{\partial\mu_o} = \frac{1}{h_1} \quad \{- \mu_o(1-\mu_o^2)^{-1/2} \sin\xi + \frac{h_2}{h_3} [\mu-\mu_o(1-\mu_o^2)^{-1/2} \ (1-\mu^2)^{1/2} \cos\xi]\},$$

(2.52)

and

$$\frac{\partial\phi'}{\partial\xi} = \frac{1}{h_1} \quad \{(1-\mu_o^2)^{1/2} \cos\xi - \frac{h_2}{h_3} (1-\mu^2)^{1/2} \ (1-\mu_o^2)^{1/2} \sin\xi\}, \qquad (2.53)$$

where

$$h_1 = \mu_o(1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2} \cos\xi, \qquad (2.54)$$

$$h_2 = (1-\mu_o^2)^{1/2} \sin\xi \ \{\mu\mu_o + (1-\mu^2)^{1/2} \ (1-\mu_o^2)^{1/2} \cos\xi\}, \qquad (2.55)$$

and

$$h_3 = (1-\mu_o^2)^{1/2} \sin^2\xi + (1-\mu^2)\mu_o^2 - 2\mu_o \ (1-\mu^2)^{1/2}$$

$$(1-\mu_o^2)^{1/2} \cos\xi + \mu^2(1-\mu_o^2) \cos^2\xi. \qquad (2.56)$$

Upon substituting Eqs. (2.50)-(2.53) in Eq. (2.47), and after some algebra, one obtains (See Appendix A)

$$J = -1. \qquad (2.57)$$

Using Eq. (2.57) in Eq. (2.46) one finally obtains

$$S_{g'\to g}(x,\mu,\phi) = \int_{-1}^{+1} d\mu_o \ \sigma_{g'\to g}(\mu_o) \int_0^{2\pi} d\xi \ \Psi_{g'} \ (x,g_1,g_2) \qquad (2.58)$$

where g_1 and g_2 are given by Eq. (2.48) and Eq. (2.49), respectively.

For the azimuthally symmetric problem the flux is independent of the azimuthal angle, ϕ. In this case, the scattering source takes the simpler form

$$S_{g'\to g}(x,\mu) = \int_{-1}^{+1} d\mu_o \ \sigma_{g'\to g}(\mu_o) \int_0^{2\pi} d\xi \ \Psi_{g'}(x,g_1). \qquad (2.59)$$

Using the fact that $\cos\xi = \cos(2\pi-\xi)$, $0 \le \xi \le \pi$, Eq. (2.59) becomes

$$S_{g'\to g}(x,\mu) = 2\int_{-1}^{+1} d\mu_o\ \sigma_{g'\to g}(\mu_o) \int_0^{\pi} d\xi\ \Psi_{g'}[x,g_1(\mu,\mu_o,\xi)]. \qquad (2.60)$$

2.3.2 Transformation Mappings

The mappings of the boundary of the (μ',ϕ') onto the (μ_o,ξ) plane, as shown in Figs. 2.14(a)-2.14(c), are next examined. These mappings are obtained using Eqs. (2.42)-(2.45). It is necessary to consider three separate cases: (i) $\mu^2 \neq 1$, (ii) $\mu = -1$, and (iii) $\mu = +1$. It is seen that for all cases the boundaries of the (μ',ϕ') plane maps onto the boundaries of the (μ_o,ξ) plane. It is also seen that although one-to-one correspondence exists for $\mu = \pm 1$, the mapping is undefined for $\mu^2 \neq 1$ when $\mu_o = \pm 1$ and $\pm \mu$.

To find the limits of the ξ-integral, for the case when $\sigma_{g'\to g}(\mu_o)$ has a narrow angular support over the interval μ_o: $[\mu_{o,min}, \mu_{o,max}]$, the iso-$\mu_o$ curves in the (μ',ϕ') integration plane for fixed μ and the images of these curves in the (μ_o,ξ) integration plane are plotted in Fig. 2.15. It is clear from these figures that the limits of the ξ-integral are 0 and π (except when $\mu_o = \pm \mu$ and $\mu_o = \pm 1$ in which cases they are indeterminate).

2.3.3 Limits of the Scattering Source Integral When the Group to-Group Cross Sections Have Narrow Angular Support

From the transformation mapping given in the previous section, it is clear that the scattering source integral, when the group-to-group cross section, $\sigma_{g'\to g}(\mu_o)$ has a narrow angular support over μ_o: $[\mu_{o,min}, \mu_{o,max}]$, is given by

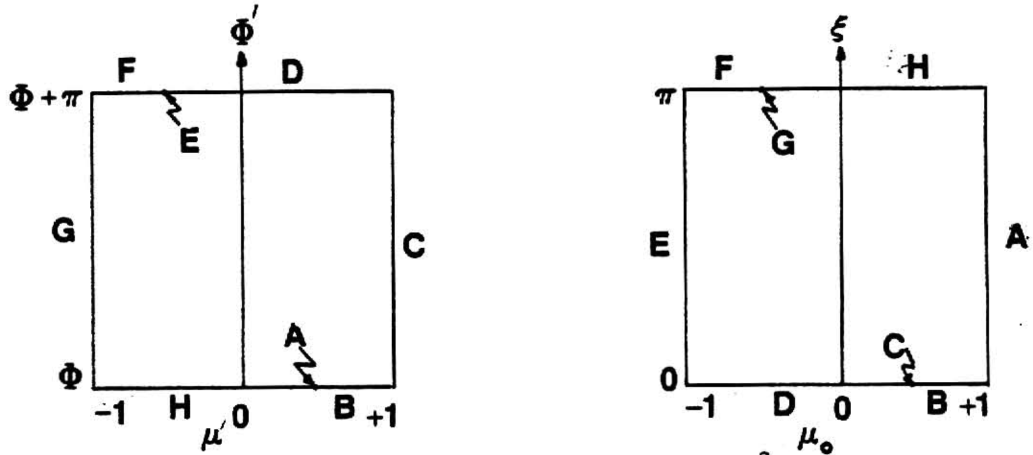

Fig. 2.14a. Transformation mappings, $\mu^2 \neq 1$.

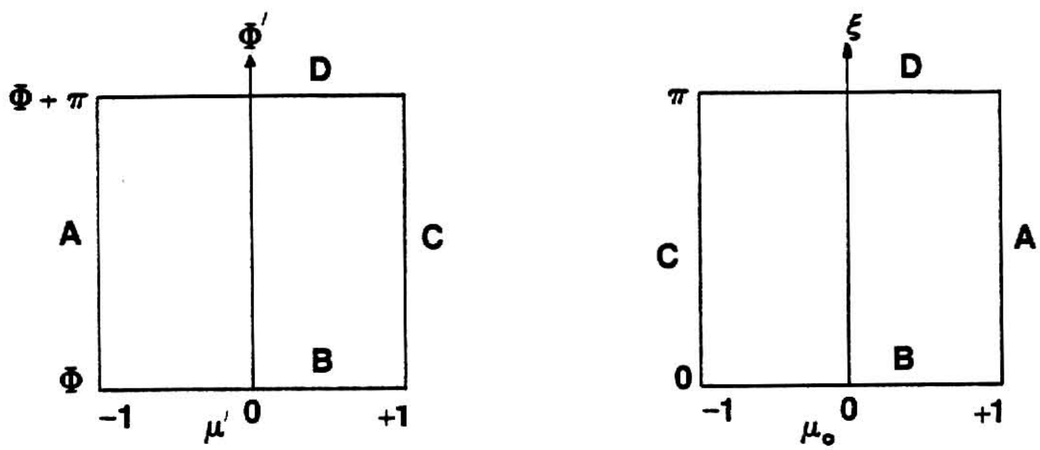

Fig. 2.14b. Transformation mappings, $\mu = -1$.

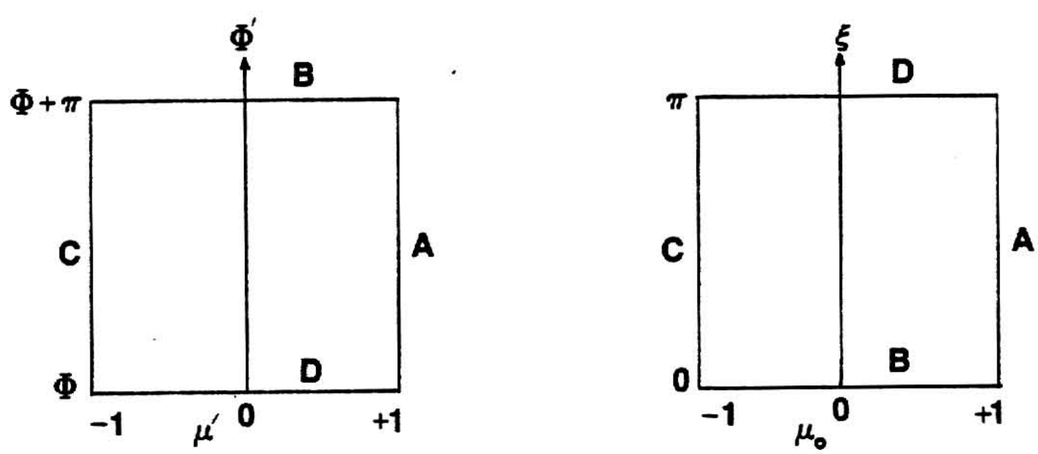

Fig. 2.14c. Transformation mappings, $\mu = +1$.

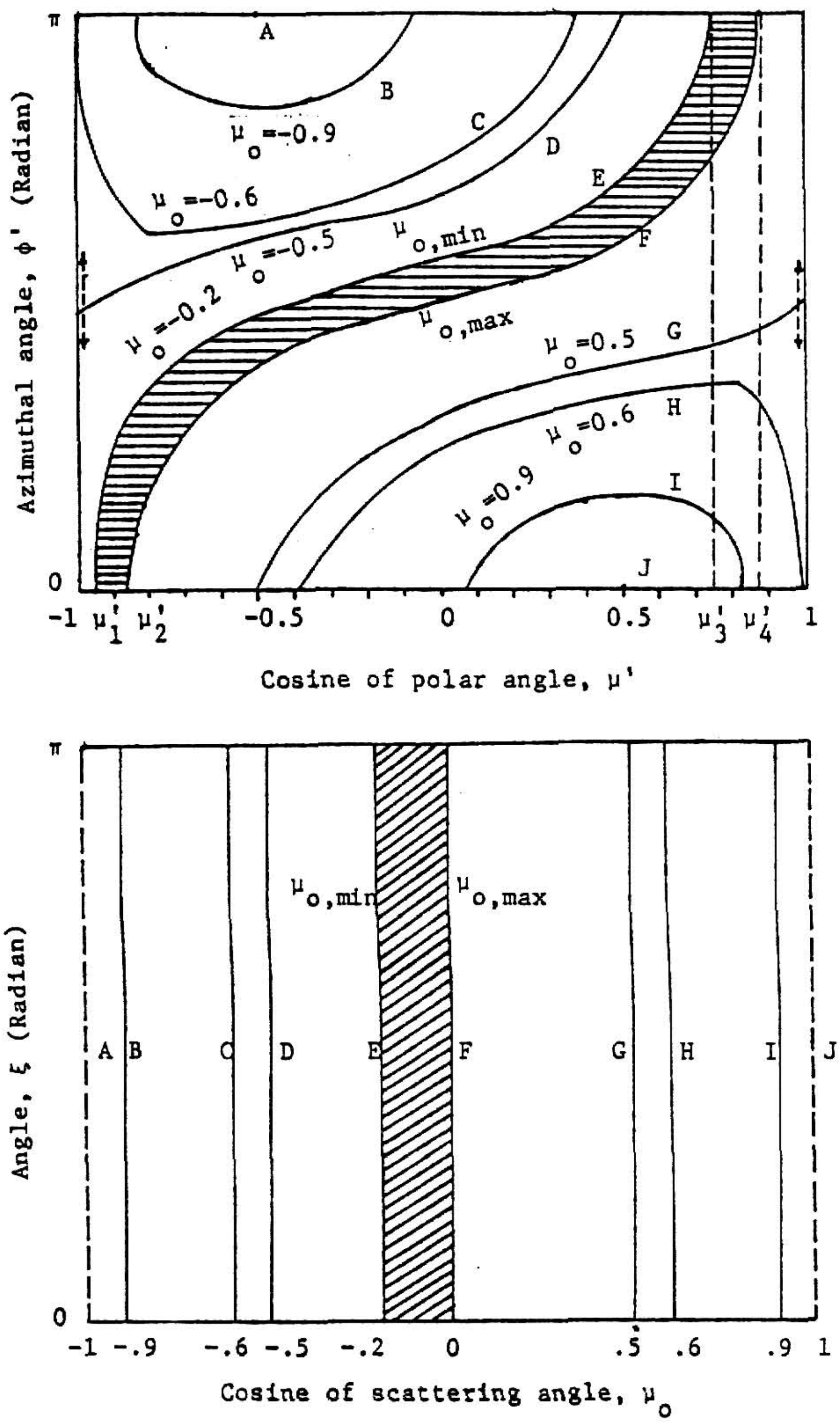

Fig. 2.15. Iso-μ_o curves in the (μ',ϕ') plane (μ=0.5), and their images in the (μ_o,ξ) plane. Shaded region shows the domain of integration when group-to-group cross section has non-zero value for $\mu_{o,min}<\mu_o<\mu_{o,max}$.

$$S_{g'\to g}(x,\mu) = 2 \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o \, \sigma_{g'\to g}(\mu_o) \int_0^{\pi} d\xi \, \Psi_{g'}$$

$$[x, \mu\mu_o + (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2} \cos\xi]. \qquad (2.61)$$

Thus it is seen that the limits of integration in the (μ_o,ξ) plane are much simpler than those in the (μ',ϕ') plane, since it is no longer necessary to split the range of integration in the outer integral and find the limits of the inner integral for each of these subranges which is quite cumbersome. However, as will be seen in the next chapter, the use of the scattering source term in the above form requires flux interpolation in the iterative solution of the neutron transport equation by the method of discrete ordinates.

3.0 METHODS OF EVALUATION OF THE SCATTERING SOURCE TERM IN THE DISCRETE ORDINATE TRANSPORT EQUATION

The multigroup form of the discrete ordinate transport equation in slab geometry (azimuthally symmetric case) can be written as [12,15]

$$\mu_i \frac{\partial \Psi_g(x,\mu_i)}{\partial x} + \sigma_g \Psi_g(x,\mu_i) = \sum_{g'} S_{g'\to g}(x,\mu_i), \tag{3.1}$$

where μ_i is the direction cosine in the i-th discrete direction, $\Psi_g(x,\mu_i)$ is the angular flux for group g at spatial point x and in direction with directed cosine μ_i, σ_g is the total cross section for group g, and $S_{g'\to g}(x,\mu_i)$ is the scattering source from group g' to group g at x and in direction μ_i. Specific forms of $S_{g'\to g}(x,\mu)$ involving highly anisotropic group-to-group cross sections have been discussed in the last chapter.

Equation (3.1) can be solved by using standard discrete ordinate techniques, i.e., by discretizing the spatial variable, replacing the spatial derivative operator by its finite difference representation, evaluating $S_{g'\to g}(x,\mu_i)$ by numerical quadrature and solving the resulting equations by iteration [12]. For an accurate solution of the discrete ordinate equations with highly anisotropic scattering, the traditional truncated Legendre function expansion method is not useful. In this chapter various methods to evaluate the scattering source term accurately are discussed. First, however, the traditional Legendre function expansion method is reviewed.

3.1 Legendre Function Expansion Method for Treating Scattering Source Term with Highly Anisotropic Cross Sections

The scattering source term in the multigroup neutron transport equation can be written as

$$S_{g'\to g}(x,\mu) = \int_{-1}^{+1} d\mu' \, \Psi_{g'}(x,\mu') \int_{0}^{2\pi} d\phi' \, \sigma_{g'\to g}(\mu_o). \qquad (3.2)$$

The group-to-group cross sections are commonly approximated by the following N+1 term Legendre polynomial expansion:

$$\sigma_{g'\to g}(\mu_o) \simeq \sum_{n=0}^{N} \frac{2n+1}{4\pi} \, C_n^{g'\to g} \, P_n(\mu_o), \qquad (3.3)$$

where $C_n^{g'\to g}$ are the expansion coefficients, and P_n are the Legendre function of the first kind [16]. Using the addition theorem [16], the expansion in Eq. (3.3) can be re-expressed as

$$\sigma_{g'\to g}(\mu_o) = \frac{1}{4\pi} \sum_{n=0}^{N} (2n+1) \, C_n^{g'\to g} \, [P_n(\mu) \, P_n(\mu') +$$

$$2 \sum_{m=1}^{n} \frac{(n-m)!}{(n+m)!} P_n^m(\mu) \, P_n^m(\mu') \cos m(\phi-\phi')], \qquad (3.4)$$

where P_n^m are the associated Legendre functions of the first kind [16]. Insertion of Eq. (3.4) in Eq. (3.2) and integration over the azimuthal angle ϕ yields

$$S_{g'\to g}(x,\mu) = \frac{1}{2} \sum_{n=0}^{N} (2n+1) \, C_n^{g'\to g} \, P_n(\mu) \int_{-1}^{+1} d\mu' \, P_n(\mu') \, \Psi_{g'}(x,\mu'). \qquad (3.5)$$

With the introduction of numerical quadratures for the integration over μ', the scattering source in the discrete direction μ_i can be approximated by

$$S_{g'\to g}(x,\mu_i) \simeq \frac{1}{2} \sum_{n=0}^{N} (2n+1)\, C_n^{g'\to g}\, P_n(\mu_i) \sum_j \omega_j P_n(\mu_j)\, \Psi_{g'}(x,\mu_j), \quad (3.6)$$

where ω_j are the quadrature weights for integration over μ'. This form of the scattering source term is widely used in discrete ordinate codes based on the Legendre expansion method [17,18].

If the group-to-group cross sections $\sigma_{g'\to g}(\mu_o)$ are highly peaked and have a narrow angular support as is the case in fine multigroup neutron and photon shielding calculations, the truncated Legendre function expansion using a reasonable number of terms (≤ 8) may introduce severe distortions in the cross sections which in turn produce negative or oscillatory angular fluxes. A high order expansion which would mitigate these effects is generally found to be practically infeasible for multigroup discrete ordinate calculations as a result of excessive computational effort.

3.2 Evaluation of the Scattering Source Integral with (μ_o,ξ) as Integration Variables

For simplicity the azimuthally symmetric case is first considered. In this case, as noted in Chapter 2, the scattering source term is given by

$$S(x,\mu) = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o\, \sigma(\mu_o) \int_0^{2\pi} d\xi\, \Psi[x,\mu\mu_o+(1-\mu^2)^{\frac{1}{2}}\, (1-\mu_o^2)^{\frac{1}{2}}\cos\xi]. \quad (3.7)$$

Here for ease of writing the energy group subscripts have been suppressed.

In the standard iterative solution of the discrete ordinate equation, the flux is assumed known at each iteration (from the previous iteration) in the discrete directions, μ_j, j=1,2,...N. Therefore, in order to evaluate the scattering source term from the above expression, it is necessary to obtain $\Psi[x,\mu\mu_o+(1-\mu^2)^{\frac{1}{2}}(1-\mu_o^2)^{\frac{1}{2}}\cos\xi]$ from $\Psi(x,\mu_j)$, j=1,2,...N using some interpolation scheme.

Upon using interpolation one may write

$$\Psi(x,\tilde{\mu}) \simeq \sum_{j=1}^{N} \Psi(x,\mu_j)\ \ell_j(\tilde{\mu}), \tag{3.8}$$

where

$$\tilde{\mu} = \mu\mu_o + (1-\mu^2)^{\frac{1}{2}}\ (1-\mu_o^2)^{\frac{1}{2}} \cos\xi, \quad \text{and}$$

$\ell_j(\tilde{\mu})$ are the interpolating functions. Various forms for $\ell_j(\tilde{\mu})$ will be considered in this work. But first it is noted that substituting Eq. (3.8) into Eq. (3.7), the scattering source term can be written in the standard discrete ordinates form as

$$S(x,\mu) = \sum_{j=1}^{N} \Psi(x,\mu_j)\ D_j(\mu), \tag{3.9}$$

where

$$D_j(\mu) = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o\ \sigma(\mu_o) \int_0^{2\pi} d\xi\ \ell_j(\tilde{\mu}). \tag{3.10}$$

The choice of the interpolating functions depends on the degree of accuracy and smoothness of the solution desired. Specific forms of $\ell_j(\tilde{\mu})$ and the evaluation of $D_j(\mu)$ using these forms will now be considered.

3.2.1 Global Lagrange Interpolation

For global Lagrange interpolation, the j-th interpolations polynomial, $\ell_j(\tilde{\mu})$, is given by

$$\ell_j(\tilde{\mu}) = \prod_{\substack{k=1 \\ k\neq j}}^{N} \frac{\tilde{\mu}-\mu_k}{\mu_j-\mu_k} , \tag{3.11}$$

where $\{\mu_k\}$, k=1,2,...N are the direction cosines used in the discrete ordinate method. The integration over $d\xi$ in Eq. (3.10) can be carried out analytically using the power series representation for $\ell_j(\tilde{\mu})$ and the binomial theorem. The result is

$$D_j(\mu) = \pi \sum_{k=0}^{N} \sum_{\ell=0}^{[k/2]} C_k^{(j)} \binom{j}{2\ell} \frac{(2\ell-1)!!}{2^{\ell-1}\ell!} \mu^{k-2} (1-\mu^2)^{\ell} \sigma_{K\ell}, \tag{3.12}$$

where

$$\sigma_{k\ell} = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o \, \sigma(\mu_o) \, \mu_o^{k-2} \, (1-\mu_o^2)^{\ell}, \tag{3.13}$$

$(2\ell-1)!! = 1.3.5........(2\ell-1)$,

$[k/2] =$ largest integer not exceeding $k/2$,

and $C_k^{(j)}$ are the power series expansion coefficients for the Lagrangian interpolation formula given by Eq. (3.11) [19].

It may be noted that if $\sigma(\mu_o)$ has a simple analytical form (e.g., piecewise polynomial), $\sigma_{k\ell}$ can also be evaluated analytically from Eq. (3.13).

3.2.2 Piecewise Lagrange Interpolation

For piecewise linear Lagrange interpolation, $\ell_j(\tilde{\mu})$ is a "hat function" given by

$$\ell_j(\tilde{\mu}) = \begin{cases} 0 & , \quad \tilde{\mu} \le \mu_{j-1} \\ (\tilde{\mu}-\mu_{j-1})/(\mu_j-\mu_{j-1}) & , \quad \mu_{j-1} \le \tilde{\mu} \le \mu_j \\ (\mu_{j+1}-\tilde{\mu})/(\mu_{j+1}-\mu_j) & , \quad \mu_j \le \tilde{\mu} \le \mu_{j+1} \\ 0 & , \quad \tilde{\mu} \ge \mu_{j+1} \end{cases} \tag{3.14}$$

In this case, $D_j(\mu)$ cannot be easily evaluated analytically even if $\sigma(\mu_o)$ is a simple function of μ_o, and recourse must be made to numerical integration. It should be noted that if the flux distribution is not smooth, a piecewise Lagrange polynomial approximation is generally more accurate than the global Lagrange polynomial approximation.

3.2.3 Spline Interpolation

The spline approximations, in addition to having more smoothness, is also more accurate than the piecewise Lagrange polynomial approximations. The procedure to evaluate the scattering source term in this case is outlined below.

If a spline polynomial approximation is used to represent the flux, then

$$\Psi(x,\tilde{\mu}) \simeq \tilde{\Psi}(x,\tilde{\mu}) \equiv \sum_{j=1}^{N} C_j(x)\ \ell_j(\tilde{\mu}), \tag{3.15}$$

where the ℓ_j is the j-th spline function, and $C_j(x)$, which are implicit functions of the flux in the discrete directions, are obtained by solving the interpolatory constraint equations,

$$\tilde{\Psi}\ (x,\mu_i) = \Psi(x,\mu_i), \qquad i=1,2,\ldots N \tag{3.16}$$

It is easily shown that the $C_j(x)$ satisfy the following matrix equation:

$$\underline{\tilde{A}}\ \underline{C} = \underline{B}\ , \tag{3.17}$$

where the matrix $\underline{\tilde{A}}$ and the vectors $\underline{B}$ and $\underline{C}$ are given by

$$\tilde{A}_{ij} = \ell_j(\mu_i), \quad \begin{array}{l} i=1,2,\ldots N \\ j=1,2,\ldots N \end{array} \tag{3.18}$$

$$B_i = \Psi(x,\mu_i), \quad i=1,2,\ldots N, \tag{3.19}$$

$$C_i = C_i(x)\ , \quad i=1,2,\ldots N. \tag{3.20}$$

As an example, consider the case of cubic splines. In this case,

$$\ell_i(\mu) = \frac{1}{h^3}\begin{cases} (\mu-\mu_{i-2})^3, & \mu_{i-2}\leq\mu\leq_{i-1} \\ h^3+3h^2(\mu-\mu_{i-1})+3h(\mu-\mu_{i-1})^2-3(\mu-\mu_{i-1})^3, & \mu_{i-1}\leq\mu\leq\mu_i \\ h^3+3h^2(\mu_{i+1}-\mu)+3h(\mu_{i+1}-\mu)^2-3(\mu_{i+1}-\mu)^3, & \mu_i\leq\mu\leq\mu_{i+1} \\ (\mu_{i+2}-\mu)^3, & \mu_{i+1}\leq\mu\leq\mu_{i+2} \\ 0\quad , & \text{otherwise} \end{cases} \tag{3.21}$$

where $h = \mu_i-\mu_{i-1}$, and $\underline{\tilde{A}}$ is given by [20]

$$\tilde{A}_{ij} = \begin{cases} 1 \ , & i=j-1 \text{ or } j+1 \\ 4 \ , & i=j \\ 0 \ , & \text{otherwise} \end{cases}\ . \tag{3.22}$$

Since the matrix $\underline{\tilde{A}}$ is diagonally dominant, it follows from Gershgorin's theorem [21] that $\underline{\tilde{A}}$ is non-singular. Hence, the system of equations

(3.17) has a unique solution, namely

$$\underline{C} = \underline{\tilde{A}}^{-1}\,\underline{B}, \tag{3.23}$$

or

$$C_j = \sum_k (\underline{\tilde{A}}^{-1})_{jk}\,\Psi(x,\mu_k). \tag{3.24}$$

Upon using Eq. (3.15) in Eq. (3.7) one obtains

$$S(x,\mu) = \sum_{j=1}^{N} C_j(x)\,D_j(\mu), \tag{3.25}$$

where

$$D_j(\mu) = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o\,\sigma(\mu_o) \int_0^{2\pi} d\xi\,\ell_j(\tilde{\mu}), \tag{3.26}$$

$$\tilde{\mu} = \mu\mu_o + (1-\mu^2)^{\frac{1}{2}}\,(1-\mu_o^2)^{\frac{1}{2}}\cos\xi, \tag{3.27}$$

and $C_j(x)$ is given by Eq. (3.24).

As in the case of piecewise Lagrange interpolation, the $D_j(\mu)$ functions must be evaluated numerically.

Next the evaluation of the scattering source term for the azimuthally dependent case will be considered. In this case, the scattering source term is given by

$$S(x,\mu,\phi) = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o\,\sigma(\mu_o) \int_0^{2\pi} d\xi\,\Psi(x,\alpha,\beta), \tag{3.28}$$

where

$$\alpha = \mu\mu_o + (1-\mu^2)^{\frac{1}{2}}\,(1-\mu_o^2)^{\frac{1}{2}}\cos\xi, \tag{3.29}$$

$$\beta = \phi + \tan^{-1}\left[\frac{(1-\mu_o^2)^{\frac{1}{2}}\sin\xi}{\mu_o(1-\mu^2)^{\frac{1}{2}} - \mu(1-\mu_o)^{\frac{1}{2}}\cos\xi}\right]. \tag{3.30}$$

Using two-way global Lagrange interpolation formula to express $\Psi(x,\alpha,\beta)$ in terms of $\Psi(x,\mu_j,\phi_k)$, the flux in the discrete directions, $\mu_i(i=1,2,...N)$ and ϕ_j $(j=1,2,...M)$, one obtains

$$\Psi(x,\alpha,\beta) = \sum_{i=1}^{N} \sum_{j=1}^{M} \ell_i(\alpha)\ \ell_j(\beta)\ \Psi(x,\mu_i,\phi_j), \tag{3.31}$$

where

$$\ell_i(\alpha) = \prod_{\substack{k=1 \\ k\neq i}}^{N} \frac{\alpha-\mu_k}{\mu_i-\mu_k}, \tag{3.32}$$

$$\ell_j(\beta) = \prod_{\substack{k=1 \\ k\neq j}}^{M} \frac{\beta-\phi_k}{\phi_j-\phi_k}. \tag{3.33}$$

Substitution of Eq. (3.31) to Eq. (3.28) gives

$$S(x,\mu,\phi) = \sum_{i=1}^{N} \sum_{j=1}^{M} \Psi(x,\mu_i,\phi_j)\ D_{ij}(\mu), \tag{3.34}$$

where

$$D_{ij}(\mu) = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o\ \sigma(\mu_o) \int_0^{2\pi} d\xi\ \ell_i(\alpha)\ \ell_j(\beta). \tag{3.35}$$

Again, $D_{ij}(\mu)$ cannot be easily evaluated analytically and recourse must be made to numerical integration.

Evaluation of the scattering source term for the azimuthally dependent case using piecewise Lagrange interpolating polynomials and the spline functions, are very complicated, and will not be pursued in this work.

3.3 Evaluation of the Scattering Source Intergral with (μ',μ_o) as Integration Variables

3.3.1 Numerical Evaluation of the Scattering Source Term: Removal of Singularity

In Section 2.2.3 of Chapter 2, it was shown that when the group-to-group cross section, $\sigma_{g'\to g}(\mu_o)$ has a narrow angular support over μ_o, i.e., $[\mu_{o,min},\mu_{o,max}]$, the scattering source term is given by

$$S(x,\mu) = 2\left[\int_{\mu_1'}^{\mu_2'} d\mu'\ \Psi(x,\mu')A_1(\mu,\mu') + \int_{\mu_2'}^{\mu_3'} d\mu'\ \Psi(x,\mu')A_2(\mu,\mu')\right.$$

$$\left. + \int_{\mu_3'}^{\mu_4'} d\mu'\ \Psi(x,\mu')\ A_3(\mu,\mu')\right], \tag{3.36}$$

where

$$A_1(\mu,\mu') = \int_{\mu_{o,min}}^{f_2} d\mu_o \frac{\sigma(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}} , \tag{3.37}$$

$$A_2(\mu,\mu') = \int_{\mu_{o,min}}^{\mu_{o,max}} d\mu_o \frac{\sigma(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}} , \tag{3.38}$$

$$A_3(\mu,\mu') = \int_{f_1}^{\mu_{o,max}} d\mu_o \frac{\sigma(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{1/2}} , \tag{3.39}$$

$$f_1 = \mu\mu'-(1-\mu^2)^{1/2}\ (1-\mu'^2)^{1/2},$$

$$f_2 = \mu\mu' + (1-\mu^2)^{1/2}\ (1-\mu'^2)^{1/2} \tag{3.41}$$

and μ_1', μ_2', μ_3' and μ_4' are given by Eqs. (2.7)-(2.11). Again for ease of notation, the energy group subscripts have been omitted. It should be noted that the integrands in Eqs. (3.37) and (3.39) are singular at $\mu_o=f_2$ and $\mu_o=f_1$, respectively. To evaluate A_1 and A_3 using numerical quadrature, it is first necessary to remove these singularities. This may be accomplished in the following manner.

Consider first Eq. (3.37). Factorizing the denominator of the integrand, this equation can be written

$$A_1(\mu,\mu') = \int_{\mu_{o,min}}^{b+a} d\mu_o \, \frac{\sigma(\mu_o)}{(a+b-\mu_o)^{\frac{1}{2}}(a-b+\mu_o)^{\frac{1}{2}}} , \tag{3.42}$$

where

$$a = (1-\mu^2)^{\frac{1}{2}}(1-\mu'^2)^{\frac{1}{2}}, \tag{3.43}$$

and

$$b = \mu\mu'. \tag{3.44}$$

Equation (3.42) can be written in a more convenient form using partial fractions. One then obtains

$$A_1(\mu,\mu') = \frac{1}{2a}\int_{\mu_{o,min}}^{b+a} d\mu_o \, \frac{\sigma(\mu_o)(a+b-\mu_o)^{\frac{1}{2}}}{(a-b+\mu_o)^{\frac{1}{2}}}$$

$$+ \frac{1}{2a}\int_{\mu_{o,min}}^{b+a} d\mu_o \, \frac{\sigma(\mu_o)(a-b+\mu_o)^{\frac{1}{2}}}{(a+b-\mu_o)^{\frac{1}{2}}} . \tag{3.45}$$

It may be noted that the first integral in Eq. (3.45) does not have any singularity, whereas the second integral has singularity at μ_o=b+a. To remove this singularity, the second integral is rewritten as

$$\frac{1}{2a}\int_{\mu_{o,min}}^{b+a} d\mu_o \, F_1(\mu,\mu',\mu_o) + \frac{1}{2a}\int_{\mu_{o,min}}^{b+a} d\mu_o \, \frac{\sigma(b+a)(2a)^{\frac{1}{2}}}{(a+b-\mu_o)^{\frac{1}{2}}} , \tag{3.46}$$

where

$$F_1(\mu,\mu',\mu_o) = \left\{\sigma(\mu_o) \, \frac{(a-b+\mu_o)^{\frac{1}{2}}}{(a+b-\mu_o)^{\frac{1}{2}}} - \frac{\sigma(b+a)(2a)^{\frac{1}{2}}}{(a+b-\mu_o)^{\frac{1}{2}}}\right\} . \tag{3.47}$$

The quantity $F_1(\mu,\mu',\mu_o)$ is finite, namely zero, at μ_o=b+a. Thus, the singularity is removed, since the second integral in expression (3.46) can be analytically evaluated to give the result

$$\frac{\sigma(b+a)}{(2a)^{1/2}}\int_{\mu_{o,min}}^{b+a} d\mu_o\ (a+b-\mu_o)^{-\frac{1}{2}} = \left(\frac{2}{a}\right)^{\frac{1}{2}}\sigma(b+a)(a+b-\mu_{o,min})^{\frac{1}{2}}. \qquad (3.48)$$

Thus,

$$A_1 = \frac{1}{2a}\int_{\mu_{o,min}}^{b+a} d\mu_o\ \frac{\sigma(\mu_o)(a+b-\mu_o)^{\frac{1}{2}}}{(a-b+\mu_o)^{\frac{1}{2}}} + \frac{1}{2a}\int_{\mu_{o,min}}^{b+a} d\mu_o\ F_1(\mu,\mu',\mu_o)$$

$$+ \left(\frac{2}{a}\right)^{\frac{1}{2}}\sigma(b+a)(a+b-\mu_{o,min})^{\frac{1}{2}}. \qquad (3.49)$$

Similarly,

$$A_3(\mu,\mu') = \frac{1}{2a}\int_{b-a}^{\mu_{o,max}} d\mu_o\ \frac{\sigma(\mu_o)(a-b+\mu_o)^{\frac{1}{2}}}{(a+b-\mu_o)^{\frac{1}{2}}} +$$

$$\frac{1}{2a}\int_{b-a}^{\mu_{o,max}} d\mu_o\ F_2(\mu,\mu',\mu_o) + \left(\frac{2}{a}\right)^{\frac{1}{2}}\sigma(b-a)(a-b+\mu_{o,max})^{\frac{1}{2}}. \qquad (3.50)$$

Free from singularities, A_1, A_2 and A_3 can now be evaluated accurately using any standard numerical quadrature formula. Finally, the integration over μ' in Eq. (3.36) can be carried out using numerical quadrature.

3.3.2 Evaluation of the Scattering Source Integral Using Piecewise Polynomial Approximations for the Angular Flux and Group-to-Group Cross Sections

A method for the evaluation of the scattering source integral using piecewise polynomial approximations for the angular flux and group-to-group cross sections is described in this section. In this method integration over both the angular variables in the scattering source integral is carried out analytically thereby eliminating the need for numerical quadrature which may be very time consuming.

It should be noted that group-to-group cross sections for scattering of neutrons can often be represented with a good approximation by low order piecewise polynomials [10] as shown in Fig. 3.1. The break points $\mu_{o,1}$, $\mu_{o,2}$, $\mu_{o,3}$ and $\mu_{o,4}$ in Fig. 3.1 are given by [2]

$$\mu_{o,1} = \mu_{o,min} = \max[-1,\ S(E_{g+1},\ E_{g'})],$$

$$\mu_{o,2} = \min\ [S(E_{g+1},\ E_{g'+1}),\ S(E_g, E_{g'})],$$

$$\mu_{o,3} = \max\ [S(E_{g+1}, E_{g'+1}),\ S(E_g, E_{g'})], \qquad (3.51)$$

and

$$\mu_{o,4} = \mu_{o,max} = \min[+1,\ S(E_g, E_{g'+1})],$$

where for elastic scattering

$$S(E,E') = \left(\frac{A+1}{2}\right)\left(\frac{E}{E'}\right)^{1/2} - \left(\frac{A-1}{2}\right)\left(\frac{E'}{E}\right)^{1/2}. \qquad (3.52)$$

Here E' is the initial energy, E is the final energy, and A is the atomic mass of the scattering nucleus. In Eq. (3.51), $E_{g'}$ and $E_{g'+1}$ are the upper and the lower energy limits of group g' respectively. Similarly, E_g and E_{g+1} are the upper and the lower energy limits of group g respectively.

Hong [11] has shown that low order piecewise polynomial approximations for the group transfer cross sections are also good when both elastic and inelastic scattering are present. In this case,

$$S(E,E') = \frac{1}{2}\left\{(A+1)\left(\frac{E}{E'}\right)^{1/2} - (A-1)\left(\frac{E'}{E}\right)^{1/2} - \frac{QA}{(EE')^{1/2}}\right\}, \qquad (3.53)$$

where Q is the "Q-value" of the inelastic scattering process.

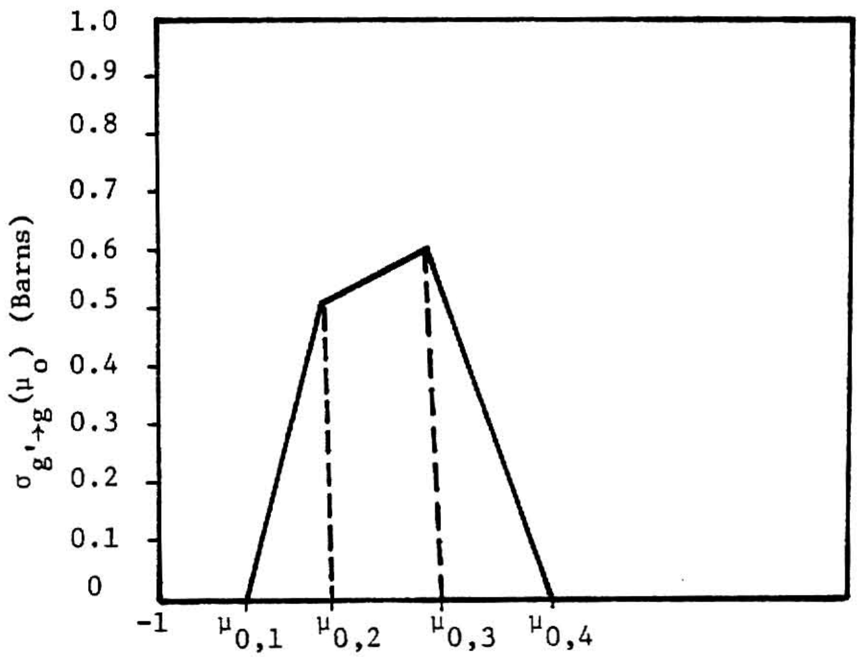

Fig. 3.1. Piecewise linear approximations for group-to-group transfer cross sections.

Consider now the evaluation of the scattering source integral given by Eq. (3.36). Let $S_n(x,\mu)$ denote the component of the scattering source integral due to the n-th segment of $\sigma_{g'\to g}(\mu_o)$. Then, the scattering source integral can be written as

$$S(x,\mu) = \sum_{n=1}^{3} S_n(x,\mu), \tag{3.54}$$

where

$$S_n(x,\mu) = 2[\int_{\mu_1'}^{\mu_2'} d\mu' \, \Psi(x,\mu') \, A_1^n(\mu,\mu') +$$

$$\int_{\mu_2'}^{\mu_3'} d\mu' \, \Psi(x,\mu') \, A_2^n(\mu,\mu') + \int_{\mu_3'}^{\mu_4'} d\mu' \, \Psi(x,\mu') \, A_3^n(\mu,\mu'), \tag{3.55}$$

with

$$A_1^n(\mu,\mu') = \int_{\mu_{o,n}}^{f_2} d\mu_o \, \frac{\sigma(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{\frac{1}{2}}} \quad , \tag{3.56}$$

$$A_2^n(\mu,\mu') = \int_{\mu_{o,n}}^{\mu_{o,n+1}} d\mu_o \, \frac{\sigma(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{\frac{1}{2}}} \, , \tag{3.57}$$

$$A_3^n(\mu,\mu') = \int_{f_1}^{\mu_{o,n+1}} d\mu_o \, \frac{\sigma(\mu_o)}{(1-\mu^2-\mu'^2-\mu_o+2\mu\mu'\mu_o)^{\frac{1}{2}}} \quad , \tag{3.58}$$

The integration limits $\{\mu_1', \mu_2', \mu_3', \mu_4'\}$ are the ordered values of $\{\bar{\mu}_1', \bar{\mu}_2', \bar{\mu}_3', \bar{\mu}_4'\}$ where

$$\bar{\mu}_1' = \mu\mu_{o,n} - (1-\mu^2)^{\frac{1}{2}}(1-\mu_{o,n}^2)^{\frac{1}{2}} \, , \tag{3.59}$$

$$\bar{\mu}_2' = \mu\mu_{o,n+1} - (1-\mu^2)^{\frac{1}{2}}(1-\mu_{o,n+1}^2)^{\frac{1}{2}}, \tag{3.60}$$

$$\bar{\mu}_3' = \mu\mu_{o,n} + (1-\mu^2)^{\frac{1}{2}}(1-\mu_{o,n}^2)^{\frac{1}{2}}, \tag{3.61}$$

$$\bar{\mu}_4' = \mu\mu_{o,n+1} + (1-\mu^2)\ (1-\mu^2_{o,n+1}) \quad , \tag{3.62}$$

and f_1 and f_2 are given by Eqs. (3.40) and (3.41), respectively.

Let

$$\bar{S}_n^1(x,\mu) = 2 \int_{\mu_1'}^{\mu_2'} d\mu'\ \Psi(x,\mu')\ A_1^n(\mu,\mu'), \tag{3.63}$$

$$\bar{S}_n^2(x,\mu) = 2 \int_{\mu_2'}^{\mu_3'} d\mu'\ \Psi(x,\mu')\ A_2^n(\mu,\mu'), \tag{3.64}$$

and

$$\bar{S}_n^3(x,\mu) = 2 \int_{\mu_3'}^{\mu_4'} d\mu'\ \Psi(x,\mu')\ A_3^n(\mu,\mu'). \tag{3.65}$$

Then one has for the n segment of $\sigma_{g'\to g}(\mu_o)$

$$S_n(x,\mu) = \sum_{k=1}^{3} \bar{S}_n^k(x,\mu). \tag{3.66}$$

Consider now the evaluation of $\bar{S}_n^i$, i=1,...3 using piecewise polynomial approximations for σ and Ψ. First, it is necessary to evaluate $A_i^n(\mu,\mu')$, i=1,...3. The piecewise polynomial approximation (of degree L) for the transfer cross section in the n-th $\mu_{o,n}$ domain can be written as

$$\sigma(\mu_o) = \begin{cases} \sum_{\ell=0}^{L} C_\ell^n\ \mu_o^\ell\ , & \mu_{o,n} \le \mu_o \le \mu_{o,n+1} \\ 0\ , & \text{otherwise} \end{cases} \tag{3.67}$$

where the C_ℓ^n are interpolatory coefficients determined by fitting Eq. (3.67) to the group transfer cross section $\sigma(\mu_o)$ (group subscripts have been dropped for simplicity of notation) at (L+1) μ_o-values between $\mu_{o,n}$ and $\mu_{o,n+1}$.

Upon substituting Eq. (3.67) in Eq. (3.56) one obtains

$$A_1^n(\mu,\mu') = \sum_{\ell=0}^{L} C_\ell^n \int_{\mu_{o,n}}^{f_2} d\mu_o \frac{\mu_o^\ell}{(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{\frac{1}{2}}} \quad . \tag{3.68}$$

By tabulated formula

$$I_\ell(\mu,\mu',\mu_o) = \int \frac{\mu_o^\ell \, d\mu_o}{(1-\mu^2-\mu'^2-\mu'^2_o+2\mu\mu'\mu_o)^{\frac{1}{2}}}$$

$$= -\frac{\mu_o^{\ell-1}}{\ell}(1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o)^{\frac{1}{2}} + \frac{(2\ell-1)}{\ell}\mu\mu' I_{\ell-1}(\mu,\mu',\mu_o)$$

$$- \frac{(\ell-1)(1-\mu^2-\mu'^2)}{\ell} I_{\ell-2}(\mu,\mu',\mu_o), \quad \ell=2,3,\ldots L \tag{3.69}$$

where

$$I_o(\mu,\mu',\mu_o) = \frac{\pi}{2} - \cos^{-1}[(\mu_o-\mu\mu')/(1-\mu^2)^{\frac{1}{2}}(1-\mu'^2)^{\frac{1}{2}}], \tag{3.70}$$

and

$$I_1(\mu,\mu',\mu_o) = \mu\mu' I_o - (1-\mu^2-\mu'^2-\mu_o + 2\mu\mu'\mu_o)^{\frac{1}{2}}. \tag{3.71}$$

Substituting Eq. (3.69) in Eq. (3.68) one obtains a closed formula for $A_1^n(\mu,\mu')$ for any value of L. Thus,

$$A_1^n(\mu,\mu') = \sum_{\ell=0}^{L} C_\ell^n I_\ell(\mu,\mu',\mu_o)\Big|_{\mu_{o,n}}^{f_2} . \tag{3.72}$$

Similarly

$$A_2^n(\mu,\mu') = \sum_{\ell=0}^{L} C_\ell^n I_\ell(\mu,\mu',\mu_o)\Big|_{\mu_{o,n}}^{\mu_{o,n+1}} , \tag{3.73}$$

and

$$A_3^n(\mu,\mu') = \sum_{\ell=0}^{L} C_\ell^n I_\ell(\mu,\mu',\mu_o)\Big|_{f_1}^{\mu_{o,n+1}} . \tag{3.74}$$

As an example, consider the case of piecewise linear approximation for the group-to-group cross section. For L=1, Eq. (3.68) can be written as

$$A_1^n(\mu,\mu') = \{C_o^n I_o + C_1^n I_1\}\Big|_{\mu_{o,n}}^{f_2} . \qquad (3.75)$$

Upon using Eq. (3.70) and (3.71) in Eq. (3.75) one obtains

$$A_1^n(\mu,\mu') = \{C_o^n + C_1^n\mu\mu'\} F_1(\mu,\mu',\mu_{o,n}) + C_1^n F_2(\mu,\mu',\mu_{o,n}), \qquad (3.76)$$

where

$$F_1(\mu,\mu',\mu_o) = \cos^{-1} [(\mu_o - \mu')/(1-\mu^2) (1-\mu'^2)], \qquad (3.77)$$

and

$$F_2(\mu,\mu',\mu_o) = (1-\mu^2-\mu'^2-\mu_o^2+2\mu\mu'\mu_o) . \qquad (3.78)$$

Similarly,

$$A_2^n(\mu,\mu') = \{C_o^n + C_1^n\mu\mu'\}\{F_1(\mu,\mu',\mu_{o,n+1}) - F_1(\mu,\mu',\mu_{o,n})\}$$

$$+ C_1^n \{F_2(\mu,\mu',\mu_{o,n}) - F_2(\mu,\mu',\mu_{o,n+1})\}, \qquad (3.79)$$

and

$$A_3^n(\mu,\mu') = \{C_o^n + C_1^n\mu\mu'\}\{\pi - F_1(\mu,\mu',\mu_{o,n+1})\} - C_1^n F_2(\mu,\mu',\mu_{o,n+1})$$

$$(3.80)$$

Once $A_i^n (\mu,\mu')$, $i=1,\ldots 3$ are evaluated, $\overline{S_n^j}(x,\mu)$, $j=1,\ldots 3$ given by Eqs. (3.63)-(3.65) can be evaluated by performing integration over μ' analytically using piecewise polynomial approximations for the angular flux. Piecewise Lagrange M-th degree polynomials that fit $\psi^j(\mu_i')$ (where $\psi^j(\mu_i')$ is the angular flux at direction μ_i' in the j-th angular interval piece with $i=0,1,2,\ldots M$) can be expressed as

$$\psi^j(x,\mu') = \sum_{i=0}^{M} L_i^j(\mu') \psi^j(x,\mu_i'),\ j=1,2,\ldots \frac{N-1}{M} , \qquad (3.81)$$

where

$$L_i^j(\mu') = \prod_{m=0}^{M} \frac{\mu'-\mu'^j_m}{\mu'^j_i-\mu'^j_m}, \quad i=0,1,\ldots M. \tag{3.82}$$

Here N is the number of discrete directions. Upon substituting Eqs. (3.81) and (3.72) in Eq. (3.63) one obtains

$$\bar{S}_n^{1}(x,\mu) = 2 \sum_j \int_j d\mu' \sum_{i=0}^{M} L_i^j(\mu')\, \Psi_i^j(x) \sum_{\ell=0}^{L} C_\ell^n \{I_\ell(\mu,\mu',f_2)$$

$$-I_\ell(\mu,\mu',\mu_{o,n})\}, \tag{3.83}$$

where $I_\ell(\mu,\mu',\mu_o)$ is given by Eqs. (3.69)-(3.71), and $\Psi_i^j(x) = \Psi^j(\mu_i',x)$. The quantity $\bar{S}_n^1(x,\mu)$ can be evaluated using numerical quadrature for any value of L. However, if the μ' integral in Eq. (3.83) is to be evaluated analytically, explicit functional form of the integrand must be known. Consideration will, therefore, be given to a specific case, for example, the piecewise linear approximation for $\sigma(\mu_o)$. For L=1 we have [using Eqs. (3.70) and (3.71) in Eq. (3.83)]

$$\bar{S}_n^{1}(x,\mu) = 2 \sum_j \int_j d\mu' \sum_{i=0}^{M} L_i^j(\mu')\, \Psi_i^j(x)\, [\{C_o^n + C_1^n\mu\mu'\}$$

$$\times F_1(\mu,\mu',\mu_{o,n}) + C_1^n\, F_2(\mu,\mu',\mu_{o,n})]. \tag{3.84}$$

To perform the integration over μ' in the above equation analytically, it is necessary to evaluate integrals of the following forms:

$$F_1^m(x) = \int x^m \cos^{-1}\left(\frac{a-bx}{(1-x^2)^{\frac{1}{2}}}\right) dx, \quad m=0,1,\ldots M+1 \tag{3.85}$$

and

$$F_2^m(x) = \int x^m (a+bx+cx^2)^{\frac{1}{2}}\, dx, \quad m=0,1,\ldots M \tag{3.86}$$

The method of integration by parts can be used to evaluate $F_1^m(x)$. One obtains, after much algebra

$$F_1^0(x) - x\, u_1(x) + a(b^2+1)^{-\frac{1}{2}}\, u_2(x) + u_3(x) + u_4(x), \qquad (3.87)$$

where

$$u_1(x) = \cos^{-1}\left(\frac{a-bx}{(1-x^2)^{\frac{1}{2}}}\right) \quad ,$$

$$u_2(x) = \sin^{-1}\left(\frac{-(b^2+1)x+ab}{(1-a^2+b^2)^{\frac{1}{2}}}\right) \quad ,$$

$$u_3(x) = \frac{1}{2}\,\frac{a+b}{|a+b|}\,\sin^{-1}\left(\frac{-(a+b)^2(x+1)^{-1}+ab+b^2+1}{(1-a^2+b^2)^{\frac{1}{2}}}\right) \quad ,$$

and

$$u_4(x) = \frac{1}{2}\,\frac{a-b}{|a-b|}\,\sin^{-1}\left(\frac{-(a-b)^9(x-1)^{-1}+ab-b^2-1}{(1-a^2+b^2)^{\frac{1}{2}}}\right).$$

$$F_1^1(x) = \frac{1}{2}\,[x^2\, u_1(x) + a\,\{-(a^2-1) + 2abx - (b^2+1)x^2\}^{\frac{1}{2}}$$

$$(b^2+1)^{-1} + \{a^2b(b^2+1)^{-1}-b\}\,(b^2+1)^{-\frac{1}{2}}\,u_2(x)-u_3(x) + u_4(x)]. \quad (3.88)$$

Integral F_2^m is tabulated [22] and may be evaluated as

$$F_2^0(x) = \int \sqrt{R}\,dx = \frac{(2cx+b)\sqrt{R}}{4c} + \frac{\Delta}{8c}\int\frac{dx}{\sqrt{R}}\,, \qquad (3.89)$$

$$F_2^1(x) = \int x\sqrt{R}\,dx = \frac{R^{3/2}}{3c} - \frac{(2cx+b)b}{8c^3}\,R^{\frac{1}{2}} - \frac{b\Delta}{16c^2}\int\frac{dx}{\sqrt{R}}\,, \qquad (3.90)$$

where

$$R = a+bx+cx^2,$$

$$\Delta = 4ac-b^2,$$

and

$$\int\frac{dx}{\sqrt{R}} = \frac{-1}{\sqrt{-c}}\,\sin^{-1}\left(\frac{2cx+b}{\sqrt{-\Delta}}\right) \quad \text{for } c<0, \quad \Delta<0.$$

Upon evaluation of the μ'-integral of Eq. (3.84) one obtains

$$\bar{S}_n^1(x,\mu) = \sum_{m'} G'_{nm'}(\mu)\ \Psi_{m'}(x), \quad m'=i+(j-1)M+1 \tag{3.91}$$

where $G^1_{nm'}(\mu)$ is a function of $F_1^m(\mu)$ and $F_2^m(\mu)$.

Proceeding in the same manner, $\bar{S}_n^2(x,\mu)$ and $\bar{S}_n^3(x,\mu)$ given by Eqs. (3.64) and (3.65) can be written as

$$\bar{S}_n^2(x,\mu) = 2 \sum_j \int_j d\mu' \sum_{i=0}^{M} L_i^j(\mu')\ \Psi_i^j(x)\ [\{C_o^n+C_1^n\mu\mu'\}$$

$$\{F_1(\mu,\mu',\mu_{o,n+1}) - F_1(\mu,\mu',\mu_{o,n})\} + C_1^n\ \{F_2(\mu,\mu',\mu_{o,n}) -$$

$$F_2(\mu,\mu',\mu_{o,n+1})\}] = \sum_{m'} G^2_{nm'}(\mu)\ \Psi_{m'}(x), \tag{3.92}$$

and

$$\bar{S}_n^3(x,\mu) = 2 \sum_j \int_j d\mu' \sum_{i=0}^{M} L_i^j(\mu')\ \Psi_i^j(x)\ [\{C_o^n + C_1^n\mu\mu'\}\{\pi-$$

$$F_1(\mu,\mu',\mu_{o,n+1})\} - C_1^n\ F_2(\mu,\mu',\mu_{o,n+1})] = \sum_{m'} G^3_{nm'}(\mu)\ \Psi_{m'}(x) \tag{3.93}$$

With these results, the inscattering source term at $\mu=\mu_m$ can finally be written as

$$S(x,\mu_m) = \sum_{n=1}^{3} S_n(x,\mu_m) = \sum_{m'=1}^{N} G_{m'm}\ \Psi_{m'}(x) \tag{3.94}$$

where

$$G_{mm'} = \sum_{n=1}^{3} \sum_{k=1}^{3} G^k_{nm'}\ (\mu_m). \tag{3.95}$$

It may be noted that this final form of the scattering source term is of the same form as that in the exact kernel method. Hence any discrete ordinate code using the exact kernel method can also be used with the above method.

Hong [11] has also derived the above result. He worked in the (μ',ϕ') integration plane while in this study it is found more convenient to work in the (μ',μ_o) integration plane.

The above method has the advantage that it is not necessary to use the directions prescribed by the quadrature scheme - any discrete directions may be used. Also, by eliminating the need for numerical quadrature the computational efforts can be greatly reduced.

The limiting case of isotropic scattering will now be considered. In this case the scattering source is given by

$$S(x,\mu) = \frac{\sigma_s}{4\pi} \int_{-1}^{+1} d\mu' \, \Psi(x,\mu') \int_{f_1}^{f_2} \frac{d\mu_o}{(1-\mu^2-\mu'^2-\mu^2+2\mu\mu'\mu_o)^{\frac{1}{2}}} \quad , \tag{3.96}$$

where $\sigma_s = 4\pi\sigma(\mu_o)$ is the total scattering cross section, and, f_1 and f_2 are given by Eqs. (3.40) and (3.41) respectively. Performing the integration over $d\mu_o$ one obtains,

$$S(x,\mu) = \frac{\sigma_s}{2} \int_{-1}^{+1} d\mu' \, \Psi(x,\mu'). \tag{3.97}$$

For piecewise linear approximation for the angular flux one can write

$$\Psi(x,\mu') = \sum_{j=1}^{N} \Psi(x,\mu_j) \, \ell_j(\mu'), \tag{3.98}$$

where

$$\ell_j(\mu) = \begin{cases} 0 \quad , & \mu \le \mu_{j-1} \\ (\mu-\mu_{j-1})/(\mu_j-\mu_{j-1}), & \mu_{j-1} \le \mu \le \mu_j \\ (\mu_{j+1}-\mu)/(\mu_{j+1}-\mu_j), & \mu_j \le \mu \le \mu_{j+1} \\ 0 \quad , & \mu \ge \mu_{j+1} \end{cases} \tag{3.99}$$

Substitution of Eq. (3.98) in Eq. (3.97) gives

$$S(x,\mu) = \sum_{j=1}^{N} \Psi(x,\mu_j)\, D_j(\mu), \tag{3.100}$$

where

$$D_j(\mu) = \frac{\sigma_s}{2}\int_{-1}^{+1} d\mu'\, \ell_j(\mu'). \tag{3.101}$$

Using Eq. (3.99) in Eq. (3.101), the integration over μ' can be readily performed. The result is (for uniform angular mesh spacing)

$$D_j = \begin{cases} 0.25\ \sigma_s\ h, & j=1 \text{ or } N \\ 0.5\ \sigma_s\ h, & j=2,3,\ldots N-1. \end{cases} \tag{3.102}$$

where h is the uniform angular mesh spacing.

With a cubic spline approximation for the angular flux, the scattering source can be written

$$S(x,\mu) = \sum_{j=1}^{N} C_j(x)\, D_j(\mu), \tag{3.103}$$

where $C_j(x)$ is given by Eq. (3.24), and $D_j(\mu)$ is given by

$$D_j(\mu) = \frac{\sigma_s}{2}\int_{-1}^{+1} d\mu'\, \ell_j(\mu'), \tag{3.104}$$

with

$$\ell_j(\mu) = \frac{1}{h^3}\begin{cases} (\mu-\mu_{j-2})^3 & , \quad \mu_{j-2} \le \mu \le \mu_{j-1} \\ h^3+3h^2(\mu-\mu_{j-1})+3h(\mu-\mu_{j-1})^2-3(\mu-\mu_{j-1})^3, & \mu_{j-1} \le \mu \le \mu_j \\ h^3+3h^2(\mu_{j+1}-\mu)+3h(\mu_{j+1}-\mu)^2-3(\mu_{j+1}-\mu)^3, & \mu_j \le \mu \le \mu_{j+1} \\ (\mu_{j+2}-\mu)^3 & , \quad \mu_{j+1} \le \mu \le \mu_{j+2} \\ 0 & , \quad \text{Otherwise} \end{cases} \tag{3.105}$$

Substituting Eq. (3.105) in Eq. (3.104), the integration over μ' can be analytically performed. The result is

$$D_j = \begin{cases} 1.5\ \sigma_s h & , \quad j=1 \text{ or } N \\ 2.875\ \sigma_s h & , \quad j=2 \text{ or } N-1. \\ 3\ \ \sigma_s h & , \quad \text{Otherwise} \end{cases} \tag{3.106}$$

3.4 Numerical Results for Isotropic Scattering

A detailed numerical investigation of the various methods of evaluating the scattering source integral involving anisotropic group-to-group cross sections presented in this chapter is quite involved, and is suggested for further study along these lines. In this section, some numerical results are presented for the simple case of isotropic scattering. In particular, the accuracy of the low-order piecewise polynomial approximations for the angular flux in the evaluation of the scattering source is examined.

The one-speed slab albedo problem having the following parameters was solved using the discrete ordinate method [12,7]. Slab thickness = 1 mean free path, mean number of secondary neutrons per collision, c = 0.95, unit current source incident on the left hand face of the slab, and isotropic scattering. The scattering source was analytically evaluated using piecewise linear and cubic spline approximations for the angular flux [see Eqs. (3.98)-(3.106)]. Values of the transmitted and reflected angular fluxes obtained using the above approximations as well as the exact results are listed in Table (3.1). The exact results were obtained from the tabulated (exact) values of Chandrasekhar X and Y functions [23,24] which are defined by and

$$\left.\begin{aligned} X(\mu) &= 1.0 + \mu\ \Psi(0,-\mu) \\ Y(\mu) &= \mu\ \Psi(1,\mu) \end{aligned}\right\} \quad \mu>0.$$

From the numerical results it is seen that there is good agreement between the computed and the exact values of the angular fluxes for both piecewise linear and cubic spline approximations. It is also not suprising to find that the cubic spline approximation is more accurate than the piecewise linear approximation.

Table 3.1. Comparison of angular fluxes calculated using piecewise linear (P.L.A.) and cubic spline (C.S.A.) approximations with the exact result (spatial mesh = 0.05 mean free path).

Transmitted Angular Flux

μ	$\Psi(1,\mu)$ P.L.A.	$\Psi(1,\mu)$ C.S.A.	$\Psi(1,\mu)$ Exact
0.2	0.5809	0.5930	0.5640
0.6	0.9264	0.9483	0.9333
1.0	0.8850	0.9019	0.8913

Reflected Angular Flux

μ	$\Psi(0,\mu)$ P.L.A.	$\Psi(0,\mu)$ C.S.A.	$\Psi(0,\mu)$ Exact
-0.2	1.3758	1.4610	1.4740
-0.6	0.8995	0.9245	0.9283
-1.0	0.6549	0.6691	0.6717

4.0 CONCLUSIONS AND SUGGESTIONS FOR FURTHER STUDY

In this work we have studied various transformations of the scattering source term in the discrete ordinate transport equation which facilitate accurate evaluation of the scattering source term containing highly anisotropic cross sections, such as those occur in fine multi-group shielding calculations. Of the two variable transformations discussed, i.e., (μ_o,ξ) and (μ',μ_o') (see Chapter 2), the latter appears to be more promising, since it is not necessary to use interpolation in flux values in the iterative evaluation of the scattering source term in the solution of discrete ordinate transport equation.

In chapter 3, methods for the numerical evaluation of the scattering source term in the discrete ordinate transport equation are discussed for both the above transformations. For a typical slab albedo problem, it is found that low-order piecewise linear approximation and cubic spline approximation for the angular flux are quite satisfactory. Also, as might be expected, the cubic spline approximation is found to yield more accurate values of the angular flux than the piecewise linear approximation.

A method is also discussed for the analytical evaluation of the scattering source term using piecewise polynomial approximations for the angular flux and cross sections. This method has the advantage that it is not necessary to use the discrete directions prescribed by the quadrature scheme - any discrete directions may be used. Also, by eliminating the need for numerical quadrature, the computational efforts can be greatly reduced. Further work along these lines should include development of methods of evaluation of the scattering source term using spline functions for the flux and cross sections. Further work is also desirable to investigate numerically the accuracy of low-order piecewise polynomial approximations for the angular flux and the group transfer cross sections in the solution of fast neutron shielding problems.

5.0 ACKNOWLEDGEMENTS

I am indebted to Professor J. K. Shultis for guiding me throughout the course of this work and for many valuable suggestions. I would like to thank Dr. Z. Weiss for many hours of stimulating discussions. I would also like to thank Professor R. E. Faw, Professor G. G. Simons, and Professor F. A. Tillman for acting as members of my supervisory committee. I am grateful to the National Science Foundation and the Department of Nuclear Engineering for providing me the financial support. Thanks are also due to Ms. Shelly Kemnitz and Mr. H. Zamani for excellent typing and drawing, respectively. Last but not the least, I would like to thank my wife for being a constant source of inspiration.

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APPENDIX A

Evaluation of the Jacobian for Change of Variables from (μ',ϕ') to (μ_o,ξ) in the Scattering Source Integral

The Jacobian for the change of variables from (μ',ϕ') to (μ_o,ξ) in the scattering source integral was discussed in Section 2.3. In this appendix, the detailed evaluation of the Jacobian is given.

The Jacobian of transformation is defined by

$$J = \begin{vmatrix} \frac{\partial\mu'}{\partial\mu_o} & \frac{\partial\mu'}{\partial\xi} \\ \frac{\partial\phi'}{\partial\mu_o} & \frac{\partial\phi'}{\partial\xi} \end{vmatrix} = \frac{\partial\mu'}{\partial\mu_o}\frac{\partial\phi'}{\partial\xi} - \frac{\partial\mu'}{\partial\xi}\frac{\partial\phi'}{\partial\mu_o} . \tag{A.1}$$

From section 2.3 the transformation equations, given by Eqs. (2.42)-(2.44), are rewritten as

$$\mu' = \mu\mu_o + (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2} \cos\xi, \tag{A.2}$$

$$(1-\mu'^2)^{1/2} \sin(\phi-\phi') = (1-\mu_o^2)^{1/2} \sin\xi, \tag{A.3}$$

and

$$(1-\mu'^2)^{1/2} \cos(\phi-\phi') = \mu_o(1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2} \cos\xi. \tag{A.4}$$

In order to find the Jacobian it is necessary to evaluate the partial derivatives in Eq. (A.1). From Eq. (A.2) one obtains

$$\frac{\partial\mu'}{\partial\mu_o} = \mu - \mu_o(1-\mu_o^2)^{-1/2} (1-\mu^2)^{1/2} \cos\xi, \tag{A.5}$$

and

$$\frac{\partial\mu'}{\partial\xi} = - (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2} \sin\xi. \tag{A.6}$$

From Eq. (A.3) one finds

$$(1-\mu'^2)^{1/2}\cos(\phi'-\phi)\frac{\partial\phi'}{\partial\mu_o} - \mu'(1-\mu'^2)^{1/2}\sin(\phi'-\phi)\frac{\partial\mu'}{\partial\mu_o}$$

$$= \mu_o(1-\mu_o^2)^{-1/2}\sin\xi. \qquad (A.7)$$

Substituting the values of $\sin(\phi'-\phi)$ and $\cos(\phi'-\phi)$ from Eqs. (A.3) and (A.4) in Eq. (A.7) one obtains

$$\{\mu_o(1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2}\cos\xi\}\frac{\partial\phi'}{\partial\mu_o} = (1-\mu_o^2)^{1/2}\sin\xi\ .$$

$$(1-\mu'^2)^{-1}\mu'\frac{\partial\mu'}{\partial\mu_o} - \mu_o(1-\mu_o^2)^{-1/2}\sin\xi. \qquad (A.8)$$

Eliminating μ' and $\frac{\partial\mu'}{\partial\mu_o}$ from Eq. (A.8), using Eqs. (A.2) and (A.5), and solving for $\frac{\partial\phi'}{\partial\mu_o}$ yields

$$\frac{\partial\phi'}{\partial\mu_o} = \frac{1}{h_1}\{-\mu_o(1-\mu_o^2)^{-1/2}\sin\xi + \frac{h_2}{h_3}[\mu-\mu_o(1-\mu_o^2)^{-1/2}(1-\mu^2)^{1/2}\cos\xi]\}\ , \qquad (A.9)$$

where

$$h_1 = \mu_o(1-\mu^2)^{1/2} - \mu(1-\mu_o^2)^{1/2}\cos\xi\ , \qquad (A.10)$$

$$h_2 = (1-\mu_o^2)^{1/2}\sin\xi\ \{\mu\mu_o + (1-\mu^2)^{1/2}(1-\mu_o^2)^{1/2}\cos\xi\}, \qquad (A.11)$$

and

$$h_3 = (1-\mu_o^2)^{1/2}\sin^2\xi + (1-\mu^2)\mu_o^2 - 2\mu\mu_o(1-\mu^2)^{1/2}$$

$$(1-\mu^2)^{1/2}\cos\xi + \mu^2(1-\mu_o^2)\cos^2\xi. \qquad (A.12)$$

Similiarly,

$$\frac{\partial\phi'}{\partial\xi} = \frac{1}{h_1}\{(1-\mu_o^2)^{1/2}\cos\xi - \frac{h_2}{h_3}(1-\mu^2)^{1/2}(1-\mu_o^2)^{1/2}\sin\xi. \qquad (A.13)$$

Substituting the values of the partial derivatives in Eq. (A.1) from Eqs. (A.5), (A.6), (A.12) and (A.13) one obtains

$$J = \frac{1}{h_1} \{\mu-\mu_o(1-\mu_o^2)^{-1/2} (1-\mu^2)^{1/2} \cos\xi\}\{(1-\mu_o^2)^{1/2} \cos\xi$$

$$- \frac{h_2}{h_3} (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2} \sin\xi\} + \frac{1}{h_1} (1-\mu^2)^{1/2} (1-\mu_o^2)^{1/2} \sin\xi$$

$$\{-\mu_o (1-\mu_o^2)^{-1/2} \sin\xi + \frac{h_2}{h_3} [\mu-\mu_o(1-\mu_o^2)^{-1/2} (1-\mu^2)^{1/2} \cos\xi]\},$$

or

$$h_1 J = (1-\mu_o^2)^{1/2} \cos\xi \{\mu-\mu_o(1-\mu_o^2)^{-1/2} (1-\mu^2)^{1/2} \cos\xi\}$$

$$- \mu_o(1-\mu^2)^{1/2}\sin^2\xi$$

$$= \mu(1-\mu_o^2)^{1/2} \cos\xi - \mu_o(1-\mu^2)^{1/2} . \qquad (A.14)$$

Using Eq. (A.10) in Eq. (A.14) gives

$$h_1 J = - h_1 .$$

Thus, $J = -1$. (A.15)

SOME TECHNIQUES TO EVALUATE THE SCATTERING SOURCE IN THE DISCRETE ORDINATE TRANSPORT EQUATION WITH HIGHLY ANISOTROPIC SCATTERING

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AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

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ABSTRACT

Various transformations of the scattering source term in the discrete ordinate transport equation have been studied, which facilitate accurate evaluation of the scattering source term containing highly anisotropic cross sections such as those occur in fine multigroup shielding calculations. Of the two variable transformations discussed, i.e., (μ_o,ξ) and (μ',μ_o), the latter appears to be more promising, since it is not necessary to use flux interpolation in the iterative evaluation of the scattering source term in the solution of the discrete ordinate transport equation.

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A method is also discussed for the analytical evaluation of the scattering source term using piecewise polynomial approximations for the angular flux and cross sections. This method has the advantage that it is not necessary to use the discrete directions prescribed by the quadrature scheme - any discrete directions may be used. Also, by eliminating the need for numerical quadrature, the computational efforts can be greatly reduced.