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Applications of the transmission matrix method to neutron and gamma transport

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APPLICATIONS OF THE TRANSMISSION MATRIX METHOD
TO NEUTRON AND GAMMA TRANSPORT

by

Ervin Thomas Boulette

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INTRODUCTION

In 1967, during a special panel discussion presented at the Thirteenth Annual Meeting of the American Nuclear Society, Edwards (1) described several major problems still encountered in shielding analysis today. He stated that "the major weakness . . . is that inexpensive reasonably accurate direct design methods and computer programs are not available" for shielding analysis. He further went on to say that "we need to be able to calculate the spatial and energy distributions of neutrons and gamma rays, including secondary gamma rays, within reactor-shield assemblies and the spatial, energy, and angular distributions of leakage neutrons and gamma rays."

The termination of his talk was concerned with his suggestions for improving the current shielding analysis status. It is interesting to cite his closing remarks because of their relationship to this work. He said, "A method which I believe deserves renewed attention is the operator matrix method. Existing rigorous transport programs, both discrete-ordinate and Monte Carlo, could either be used directly or modified slightly for use in calculating reflection, transmission, and internal response matrices for incident matrices of neutrons and gamma rays on infinite slabs of finite thickness. These operator matrices could very well include the effect of internal secondary sources. These operator matrices could then be applied cheaply in a detailed matrix analysis of multilayered shields of different materials. The additional input required would be neutron and gamma ray matrices incident on each face."

One such operator matrix method is the transmission matrix method developed by Yarmush, Zell, and Aronson (2). This is the method employed in this investigation, and much of the general theory presented herein is based on their development.
The transmission matrix method computes transmission and reflection matrix operators for a homogeneous slab of arbitrary thickness from the transmission and reflection functions of an infinitesimally thin slab of the same material. To a first order approximation in the thickness variable, only the uncollided flux and the once-scattered flux need be considered in calculating the transmission and reflection functions for a very thin slab. Because of this approximation, these functions may be obtained directly in terms of basic cross sections. Thus, if one defines an incoming flux vector whose components define the energy and angular distribution of the flux, the transmission and reflection matrix operators will transform this incoming vector into an outgoing vector in energy and angle.

In this investigation, the transmission matrix method is applied to the transport of gamma radiation through three different materials: water, lead, and uranium. In all cases, the geometry is one-dimensional. To verify the results obtained by this method, differential energy spectra and buildup factors for the three materials are calculated from the transmitted flux vectors and compared with results tabulated in Goldstein (3).

In addition to the investigation of gamma radiation transport in homogeneous slabs, the method is applied to two-layer slabs made up of lead and water. Calculations of gamma ray transmission through heterogeneous slabs have been mainly calculated by the Monte Carlo method. Using this method, Bowman and Trubey (4) obtained the buildup factors for perpendicular gamma ray sources incident upon lead-water stratified slabs. From these results, Kalos (5) developed a semi-empirical formula to approximate the buildup factors in a two-layer slab by using the buildup factors and absorption factors of the individual layers. Broder, Kayurin, and Kutuzov (6) have
derived a comparatively simple semi-empirical formula for obtaining the buildup factors for isotropic point gamma sources incident upon laminated slabs in terms of the buildup factors of the individual laminae. The buildup factors for two-layer slabs obtained in this report are compared with those obtained by the formula derived by Broder, et al.

To culminate this investigation, the transmission of secondary gamma radiation due to thermal neutron capture is calculated. The volume distributed secondary gamma source is approximated by a finite number of plane sources, and the transmission matrix method is applied to each source individually. The total transmitted flux is then simply the sum of the transmitted components due to each plane source.
GENERAL THEORY

The H and W Matrices

A one-dimensional slab of thickness \( t \) is considered

\[
\begin{pmatrix}
\phi_1 \\
\psi_1
\end{pmatrix}
\xrightarrow{t}
\begin{pmatrix}
\phi_2 \\
\psi_2
\end{pmatrix}
\]

where \( \phi_1 \) and \( \psi_1 \) are respectively the incoming and outgoing distributions in angle and energy on the left face of the slab, and \( \phi_2 \) and \( \psi_2 \) are the outgoing and incoming distributions on the right. If one excludes photon-photon reactions, there is a linear operator \( H(t) \) such that

\[
\begin{pmatrix}
\phi_2 \\
\psi_2
\end{pmatrix} = H(t) \begin{pmatrix}
\phi_1 \\
\psi_1
\end{pmatrix}, \tag{1}
\]

where \( \begin{pmatrix}
\phi_2 \\
\psi_2
\end{pmatrix} \) and \( \begin{pmatrix}
\phi_1 \\
\psi_1
\end{pmatrix} \) are two-component vectors and \( H(t) \) is a two by two matrix of operators. The \( H(t) \) operator is characteristic of the slab, and contains all the information of interest.

It can be seen that if there is a second slab contiguous to the original slab on the right, then the appropriate \( H \) operator for this combination is

\[
H = H_2 H_1, \tag{2}
\]
where \( H_1 \) is the \( H \) operator for the first slab (the one on the left) and \( H_2 \) is the \( H \) operator for the second slab. In general, if there are \( n \) adjacent slabs, then the appropriate \( H \) operator for the system is

\[
H = H_n H_{n-1} \ldots H_2 H_1
\]

where \( H_i \) is the \( H \) operator for the \( i \)-th slab counting from the left.

To find the form of the \( H \) operator of a slab in terms of the usual transmission and reflection operators, one has

\[
\varphi_2 = T \varphi_1 + R^* \psi_2
\]

\[
\psi_1 = R \varphi_1 + T^* \psi_2
\]

where

\( T = \) the transmission operator for radiation incident on the left
\( T^* = \) the transmission operator for radiation incident on the right
\( R = \) the reflection operator for radiation incident on the left
\( R^* = \) the reflection operator for radiation incident on the right.

For simplicity one may define \( U = T^{-1} \) and \( U^* = T^{*-1} \). If the slab is symmetric between left and right, and if it is homogeneous, then \( T = T^* \) and \( R = R^* \); however, in the case of adjacent slabs of different materials, these equalities do not hold.

Equations 4 and 5 may be solved for \( \varphi_2 \) and \( \psi_2 \), the results are

\[
\psi_2 = T^{*-1} (\psi_1 - R \varphi_1) = - U^* R \varphi_1 + U^* \psi_1
\]

and

\[
\varphi_2 = T \varphi_1 + R^* (-U^* R \varphi_1 + U^* \psi_1)
\]

\[
= (T - R^* U^* R) \varphi_1 + R^* U^* \psi_1
\]
In terms of the vectors $\begin{bmatrix} \phi_2 \\ \psi_2 \end{bmatrix}$ and $\begin{bmatrix} \phi_1 \\ \psi_1 \end{bmatrix}$, equations 6 and 7 may be represented in matrix notation as

$$
\begin{bmatrix}
\phi_2 \\
\psi_2 
\end{bmatrix} =
\begin{bmatrix}
T^* R^* R & R^* U^* \\
-U^* R & U^* 
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\psi_1 
\end{bmatrix}.
$$

Comparing equations 7 and 1, one can see that

$$
H =
\begin{bmatrix}
T^* R^* R & R^* U^* \\
-U^* R & U^* 
\end{bmatrix}.
$$

Therefore, considering only homogeneous laminated slabs, the $H$ operator becomes

$$
H =
\begin{bmatrix}
T-RUR & RU \\
-UR & U 
\end{bmatrix}.
$$

Now, one may consider power series expansions of $T$, $R$ and $U$ in terms of the slab thickness $t$.

$$
T(t) = 1 - \alpha t + \ldots
$$

$$
R(t) = \beta t + \ldots
$$

and

$$
U(t) = 1 + \alpha t + \ldots
$$

In these equations, $\alpha$ and $\beta$ are matrix operators and $I$ represents the unit operator. The constant term in the expansion of $T$ is unity because for a vanishingly thin slab, the flux is unaffected. Likewise, the constant term
in the expansion for $R$ is zero since for a vanishingly thin slab there is no reflection. The linear term for $T$ is chosen to be negative by analogy with the case of the unscattered flux along the slab normal, for which

$$T = e^{-\alpha t}.$$ 

The operator $\beta$ involves the differential cross section, since for a very thin slab, only first order scattering contributes to the reflected flux. The operator $\alpha$ involves the total cross section in addition to the differential cross section, since it must include the part of the attenuation of the radiation linear in the thickness $t$. The attenuation part of $\alpha$ is diagonal in the angle and energy variables since it refers only to a reduction in intensity of each component of the incident beam separately.

One may now consider the case of two homogeneous slabs of the same material which are adjacent to each other. The $H$ operator for this system is

$$H(t_2 + t_1) = H(t_2)H(t_1)$$

where $t_1$ and $t_2$ are slab thicknesses. From equation 14 it is obvious that the form of $H$ is

$$H(t) = \exp(-Wt)$$

where $W$ is a constant matrix. It should be noted that equation 15 implies that for any matrix $A$

$$AH(t)A^{-1} = \exp(-AWA^{-1}t)$$

that is, the same transformation that diagonalizes $W$ will also diagonalize the matrix $H$.

Equation 15 may be rewritten as
\[ H(t) = \exp(-Wt) = 1 - Wt + \frac{1}{2!} (Wt)^2 - \ldots \]  

(17)

and to first order in \( t \)
\[ H(t) \approx 1 - Wt \quad . \]

(18)

Also, to first order in \( t \),
\[ RU \approx \beta t (1 + \alpha t) \approx \beta t \]

(19)

and
\[ UR \approx -(1 + \alpha t) \beta t \approx -\beta t \]

(20)

Thus to first order in \( t \), \( H(t) \) becomes
\[
H(t) = \begin{bmatrix}
1 - \alpha t & \beta t \\
-\beta t & 1 + \alpha t
\end{bmatrix} + \begin{bmatrix}
-\alpha & \beta \\
-\beta & \alpha
\end{bmatrix} t
\]

(22)

Comparing equations 18 and 22, one can see that
\[
W = \begin{bmatrix}
\alpha & -\beta \\
\beta & -\alpha
\end{bmatrix}
\]

(23)

Diagonalization of \( W \)

The transfer matrix \( H \) can be computed by diagonalizing \( W \). The diagonalization of \( W \) can in turn be reduced to the diagonalization of matrices of lower order.

In the following discussion, it will be assumed that all the eigenvalues of the matrix \( W \) are real and distinct. If \( P \) is the matrix
\[ P = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad (24) \]

then

\[ \overline{W} = P^{-1}WP = \begin{bmatrix} 0 & \sigma \\ \delta & 0 \end{bmatrix}, \quad (25) \]

where

\[ \sigma = \alpha + \beta \]
\[ \delta = \alpha - \beta \quad . \quad (26) \]

It should be noted that \( P^{-1} = \frac{1}{2}P \).

If \( \xi \) is an eigenvector of the matrix \( A \), where \( A = \sigma \delta \), which corresponds to the eigenvalue \( \gamma \), then, setting \( \lambda \) equal to a square root of \( \gamma \), the vector

\[ Z = \begin{bmatrix} \xi \\ \delta \xi / \lambda \end{bmatrix}, \quad (28) \]

can be shown to be an eigenvector of the matrix \( \overline{W} \). Then, if \( X \) is the matrix of column eigenvectors of \( A \), \( Y \) the matrix of row eigenvectors of \( A \), suitably normalized so that \( YX = I \), the \( W \) matrix is diagonalized by the transformation

\[ \frac{1}{\lambda} \begin{bmatrix} C_+ & C_- \\ C_- & C_+ \end{bmatrix} \overline{W} \begin{bmatrix} B_+ & B_- \\ B_- & B_+ \end{bmatrix} = \begin{bmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{bmatrix}, \quad (29) \]

where
\[
\Lambda = \begin{bmatrix}
\lambda_1 & & \\
& \lambda_2 & \\
& & \ddots \\
& & & \lambda_{ML}
\end{bmatrix}
\]

and \( \lambda_j = \frac{1}{2} \gamma_j \); \( \gamma_j \) is an eigenvalue of \( A \).

\[
B_+ = X + \delta X \Lambda^{-1}
\]

(31)

\[
B_- = X - \delta X \Lambda^{-1}
\]

(32)

\[
C_+ = Y + \Lambda^{-1} Y \sigma
\]

(33)

\[
C_- = Y - \Lambda^{-1} Y \sigma
\]

(34)

Here ML is the order of the \( \alpha \) and \( \beta \) matrices. If one sets

\[
B = \begin{bmatrix}
B_+ & B_- \\
B_- & B_+
\end{bmatrix}
\]

and \( C = \begin{bmatrix} C_+ & C_- \\
C_- & C_+
\end{bmatrix} \)

(35)

then every column of \( B \) has the form

\[
PZ = \begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
\begin{bmatrix}
\xi \\
-\delta \xi \Lambda
\end{bmatrix} = \begin{bmatrix}
\xi + \delta \xi \Lambda \\
\xi - \delta \xi \Lambda
\end{bmatrix}
\]

(36)

since \( PZ \) is an eigenvector of \( W \) and \( \frac{1}{2} C = (\frac{1}{2} B)^{-1} \).

Relation to the Transport Equation

The one-dimensional transport equation is

\[
\frac{\partial \bar{\phi}(x, w, V)}{\partial x} = -\mu(V) \bar{\phi}(x, w, V)
\]

\[+
\int_{-1}^{1} dw' \int_{-\pi}^{\pi} dV' \int_{0}^{2\pi} -d\xi' \sigma(\Omega, \Omega'; V, V') \bar{\phi}(x, w', V')
\]

(37)

for \(-1 \leq \xi \leq 1\).
where
\[ V' = \text{wavelength or lethargy before collision}; \]
\[ V = \text{wavelength or lethargy after collision}; \]
\[ x = \text{depth in the medium}; \]
\[ \delta(x,\omega,V) = \text{differential flux per unit } V\text{-interval, at depth } x, \text{in any direction making the angle } \arccos \omega \text{ with the forward normal}; \]
\[ \mu(V) = \text{total macroscopic cross section at } V; \]
\[ \sigma(\Omega,\Omega';V,V') = \text{macroscopic differential cross section, as a function of the direction } \Omega \text{ and } \Omega' \text{ of the emergent and incident rays respectively, and of } V \text{ and } V'. \]

\( \Omega \) represents a direction and is specified by the pair of angles \((\theta, \xi)\), where \( \xi \) is the polar angle, \( \theta = \arccos \omega \), and \( \omega \) is the azimuthal angle of the coordinate system.

The integration over \( \omega' \) in equation 37 can be broken up into two ranges; \(-1 \leq \omega' \leq 0 \) and \( 0 \leq \omega' \leq 1 \). For convenience, the following notation is introduced:

\[ \beta(x,\omega',V') \rightarrow \{ \delta(x,\omega',V'); \, 0 \leq \omega' \leq 1 \} \]
\[ \omega(x,\omega',V') \rightarrow \{ \delta(x,\omega',V'); \, -1 \leq \omega' \leq 0 \} \]
\[ = \{ \delta(x,-\omega',V'); \, 0 \leq \omega' \leq 1 \} \]

and

\[ K(\omega,\omega') = \frac{V}{2\pi} \int_{0}^{\pi} \frac{1}{2\pi} \int_{0}^{\pi} \sigma(\Omega,\Omega';V,V') \, d\Omega \, d\Omega'. \]

Since \( \sigma \) actually depends only on the angle \( \arccos \gamma \) between the directions \( \Omega \) and \( \Omega' \), where \( \gamma = \cos \omega \cos \omega' + \sin \omega \sin \omega' \cos (\xi - \xi') \), it follows that \( K(-\omega,\omega') = K(\omega,\omega') \). If one uses these conventions, equation
37 can be separated into two equations. For the forward hemisphere, one has
\[
\frac{\partial \psi(x, \omega)}{\partial x} = -\mu \psi(x, \omega) + \int_0^1 d\omega' K(\omega, \omega') \psi(x, \omega') + \int_0^1 d\omega' K(-\omega, \omega') \psi(x, \omega') ; \quad 0 \leq \omega \leq 1
\]
and for the backward hemisphere, one has
\[
-\omega \frac{\partial \psi(x, \omega)}{\partial x} = -\mu \psi(x, \omega) + \int_0^1 d\omega' K(-\omega, \omega') \psi(x, \omega') + \int_0^1 d\omega' K(\omega, \omega') \psi(x, \omega') ; \quad 0 \leq \omega \leq 1
\]

The operators \(\alpha\) and \(\beta\) were defined in terms of the properties of an infinitely thin slab, and the thin layer of material between two parallel planes whose coordinates are \(x\) and \(x + dx\) is a slab of thickness \(dx\). The forward moving radiation \(\psi(x + dx)\) coming out of the face at \(x + dx\) is the sum of a transmission and a reflection term:
\[
\psi(x + dx) = (1 - \alpha dx) \psi(x) + \beta dx \psi(x + dx)
\]
and taking the limit as \(dx\) approaches zero one has
\[
\frac{\partial \psi(x)}{\partial x} = -\alpha \psi(x) + \beta \psi(x).
\]

Comparing equations 38 and 41, one obtains equations defining \(\alpha\) and \(\beta\) as integral operators on functions of angle \(\theta = \arccos \omega\) and wavelength (or lethargy) \(\nu\);
\[
\omega \alpha \psi(x, \omega) = \mu \psi(x, \omega) - \int_0^1 d\omega' K(\omega, \omega') \psi(x, \omega')
\]
and
\[ \omega \psi(x, \omega) = \int_0^1 d\omega' K(\omega, \omega') \psi(x, \omega') . \]  

The operator formalism in equation 15 involving \( H \) and \( W \) may be viewed as a way of expressing the integration of the linear Boltzmann equation.

**Expressions for \( \alpha \) and \( \beta \) in Terms of Collision Cross Sections**

One may consider distributions \( \phi \) which are symmetrical about the slab normal at each point and are given by the same function of angle at each point.

Since one is concerned with extremely thin slabs, the calculation of \( \alpha \) and \( \beta \) will involve only unscattered and singly scattered radiation to first order in the thickness \( t \). For \( x < t \) one has for the singly scattered radiation

\[ \varphi_1(x, \epsilon, \omega) = \frac{1}{\omega} \int_{\Omega} d\Omega' \int_0^{\epsilon} d\epsilon' \int_0^x dx' \varphi_0(\epsilon', \omega') \exp\left[ \frac{\mu(\epsilon') x'}{\omega'} \right] \cdot \sigma(\Omega, \Omega'; \epsilon, \epsilon') \exp\left[ -\frac{\mu(\epsilon)(x-x')}{\omega} \right]. \]

where

- \( x \) = distance from incidence face of the slab
- \( x' \) = distance from incidence face at a collision point
- \( \omega \) = cosine of the angle with the slab normal
- \( \omega' \) = cosine for incident radiation
- \( \varphi_1(x, \epsilon, \omega) \) = singly scattered flux density at distance \( x \) per unit energy range at \( \epsilon \) per unit solid angle at \( \omega \)
- \( \varphi_0(\epsilon', \omega') \) = incident flux density at \( (\epsilon', \omega') \) per unit energy range and unit solid angle
- \( \mu(\epsilon) \) = total macroscopic linear cross section at \( \epsilon \)
- \( \Omega = \) direction after scattering; \( \Omega' = \) direction before scattering
- \( \sigma(\Omega, \Omega'; \epsilon, \epsilon') \) = differential scattering cross section from \( (\epsilon', \Omega') \) to
Equation 44 is determined from the probability that a particle emitted at the source will reach a point \( x \) after one and only one collision. This probability may be expressed as the product of four probabilities (7). The diagram in Figure 2 serves to clarify the derivation of these four probabilities.

The first probability, \( \exp(-\mu(E') x'/\omega') \), is that the particle will travel a distance \( x'/\omega' \) before interacting with the scattering medium. The probability that an interaction takes place in an interval of scattered path length is \( \mu(E') \text{d}x'/\omega \). Furthermore, the probability that such an interaction results in the particle being scattered into the direction \( \Omega \) with energy \( E \) is \( \sigma(\Omega' \Omega; E, E')/\mu(E') \). Finally the probability that the scattered particle
reaches a distance $x$ from the source is $\exp(-\mu(E)(x-x')/\omega)$. Thus the probability that a particle having energy $E'$ and traveling in direction $\Omega'$ will reach point $x$ with energy $E$ and direction $\Omega$ after one and only one collision is

$$d\theta_1(x,E,\omega) = \theta_0(E',\omega') \exp\left(-\mu(E')x'/\omega'\right) \exp\left(-\mu(E)(x-x')/\omega\right).$$  \hspace{1cm} (45)$$

Integration of equation 45 over all incoming energies and directions and over the thickness $x'$ results in equation 44.

The uncollided flux at $x'$ having energy $E$ and angle $\omega = \arccos \omega$ with the normal is simply

$$\theta_u(E,\omega) = \theta_0(E,\omega) \exp\left(-\frac{\mu(E)x'}{\omega}\right).$$  \hspace{1cm} (46)$$

If one considers only first order terms in $t$, the total transmitted flux at $t$ is the sum of the uncollided flux at $t$ and the first scattered flux at $t$. Thus

$$\theta(t,E,\omega) = \exp\left(-\frac{\mu(E)t}{\omega}\right) \theta_0(E,\omega)$$

$$+ \frac{1}{2\pi\omega} \int_{0}^{2\pi} \text{d}\xi \int_{E}^{E'} \text{d}E' \int_{\Omega}^{\Omega'} \sigma(\Omega,\Omega';E,E') \exp\left(-\frac{\mu(E')}{\omega'}\right) \theta_0(E',\omega') \cdot$$

$$\cdot \int_{0}^{t} \exp\left[-\frac{\mu(E')}{\omega'} - \frac{\mu(E)}{\omega} x'\right] \text{d}x'.$$  \hspace{1cm} (47)$$

It should be noted that the scattering integral is an average over $\xi$ the polar angle after scattering. However, since $\sigma(\Omega,\Omega';E,E')$ depends only upon the scattering angle, the integral over $d\Omega'$ is already independent of $\xi$. To show this, the $(E,E')$ dependence of $\sigma(\Omega,\Omega';E,E')$ is suppressed and
it is noted that
\[ \sigma(\Omega, \Omega') = \sigma(\cos \psi) \] (48)
where \( \cos \psi \) is the cosine of the scattering angle. Thus
\[ \sigma(\Omega, \Omega') = \sigma[\omega' + \sqrt{1-\omega^2}, \sqrt{1-\omega'^2} \cos(\xi-\xi')] \] (49)

Letting \( \xi' \) become the change in polar angles \( \xi-\xi' \), one obtains
\[
\frac{1}{2\pi} \int_0^{2\pi} d\xi \int d\Omega' \sigma(\Omega, \Omega') \varrho(E', \omega') = \frac{1}{2\pi} \int_0^{2\pi} d\xi \int_0^{2\pi} [-\int_0^{2\pi} d\omega' \sigma(\xi') \varrho(E', \omega')] d\xi' \\
= \frac{1}{2\pi} \int_0^{2\pi} d\xi \int_0^{2\pi} [-d\xi' \int_0^{2\pi} d\omega' \sigma(\xi') \varrho(E', \omega')] \\
= \int d\Omega' \sigma(\xi') \varrho(E', \omega') 
\] (50)
The variable \( \xi' \) is now defined as the change in polar angle after scattering.

Substituting equation 50 into equation 47 and approximating to first order in \( t \), one obtains
\[
\varrho(t, E, \omega) \approx \varrho_0(E, \omega) - \frac{t}{\omega} \left\{ \mu(E) \varrho_0(E, \omega) - \int dE' \int d\omega' \left\{ \sum_{\Omega, \Omega'} \sigma(\Omega, \Omega'; E, E') \varrho_0(E', \omega') \right\} \right\} \\
= \varrho_0(E, \omega) - \frac{t}{\omega} \int dE' \int d\omega' \left\{ \sum_{\Omega, \Omega'} \sigma(\Omega, \Omega'; E, E') \varrho_0(E', \omega') \right\} \varrho_0(E', \omega') 
\] (51)

By the definition of the transmission matrix \( T \) and equation 11, one obtains
\[
\varrho = T\varrho_0 = (1 - \alpha t)\varrho_0 = \varrho_0 - \alpha t\varrho_0 
\] (52)
and comparing equation 52 with equation 51 one can determine \( \alpha \) as the
integral operator.

\[ \alpha \varphi_o = \frac{1}{\omega} \int dE' \int d\omega' \left\{ \mu (E') \delta (E-E') \delta (\omega-\omega') \right\} \varphi_o (E', \omega') \]  

(53)

The kernel corresponding to \( \alpha \) is

\[ K_{\alpha} (E, \omega; E', \omega') = \frac{1}{\omega} \left\{ \mu (E) \delta (E-E') \delta (\omega-\omega') \right\} \phi_o (E', \omega') \]  

(54)

Similarly, the reflected flux is

\[ \psi (0, E, \omega) = \frac{1}{\omega} \int dE' \int d\omega' \phi_o (E', \omega') \phi (E', \omega) \int_0^t \exp \left\{ -\frac{\mu (E')}{\omega} \right\} d\gamma \]

(55)

so that the relation

\[ \psi = R \phi_o = t \beta \phi_o \]  

(56)

indicates that the \( \beta \) operator is

\[ \beta \phi_o = \frac{1}{|\omega|} \int dE' \int d\omega' \int_0^{2\pi} d\Omega' \sigma (\Omega, \Omega'; E, E') \varphi_o (E', \omega') \]  

(57)

The kernel corresponding to \( \beta \) is

\[ K_{\beta} (E, \omega; E', \omega') = \frac{1}{|\omega|} \int_0^{2\pi} d\Omega' \sigma (\Omega, \Omega'; E, E') \]  

(58)

In the one-velocity problem with isotropic scattering, equations 54 and 58 become respectively

\[ K_{\alpha} (\omega, \omega') = \frac{1}{\omega} \left\{ \mu \delta (\omega-\omega') - \frac{\sigma_s}{2} \right\} \]  

(59)

\[ K_{\beta} (\omega, \omega') = \frac{1}{|\omega|} \frac{\sigma_s}{2} \]  

(60)

where \( \sigma_s \) is the total macroscopic scattering cross section.
It will be convenient to employ as an energy variable not the energy itself, but another variable, monotonic in energy. This variable will be represented by $V$. Then all the previous equations will hold by replacing $E$ by $V$ and $E'$ by $V'$.

For gamma ray work, it is conventional to select for $V$ the gamma ray wavelength in Compton units, so that $V = \lambda/E$, when $E$ is expressed in units of the rest energy of the electron. For neutrons, the customary choice for $V$ is the neutron lethargy, defined as $V = \ln(E_o/E)$, where $E_o$ is some reference energy, usually the largest energy of interest.

For elastic collisions, to which this investigation is restricted, there is a relationship of the form $\cos \psi = \gamma(V-V')$, where $\gamma$ is a function of the difference $(V-V')$ in $V$ before and after the collision, and $\psi$ is the angle of scattering in the laboratory system.

For gamma rays, $\gamma$ takes the form

$$\gamma(V-V') = 1 - (V-V')$$

(61)

and for neutrons

$$\gamma(V-V') = \cosh\left(\frac{V-V'}{2}\right) - A \sinh\left(\frac{V-V'}{2}\right)$$

(62)

where $A$ is the nuclear mass of the scattering nucleus.

For further simplicity, a function $\sigma(V-V')$ is introduced by the relation

$$\int d\Omega \sigma(\Omega,\Omega';V,V') = \sigma(V,V')$$

(63)

Now, if $\cos \psi = \gamma(V-V')$, then

$$\sigma(\Omega,\Omega';V,V') = \sigma(V,V') \frac{\delta[\cos \psi - \gamma(V-V')]}{2\pi}$$

(64)

where $\sigma(V,V')$ is the Klein-Nishina formula (8).
\[
\sigma(V,V') = \frac{1}{2} r^2_0 \left( \frac{V'}{V} \right)^2 \left[ \frac{V'}{V} + \frac{V}{V'} + 2(V' - V) + (V' - V)^2 \right]
\]

and \( r_0 \) is the classical electron radius. Rewriting equation 51 with \( E \) and \( E' \) replaced by \( V \) and \( V' \), one obtains

\[
\alpha_0(V',\omega') = \frac{1}{\omega} \int dV' \int d\omega' \left\{ \mu(V') \delta(V-V') \delta(\omega-\omega') \right\}
\]

\[
-\frac{1}{2\pi} \int d\xi' \sigma(V,V') \delta[\cos \psi - \gamma(V-V')] \theta_0(V',\omega') .
\]

The \( \xi' \) integration can be carried out explicitly. If one considers the following scattering diagram,

![Figure 3. The scattering geometry](image)

then

\[
\cos \psi = -\cos \theta \cos \theta' + \sin \theta \sin \theta' \cos \xi'
\]

(66)

where \( \theta = \arccos \omega \), and \( \xi' \) is the change in polar angles after scattering. For fixed \( \theta \) and \( \theta' \)

\[
d(\cos \psi) = -\sin \theta \sin \theta' \sin \xi' \, d\xi' .
\]

(67)
However, equation 66 also yields

\[
\begin{align*}
(sin \theta sin \theta' sin \xi')^2 &= sin^2 \theta sin^2 \theta' - sin^2 \theta sin^2 \theta' cos^2 \xi' \\
&= sin^2 \theta sin^2 \theta' - (cos \psi - cos \theta cos \theta')^2 \\
&= -(cos \psi - cos \theta cos \theta' + sin \theta sin \theta')(cos \psi - cos \theta cos \theta' - sin \theta sin \theta') \\
&= [cos(\theta - \theta') - cos \psi][cos \psi - cos(\theta + \theta')] \\
\end{align*}
\]

and so, by equation 67

\[
\begin{align*}
\frac{2\pi}{\xi'} d\xi'[cos \psi - \gamma(V-V')] \\
&= 2\int_0^{\xi'} d(cos \psi)[[cos(\theta - \theta') - cos \psi][cos \psi - cos(\theta + \theta')]]^{1/2} \\
&= 2\cos(\theta - \theta') \\
&= 2Re \frac{1}{S} \\
\end{align*}
\]

where \( S \) is given by

\[
S^2 = [cos(\theta - \theta') - \gamma(V-V')][\gamma(V-V') - cos(\theta + \theta')] \\
\]

The factor 2 appears in equation 70 because of the symmetry of the left-hand side about \( \xi' = \pi \). Equation 65 may now be written as

\[
\alpha G(V',\omega') = \frac{1}{\omega} \int dV' \int d\omega' \delta(V') \delta(\omega') - \sigma(V',V')Re \frac{1}{n}S; \ 0 \leq \omega \leq 1 \\
\]

where

\[
\begin{align*}
S^2 &= (sin \theta sin \theta')^2 - (\gamma - cos \theta cos \theta')^2 \\
&= (1-\omega^2)(1-\omega'^2) - \gamma^2 + 2\gamma \omega \omega' - \omega \omega'^2 \\
&= 1 - \omega^2 - \omega'^2 - \gamma^2 + 2\gamma \omega \omega' \\
\end{align*}
\]
In a similar manner, equation 57 may be simplified to the following expression

$$\beta_o(V',\omega) = \frac{1}{|\omega|} \int dV' \int_0^1 d\omega' \sigma(V, V') \Re \int_{\pi S} \beta_o(V', \omega') \quad -1 \leq \omega \leq 0 \quad (73)$$

where $\omega$ is measured from the forward normal.

**Matrix Representation**

The distributions $\phi$ and $\alpha \phi$ are to be expanded at each wavelength of interest as linear combinations of basis functions $F_o(\omega), F_1(\omega), \ldots$, which form a complete, but not necessarily orthogonal, set on the interval $0 \leq \omega \leq 1$.

Then $\phi$ can be written in the form

$$\phi(\omega) = \sum_n \phi_n F_n(\omega) \quad (74)$$

If one defines $\psi_m = \alpha \phi$, then the matrix element $\alpha_{mn}$ is the integral operator in $V$ which transforms $\phi_n$ into $\psi_m$. Thus

$$\psi_m = \sum_n \alpha_{mn} \phi_n \quad (75)$$

Similarly,

$$\psi(\omega) = \sum_m \psi_m F_m(\omega) \quad$$

In order to weight the errors in a finite angular representation, the weighting function $g(\omega)$ is introduced. If equation 71 is now multiplied by $g(\omega)F_k(\omega)\omega$ and integrated over $\omega$ from 0 to 1; one obtains
\[
\int_0^1 \omega g(\omega) F_k(\omega) \alpha \beta \omega^0 d\omega = \int_0^1 \omega g(\omega) F_k(\omega) \psi(\omega) d\omega
\]

\[
= \sum_{m} \int_0^1 \omega g(\omega) F_k(\omega) F_m(\omega) \psi_m(\omega) d\omega
\]

\[
= \sum_{m} \int_0^1 g(\omega) \omega F_k(\omega) F_m(\omega) \alpha \beta n \psi_n(\omega) d\omega
\]

and thus

\[
\int_0^1 \omega g(\omega) F_k(\omega) \alpha \beta \omega^0(\omega) = \int_0^1 \omega d\omega \int_0^1 dV \int_0^1 d\omega' \left\{ g(\omega) F_k(\omega) \nu(V) \delta(V-V') \delta(\omega-\omega') \right\}
\]

\[
- g(\omega) F_k(\omega) \sigma(V,V') Re \frac{1}{\pi S} \beta_n(V') F_n(V')
\]

Because of the \(\delta\)-function factor, the integral over the first term on the right is

\[
\int_0^1 \omega g(\omega) F_k(\omega) F_n(\omega) d\omega \beta_n(V) \nu(V) = z_{kn} \beta_n(V) \nu(V)
\]

where

\[
z_{kn} = \int_0^1 g(\omega) F_k(\omega) F_n(\omega) d\omega
\]

The integral over the second term on the right can be conveniently expressed in terms of the functions

\[
d_{mn}(\gamma) = \int_0^1 \int_0^1 \omega m \omega^0 \omega^0 \Re e \frac{1}{\pi S(\omega,\omega',\gamma)} d\omega d\omega'
\]

Explicit formulas for the \(d_{mn}\) terms are given in WADC Technical Report 59-772, and will be employed for all further calculations (2). It should be noted that because of the symmetry of \(S\) in \(\omega\) and \(\omega'\), \(d_{mn} = d_{nm}^*\).

If one assumes that there are power series expansions for the basis
functions \( F_1(\omega) \) and for \( g(\omega) \):

\[
F_m(\omega) = \sum_{n} q_{mn} \omega^n ; \quad m = 0, 1, 2, \ldots \tag{82}
\]

\[
g(\omega) = \sum_{i} g_i \omega^i ; \quad i = 0, 1, 2, \ldots \tag{83}
\]

and one sets

\[
e_{km} = \frac{1}{k} \int_0^k g(\omega) F_k(\omega) F_m(\omega) d\omega , \tag{84}
\]

then equation 78 may be written in the form

\[
\sum m e_{km} \alpha \phi_n(V) = \mu_n(V) z_{kn} \phi_n(V)
\]

\[
\quad \int_0^V \sigma(V, V') \sum_{i} g_i \sum_{s} q_{is} \sum_{r} q_{nr} d_{r+s+i,r} [\gamma(V-V')] \phi_n(V') . \tag{85}
\]

The corresponding operator for \( \alpha_{mn} \) is formed from this by suppressing the function \( \phi_n \) on the right of each term.

This operator equation may be written in matrix notation by defining

\( E = \) matrix of the \( e_{mn} \)

\( Z = \) matrix of the \( z_{mn} \)

\( Q = \) matrix of the \( q_{mn} \)

\( D = \) matrix of the \( d_{mn} \)

\( G = \) matrix whose \( (i,j) \)-th element is \( g_{j-i} \) if \( j \leq i \), and zero if \( j > i \);

and by recalling that \( \alpha \) can be interpreted as the matrix of the \( \alpha_{mn} \). If these conventions are employed, then

\[
E \phi(V) = \mu(V) Z \phi(V) - \int_0^V \sigma(V, V') Q G D [\gamma(V-V')] \phi(V') dV' . \tag{86}
\]

in this expression \( E, Z, Q, \) and \( G \) are infinite matrices of constants. The elements of \( D \) are functions of \( \gamma(V-V') \), thus equation 86 may be rewritten
as

\[ E\alpha\beta(V) = \mu(V)Z\alpha(V) - QG \int_{V}^{V'} \sigma(V,V')D[\gamma(V-V')]\beta(V')dV'Q^T. \]  

(87)

The matrix representation for the reflection operator \( \beta \) will employ the same basis functions \( F_\alpha(\omega), F_\beta(\omega), \ldots \), as for \( \alpha \), but \( \omega \) is now measured from the backward normal. Thus

\[ E\beta\beta(V) = QG \int_{V}^{V'} \sigma(V,V')D^*\gamma(V-V')\beta(V')dV'Q^T. \]  

(88)

Here the elements \( d^*_{nm} \) of \( D^* \) are given by

\[ d^*_{mn}(\gamma) = (-1)^m \int_{-\pi}^{\pi} d\omega \int_{-\pi}^{\pi} d\omega' \omega^m \omega'^n \text{Re} \frac{1}{\pi S}. \]  

(89)

where \( S \) has been defined earlier. The \((-1)^m\) factor appears because the \( \omega \) of the integration is the cosine of the angle measured from the forward normal. By virtue of the symmetric form of \( S \), substitution of \(-\omega \) for \( \omega \) and \(-\gamma \) for \( \gamma \) in equation 89 yields

\[ d^*_{mn}(-\gamma) = d_{mn}^{*\gamma}(\gamma) ; \quad -1 \leq \gamma \leq 1 \]  

(90)

and thus \( D^* \) may be found from \( D \).

For simplicity, the distribution function within an energy group is taken as independent of angle, and so can be written as \( f_\omega(V) \). Also, in any calculation it is necessary to cut-off the infinite expansion in angle and to discretize the continuous variable \( V \). One possible discretized form of equation 87 is

\[ E\alpha\beta_{\omega\omega'} = \delta_{\omega\omega'} \int_{V_{\omega-1}}^{V_{\omega}} f_\omega(V')dV'Z \]

\[ - QG \int_{V_{\omega-1}}^{V_{\omega}} dV' \int_{V_{\omega-1}}^{V_{\omega}} dV' f_\omega(V')\sigma(V,V')D[\gamma(V,V')Q^T. \]  

(91)
Similarly, for the reflection operator,
\[
E \mathcal{S}_{\mathcal{L},1} = Q \int \frac{dV'}{V_{\mathcal{L'}}-V_{\mathcal{L}}-1} \int \frac{dV}{V_{\mathcal{L}}-1} f_\mathcal{L}(V') \sigma(V,V')D[-\gamma(V-V')] Q^{T} .
\]  
(92)

An appropriate form of \( f_\mathcal{L}(V') \) is
\[
f_\mathcal{L}(V') = \frac{V_{\mathcal{L}}V_{\mathcal{L}-1}}{(V_{\mathcal{L}}-V_{\mathcal{L}-1})V_{\mathcal{L}}^{2}} .
\]  
(93)

Multiplying equations 91 and 92 by \( E^{-1} \) yields the expressions for the \( \alpha_{\mathcal{L},1} \), and \( \beta_{\mathcal{L},1} \) blocks.

**Determination of \( E, Z, Q, G \) and \( D \)**

The basis functions to be employed are the half-range Legendre polynomials. These polynomials satisfy the following relationships:
\[
F_1^\pm(\omega) = F_1(2\omega - 1) ; 0 \leq \omega \leq 1
\]
\[
= 0 ; \omega < 0
\]
\[
F_1^\mp(\omega) = F_1(2\omega + 1) ; -1 \leq \omega \leq 0
\]
\[
= 0 ; \omega > 0
\]  
(94)

(95)

where \( F_1(2\omega \pm 1) \) is the Legendre polynomial of order 1. The orthogonality relations satisfied by the half-range Legendre polynomials are
\[
\int_{0}^{1} d\omega \ F_{1}^{\pm}(\omega) F_{j}^{\pm}(\omega) = \int_{-1}^{0} d\omega \ F_{1}^{-}(\omega) F_{j}^{-}(\omega) = \frac{\delta_{j1}}{2i+1} .
\]  
(96)

Since this investigation is concerned only with the range of \( \omega \) from 0 to 1, equation 95 may be ignored. From equation 94, therefore, one obtains the coefficients of the power series expansions for \( F_1^\pm(\omega) \).

The power series expansions of the first three Legendre polynomials (9) are as follows:
Thus, from equation 14, the power series expansions for the first three half-range Legendre polynomials basis functions are

\[ F_0^+(w) = F_0(2w-1) = 1 \]
\[ F_1^+(w) = F_1(2w-1) = 2w-1 \]
\[ F_2^+(w) = F_2(2w-1) = 6w^2 - 6w + 1 \]

For this investigation, \( g(w) = 1 \), thus the \( Z \) matrix is readily obtained from the orthogonality relationship indicated in equation 96.

\[
Z = \begin{bmatrix}
1.0000 & 0 & 0 \\
0 & 0.3333 & 0 \\
0 & 0 & 0.2000
\end{bmatrix}
\] (97)

The elements of the \( Q \) matrix may be obtained from equation 82 and the coefficients of the half-range Legendre polynomials. Thus

\[
Q = \begin{bmatrix}
1 & 0 & 0 \\
-1 & 2 & 0 \\
1 & -6 & 6
\end{bmatrix}
\] (98)

Since \( g(w) \) is set equal to 1, the \( G \) matrix is simply the identity matrix 1.

The \( i,j \)-th element of the matrix \( E \) is defined in equation 84. Substitution of the basis functions into this equation and integrating over the variable \( w \), one obtains

\[
E = \begin{bmatrix}
0.50000 & 0.16667 & 0 \\
0.16667 & 0.16667 & 0.26667 \\
0 & 0.26667 & 0.10000
\end{bmatrix}
\] (99)
The elements of the D matrix are functions of $\gamma(V-V')$ and formulas for the individual elements are supplied by WADC Technical Report 59-772. Since this investigation is concerned with a third order polynomial approximation of the angular variable, the D matrix takes the following form:

$$D = \begin{bmatrix}
    C & 0 & 0 \\
    \frac{1}{2} \left( 1 + \frac{1}{2} \right) & \frac{\gamma C}{3} + \frac{R}{3} & 0 \\
    \frac{C}{3} + \frac{\gamma R}{3} & \frac{1}{4} \left[ \frac{1 + \gamma^2}{4} \right] & \frac{(1 + 2 \gamma^2) C}{15} + \frac{\gamma R}{5}
\end{bmatrix}$$

where

$$C = 1 - \frac{1}{\pi} \arccos \gamma ; \quad 0 \leq C \leq 1$$

$$R = \frac{1}{\pi} (1 - \gamma^2)^{1/2}$$

$$\gamma = 1 - (V-V')$$

It should be noted that the matrix $D^*$ is of the same form as $D$ except that $\gamma$ is replaced by $-\gamma$ in $D^*$.

Integration Scheme

Gauss' formula for arbitrary intervals is employed for numerical integration of equations 86 and 87 (9). A five-point mesh is employed for both integrals. Gauss' formula is

$$\int_{a}^{b} f(y) \,dy = \frac{b-a}{2} \sum_{i=1}^{n} w_i \,f(y_i) + R_n$$

(101)

where $w_i$, the weighting factor is defined as

$$w_i = \frac{2}{(1-x_i)^2} \left[ \frac{p_n'(x_i)}{p_n(x_i)} \right]^2$$

(102)

and

$$y_i = \left( \frac{b-a}{2} \right) x_i + \frac{b+a}{2}$$

(103)
The absissas $x_i$ is the $i$-th zero of the Legendre polynomial. Tables of $x_i$ and $w_i$ are found in the Handbook of Mathematical Functions, AMS 55 (9).

For the double integral, Gauss' formula becomes

$$\int_a^b \int_c^d f(y, y') dy dy' = \frac{(b-a)}{2} \frac{(d-c)}{2} \left[ \sum w_i \sum w_j f(y_i, y'_j) \right]$$

Diagonalization of $A = \sigma \delta = (\alpha + \beta)(\alpha - \beta)$

The matrices representing $\alpha$ and $\beta$ may be considered to be matrices in energy whose elements are matrices in angles, or blocks. Because of the scattering condition, all blocks above the main diagonal are zero. Thus $\alpha$ and $\beta$ are block lower triangular matrices, and their elements may be denoted by four subscript symbols

$$\alpha = \begin{bmatrix} \alpha^{mm'} \\
\alpha^{m'm'} \end{bmatrix} ; \quad \beta = \begin{bmatrix} \beta^{mm'} \\
\beta^{m'm'} \end{bmatrix}$$

where $\ell$ is the energy row index, $\ell'$ is the energy column index, $m$ is the angle row index and $m'$ is the angle column index. For convenience, the following matrix notational conventions will be employed (10):

$A_{\ell \ell'}^{m} = $ column vector consisting of all elements $A^{mn'}_{\ell \ell'}$ whose second indices are fixed values of $m'$ and $\ell'$

$A_{\ell \ell'}^{m'} = $ row vector consisting of all elements $A^{mn}_{\ell \ell'}$ whose first indices are fixed values of $m$ and $\ell$

$A_{\ell \ell'} = $ block consisting of elements $A^{mn}_{\ell \ell'}$ whose energy indices are the fixed values $\ell$ and $\ell'$

$A_{\ell \ell'}^{m} = m^{t}$-th column of the $A_{\ell \ell'}$ block
The diagonalization of the matrix $A$ is simplified by considering the following properties of this matrix. Since $\alpha$ and $\beta$ are block lower triangular matrices, it follows that $A$ will also be of this form. Furthermore, the characteristic equation of $A$

$$|A - \gamma I| = 0$$

is also block lower triangular. However, the determinant of a block triangular matrix is the product of the determinants of the blocks along the main diagonal, so that

$$|A - \gamma I| = \prod_{\ell=1}^{L} |A_{\ell\ell} - \gamma I| \quad (105)$$

In other words, the set of eigenvalues of $A$ is made up of the sets of eigenvalues of each block $A_{\ell\ell}$, $\ell = \ell' = 1, 2, \ldots, L$.

If $X_{\ell \ell}^{m}$ is a column of $X$, it will be an eigenvector of $A$ corresponding to an eigenvalue $\gamma_{j}$, $\gamma_{m}^{l}$. Reducing the matrix-column product

$$AX_{\ell \ell}^{m} = X_{\ell \ell}^{m} \gamma_{j} \quad (106)$$

to the block-component equations

$$\sum_{k=1}^{L} A_{\ell \ell}^{k} X_{k \ell}^{m} = X_{\ell \ell}^{m} \gamma_{j} = X_{\ell \ell}^{m} \gamma_{m}^{l} \quad (107)$$
or

$$\sum_{k=1}^{L-1} A_{\ell \ell}^{k} X_{k \ell}^{m} = (\gamma_{m}^{l} I - A_{\ell \ell}) X_{\ell \ell}^{m} \quad (108)$$

Thus, if the eigenvectors and eigenvalues of $A_{\ell \ell}$ are known, the other block components of $X_{\ell \ell}^{m}$ are determined recursively by
\[ X_{\ell' \ell}^m = (\gamma_{\ell, \ell'}^m 1 - A_{\ell, \ell'})^{-1} \sum_{k=\ell'}^{\ell-1} A_{\ell, k} X_{k \ell}^m \quad ; \quad \ell > \ell' \quad . \] (109)

By similar arguments, the components of \( Y \) (the matrix of row eigenvectors) are found to be

\[ Y_{\ell' \ell}^m = \sum_{k=\ell'+1}^{\ell} Y_{\ell' \ell}^m A_{\ell, k} (\gamma_{\ell, \ell'}^m 1 - A_{\ell, \ell'})^{-1} \quad . \] (110)

### Diagonalization of Blocks on the Energy Diagonal

Diagonalization of the block matrices along the energy diagonal is performed by employing the power method\((11)\). The simple power method is modified to take into account the possibility of repeated roots, or roots whose magnitude are nearly equal.

### Final Computation of T and R

Once the eigenvalues and the row and column eigenvectors of \( A \) are found, they may be adjusted to form a set of transforming matrices which will diagonalize \( W \), where

\[ W = \begin{bmatrix} \alpha & -\beta \\ \beta & -\alpha \end{bmatrix} \quad . \]

In particular, the following relationship is obtained:

\[ \frac{1}{\lambda} \begin{bmatrix} C_+ & C_- \\ C_- & C_+ \end{bmatrix} \begin{bmatrix} \alpha & -\beta \\ \beta & -\alpha \end{bmatrix} \begin{bmatrix} B_+ & B_- \\ B_- & B_+ \end{bmatrix} = \begin{bmatrix} \Lambda & 0 \\ 0 & -\Lambda \end{bmatrix} \] (111)

where \( \Lambda \) is defined in equation 30 and \( B_\pm \) and \( C_\pm \) are defined in equations 31 through 34. Since, as was indicated above, the matrices which diagonalize \( W \) also diagonalizes the transfer matrix \( H(t) \); then
The above matrix equation may be solved for \( T \) and \( R \). Thus

\[
\begin{align*}
T &= 4\left( B_+ e^{A t} C_+ + B_- e^{-A t} C_- \right) - 1 \\
RT^{-1} &= \frac{1}{4} \left( B_+ e^{A t} C_+ + B_- e^{-A t} C_- \right) \\
R &= RT^{-1} T
\end{align*}
\]

where

\[
e^{\pm A t} = \begin{bmatrix}
\pm \lambda_1 t \\
e^t \\
\pm \lambda_2 t \\
e^t \\
\cdots \\
\pm \lambda_M t \\
e^t
\end{bmatrix}
\]
RESULTS AND DISCUSSION OF PRIMARY GAMMA TRANSPORT

A computer program was written to compute the \( \alpha \) and \( \beta \) matrices, diagonalize the A matrix and obtain the transmission and reflection matrix operators. The gamma ray source under investigation was a 2 Mev plane isotropic source. To approximate a 2 Mev source, the upper energy group limits were 2.001 Mev to 1.999 Mev. Because of such a narrow group, it was assumed that the energy flux transmitted into that group was entirely uncollided.

The input data to the program were the constant matrices \( Q, Z, E^{-1}, \) and \( G, \) which were defined above; the number of energy groups, five; and gamma radiation attenuation data for each material of interest. The gamma attenuation data consisted of tables of total cross sections and the corresponding gamma energy for each value of the cross section (12). With the use of Lagrange's interpolation formula (13) a cross section was obtained for all energies which the scattered gamma ray might have.

The initial selection of the individual energy group limits was determined by examining the differential energy spectra found in Goldstein (3). From these spectra, an estimation was made for the "cut-off" energy of each material being investigated. The "cut-off" energy corresponds to the lower energy limit of the lowest energy group in the analysis. Therefore, all transmitted gamma rays having energies less than the "cut-off" energy were ignored. In the case of dense materials such as lead and uranium, the "cut-off" energy is in the vicinity of 0.5 Mev. For less dense materials such as water, however, the "cut-off" energy is quite a bit lower; i.e., the differential energy spectrum for water reaches a maximum at a
relatively low energy. For water, this peak is located between 0.05 to 0.1 Mev. However, if one wishes to calculate energy flux transmission through lead-water laminated slabs, the energy grouping in each material must be the same. To resolve this problem, a search was made to locate the highest possible "cut-off" energy for water and still retain a fair degree of accuracy.

The initial grouping was selected to yield groups of approximately equal widths for the scattered groups, and a very narrow group for the source in order to approximate the 2 Mev monoenergetic problem. The grouping, from the highest group to the lowest was as follows:

- first group: 2.001 to 1.999 Mev
- second group: 1.999 to 1.5 Mev
- third group: 1.5 to 1.0 Mev
- fourth group: 1.0 to 0.5 Mev
- fifth group: 0.5 to 0.15 Mev.

Since 0.15 Mev is well below the "cut-off" energies of lead and uranium, as indicated in the differential energy spectra, it was expected that the results obtained for these materials using this energy grouping arrangement would be fairly accurate. However, in the case of water, the accuracy of the results was questionable. In order to check the results obtained for this choice of energy groups, the energy buildup factor as a function of slab thickness was calculated for each material.

The energy buildup factor $B_E$ is defined as

$$B_E = \frac{\text{Total energy flux transmitted}}{\text{Uncollided energy flux transmitted}}.$$

As has been indicated above, the uncollided flux transmitted is the energy
flux transmitted in the upper energy group, from 2.001 Mev to 1.999 Mev. To obtain the total energy flux transmitted, the form of the transmission matrix $T$ should be taken into account. As has been indicated above, the form of the transmission matrix is lower block triangular. The $LL'$ block corresponds to the transmitted energy flux in the $\ell$-th group due to an incoming energy flux in the $\ell'$-th group. The elements in the $LL'$ block transform the incoming angular distribution. Thus, the transmitted energy flux vector $\Phi_T^m$ whose components specify the energy and angular distributions of the transmitted flux, is simply the matrix product of $T$ and the source vector $\Phi_S^m$.

$$\Phi_T^m = \sum_{\ell',m'} T_{\ell',m'}^{m,m'} \Phi_S^{m'} .$$

Because of the orthogonality property of the half-range Legendre polynomials, and since the source is assumed to be isotropic, the total energy flux transmitted in the $\ell$-th group is $\Phi_T^\ell$, and the total energy flux transmitted through the slab is $\sum_{\ell=1}^L \Phi_T^\ell$, where $L$ is the number of energy groups in the analysis. Thus

$$B_{Le} = \frac{\sum_{\ell=1}^L \Phi_T^\ell}{\Phi_S^1} .$$

Buildup factors were calculated for all three materials under consideration and the results are plotted in Figure 4. For comparison purposes, the energy buildup factors for lead and water calculated by the moments method (3) are plotted on the same graph. Unfortunately, these energy buildup factors were calculated for slabs of infinite thickness. However, in Goldstein (3) correction factors for lead and water have been plotted;
Figure 4. Energy buildup factor, $B_E$, of water, lead, and uranium for a 2 Mev plane isotropic source.

- : adjusted Moments Method calculations
- : present calculations
these can be used to adjust infinite energy buildup factors to finite energy buildup factors. The results plotted in the graph are thus adjusted energy buildup factors calculated by the moments method.

In order to determine whether a "cut-off" energy of 0.15 Mev was accurate enough for energy flux transmission calculations through a water slab, it was decided to reduce the lower limit of the lowest energy group to 0.10 Mev, and see if this reduction in "cut-off" energy resulted in a significant change in the energy buildup factors. When this was done, large errors were introduced in the transmission matrix. After some deliberation, it was discovered that the error was introduced because of the method of numerical integration. An energy group whose upper and lower energy limits are 0.5 Mev and 0.1 Mev respectively introduced too many zero grid points that were weighted as heavily as non-zero grid points in the numerical integration scheme. The reason for this is that a gamma ray whose energy is 0.5 Mev cannot suffer a 0.4 Mev reduction in energy after only one collision even if the scattering angle of the interaction is $2\pi$. To resolve this difficulty, it was decided that the lower energy limits of each energy group should be selected according to the Compton law (14) with a scattering angle of $\pi$. That is, the upper limit of any group determines the lower limit of that group, as well as the upper limit of the next group, through the following relationship:

$$E_{\text{lower}} = 0.511 \frac{E_{\text{upper}}}{(0.511 + E_{\text{upper}})}$$  \hspace{1cm} (119)

where $E$ is measured in Mev. For five energy groups, this resulted in the following grouping:

- first group: 2.001 to 1.999 Mev
second group: 1.999 to 0.407 Mev
third group: 0.407 to 0.227 Mev
fourth group: 0.227 to 0.157 Mev
fifth group: 0.157 to 0.120 Mev.

The energy buildup factors for water employing this grouping differed by only a few percent when compared to those calculated with a "cut-off" energy of 0.15 Mev. As a final check on the "cut-off" energy for water, an eight energy group analysis was made. As in the above case, the group limits were determined by the Compton law with a scattering angle of \( \pi \).

The resulting energy grouping was

- first group: 2.001 to 1.999 Mev
- second group: 1.999 to 0.407 Mev
- third group: 0.407 to 0.227 Mev
- fourth group: 0.227 to 0.157 Mev
- fifth group: 0.157 to 0.120 Mev
- sixth group: 0.120 to 0.097 Mev
- seventh group: 0.097 to 0.082 Mev
- eighth group: 0.082 to 0.070 Mev.

The energy buildup factors obtained with this grouping compared very closely with the five energy group analysis. Thus, it was concluded that the five energy group case with a "cut-off" energy of 0.15 Mev was appropriate for this analysis and thereby rendering possible the investigation of lead-water and water-lead laminated slabs with only five energy groups.

Differential energy spectra for lead and water for a variety of slab thicknesses were calculated, and the results are plotted in Figures 5 through 12. The spectrum characteristics exhibited by these curves are
Figure 5. Differential energy spectrum for a 2 Mev plane isotropic source incident upon one mean free path of water.
Figure 6. Differential energy spectrum for a 2 Mev plane isotropic source incident upon two mean free paths of water.
Figure 7. Differential energy spectrum for a 2 Mev plane isotropic source incident upon four mean free paths of water
Figure 8. Differential energy spectrum for a 2 Mev plane isotropic source incident upon seven mean free paths of water.
Figure 9. Differential energy spectrum for a 2 Mev plane isotropic source incident upon one mean free path of lead.
Figure 10. Differential energy spectrum for a 2 Mev plane isotropic source incident upon two mean free paths of lead.
Figure 11. Differential energy spectrum for a 2 Mev plane isotropic source incident upon four mean free paths of lead.
Figure 12. Differential energy spectrum for a 2 Mev plane isotropic source incident upon seven mean free paths of lead.
substantiated by the spectra from Goldstein (3). That is, in the case of lead, the maximum of the spectrum shifts toward lower energies as the slab thickness is increased; whereas in the case of water, the minimum shifts toward higher energies as the slab thickness increases. The spectra for water in this investigation have been obtained from the five energy grouping with a "cut-off" energy of 0.12 Mev so as to emphasize the buildup of a peak in the spectra at low energies.

Included in the results are plots of the angular distributions of the transmitted energy flux for water, lead, and uranium. These distributions are indicated in figures 13 through 15. The major point to be noted here is the forward peaking of the transmitted flux with increasing slab thickness.

Also included in the homogeneous slab transmission calculations are plots of the total energy flux transmitted as a function of slab thickness. These are illustrated in figures 16 through 18. Plotted on the same graphs are the contributions of the individual energy groups to the total energy flux transmitted. Thus, ascribed to each curve on the graph is the upper limit of the corresponding energy group. To obtain the energy transmitted within a certain energy interval determined by the energy group limits, one has only to find the difference between the curves corresponding to the energy limits of interest. It should be noted that all curves except the highest go to zero as the slab thickness goes to zero. This means that for a vanishingly thin slab, the scattered gamma ray energy flux goes to zero. On the other hand, the highest curve which corresponds to the total energy flux transmitted has a value of 2 Mev at a zero slab thickness. In other words, the total energy transmitted as the slab thickness goes to zero is
Figure 13. The angular distributions \( \phi_i \) of the transmitted energy flux due to a 2 Mev plane isotropic gamma source incident upon mean free paths of water.
Figure 14. The angular distributions $\theta_i$ of the transmitted energy flux due to a 2 Mev plane isotropic source incident upon i mean free paths of lead.
Figure 15. The angular distributions $\varphi_i$ of the transmitted energy flux due to a 2 Mev plane isotropic gamma source incident upon i mean free paths of uranium.
Figure 16. The energy-group components of the transmitted energy flux through water
Cut-off Energy: 0.12 Mev
Figure 17. The energy-group components of the transmitted energy flux through lead
Figure 18. The energy-group components of the transmitted energy flux through uranium
Transmitted Energy Flux $\beta (\text{MeV/cm}^2 \cdot \text{sec})$

Cut-off Energy: 0.15 MeV

Cut-off Energy: 0.500 Mev
is simply the source strength.

To further investigate the usefulness of the transmission matrix method to radiation shielding problems, transmission calculations were made for two-layer slabs. In one case, the slab was made up of a layer of water followed by a layer of lead, H\textsubscript{2}O-Pb slab; and in the other case, the materials were reversed, Pb-H\textsubscript{2}O slab. Energy buildup factors were calculated for a variety of water and lead thicknesses and the results are plotted in Figures 19 and 20. The general shapes of the curves are very similar to those obtained by Shimizu (15) and Bowman and Trubey (4). However, since the gamma sources in these investigations were different from the one employed here, actual magnitudes of the energy buildup factors could not be compared. To check the magnitude of the two-layer energy buildup factors, use was made of the semi-empirical formula derived by Broder, Kayurin, and Kutuzov (6). The formula for two-layer slabs is

\[ B(x_1, x_2) = B_1(x_1) + B_2(x_1 + x_2) - B_2(x_1) \]  

(120)

where the indices 1 and 2 refer to the first and second materials respectively, and \( x_i \) is the thickness of the \( i \)-th lamina. Table 1 indicates the accuracy of the transmission matrix method for calculating energy buildup factors for laminated heterogeneous slabs. The buildup factors for the individual laminae employed in equation 120 were taken from this investigation.

Overall, the results obtained by the transmission method agree quite well with those obtained by other methods. It should be noted that the major source of error is probably due to the angular approximation.

According to Yarmush, Zeli, and Aronson (2), to obtain a high degree of
Figure 19. Energy buildup factor of water followed by lead for a 2 Mev isotropic plane source.
Figure 20. Energy buildup factor of lead followed by water for a 2 Mev plane isotropic source.
Table I. Energy buildup factors of lead followed by water for a 2 Mev isotropic plane source. \( T_1 \) refers to the lead thickness in mean free paths and \( T_2 \) refers to the water thickness.

<table>
<thead>
<tr>
<th>Pb-H(_2)O Slab ( T_1 ) (mfp) - ( T_2 ) (mfp)</th>
<th>Transmission Matrix Method</th>
<th>Broder, et al. Formula</th>
<th>Percent Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 1</td>
<td>2.48</td>
<td>2.37</td>
<td>+4.6</td>
</tr>
<tr>
<td>2 3</td>
<td>3.21</td>
<td>3.14</td>
<td>+2.2</td>
</tr>
<tr>
<td>2 5</td>
<td>3.92</td>
<td>3.84</td>
<td>+2.1</td>
</tr>
<tr>
<td>4 1</td>
<td>3.04</td>
<td>2.86</td>
<td>+6.3</td>
</tr>
<tr>
<td>4 5</td>
<td>6.19</td>
<td>5.90</td>
<td>+4.8</td>
</tr>
</tbody>
</table>

Accuracy at least a seven order half-range Legendre polynomial expansion for the angular variable is required. The effect of the order of the angular polynomial is even more critical as the slab increases in thickness. This would account for the increasing deviation in the energy buildup factor curves as the slab thickness increases.
SECONDARY GAMMA TRANSMISSION THEORY

In the preceding chapter an expression was derived for the transmission operator $T$ as a function of the slab thickness, the number of energy groups, and the order of the angular polynomial expansion approximation. Thus, given an infinite plane source vector, $\phi_0$, the transmitted flux vector may be obtained by the relationship

$$\phi_T = T(t)\phi_0$$  \hspace{1cm} (121)

In the calculation of the transmission of secondary gamma rays, the contribution to the total transmitted flux vector of reflected gamma rays will be ignored since it involves the product of $R$ and $T$, and the elements of the $R$ matrix are very much smaller than those of the matrix $T$. If this consideration is taken into account, it can be shown that the matrix $T$ satisfies the same relation as the transfer matrix $H$, that is,

$$T(nt) = T^n(t)$$  \hspace{1cm} (122)

where $n$ is the number of laminae of thickness $t$ which make up the slab.

In order to apply the $T$ operator to a distributed source, such as the secondary gamma source produced by thermal neutron capture, the distributed source must be approximated by a finite number of infinite plane sources. Once the magnitudes of the infinite plane source vectors are determined, as well as their effective locations in the slab, the total transmitted flux due to all of the sources will simply be the sum of the transmitted vectors of each of the individual plane sources. In other words,

$$\phi_T = \sum_i T_i \phi_{0i} = \sum_i T(t_i)\phi_{0i}$$  \hspace{1cm} (123)
where \( i \) indicates the number of infinite planes sources approximating the distributed source.

**Secondary Gamma Source**

Although only secondary gamma sources produced by thermal neutron captures will be considered, there is no reason to believe that the same approximations will not hold for other types of reactions yielding secondary gammas.

Secondary gammas produced by thermal neutron captures are generally considered to be produced isotropically. This assumption will be made in this investigation. Thus, the number of secondary gammas produced in the thickness \( \Delta t = t_2 - t_1 \) having energy \( E' \) and traveling in the direction such that the cosine of the angle with the slab normal is \( \omega' \) is

\[
\mathcal{G}_S(\omega',E') = \frac{1}{2} \int_{t_1}^{t_2} K \tilde{\varphi}(t) \sigma_{n,\gamma} f(E') \, dt
\]

(124)

where \( \tilde{\varphi}(t) \) is the thermal neutron flux distribution as a function of the distance \( t \), \( \sigma_{n,\gamma} \) is the macroscopic thermal neutron capture cross section, \( f(E') \) is the secondary gamma energy spectrum, and \( K \) is the number of secondary gammas produced per thermal neutron captured (15).

This source will be approximated by an infinite plane source of gammas located at an effective position in the slab, \( z_{eff} \), which is weighted with the secondary gamma source \( \mathcal{G}_S(\omega',E') \). Thus
A slab made up of \( n \) laminae all of thickness \( T \) is depicted in Figure 21.

For simplification, the distributed source is assumed to be approximated by only one infinite plane source, located in the first lamina. The thickness of the individual laminae should be less than or equal to one gamma scattering mean free path of the material.

In order to take advantage of the property of the \( T \) operator indicated
in equation 122, the infinite plane secondary gamma source must be adjusted so that it coincides with the face of a lamina, in this case, the interface between the first and second laminae. The source adjustment involves two factors. First, there is the simple exponential attenuation factor, \( \exp(-\bar{T} - t_{\text{eff}}) \); and secondly, there is the distortion of the angular dependence of the flux. With the assumption that there are no scattering events taking place while the gammas travel through the thickness \( \bar{T} - t_{\text{eff}} < I \) mean free path, the angular dependence will be transformed from isotropic to cosine in nature. Thus the adjusted source at the interface is

\[
\mathcal{G}_{\text{adj}}(\omega',E') = \omega' \exp(t_{\text{eff}} - \bar{T}) \mathcal{G}_S(\omega',E')
\]  

or, in terms of the half-range Legendre polynomials,

\[
\mathcal{G}_{\text{adj}}(\omega',E') = \frac{1}{2L} \bigg[ (2\omega'-1) \bigg] \exp(t_{\text{eff}} - \bar{T}) \mathcal{G}_S(\omega',E')
\]  

The transmitted vector due this source is then

\[
\mathcal{G}_T = T[(n-1)I] \mathcal{G}_{\text{adj}} = T^{n-1}(I) \mathcal{G}_{\text{adj}}
\]  

Of course, if the slab in question is not very thin, more than one infinite plane secondary gamma source will be required to approximate the distributed source. To determine the number of infinite plane sources required, an iterative process was adopted. At each iteration, the number of infinite plane sources was doubled. This process was then continued until convergence of the transmitted flux vector was obtained.

A sample run was made using the transmission matrix for lead. To simplify the problem, the following assumptions were made:
\[ K = 1 \]
\[ \psi(t) = e^{-t}; \ t \text{ in mean free paths} \]
\[ \sigma_{n,\gamma} = 1 \text{ cm}^{-2} \]
\[ f(E) = 2 \text{ Mev} \]

The shield thickness was selected to be eight mean free paths thick. In Figure 22 is indicated the transmitted energy flux through eight mean free paths of lead as a function of the number of infinite plane gamma sources which approximate the distributed secondary gamma source. As can be seen in the figure, there is convergence of the transmitted energy flux at eight infinite plane sources.
Figure 22. Transmitted energy flux due to secondary gamma sources in eight mean free paths of lead
Possibly the most important advantage of the transmission matrix method is that various intermediate results are common to problems for different shields. A large portion of the computing time goes into the calculation of the $A_1$, $B_2$, and $C_3$ matrices which are employed in the diagonalization of the matrix $W$. These are specific to the material and do not involve the slab thickness. The $H$, $T$, $U$, and $R$ matrices for a slab are characteristic only of the material and slab thickness, and in a laminated shield, these matrices are independent of other laminae in the shield. The matrices for the overall shield are obtained by simple algebraic operations on the matrices of the individual laminae.

This property of the transmission matrix method makes it particularly attractive to machine computation. Intermediate results such as the $A_1$, $B_2$, and $C_3$ matrices as well as the $H$, $T$, and $R$ matrices for laminae of a standard thickness, such as one mean free path, may be stored on magnetic tape. They need never be computed again. Thus once the $A_1$, $B_2$, and $C_3$ matrices for water have been computed, they may be used in any shield that contains water laminae. Once the $H$, $T$, and $R$ matrices for one mean free path water slabs have been computed, they may be used in any shield that contains one mean free path water laminae. No competitive method is able to use intermediate results to any comparable extent. The energy buildup factors obtained in this work for lead-water shields employed this property of the transmission matrix method. Transmission matrices for one mean free path lead and water laminae were first calculated and served as input data for the two-layer shield program. The total computer time required to
generate the data for the curves in Figures 19 and 20 was about eight seconds of 360/65 time.

Another important advantage of the transmission matrix method is the fact that the transmission matrix contains the solutions to a large variety of problems. For instance, the first column of the first block column of the transmission matrix gives the energy and angular distributions of the transmitted flux due to an isotropic source in the uppermost group. The second column corresponds to a source whose angular dependence is defined by the second half-range Legendre polynomial, \(2\omega - 1\). Similarly, the third column corresponds to a source whose angular dependence is defined by the third half-range Legendre polynomial, \(6\omega^2 - 6\omega + 1\). In general, then, the first block column of the transmission matrix determines the transmitted flux vector due to a source in the upper energy group whose angular dependence is defined in the following manner:

\[
S(\omega) = a(1) + b(2\omega - 1) + c(6\omega^2 - 6\omega + 1),
\]

where \(a\), \(b\), and \(c\) are constants selected to describe the angular dependence of the source. For instance,

\[
\begin{align*}
a &= 1, & b &= c &= 0 & \text{corresponds to an isotropic source;} \\
a &= \frac{1}{2}, & b &= \frac{1}{2}, & c &= 0 & \text{corresponds to a cosine source.}
\end{align*}
\]

Thus, one of the advantages of this method is that the transmission matrix is determined for a source whose angular dependence is a polynomial in the cosine of the angle with the slab normal; and therefore, a large variety of problems are solved simultaneously. The above arguments may be applied to other block columns as well, so that one may obtain calculations for an energy distributed source as well as an angular distributed one.
From the foregoing discussion, it is clear that the transmitted vector will be a function of both the energy of the gamma and the angle with the slab normal. The three components in each energy group of the transmitted vector are simply the coefficients of the three half-range Legendre polynomials. Thus, a transmitted vector yields not only an energy spectrum, but an angular spectrum as well. It should be noted at this point that the orthogonality property of the half-range Legendre polynomials simplifies the problem greatly. For instance, if an isotropic source is being considered, the first component in each energy group of the transmitted vector corresponds to the total flux transmitted in that group. Similarly, one-half the sum of the leading components in the first two columns of an energy block corresponds to the flux transmitted in that energy group due to a cosine source. Similar rules may be derived for higher order sources.
SUGGESTIONS FOR FURTHER STUDY

As has been indicated previously the major source of error in this investigation is the order of the half-range Legendre polynomial expansion of the angular variable. A higher order polynomial should be used for better accuracy. Of course, this would increase the size of the problem considerably. As an alternative, one might attempt to expand the angular dependence by means of other polynomials; for instance, Chebychev polynomials.

Another approximation employed in this work was the energy dependence of the flux in each energy group. The flux was assumed to be constant with energy in each group. A better choice for the energy dependence of the flux could be obtained from differential energy spectra. Although this point is not significant when dealing with narrow energy groups, the energy dependence of the flux within the groups becomes important as the group widths become larger.

Although neutron transmission calculations have not been made in this report, the theory of neutron transport has been included. The major problem here would be to obtain appropriate group cross sections for neutrons. However, transmission calculations for neutrons would be valuable, not only for neutron shielding, but also for the calculation of secondary gamma ray attenuation. With the fast neutron distribution obtained with the transmission matrix method, one could then calculate the secondary gamma sources due to inelastic scattering of fast neutrons. Coupling this secondary gamma source with that one due to thermal neutron capture, would yield a good approximation to the production and
transmission of secondary gammas in a slab. Also, since the thermal neutron distribution is dependent upon the fast neutron distribution, the transmission matrix method would serve to obtain the thermal distribution as well.

A final suggestion for investigation is the possibility of applying the transmission matrix method to more complex geometries. For instance, instead of dealing with infinite plane laminae, one might consider concentric shells.
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