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Applications of collision probabilities in reactor physics

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APPLICATIONS OF COLLISION PROBABILITIES IN REACTOR PHYSICS

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ABSTRACT

The traditional applications of collision probabilities in reactor physics are the solution of the integral form of the neutron transport equation and in the derivation of equivalence relations connecting heterogeneous and homogeneous resonance integrals.

An alternative method of solving the multigroup flux equations is presented. The method is well suited to few region, many group condensation calculations particularly if the resonance treatment requires a group by group flux solution.

A review is given of existing methods of computing collision probabilities in slab, annular and cluster geometry. Developments include anisotropic scattering representation, \( \exp(iBz) \) leakage representation and a rapid approximate cluster geometry routine.

Finally a method of computing heterogeneous resonance integrals is discussed. The method combines the Russian subgroup formulation of homogeneous resonance integrals and equivalence relations based entirely on numerical collision probabilities.
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Neutronics calculations of power reactors are customarily divided into two stages, a cell calculation and a whole reactor calculation. Finite difference diffusion codes are employed in the whole reactor calculation, which is restricted by present computer capabilities to a relatively coarse spatial mesh and a small number of neutron energy groups. The function of the cell calculation is to provide cross sections and diffusion coefficients, suitably averaged over space and energy, as input to the whole reactor calculation. The two calculations are usually assumed independent in that the gross flux shape across the reactor is ignored when the cell calculation is performed. The cell is treated as one of an infinite array, so that neutrons leaving the cell are exactly matched by those entering the cell from its neighbours. The axial dependence of the cell flux is commonly ignored, and the geometry is often simplified, if necessary, to reduce the cell calculation to a one dimensional calculation.

Methods which have been used for the cell calculation include finite difference diffusion, spherical harmonics expansions ($P_n$), discrete ordinates ($S_n$), and collision probabilities. The presence of strongly absorbing fuel elements implies a violation of the assumptions on which the diffusion approximation is based, and significant errors have arisen in attempts to apply diffusion theory in the cell situation. $P_n$ methods are often slow to converge with increasing order of $n$, and applying the boundary conditions involves computation of quantities subject to round-off when $n$ becomes large. $P_n$ methods are therefore less attractive than
S\textsubscript{n} methods where increasing the order \(n\) is simply increasing the number of angles in a quadrature scheme.

The S\textsubscript{n} method satisfies the requirements for a cell calculation. In principle the S\textsubscript{n} method can be made to yield as accurate an answer as one wishes, simply by increasing the order \(n\) and the number of spatial mesh intervals in the problem. Some difficulties may be encountered in slab geometry, but these can be overcome by the selection of an appropriate set of angles (corresponding to a double P\textsubscript{n} solution) and retaining, if necessary, the exponential form of the angular flux across each mesh interval. In cylindrical geometry the outer boundary of the cell will be square or hexagonal. This boundary is replaced by a circular one enclosing the same volume and the boundary condition is altered from mirror reflection to isotropic reflection to compensate for the deformation. Cluster geometry can be treated by a one dimensional S\textsubscript{n} calculation only if the fuel rods are smeared into the surrounding material to form homogeneous annuli. Elaborate smearing procedures which have been devised will normally give satisfactory accuracy but the smearing imposes a limit on the accuracy of the calculation. Spherical geometry, which is of little practical interest in this context, can be handled without difficulty.

The S\textsubscript{n} method, which is based on the differential form of the transport equation, computes the angular flux in each mesh interval for a set of discrete directions in addition to the scalar fluxes which would suffice to calculate reaction rates in the cell. Because of this it is possible to incorporate anisotropic scattering into the S\textsubscript{n} method without undue difficulty. However most cell calculations for thermal reactors
are currently performed using isotropic scattering and a transport corrected total cross section. In this approximation the method of collision probabilities, which is based on the integral form of the transport equation, provides an alternative means of computing the scalar fluxes in each mesh interval.

The collision probability method as normally applied rests on two main assumptions. Firstly neutrons emitted from fission or scattering are assumed to be emitted isotropically in the laboratory reference frame and secondly, that the emission density is uniform across each mesh interval. The collision probability $P_{ij}$ is defined to be the probability that a neutron born uniformly in volume and isotropically in angle in region $i$ will have its next collision in region $j$. This probability can be evaluated without knowledge of the flux level in each region, and the fluxes can be determined subsequently by solution of the multigroup neutron conservation equation.

From a computational standpoint the collision probability method lies between diffusion theory and $S_n$ methods. Each method involves the solution of a multigroup matrix equation, and for the purposes of this argument we shall suppose that the same basic outer-inner iteration scheme is common to all three. The outer iteration consists of a pass through all the energy groups with the fission source fixed while an inner iteration solves for the scalar fluxes in one group assuming the scattering sources from other groups remain fixed. The inner iteration equation may be written

$$A\phi = S \tag{1.1}$$
1.4.

where $\vec{0}$ and $S$ are vectors of length equal to the number of spatial regions in the problem.

In finite difference diffusion codes the matrix $A$ has a particularly simple form. In one dimensional geometries $A$ is tridiagonal and forward elimination, backward substitution provides an efficient method of solution. In more than one dimension the number of non-zero off-diagonal elements in a row of $A$ is usually the number of mesh regions immediately surrounding a typical mesh region. For X-Y geometry this number is 4, for hexagonal geometry 6, for X-Y-Z geometry 6. Thus the group diffusion matrix $A$ is always sparsely populated. This fact is responsible for the widespread use of diffusion theory in situations where the approximation is adequate to describe the physical processes. Only the non-zero elements of $A$ need be stored, and the solution of equation 1.1 by iteration involves few arithmetic operations per iteration. Thus very large problems can be accommodated in present day computers, and the solution times are not prohibitive.

$S_n$ methods do not solve the equation 1.1 in the normal matrix manner. $\vec{0}$ is divided into angular components along a number of fixed directions and the differential equation along each direction is solved, again usually with a finite difference representation of the differential operator. The scalar flux $\vec{0}$ is reconstituted by integrating over the angular directions along which the equation is solved. Compared with an iteration of the group diffusion process, the $S_n$ solution of equation 1.1 is computationally slow. Since angular fluxes are required in each mesh interval, storage requirements are increased if the iteration is to proceed efficiently. This storage penalty is not excessive, as it is
necessary only to store the starting values of the angular fluxes at the cell boundaries, so that on storage requirements $S_n$ methods can compete on roughly equal terms with diffusion theory. In length of calculation the $S_n$ codes are hampered by an intrinsically slow inner iteration, and often in practice by outer iteration convergence schemes less sophisticated than their diffusion code counterparts.

In collision probability calculations, the matrix $A$ of equation 1.1 is a full matrix which is simply related to the collision probability elements $P_{ij}$. The storage requirement of such a calculation thus increases as the square of the number of mesh intervals, becoming barely tolerable for two dimensional calculations and impossible for three dimensional calculations with realistic mesh subdivisions. We can therefore regard the method essentially as one dimensional and confine our comparison to that situation. The calculation is divided into two stages, one being the computation of the matrix $A$ and the other the solution of the matrix equation.

The time taken to compute the matrix $A$, or more precisely the collision probability matrix $P$, depends on the geometry of the situation and on the degree of approximation which can be tolerated, while the time for solution of the matrix equation is independent of geometry. On the IBM 360/50 the solution of a typical 20 region, 20 group flux problem takes one or two minutes, while the collision probability calculation time ranges from a few seconds for slab geometry to a few hours for numerical integration in cluster geometry. If the collision probability routine is fast and accurate, the method falls between diffusion codes and $S_n$ codes in computational speed. This situation
occurs in those geometries for which one dimensional $S_n$ is applicable. For other geometries, and clusters in particular, the length of the calculation is tolerated for the improved spatial representation which the method affords.

Another traditional application of the collision probability method has been in formulating equivalence relations which enable resonance absorption in heterogeneous cells to be computed using the formalism already well developed for homogeneous systems. Most previous equivalence relations have been based on simple approximations to the collision probabilities which arise naturally in the formulation of the slowing down equations. The method presented here differs in that the numerical collision probabilities are used in conjunction with the recently developed subgroup method for homogeneous resonance calculation.

The thesis consists of three sections. The first is devoted to the solution of the multigroup flux equations, the second to the methods of computing collision probabilities in different geometries, and the third to the formulation of heterogeneous resonance absorption calculations. Before proceeding to details of the work we present an outline of the collision probability method and its variants.

(b) The Collision Probability Method

The collision probability method is based on the integral form of the stationary neutron transport equation which has been discussed in detail by several authors, for example Davison (1957). We shall first exhibit the general form of the equation with the angular dependence explicitly retained.
\[ \phi(r, E, \Omega) = \int du \exp \left[ -\int_0^u dt \, \Sigma(r - \Omega t, E) \right] \{ S(r - \Omega u, E, \Omega) \]
\[ + \int d\Omega' \int dE' \, \Sigma(r - \Omega u ; E', \Omega' \rightarrow E, \Omega) \phi(r - \Omega u, E', \Omega') \} \]

where

\[ \phi(r, E, \Omega) \]

is the angular flux at energy \( E \) and angle \( \Omega \) at the point \( r \),

\[ \Sigma(r, E) \]

is the total cross section at energy \( E \) for the material at \( r \),

\[ \Sigma(r ; E', \Omega' \rightarrow E, \Omega) \]

is the scattering cross section from energy \( E' \) and angle \( \Omega' \) to energy \( E \), angle \( \Omega \) for the material at \( r \),

\[ S(r, E, \Omega) \]

is the angular source at \( r \) for energy \( E \) and angle \( \Omega \).

(This term may include a fission source which depends on \( \phi \)).

\[ \exp \left[ -\int_0^u dt \, \Sigma(r - \Omega t, E) \right] \] is the transmission probability at energy \( E \) for a neutron travelling from \( r - \Omega u \) to \( r \).

The scalar flux \( \phi(r, E) \) is given by the integral:

\[ \phi(r, E) = \int d\Omega \, \phi(r, E, \Omega) \] \( \ldots(1.3) \)
In most applications of the collision probability method, the source, flux, and scattering are assumed to be isotropic, leading to the following simplifications:

\[ \phi(r, E, \Omega) = \frac{1}{4\pi} \phi(r, E) \quad \ldots(1.4) \]

\[ S(r, E, \Omega) = \frac{1}{4\pi} S(r, E) \quad \ldots(1.5) \]

\[ \int d\Omega' \Sigma(r; E', \Omega' \rightarrow E, \Omega) \phi(r, E', \Omega') = \frac{1}{4\pi} \phi(r, E') \Sigma(r; E' \rightarrow E) \quad \ldots(1.6) \]

Substituting in equation 1.2 and integrating with respect to \( \Omega \) we obtain

\[ \phi(r, E) = \int d\Omega \int du \exp \left[ - \int_0^u dt \Sigma(r - \Omega t, E) \right] \left\{ \frac{S(r - \Omega u, E)}{4\pi} \right. \]

\[ + \frac{1}{4\pi} \int dE' \phi(r - \Omega u, E') \Sigma(r - \Omega u; E' \rightarrow E) \right\} \ldots(1.7) \]

A further change of integrating variable gives the familiar form

\[ \phi(r, E) = \int dr' \frac{1}{4\pi \sqrt{r - r'}^2} \exp \left[ - \int_{r'}^r dr \Sigma(r, E) \right]\]

\[ \left\{ S(r', E) + \int dE' \phi(r', E') \Sigma(r', E' \rightarrow E) \right\} \ldots(1.8) \]

An alternative statement in terms of reaction rate is obtained by multiplying throughout by \( \Sigma(r, E) \)
\[ \Sigma(r, E) \phi(r, E) = \int dr' P(r' \rightarrow r) \left\{ S(r', E) + \int dE' \phi(r', E') \Sigma(r', E' \rightarrow E) \right\} \]

...(1.9)

where

\[ P(r' \rightarrow r) = \frac{1}{4\pi |r - r'|^2} \Sigma(r, E) \exp \left[ - \int_0^1 dt \Sigma(r - (r-r')t, E) \right] \]

...(1.10)

The quantity \( P(r' \rightarrow r) \) is the probability that a neutron born at \( r' \) with energy \( E \) will have its next collision at \( r \). The reactor, or reactor cell, is divided into regions over which the material compositions and hence the cross sections are constant. For calculation purposes the regions of constant cross section are assumed capable of further subdivision into subregions \( R_i \) where the variation of \( \phi \) with \( r \) can be neglected. This assumption is central to the development of the method and is discussed in detail in later chapters. If we accept the assumption then we may write equation 1.9 in the form

\[ \Sigma(r, E) \phi(r, E) = \sum_j \int_{R_j} dr' P(r' \rightarrow r) \left\{ S(r', E) + \int dE' \phi(r', E') \Sigma(r', E' \rightarrow E) \right\} \]

...(1.11)

Integrating over region \( R_i \) we obtain

\[ V_i \Sigma(R_i, E) \phi(R_i, E) = \sum_j V_j P(R_j \rightarrow R_i) \left\{ S(R_j, E) + \right. \]

\[ + \int dE' \phi(R_j, E') \Sigma(R_j, E' \rightarrow E) \right\} \]

...(1.12)
where

\[ P(R_j \rightarrow R_i) = \frac{1}{V_j} \int_{R_i} \int_{R_j} dr \, \int_{R_j} dr' \, P(r' \rightarrow r) \] \hspace{1cm} \ldots(1.13) \]

From the definition of \( P(r' \rightarrow r) \) in equation 1.10 it follows immediately that

\[ V_j \sum_i P(R_i \rightarrow R_j) = V_j \sum_j P(R_j \rightarrow R_i) \] \hspace{1cm} \ldots(1.14) \]

An interesting departure from the conventional collision probability formulation has been developed by Carlvik (1966) from the earlier work of Kobayashi and Nishihara (1964). In annular geometry the region to region probabilities \( P(R_j \rightarrow R_i) \) are replaced by radius to radius probabilities \( P(r_j \rightarrow r_i) \). This simplifies the calculation of the off-diagonal elements of the matrix and complicates the evaluation of the diagonal elements. The radii \( r_j \) are chosen so that they are the ordinates for a Gaussian integration scheme over each annulus of different material. Thus the volume averaged flux is obtained by performing the Gaussian integration over the volume rather than summing over the subregions of the conventional collision probability approach.

This procedure has been labelled 'Discrete Integral Transport' by Carlvik who claims that it is more accurate than collision probabilities when the same computer time is invested in each. Despite the difficulties involved in the calculation of the diagonal elements in Carlvik's method there is no doubt that his formulation is superior. In this thesis, however, we have retained the normal collision probability formulation for a number of reasons. The first is that the usual collision probabilities can be used in cluster geometry while the discrete method cannot.
Secondly we were interested in some applications such as the \( \exp(iBz) \) representation of leakage where the interpretation of the diagonal elements of Carlvik's method would be difficult. Finally the approach we have adopted enables the same routines to be used both in multigroup calculations and in the determination of heterogeneous equivalence relations.

We shall first examine the use of the collision probability method in the computation of multigroup fluxes in various types of reactor cell. The multigroup approximation can be obtained by dividing the energy range into a set of groups and integrating equation 1.12 over each group \( g \).

\[
\int \Sigma(R_j,E) \phi(R_j,E) \, dE = \sum_j \int \frac{dE}{\Sigma_j} \frac{\phi_j(R_j,E) \Sigma_j(R_j,E)}{\phi_j} + \int \phi_j(R_j,E') \Sigma_j(R_j,E' \rightarrow E) \, dE' \]

...(1.16)

The group flux and group cross sections are defined as follows:

\[
\phi_g = \int \phi(R_j,E) \, dE \]

...(1.17)

\[
\Sigma_g = \int \phi(R_j,E) \Sigma(R_j,E) \, dE/\phi_g \]

...(1.18)

\[
\Sigma_{g',g} = \int \frac{dE}{\Sigma_g} \frac{\phi_j(R_j,E') \Sigma_j(R_j,E' \rightarrow E) / \phi_j}{\phi_{g',j}} \]

...(1.19)

It is tacitly assumed in setting down the above equations that the detailed shape of \( \phi(R_j,E) \) is determined. In practice we may know the approximate form of the spectrum in each region, thus enabling
the group constants to be computed with sufficient accuracy. Alternatively we may evaluate the group constants on a fine energy mesh, so that the detail in the spectrum is less important, and then perform a homogeneous or few region calculation to obtain a condensing spectrum. Unless we are prepared to go to the very fine energy mesh of a code such as SDR (Brissenden and Dunston 1965), the spectrum shape in the resonance region will never be sufficiently well determined and we rely therefore on analytic techniques in this energy region. The collision probability method is ideally suited to the few region, many group calculation often undertaken in the course of multigroup cross section preparation and we shall return to this point later. For the present we shall assume that the group constants defined by equations 1.18 and 1.19 can be determined.

Equation 1.16 can be written in the form

$$V_i \Sigma g_i \phi_i = \sum_j V_j \left[ S_{g_j} + \sum_{g',g} \sum_{g'j} \phi_j g' \right] p_{gji} \quad \ldots (1.20)$$

where $p_{gji}$ is $P(R_j \rightarrow R_i)$ of equation 1.13 evaluated with $\Sigma(R_j, E) = \Sigma_{gj}$.

If the reactor cell contains fissionable material and no external source then equation 1.20 may be written

$$V_i \Sigma g_i \phi_i = \sum_j V_j \left[ \frac{1}{\lambda} \chi_g \sum_{g',g} \phi_j g' \Sigma^F_{g'j} + \sum_{g',ggj} \phi_j g' \right] p_{gji} \quad \ldots 1.21$$

where
\[ \lambda \] is the multiplication of the reactor cell,

\[ \nu \Sigma^F_g \] is the average number of neutrons per fission times the fission cross section in group \( g \), region \( i \),

and \( \chi_g \) is the proportion of fission neutrons born in group \( g \).

Thus a typical collision probability flux calculation consists of the computation of the region to region probabilities of equation 1.13 for each energy group followed by the solution of equation 1.20 or 1.21 for the multigroup fluxes.
CHAPTER 2

SCOPE OF THE PRESENT WORK

Methods of solution of the matrix equations 1.20 and 1.21 have been developed by a number of authors. Pull (1963) proposed a method of solution based on successive over-relaxation (SOR) which was subsequently implemented in the PIP code by Clayton (1964). In Chapter 3 a block relaxation process developed by the candidate is discussed in some detail. This solution method is well suited either to the few region, many group condensing calculation or to eigenvalue problems where the energy transfers are purely downscattering. It becomes less attractive for few group, many region calculations but it is not clear that one would wish to use the collision probability method on this type of problem. It has the further advantage that solving a group at a time enables flux depression factors in the resonance region to be incorporated in the cross section calculation with minimum effort.

A large volume of literature has been published on the evaluation of collision probabilities in the various geometries. The candidate has prepared an extensive set of FORTRAN subroutines for the IBM 360 computer which are listed below under geometry.

Slab geometry:

Free slabs $P_0$ and $P_1$ scattering
Reflected slabs $P_0$ and $P_1$ scattering
Periodic slabs $P_0$ and $P_1$ scattering
Annular geometry:

Numerical integration, free outer boundary, $P_0$ and $P_1$ scattering

Numerical integration, white circular reflecting boundary, $P_0$ and $P_1$ scattering

Bonalumi method, free and white reflecting boundary, $P_0$ scattering

Numerical integration, specular circular reflecting boundary, $P_0$ scattering

Numerical integration, square reflecting boundary, $P_0$ scattering

Numerical integration, hexagonal reflecting boundary, $P_0$ scattering

Numerical integration, free and white reflecting boundary, $\exp(iBz)$ leakage representation

Spherical geometry:

Numerical integration, free and white reflecting boundary, $P_0$ and $P_1$ scattering

Cluster geometry:

Monte Carlo

PIJ type numerical integration

PIJ type numerical integration, Bonalumi in moderator

Synthetic Bonalumi approximation

These routines are discussed in Chapters 4, 5 and 6 and more fully by Doherty (1969A, 1969B, 1970, 1971A, 1971B). As numerical comparisons have been given in the reports cited we have refrained from incorporating them in the present work. The routines are intended to be used in a cell calculation code which ultimately will use large amounts of computer time and considerable effort has been invested in optimal coding of the equations. Prime considerations
in the present reactor physics environment are speed of computation and accuracy of results and the viability of a particular calculation method may well depend on a practical detail such as the choice of a quadrature scheme for an integral. The coding is therefore considered by the candidate to be an integral part of the work presented, though no further reference to it will be made.

In Chapter 4 results are presented for reflected slabs with $P_1$ scattering. Slab geometry shows the collision probability method to best advantage and also allows anisotropic scattering to be introduced with a minimum of difficulty. Reasons are given for preferring $S_n$ methods when anisotropic scattering must be included in a calculation. In view of this preference and the fact that the transport corrected isotropic scattering approximation is usually adequate for cell calculations anisotropic scattering in other geometries has not been discussed.

Chapter 5 is devoted to annular geometry and in particular to the inclusion of the $\exp(iBz)$ representation of leakage proposed by Brissenden and Green (1968). This representation involves the computation of complex angular fluxes in the $S_n$ method of solution and the possibility of computing only the real scalar fluxes by the collision probability method seemed an attractive alternative. When the two methods were finally compared on realistic problems the $S_n$ method was found to be more efficient. Various approximate methods of computing annular collision probabilities, an interpolation scheme for the $K_{13}$ function, and the outer boundary condition for cylindricalised cells are also discussed in Chapter 5.
Chapter 6 contains an outline of the Bonalumi (1961) approximate method of computing annular collision probabilities and a description of a cluster geometry routine based on this method. Routines using the smeared subcell approach were developed by Doherty (1970), Bollacasa and Bonalumi (1970) and Yamamoto and Ishida (1971). These are shown to be identical except in the definition of the smeared cross section of the subcell annulus where the Yamamoto and Ishida (1971) formulation is preferred. Subcell smearing offers sufficient accuracy for many calculations with computer times which are roughly similar to Bonalumi annular calculations. It is well suited to condensation calculations and to equivalence relations based on numerical collision probabilities.

A method of combining numerical collision probabilities and the subgroup formulation of homogeneous resonance integrals (Nikolaev et al. 1971) to obtain effective resonance integrals is presented in Chapter 7. Results are given of calculations testing various facets of the model for cells consisting of a single $^{238}\text{U}$ rod surrounded by moderator. Narrow resonance theory is used throughout Chapter 7 to simplify the presentation. In Chapter 8 the complications of performing practical resonance calculations with the model are considered. Implementation of the detailed calculation scheme proposed in Chapter 8 requires preparation of libraries and a large programming effort. This work is currently being undertaken within the A.A.E.C. theoretical reactor physics section, but will not be complete for some time. We are therefore unable to present a complete assessment of the model in practical situations but the results presented in Chapter 7 are promising.
Askew (1967) compared in detail the computational efficiencies of the discrete Sn code WDSN (Green 1967) and the collision probability code PERSEUS (Green 1964). The results indicated, rather surprisingly, that the Sn code, as well as being more accurate on a coarse spatial mesh, was actually faster than the collision probability code on the same size problem. The solution of the multigroup flux equations, which was performed using the SOR method of solution outlined by Pull (1963), occupied most of the time spent on the collision probability code. The method of this chapter was devised in the hope of reducing the computer time involved in this step. It subsequently became clear that the advantage apparently enjoyed by WDSN was limited to calculations in very few groups, while for many group problems the collision probability method was already substantially faster. We have not programmed the method of Honeck (1960) for the eigenvalue problem, but from the available evidence there is little difference between Honeck's method and SOR when fission source iterations must be performed. The method presented below is less efficient than SOR for many region, few group problems and superior for few region, many group problems. As the many group problem is solved in condensation calculations there is some justification for the use of the scheme we shall describe.

The matrix equations which must be solved can be written in the most general form by combining equations 1.20 and 1.21
Firstly we shall briefly summarise the salient features of the SOR method so that differences from our method will be obvious.

Following Pull (1963) we define a collision rate vector \( \mathbf{x} \) for a system of \( k \) regions and \( n \) groups by the equations:

\[
\begin{align*}
  x_1 &= V_1 \sum_{g'} \phi_{11} \\
  x_2 &= V_2 \sum_{g'} \phi_{12} \\
  &\vdots \\
  x_k &= V_k \sum_{g'} \phi_{1k} \\
  x_{k+1} &= V_1 \sum_{g'} \phi_{21} \\
\end{align*}
\]

...(3.2)

so that \( \mathbf{x} \) is a vector of length \( kn \) whose first \( k \) elements are the group 1 collision rates, second \( k \) elements are the group 2 collision rates, and so on.

We also define an emission rate vector \( \mathbf{y} \) with similar partitioning by the equations:

\[
\begin{align*}
  y_1 &= \sum_{g'} V_1 \sum_{g'} \phi_{11} g_{11} + z_1 \\
  y_2 &= \sum_{g'} V_2 \sum_{g'} \phi_{12} g_{12} + z_2 \\
  &\vdots \\
  y_k &= \sum_{g'} V_k \sum_{g'} \phi_{1k} g_{1k} + z_k \\
  y_{k+1} &= \sum_{g'} V_1 \sum_{g'} \phi_{21} g_{21} + z_{k+1} \\
\end{align*}
\]

...(3.3)
The fission production term $z$ has been deliberately separated within
the emission vector $y$ and will be humped together with the fixed source
term to form a total source vector $z$, again with similar partitioning,
for which we shall give only the first two equations.

$$
\begin{align*}
    z_1 &= v_1 \left[ S_{11} + \frac{1}{\lambda} \chi_1 \sum \phi_{g'1} \Sigma_{g'1}^F \right] \\
    z_2 &= v_2 \left[ S_{12} + \frac{1}{\lambda} \chi_1 \sum \phi_{g'2} \Sigma_{g'2}^F \right]
\end{align*}
$$

\ldots (3.4)

With these definitions the set of equations (3.1) can be written as
a coupled set of matrix equations

$$
\begin{align*}
    x &= Py \\
    y &= Qx + z
\end{align*}
$$

\ldots (3.5)

where $P$ is the block diagonal matrix

$$
\begin{bmatrix}
    P_1 & 0 & \cdots & 0 \\
    0 & P_2 & \cdots & 0 \\
    \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & \cdots & P_n
\end{bmatrix}
$$

and $(PQ)_{ij} = P_{i\xi}Q_{\xi j}$

\ldots (3.6)

The matrix $Q$ is square and of the form

$$
\begin{bmatrix}
    D_{11} & D_{12} & \cdots & D_{1n} \\
    D_{21} & D_{22} & \cdots & D_{2n} \\
    \vdots & \vdots & \ddots & \vdots \\
    D_{n1} & D_{n2} & \cdots & D_{nn}
\end{bmatrix}
$$
where each of the submatrices $D_{ij}$ is diagonal with elements $f_{ij}$.

$$\left(D_{ij}\right)_{ll} = \sum_{j} f_{jl} / \sum_{j} f_{jl}$$  \hspace{1cm} ...(3.7)$$

The matrix equations (3.5) can be written in the form

$$\begin{pmatrix} I -P \\ -Q I \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ z \end{pmatrix}$$  \hspace{1cm} ...(3.8)$$

and the matrix

$$\begin{pmatrix} I -P \\ -Q I \end{pmatrix}$$

possesses Property A which suggests SOR as a suitable iterative method of solution. For a definition of Property A and its implications in the use of SOR the reader is referred to Varga (1962), and to Pull (1963) and Clayton (1964) for application to this particular problem.

In problems where fissionable materials are present in the system the vector $z$ contains in the term

$$\frac{1}{\lambda} \chi_{g} \sum_{g} \phi_{g,i} \sum_{g} \Sigma_{g,i} F_{g,i}$$

both the eigenvalue $\lambda$ and a guess at the initial flux distribution. The process of solution is divided into an outer-inner scheme. During an outer iteration the $z$ vector remains unchanged while a number of inner iterations are performed to determine the $x$ and $y$ vectors. After a specified number of inner iterations a new estimate of the eigenvalue of the system is made from overall neutron balance, the latest fluxes
are used to compute a new source vector \( z \), and another outer iteration begins. If no fissionable material is present, the vector \( z \) remains unaltered and the solution process consists only of inner iterations.

Restricting our attention to the fixed source problem, we start the SOR scheme with a guess \( x^1 \) of the collision rate vector \( x \) and use the second of equations 3.5 to obtain a starting value of \( y \).

\[
y^1 = Q \cdot x^1 + z \tag{3.9}
\]

The iteration scheme of SOR can be written

\[
x^{n+1} = w \cdot P \cdot y^n + (1-w) x^n
\]

\[
y^{n+1} = w \cdot Q \cdot x^{n+1} + wz + (1-w) y^n \tag{3.10}
\]

where \( w \) is the over-relaxation parameter and \( x^{n+1} \) and \( x^n \) are the \( n+1 \)th and \( n \)th iterates respectively.

After one iteration has been completed

\[
x^2 = w \cdot P \cdot y^1 + (1-w) x^1
\]

\[
y^2 = w \cdot Q \cdot x^2 + wz + (1-w) y^1 \tag{3.11}
\]

Note that all the values of \( x^2 \) were computed from the old vectors \( x^1 \) and \( y^1 \). This means that the method is inefficient for problems where the neutron transfers from group to group are purely downscatters. The difficulty is analogous to the use of the Jacobi iteration scheme for lower triangular matrices. A simple 3 x 3 matrix will serve to illustrate the problem.
Using the Jacobi scheme this becomes

\[ x_{1}^{n+1} = b_{1} \]
\[ x_{2}^{n+1} = b_{2} - a_{21} x_{1}^{n} \]
\[ x_{3}^{n+1} = b_{3} - a_{31} x_{1}^{n} - a_{32} x_{2}^{n} \] \hspace{1cm} ...(3.13)

Starting from an initial guess \( x^{1} \) three iterations are required before the correct answers are obtained. If instead the Gauss-Seidel scheme:

\[ x_{1}^{n+1} = b_{1} \]
\[ x_{2}^{n+1} = b_{2} - a_{21} x_{1}^{n+1} \]
\[ x_{3}^{n+1} = b_{3} - a_{31} x_{1}^{n+1} - a_{32} x_{2}^{n+1} \] \hspace{1cm} ...(3.14)

had been employed, then the correct result would be obtained from one iteration. It is evident that a solution scheme similar to equations 3.14 can be designed for the purely downscattering problem, and this we now proceed to do. Consider the one-group form of equation 3.1. Dropping the group index \( g \) we obtain \( k \) equations of the form
\[ V_i \sum_i \phi_i = \sum_j V_j \left[ T_j + \sum_j^S \phi_j \right] \rho_{ji} \]  
\[ \text{where} \quad T_j = S_{gj} + \frac{1}{\lambda} \sum_g \left( \sum_{g'j}^F \phi_{g'j} \sum_{g'g}^F \phi_{g'g} \right) + \sum_g \sum_{g'g} \phi_{g'g} \phi_{g'j} \]  
\[ \text{and} \quad \sum_j^S = \sum_{gj} \]  

Writing equation 3.15 in matrix form we have

\[ A \mathbf{x} = B \mathbf{y} \]  
\[ \text{where} \quad x_i = V_i \phi_i \]  
\[ y_i = V_i T_i \]  
\[ B_{ij} = \rho_{gji} \]  
\[ A_{ij} = \sum_i \delta_{ij} - \sum_j^S B_{ij} \]  

Applying the physical restrictions \( \sum_j^S > \sum_j^F \) and \( \sum_{gj} B_{ij} \leq 1 \) it can be seen that the transpose of \( A \) is an M-matrix (Varga 1962) with a positive inverse and hence that \( A^{-1} \) exists with all elements positive.

We may therefore write

\[ C = A^{-1} B \]  

and equation 3.18 reduces to

\[ \mathbf{x} = C \mathbf{y} \]
The matrix \( C \) is the same size as the original collision probability matrix. If \( C \) is evaluated explicitly for each group, then solving equation 3.24 for each group and updating the \( y \) vector of lower groups is simply the partitioned equivalent of the Gauss-Seidel scheme 3.13. If the problem is a purely downscatter problem the flux is obtained from one iteration. If upscatter is present then inner iterations will be required, and we will need to retain the group index \( g \). The set of one group equations 3.18 can then be written

\[
A^g x^g = B^g y^g \quad \text{...(3.25)}
\]

For the non-fissionable case

\[
y^g = V^g S + \sum_{g'} D^{g'g} x^{g'} \quad \text{...(3.26)}
\]

where \( D^{g'g} \) is a diagonal submatrix with elements

\[
(D^{g'g})_{ll} = \sum_{g'} g' l \quad \text{...(3.27)}
\]

Hence the equations 3.25 and 3.26 can be written

\[
A^g x^g = B^g (V^g S^g) + \sum_{g'} B^g D^{g'g} x^{g'} \quad \text{...(3.28)}
\]

\[= b^g + \sum_{g'} E^{g'g} x^{g'} \quad \text{...(3.29)}
\]

and ultimately as

\[
F x = b \quad \text{...(3.30)}
\]

where

\[
F^{gg} = A^g \quad \text{...(3.31)}
\]

\[
F^{gg'} = -E^{gg'} \quad \text{...(3.32)}
\]
For downscattering problems $F_{g'g} = 0$, $g' > g$ and we have the block lower triangular form. In the more general problem some of the lower energy groups do have upscattering and the matrix $F$ can then be written in the reducible (Varga 1962) form:

$$
\begin{pmatrix}
F_{11} & 0 \\
F_{21} & F_{22}
\end{pmatrix}
\begin{pmatrix}
x_1 \\
x_2
\end{pmatrix}
=
\begin{pmatrix}
b_1 \\
b_2
\end{pmatrix}
\quad \ldots (3.33)
$$

where $x_2$ in this partitioning contains all the groups to which upscattering is permitted. This equation is solved in the order

$$F_{11} x_1 = b_1 \quad \ldots (3.34)$$

which requires no iteration since $F_{11}$ is lower triangular, and

$$F_{22} x_2 = b_2 - F_{21} x_1 \quad \ldots (3.35)$$

The matrix $F_{22}$ is irreducible and equation 3.35 must be solved iteratively. $F_{22}$ is no longer 2-cyclic, which is a prerequisite for Property A (Varga 1962), so we cannot find a $w$ for an SOR solution in the manner normally used. Instead we use a simple accelerated Gauss-Seidel scheme.

If fissionable material is present in the system then the problem will either be an eigenvalue problem or a subcritical source problem. The latter problem can be solved by regarding fission as another form of scattering. In the eigenvalue problem equation 3.28 becomes

$$A_g \cdot x = \sum_{g' > g} B_{g'g} D_{gg'} x_{g'} + \frac{1}{\lambda} \sum_{g' > g} B_{g'g} G_{gg'} x_{g'} \quad \ldots (3.36)$$

where $G_{gg'}$ is diagonal with
Equation 3.36 can be written

\[ F \mathbf{x} = \frac{1}{\lambda} H \mathbf{x} \]  

...(3.38)

where \( F_{gg} = A_g \) as in equation 3.31 

...(3.39)

\( F_{gg'} = -E_{gg'} \) as in equation 3.32 

...(3.40)

and \( H_{gg'} = B_g G_{gg'} \) 

...(3.41)

Writing equation 3.38 in the familiar eigenvalue form

\[ T \mathbf{x} = F^{-1} H \mathbf{x} = \lambda \mathbf{x} \]  

...(3.42)

we see that an application of the matrix \( T \) corresponds to the process of obtaining a new flux iterate from the previous outer iteration.

In downscattering problems one pass through the groups produces precisely the result

\[ x^{n+1} = T x^n / \lambda^n \]  

...(3.43)

where

\[ \lambda^n = \frac{\| T x^n \|}{\| x^n \|} \]  

...(3.44)

and \( \| x \| \) is some suitable norm of \( x \). The usual norm is based on the fission production rate at each iteration since this quantity is needed to preserve neutron balance in the course of the calculation.

When upscattering problems are being solved equation 3.43 is not solved exactly, because we employ an iterative scheme in its solution. We nevertheless assume that the relation is exactly satisfied and proceed
to describe a simple method of accelerating convergence of the outer iterations. The matrix $T$ can be shown to be non-negative and irreducible. Hence from the Perron-Frobenius results for non-negative matrices (Varga 1962), $T$ has a largest real eigenvalue with an associated real positive eigenvector - the persistent flux distribution which we seek to establish. The non-negative property follows from the fact that the elements of $H$ and $F^{-1}$ are non-negative, the latter result being established with the aid of a Newmann expansion of $F^{-1}$ in block diagonal form. The irreducibility of $T$ can be asserted on physical grounds because fission neutrons are emitted in the topmost energy groups and cause further fissions in all lower energy groups.

In practice the outer iterations converge very rapidly on the cell calculations to which the method has been applied, indicating a large dominance ratio for the iteration matrix. Elaborate devices such as Chebyshev extrapolation, which are necessary in diffusion calculations on whole reactors, are not required for this problem. We here describe a simple Aitken procedure which suffices on the very few problems which require acceleration of the outer iterations.

Let the eigenvalues of $T$ be $\lambda_1, \lambda_2, \ldots$ such that

$$\lambda_1 \geq |\lambda_2| \geq |\lambda_3|$$

with corresponding eigenvectors

$$Tx_1 = \lambda_1 x_1$$

Let $y$ be a given starting vector and decompose $y$ into the eigenvectors of $T$ (which are assumed to span the space)
\[ y = \sum a_i x_i \]  \hspace{1cm} \ldots(3.46)

\[ Ty = \sum a_i \lambda_i x_i \]  \hspace{1cm} \ldots(3.47)

\[ T^m y = \sum a_i \lambda_i^m x_i \]

\[ = \lambda_1^m \left[ a_1 x_1 + \left( \frac{\lambda_2}{\lambda_1} \right)^m a_2 x_2 + \left( \frac{\lambda_3}{\lambda_1} \right)^m a_3 x_3 + \cdots \right] \]  \hspace{1cm} \ldots(3.48)

Since \( \lambda_1 \) \( \neq \) \( \lambda_i \) for \( i \neq 1 \) the simple powering procedure will ultimately yield \( \lambda_1 \) and \( x_1 \) alone. The Aitken procedure has been outlined by Fox (1964). The underlying assumption is that the subdominant eigenvalue is real and that the presence of its associated eigenvector is the main hindrance to convergence.

\[ T^ny = a_1 \lambda_1^n x_1 + a_2 \lambda_2^n x_2 + \cdots \]  \hspace{1cm} \ldots(3.49)

\[ T^{n+1}y = a_1 \lambda_1^{n+1} x_1 + a_2 \lambda_2^{n+1} x_2 + \cdots \]  \hspace{1cm} \ldots(3.50)

The estimate of the eigenvalue obtained at this point, which we denote by \( \mu^n \) is simply

\[ \mu^n = \frac{T^{n+1}y}{T^ny} = \lambda_1 \left\{ \frac{a_1 x_1 + \left( \frac{\lambda_2}{\lambda_1} \right)^{n+1} a_2 x_2 + \cdots}{a_1 x_1 + \left( \frac{\lambda_2}{\lambda_1} \right)^n a_2 x_2 + \cdots} \right\} \]  \hspace{1cm} \ldots(3.51)

Expanding equation 3.51 we obtain
From equation 3.54, \( \lambda_1 \) and \( \lambda_2 \) can be determined. The eigenvector \( x_2 \) can be eliminated from the solution by noting that

\[
T^{n+1} y - \lambda_2 T^n y \approx (\lambda_1 - \lambda_2) \frac{\lambda_1^n}{\lambda_2} x_1
\]

We have arbitrarily elected to accelerate after ten outer iterations. Very few problems reach ten iterations and for those few convergence usually follows within one or two iterations after acceleration. The convergence of the outer iterations in collision probability calculations is evidently much simpler than the same problem in diffusion theory. The reason lies in the physical characteristics of the different systems to which the methods are applied. Diffusion calculations are usually performed on large systems with fissile material spread through the system and loosely coupled, while collision probabilities are used in the cell situation where the fissile material is tightly packed and strongly coupled. The dominant eigenvalue and its associated eigenvector are therefore more easily separated in the collision probability calculation.

The method we have used involves the computation of the matrix \( C \) in equation 3.23. If the number of space points is large the inversion
is comparatively slow and a fully iterative solution would be quicker. On the other hand, for a few space points the matrix inversion is trivial and the improvement in iteration speed more than compensates for the labour of precomputing the inverse. Typical solution times on an IBM 360/50 are 20 seconds for a 3 region, 69 group (40 upscatter) problem and 4.5 minutes for a 32 region, 16 group (10 upscatter) problem. No convergence difficulties have arisen in routine use of the method and because double precision (64 bit) arithmetic is employed in the coding, any desired accuracy is readily obtainable. The choice of a strategy which is optimal for few region calculations seems reasonable in view of the extensive use of the collision probability method for condensation calculations.
CHAPTER 4
SLAB GEOMETRY AND ANISOTROPIC SCATTERING

We shall restrict ourselves to an infinite periodic slab array with $P_1$ scattering. Free and reflected slabs, together with the extension to $P_n$ scattering are discussed by Doherty (1971B). As the storage requirements increase as $(n+1)^2$ these will be little incentive to proceed beyond $P_1$ scattering with the collision probability method. In the $S_n$ method the increase in storage is proportional to $n$ and extra calculation is required only in the evaluation of the angular source in each direction. For shielding calculations, where higher order anisotropy must be considered, the $S_n$ method is the logical choice.

The starting point of our development is the multigroup form of the integral transport equation which is derived from equation 2.1 by the method outlined in Chapter 2.

\[
\phi_g (\mathbf{r}, \Omega) = \int dy \exp \left[ -\int_0^y dt \sum_g \phi_g (\mathbf{r} - \Omega t) \right]
\]

\[
\{ S_g (\mathbf{r} - \Omega y, \Omega') + \sum_{\Omega'} \int d\Omega' \sum_g \phi_g (\mathbf{r} - \Omega y; \Omega \rightarrow \Omega') \}
\]

\[
\phi_g (\mathbf{r} - \Omega y, \Omega')
\]

...\(4.1\)

where

\[
\phi_g (\mathbf{r}, \Omega) \text{ is the group } g \text{ angular flux at } \mathbf{r} \text{ in direction } \Omega \text{ etc.}
\]

In slab geometry we define $\Theta$ to be the angle between $\Omega$ and the normal to the slab interfaces and $\Psi$ to be the polar angle. From symmetry considerations $\phi$ does not depend on the angle $\Psi$ so we may consider
\[ \phi_g(\mathbf{r}, \mu) = \int_0^{2\pi} d\psi \, \phi_g(\mathbf{r}, \Omega) \quad \ldots(4.2) \]

with \( \mu = \cos \theta \).

Thus equation 4.1 can be rewritten

\[ \phi_g(\mathbf{r}, \mu) = \int dy \, \exp \left[ - \int_0^y dt \, S_g(\mathbf{r} - \Omega t) \right] \]

\[ \left\{ \int_0^{2\pi} d\psi \, S_g(\mathbf{r} - \Omega y, \Omega) + \sum_{g'} \int_0^{2\pi} d\psi \int d\Omega' \right. \]

\[ \sum_{g', g} \phi_g(\mathbf{r} - \Omega y; \Omega' \rightarrow \Omega) \phi_g(\mathbf{r} - \Omega y, \Omega') \left\} \quad \ldots(4.3) \]

The scattering cross section \( \Sigma_{g', g}(\mathbf{r}, \Omega' \rightarrow \Omega) \) can be approximated by the Legendre polynomial expansion

\[ \Sigma_{g', g}(\mathbf{r}; \Omega' \rightarrow \Omega) = \sum_{g, \ell} \frac{2\ell+1}{4\pi} \, P_{\ell}(\Omega' \cdot \Omega) \quad \ldots(4.4) \]

Using the addition theorem for Legendre polynomials

\[ P_{\ell}(\Omega' \cdot \Omega) = P_{\ell}(\mu') P_{\ell}(\mu) + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} \, P_{m}^{(\mu')}(\mu') P_{m}^{(\mu)} \cos m(\psi' - \psi) \quad \ldots(4.5) \]

A considerable simplification of the scattering term in equation 4.3 can be effected. Thus

\[ \int_0^{2\pi} d\psi \, \sum_{\ell} \frac{2\ell+1}{4\pi} \, P_{\ell}(\Omega' \cdot \Omega) = \sum_{\ell} \frac{2\ell+1}{2} \, P_{\ell}(\mu') P_{\ell}(\mu) \quad \ldots(4.6) \]

Substitution into equation 2.3 yields

\[ \phi_g(\mathbf{r}, \mu) = \int dy \, \exp \left[ - \int_0^y dt \, S_g(\mathbf{r} - \Omega t) \right] \left\{ S_g(\mathbf{r} - \Omega y, \mu) \right. \]

\[ + \sum_{g'} \sum_{\ell} \frac{2\ell+1}{2} \, P_{\ell}(\mu') P_{\ell}(\mu) \phi_{g'}(\mathbf{r} - \Omega y, \mu') \left. \right\} \quad \ldots(4.7) \]
The flux $\phi_g(r, \mu)$ and the source $S_g(r, \mu)$ can also be expanded in a series of Legendre polynomials in $\mu$:

\[
\phi_g(r, \mu) = \sum_{\ell} \frac{2\ell+1}{2} \phi_{g,\ell}(r) P_\ell(\mu) \quad \ldots(4.8)
\]

\[
S_g(r, \mu) = \sum_{\ell} \frac{2\ell+1}{2} S_{g,\ell}(r) P_\ell(\mu) \quad \ldots(4.9)
\]

The coefficients of the expansions are, as usual, obtained from the orthogonality relations:

\[
\phi_{g,\ell}(r) = \int_{-1}^{+1} d\mu \, P_\ell(\mu) \phi_g(r, \mu) \quad \ldots(4.10)
\]

\[
S_{g,\ell}(r) = \int_{-1}^{+1} d\mu \, P_\ell(\mu) S_g(r, \mu) \quad \ldots(4.11)
\]

Inserting the expansions in equation 4.7 and integrating over $\mu$ yields the following result:

\[
\phi_{g,\ell}(r) = \sum_m \frac{2m+1}{2} \int_{-1}^{+1} d\mu \, P_\ell(\mu) \int dy \exp \left[- \int_0^y dt \frac{1}{2} (r - Q t) \right]
\]

\[
\left\{ S_{g, m}(r - Q y) + \sum_{g', gm} \phi_{g', gm}(r - Q y) \right\} P_m(\mu) \quad \ldots(4.12)
\]

The flux depends only on $x$ measured along the normal to the slab interfaces, as the slabs are assumed infinite in the directions orthogonal to $x$. Thus equation 4.12 can be rewritten

\[
\phi_{g,\ell}(x) = \sum_m \frac{2m+1}{2} \int_{-1}^{+1} d\mu \, P_\ell(\mu) \int dx' \frac{1}{|\mu|} \exp \left[- \frac{1}{2} \int_{x'}^x dt \frac{1}{2} (x' - Q t) \right]
\]

\[
\left\{ S_{g, m}(x') + \sum_{g', gm} \phi_{g', gm}(x') \right\} P_m(\mu) \quad \ldots(4.13)
\]
The use of Legendre polynomial expansions of the flux and scattering matrix is now widespread in applications of transport theory. The representation of the angular source in a particular direction by this method is surprisingly good even in situations where the expansion is not a good representation of the scattering matrix. This point is discussed in detail, in the context of $S_n$ methods, by Clancy (1970).

At this stage the conventional collision probability method and the discrete method of Kobayashi and Nishihara (1964) diverge. In the latter for each region $R_i$ with volume $V_i$ a set of discrete values $x_{ij}$ are chosen as the ordinates in a Gaussian quadrature over the region. The corresponding weights in the integration are $w_{ij}$. Defining the matrix element $T_{glijmi'j'}$, by the relation

$$T_{glijmi'j'} = \frac{2m+1}{2} \int_{-1}^{+1} d\mu \ell (\mu) P_m (\mu) \frac{w_{ij}}{\mu} \exp \left[ -\frac{1}{|\mu|} \int_{x_{i'j'}}^{x_{ij}} dt \Sigma_g (t) \right],$$

...$(4.14)$

equation 4.13 can be written

$$\phi_{g} (x_{ij}) = \sum_{m,i',j'} T_{glijmi'j'} \left\{ \sum_{g'} g' \Sigma_{g'm} (x_{i'j'}) + \sum_{g'} g' \Sigma_{g'm} (x_{i'j'}) \right\}$$

...$(4.15)$

The flux in region $R_i$ is simply interpreted as

$$\phi_{ig} = \frac{1}{V_i} \int_{R_i} \phi_{g} (x) \, dx$$

$$= \frac{1}{V_i} \sum_{ij} w_{ij} \phi_{g} (x_{ij})$$

...$(4.16)$

where $V_i$ is the volume of region $R_i$. 

In the collision probability method we assume that the flux (or more precisely the source term on the right of equation 4.13) is flat and in region \( i \) we replace \( \phi_{g\ell}(x) \) by \( \phi_{g\ell}^i \). The matrix element \( Q \) is defined by

\[
Q_{ijg\ell} = \frac{2m+1}{2V_j} \int_{-1}^{1} d\mu \, P_{\ell}(\mu) \, P_{m}(\mu) \int_{R_j} \frac{dx}{\mu} \int_{R_i} dx \exp \left[ -\frac{1}{|\mu|} \int_{x'}^{x} g(t) dt \right]
\]

\[\ldots(4.17)\]

Integrating equation 4.13 over region \( R_i \) and using the relation

\[
\int \phi_{g\ell}(x) \, dx = V_i \phi_{ig\ell}
\]

\[\ldots(4.18)\]

we obtain the alternative matrix formulation

\[
\phi_{ig\ell} = \sum_j V_j \sum_m Q_{ijg\ell m} \left[ S_{jgm} + \sum_{g'} j_{g'gm} \phi_{jg'm} \right]
\]

\[\ldots(4.19)\]

Equations 4.15 and 4.19 both involve the solution of the same type of multigroup equation as we have discussed in Chapter 3. The additional indexing used in equation 4.15 may be misleading in that it may suggest that the matrix of 4.15 is larger than that of 4.19. In practice however the number of discrete points or slab subdivisions in the two representations will be about the same. A fairly detailed discussion of the relative merits of the two methods is given by Carlvik (1967). In situations where the flux changes sharply from region to region the discrete approach is better, when the change is small the volume method is better. With the aim of performing resonance equivalence calculations in mind we have preferred the conventional volume approach.

The isotropic approximation, which is usually adequate for cell
calculations, truncates the summation over \( m \) in equation 4.19 at the first term \( m = 0 \). It is conventional when using this approximation to replace the total cross section appearing in equation 4.17 by the transport correction \( \Sigma - \bar{\mu} \Sigma_s \). This represents an attempt to correct for neutrons which are preferentially forward scattered. The origin of the correction is in one group theory but it is commonly employed in multigroup theory where the justification for its use is largely empirical. In this chapter we will consider \( P_1 \) scattering where the \( m = 1 \) term is retained in the sum.

The group index \( g \) is dropped from equation 4.17 on the understanding that the matrix will be evaluated for each group in turn.

\[
Q_{ij}^m = \frac{2^{m+1}}{2V_j} \int_{-1}^{+1} \int_{R_j}^{R_i} dx' \int_{\Sigma_j}^{\Sigma_i} \left[ \frac{1}{|\mu|} \int_{x'}^{x} \Sigma(t) \, dt \right]
\]

...(4.20)

A periodic slab system consists of slab 1 of thickness \( x_1 \) and cross section \( \Sigma_1 \), slab 2 of thickness \( x_2 \) and cross section \( \Sigma_2 \), and so on to slab \( k \) of thickness \( x_k \) and cross section \( \Sigma_k \), and then repeats with slab 1 etc.

Define

\[
T_i = \exp(- \Sigma_i x_i / \mu) \]

...(4.21)

and

\[
U = \prod_{i=1}^{k} T_i \]

...(4.22)
4.7

The elements of Q then become

\[ Q_{11lm} = \frac{2m+1}{2x_1} \int_0^1 d\mu \left[ P_l(\mu) P_m(\mu) + P_l(-\mu) P_m(-\mu) \right] \]

\[ \left\{ \frac{1}{\Sigma_1} - \frac{\mu}{\Sigma_1^2} \left[ 1 - T_1 \right] \left[ 1 - \frac{1 - T_1}{1 - U} \right] \right\} \]

\[ \cdots (4.23) \]

\[ Q_{21lm} = \frac{2m+1}{2x_1} \int_0^1 d\mu \frac{P_l(\mu) P_m(\mu)}{\Sigma_1 \Sigma_2 [1 - U]} \frac{\mu [1 - T_1] [1 - T_2]}{1 - U} \]

\[ + \frac{2m+1}{2x_1} \int_0^1 d\mu \frac{P_l(-\mu) P_m(-\mu)}{\Sigma_1 \Sigma_2 [1 - U]} \frac{\mu [1 - T_1] T_3 T_4 \cdots T_k [1 - T_2]}{1 - U} \]

\[ \cdots (4.24) \]

\[ Q_{j1lm} = \frac{2m+1}{2x_1} \int_0^1 d\mu \frac{P_l(\mu) P_m(\mu)}{\Sigma_1 \Sigma_j [1 - U]} \frac{\mu [1 - T_1] T_2 \cdots T_{j-1} [1 - T_j]}{1 - U} \]

\[ + \frac{2m+1}{2x_1} \int_0^1 d\mu \frac{P_l(-\mu) P_m(-\mu)}{\Sigma_1 \Sigma_j [1 - U]} \frac{\mu [1 - T_1] T_{j+1} \cdots T_k [1 - T_j]}{1 - U} \]

\[ \cdots (4.25) \]

\[ Q_{klm} = \frac{2m+1}{2x_1} \int_0^1 d\mu \frac{P_l(\mu) P_m(\mu)}{\Sigma_1 \Sigma_k [1 - U]} \frac{\mu [1 - T_1] T_2 \cdots T_{k-1} [1 - T_k]}{1 - U} \]

\[ + \frac{2m+1}{2x_1} \int_0^1 d\mu \frac{P_l(-\mu) P_m(-\mu)}{\Sigma_1 \Sigma_k [1 - U]} \frac{\mu [1 - T_1] [1 - T_k]}{1 - U} \]

\[ \cdots (4.26) \]
Equations for neutrons originating in slabs other than the first can be deduced by relabelling the slabs. To reduce the number of elements which must be evaluated by quadrature we can employ the following reciprocity relations:

\[(2\ell+1) Q_{ij\ell m} = (2m+1) Q_{jim\ell} \quad \ldots(4.27)\]

\[V_i Q_{jim\ell} = (-1)^{\ell+m} V_j Q_{ij\ell m} \quad \ldots(4.28)\]

Equation 4.28 with \(\ell = m = 0\) is the usual volume reciprocity relation found throughout the literature. These relations may be verified by writing down the general elements and comparing term by term.

The integration over \(\mu\) in equations 4.23 to 4.26 is performed using Gauss quadrature on the interval \([0,1]\). In slab geometry it is pleasing that the integrand is the product of a term depending on \(\ell\) and \(m\) and a term independent of \(\ell\) and \(m\). By far the largest part of the total computer time is spent in evaluating the exponential products in the term independent of \(\ell\) and \(m\). The additional transfer elements needed to incorporate \(P_1\) scattering are obtained for a nominal increase in computer time.

Unfortunately the same cannot be said of the solution process because the transfer matrix with \(P_1\) scattering is four times that of the \(P_0\) case. The block relaxation process discussed in Chapter 3 involves an inversion of the group matrix which takes 8 times longer and a series of matrix-vector multiply operations which take 4 times longer. The latter predominate so the overall increase in solution time for \(P_1\) problems on
the same mesh is a factor slightly larger than 4. This highlights the superiority of $S_n$ methods in this context because the corresponding factor in an $S_n$ calculation would be somewhat less than 2.

The evaluation of the $\ell = m = 0$ matrix elements was reported by Newmarch (1959) who performed the integration in $\mu$ by trapezoidal rule with 50 values of $\mu$. We have found that sufficient accuracy can always be obtained with 16 point Gauss quadrature with a consequent saving of a factor of 3 in computer time. In fact for many applications Gauss quadrature of lower order will suffice and the FORTRAN routines allow the order of the integration to be specified.

The important feature of the integration is that the interval is $[0,1]$ and not $[-1,1]$. Both the trapezoidal integration of Newmarch and the Gauss quadrature contain a cluster of values around $\mu = 0$ which are needed to estimate correctly the flux variation in thin slab cells. The difficulties associated with $S_n$ solutions to this type of problem were pointed out by Meneghetti (1961). The 16 point quadrature we are using corresponds closely to a $\text{DP}_{16}$ solution which will be quite adequate for the problems discussed by Meneghetti.

It is clear that the $S_n$ difficulties can easily be resolved by using the same angles and weights as are used in the evaluation of the collision probabilities. The only difficulty which then arises is that $S_n$ codes often employ an approximation of the type:

$$\exp(-\sigma \Delta / \mu) = (1 - \sigma \Delta / 2\mu)/(1 + \sigma \Delta / 2\mu)$$ \hspace{1cm} ...(4.29)

Obviously such an approximation is undesirable if angles near $\mu = 0$ are to be used. This point is more fully discussed by Doherty (1969B),
but remedial action is not difficult to apply, and in fact the problem has been completely overcome in the recent SLABBO program (Clancy 1969).

Collision probability techniques in slab geometry appear to date back to the results for the two region periodic system published by Chernick (1955). Formulae for $n$-slab lattices were given by Newmarch (1959) and Takahashi (1960). The extension to $P_1$ scattering was included by Honeck (1964) in his description of the THERMOS code.

We conclude our discussion of slab geometry with a mention of the alternative numerical evaluation of the transfer elements in terms of the exponential integral functions. Consider $Q_{jlm}$ of equation 4.25 with $\ell = m = 0$. It consists of terms of the type:

$$I = \int_0^1 d\mu \frac{\mu \exp(-A/\mu)}{1 - \exp(-B/\mu)}$$

...(4.30)

Expanding the denominator we obtain

$$I = \int_0^1 d\mu \mu \left\{ \exp(-A/\mu) + \exp(-A+B/\mu) + \exp(-(A+2B)/\mu) + \cdots \right\}$$

...(4.31)

The exponential integral function $E_n(x)$ is defined to be

$$E_n(x) = \int_1^\infty y^{-n} e^{-xy} dy$$

...(4.32)

Change of variable in equation 4.31 yields immediately

$$I = E_3(A) + E_3(A+B) + E_3(A+2B) + \cdots$$

...(4.33)

The series may be summed rapidly if $B$ is large (i.e. the cell is several mean free paths across) but for $B$ small the series is slowly convergent. In this situation an approximate method attributed by
Carlvik (1969) to Brissenden (unpublished) has been shown to lead to a closed form for the summation.

\[ E_3(x) \text{ is approximated by a sum of exponentials} \]

\[ E_3(x) = \sum_k a_k \exp(-b_k x) \quad \ldots(4.34) \]

where the parameters \( a_k \) and \( b_k \) are chosen to minimise the error over the range of \( x \) of interest. Inserting this approximation into equation 4.33 yields

\[ I = \sum_k a_k \exp(-b_k A) / \left[ 1 - \exp(b_k B) \right] \quad \ldots(4.35) \]

From this form it is obvious that the method of approximation is identical to a quadrature evaluation of the original integral of equation 4.30. If the ordinates and weights are \( \mu_k \) and \( w_k \) quadrature integration will give

\[ I = \sum_k w_k \mu_k \exp(-A/\mu_k) / \left[ 1 - \exp(-B/\mu_k) \right] \quad \ldots(4.36) \]

The type of approximation in equation 4.35 can be used in the quadrature of the original equations 4.23 to 4.27 by choosing

\[ \mu_k = 1/b_k \quad \ldots(4.37) \]

\[ w_k = a_k / \mu_k \quad \ldots(4.38) \]

Numerical refinements in the evaluation of slab collision probabilities have recently been reported by Olson (1970). Here a tabular representation of the exponential has been used instead of the standard IBM exponential subroutine. Fixing and floating operations which are associated with tabular representations are performed in
ASSEMBLER to avoid the time-consuming FORTRAN coding. A factor of two increase in speed was achieved without significant worsening of the accuracy in the code for which the routine was written.
Quadrature integration routines for the calculation of annular collision probabilities have been described by Takahashi (1960), Di Pasquantonio (1963), Pennington (1964A and B), Carlvik (1964) and Doherty (1969A). All these routines are based on the idea of integrating along neutron paths. A neutron path is characterised by $\theta$, the angle between the path and the cylinder axis, and $x$, the closest distance of approach of the path to the cylinder axis. The integration over the angular orientation $\theta$ is performed analytically to give expressions involving the Bickley function $K_i^3$.

The general transfer element $\mathcal{Q}_{ji}$ is the sum of a term from neutron paths crossing region $1$, denoted $\mathcal{Q}_{ji}^1$, plus a term from paths crossing region $2$ but not region $1$, $\mathcal{Q}_{ji}^2$, etc. Initially we will confine our attention to the term $\mathcal{Q}_{ji}^1$. Let $r_j$ be the outer radius of annulus $j$ and $\Sigma_j$ its cross section. For paths which contribute to $\mathcal{Q}_{ji}^1$, $x < r_1$. Define

$$y_1 = \sqrt{r_1^2 - x^2} \quad \cdots (5.1)$$

$$y_j = \sqrt{r_j^2 - x^2} - y_{j-1} \quad \cdots (5.2)$$

We shall not derive the equations here but merely quote sufficient of them to illustrate the subsequent text.
\[ Q_{j1} = (Q_{j1}^1) = \frac{2}{\pi r_1^2 \Sigma_1 \Sigma_j} \int_0^{\pi_1} \left[ K_{13}(x_1) - K_{13}(x_2) - K_{13}(x_3) + K_{13}(x_4) \right] \] 

\[ Q_{j2} = \frac{2}{\pi (r_2^2 - r_1^2) \Sigma_2 \Sigma_j} \int_0^{\pi_1} \left[ K_{13}(x_5) - K_{13}(x_1) - K_{13}(x_6) + K_{13}(x_7) \right. \]

\[ + K_{13}(x_2) - K_{13}(x_8) - K_{13}(x_4) + K_{13}(x_8) \right] \]

\[ \text{(5.3)} \] 

\[ \text{where} \]

\[ x_1 = \sum_{k=2}^{j-1} \Sigma_k y_k, \]

\[ x_2 = x_1 + 2 \Sigma_1 y_1, \]

\[ x_3 = x_1 + \Sigma_j y_j, \]

\[ x_4 = x_2 + \Sigma_j y_j, \]

\[ x_5 = x_1 - \Sigma_2 y_2, \]

\[ x_6 = x_3 - \Sigma_2 y_2, \]

\[ x_7 = x_2 + \Sigma_2 y_2, \]

\[ x_8 = x_4 + \Sigma_2 y_2, \]

\[ \text{(5.5)} \]

\[ \text{(5.6)} \]

\[ \text{(5.7)} \]

\[ \text{(5.8)} \]

\[ \text{(5.9)} \]

\[ \text{(5.10)} \]

\[ \text{(5.11)} \]

\[ \text{(5.12)} \]

\[ \text{and} \]

\[ K_{in}(x) = \int_0^{\pi/2} d\theta \sin^{-1}(\theta) \exp(-x/\sin\theta) \]

\[ \text{(5.13)} \]
In equations 5.3, 5.4 no contribution from neutrons returning from the outer boundary has been included. This question will be discussed later. Equations 5.3, 5.4 can be modified to include void annuli ($\Sigma_j = 0$) so that the fluxes in these regions can be calculated without difficulty. For this reason it is preferable to work with the transfer elements rather than the conventional collision probabilities which are simply $\Sigma_j Q_{ji}$.

Making use of the relation

$$\frac{d}{dx} K_{13}(x) = - K_{12}(x) , \quad \ldots (5.14)$$

equation 5.3 reduces on the case $\Sigma_j = 0$ to

$$Q_{j1} = \frac{2}{\pi r_1^2 \Sigma_1} \int_0^{r_1} dx y_j \left[ K_{12}(x_1) - K_{12}(x_2) \right] \quad \ldots (5.15)$$

It will be apparent from the formulae quoted that the central problem of the exact results in annular geometry lies in the rapid evaluation of the functions $K_{in}(x)$. As well as $K_{12}$ and $K_{13}$ which have appeared so far, the evaluation of anisotropic transfer elements require $K_{14}$ and $K_{15}$. These functions were originally tabulated by Bickley and Nayler (1935). Their widespread use in collision probabilities has led to a variety of computer approximations being developed - including those of Danielsen et al. (1963), Clayton (1964A), Gargantini and Pomentale (1964), Makino (1967) and Anderson (1970).

In these papers the range of $x$ is broken into several subranges and the function is approximated by a ratio of polynomials over each subrange. The accuracy can be refined by including more terms in the polynomials and
solving for the coefficients by the standard Chebyshev rational fitting techniques.

The candidate has made an investigation of tabular representations of the $K_{13}$ function which trade core storage for computation time. The scope for tabular representation has widened with the trend towards larger computer cores, but as most large computers are run in a multi-programme mode the economics of core-versus-time strategies must be decided on the basis of overall system use. The modest storage requirements mentioned below will usually be available in this type of calculation.

The simplest tabular representation will utilise linear interpolation between tabular points. For $K_{13}(X)$ in the range $(0,15)$ we have tried steps of $0.001$ in the interval $(0,1)$ and $0.01$ in the interval $(1,15)$ giving a total of 2401 tabular values. The error halfway between tabular points has been taken as the maximum error in the interval. While not exact, this assumption allows a convenient assessment of errors to be made. Typical errors from linear interpolation are given in Table 5.1

<table>
<thead>
<tr>
<th>X</th>
<th>Fractional Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0005</td>
<td>$2.5 \times 10^{-7}$</td>
</tr>
<tr>
<td>0.4995</td>
<td>$1.9 \times 10^{-7}$</td>
</tr>
<tr>
<td>0.9995</td>
<td>$1.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>1.005</td>
<td>$1.7 \times 10^{-5}$</td>
</tr>
<tr>
<td>4.995</td>
<td>$1.4 \times 10^{-5}$</td>
</tr>
<tr>
<td>9.995</td>
<td>$1.4 \times 10^{-5}$</td>
</tr>
</tbody>
</table>
The definition of $K_{i3}$ in equation 5.13 suggests that between tabular points $a, b$ the function could better be approximated by an exponential:

$$f(x) = e^{-\beta(x-a)} f(a)$$  \hspace{1cm} \ldots (5.16)$$

The explicit use of the exponential in an interpolation scheme would be undesirable but since the interval is small we can replace the exponential by a commonly used approximation:

$$f(x) = \frac{2 - \beta(x-a)}{2 + \beta(x-a)} f(a)$$  \hspace{1cm} \ldots (5.17)$$

The value of $\beta$ is obtained by substituting at $x = b$

$$\beta = \frac{2}{(b-a)} \frac{f(a) - f(b)}{f(a) + f(b)}$$  \hspace{1cm} \ldots (5.18)$$

Errors on the same mesh as was used in the linear interpolation are presented in Table 5.2. It is obvious that this interpolation scheme is a substantial improvement.

TABLE 5.2

Errors in exponential Type Interpolation in $K_{i3}$

<table>
<thead>
<tr>
<th>$X$</th>
<th>Fraction Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0005</td>
<td>$4.3 \times 10^{-8}$</td>
</tr>
<tr>
<td>0.4995</td>
<td>$1.2 \times 10^{-8}$</td>
</tr>
<tr>
<td>0.9995</td>
<td>$7.2 \times 10^{-9}$</td>
</tr>
<tr>
<td>1.005</td>
<td>$7.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>4.995</td>
<td>$1.4 \times 10^{-7}$</td>
</tr>
<tr>
<td>9.995</td>
<td>$6.9 \times 10^{-8}$</td>
</tr>
</tbody>
</table>
The size of the table can obviously be tailored to produce any desired accuracy. The change in error at the mesh change point \( x = 1 \) can be used as a guide in this respect. Whether the interpolation procedure is useful or not depends on the particular computer (and on the precision of its arithmetic), and on the degree of the rational approximation which would otherwise be used. If the storage can be spared, \( \beta \) can be stored along with \( f(a) \) thus removing the arithmetic in equation 5.17. For maximum efficiency the table lookup procedure should follow that described by Olson (1960) for the exponential routine, which we discussed in Chapter 4.

Honeck (1960) assumed that the neutrons born in annulus \( j \) were emitted on the ring \( r = (r_{j-1} + r_j)/2 \) instead of uniformly in the volume \( r_{j-1} < r < r_j \). A similar approximation can be derived directly from equation 5.4 by applying equation 5.14 to first order in the Taylor expansion

\[
K_{13}(x_5) - K_{13}(x_1) \approx \sum_2 y_2 K_{12} \left[ \frac{x_5 + x_1}{2} \right] 
\]

\[
K_{13}(x_6) - K_{13}(x_3) \approx \sum_2 y_2 K_{12} \left[ \frac{x_6 + x_3}{2} \right] 
\]

\[
K_{13}(x_2) - K_{13}(x_7) \approx \sum_2 y_2 K_{12} \left[ \frac{x_2 + x_7}{2} \right] 
\]

\[
K_{13}(x_4) - K_{13}(x_8) \approx \sum_2 y_2 K_{12} \left[ \frac{x_4 + x_8}{2} \right] 
\]

and
This approximation reduces by a factor of two the number of function calls which are assumed to take the same time whether the function is $K_{12}$ or $K_{13}$. The discrete methods of Kobayashi and Nishihara (1964) and Carlvik (1966) give a further reduction of a factor of two because the integration over the final volume $j$ reduces to the evaluation of the integrand at a point. The gain of the discrete method over collision probabilities is therefore more pronounced in annular geometry than in slabs where the difference is marginal.

An alternative method which still retains the direct integration along neutron paths has recently been proposed by Lewis (1969). Instead of the assumption that the flux is flat in each annulus it is assumed instead that the flux can be represented by three point interpolating polynomials based on the values at the centre and the two boundaries of each annulus. The method shares with the discrete method the advantage of being point-to-point and not volume-to-volume but has the further virtue that the end points are common to the annuli on either side, while the Gauss quadrature ordinates are all internal. Thus 3 point quadrature in the discrete method requires $3m$ points for $m$ annuli but only $2m+1$ points in the method of Lewis. For large problems this advantage will be decisive.
The direct integration methods are capable of extension to include anisotropic scattering though for a larger increase in computer time than is required in slab geometry. The formulae for the discrete method have been given by Carlvik (1966) and the corresponding results for conventional collision probabilities by Takahashi (1966). A detailed account of anisotropic calculations undertaken with conventional collision probabilities has been given by Doherty (1971B). Here we confine ourselves to a few observations:

(a) Isotropic scattering with transport corrected total cross sections is adequate for most cell calculations.

(b) Of the two alternatives the discrete method is to be preferred to the conventional volume probabilities both for speed of computation and neatness of formulation.

(c) The $S^m_n$ code is the logical vehicle for anisotropic calculations in all geometries where it can be applied. Anisotropic collision probability formulations are therefore of little practical value.

In practical problems the physical outer boundary of the cell is usually square or hexagonal. The usual approximation is to replace the rectilinear boundary by a cylindrical one enclosing the same volume - the Wigner-Seitz equivalent cell. The early collision probability formulations of Takahashi (1960) and Honeck (1960) assumed mirror reflection at the outer boundary which was consistent with the assumption made in $S^m_n$ codes at that time.

Newmarch (1960) pointed out the error which mirror reflection introduced into $S^m_n$ calculations and two different modifications were
subsequently incorporated into $S_n$ codes. In the WDSN code (Green 1967) a mixed boundary condition is permitted in which a fraction $\lambda$ of the angular flux is mirror reflected and $1 - \lambda$ is returned isotropically. The user can specify the proportion $\lambda$ in his input data but many calculations are run with $\lambda = 0$. The alternative method of Honeck (1962) allows mirror reflection to be retained for computational convenience in the code. The cell is surrounded by an annulus of purely scattering material several mean free paths across which effectively destroys the dependence of the returned angular flux on the incident values.

In collision probability theory the white boundary condition is much simpler to include than mirror reflection and it is fortunate that the results obtained from the white boundary condition are satisfactory. The transfer element from annulus $j$ to the outer boundary can be computed from the relation

$$Q_{Bj} = 1 - \sum_k \Sigma_k Q_{kj}$$

Assuming that the reflected neutrons are emitted on the boundary with angular distribution $\sin \theta \cos \psi$ ($\psi$ being the angle between the inward radius and the projection of the neutron path on the horizontal plane) it is not difficult to establish the reciprocity relation

$$Q_{jB} = \frac{2}{\pi R} V_j Q_{Bj}$$

where $R$ is the radius of the outer boundary and $V_j$ is the volume of annulus $j$. The boundary to boundary transfer element $Q_{BB}$ is computed from

$$Q_{BB} = 1 - \sum_k \Sigma_k Q_{kB}$$
The transfer elements with the reflected boundary, labelled T, are given in terms of the free boundary elements Q by the relation

$$T_{ij} = Q_{ij} + Q_{Bj} Q_{iB} / (1 - Q_{BB})$$

...(5.27)

The white boundary condition can be checked against exact calculations in which the physical outer boundary is explicitly retained. Such calculations have been performed for the two region square cell by Fukai (1963) and Sauer (1964) and for the general n region cell with both square and hexagonal boundaries by the candidate (Doherty 1969B). All the available evidence indicates that this approximation gives adequate accuracy for practical computation.

In addition to the direct integration techniques, a number of rapid approximate methods have been developed for annular geometry. The most widely used of these is the method of Bonalumi (1961) with improvements by Jonsson (1963). Applications of the Bonalumi method to multigroup cluster calculations, and to the determination of resonance equivalence relations, are discussed in Chapters 6 and 7, and more details may be obtained from the original papers. Comparisons of the Bonalumi method and direct integration are given by Doherty (1969B). Some improvements in the rational polynomial approximations required in the method are quoted by Green (1964).

An extension to anisotropic scattering has been made by Hyslop (1963). The transfer term which can be computed using this extension is $Q_{jB01}$ i.e. the contribution to the $P_o$ flux in annulus $j$ from the $P_1$ component of the flux incident on boundary $B$. Actual flux computations depend on a supplementary evaluation of the flux incident on boundary $B$ (which is the
inner moderator boundary in Hyslop's calculations) by blackness or boundary extrapolation methods.

Finally, in connection with annular geometry we will discuss briefly an extension of collision probabilities to include the exp(iBz) representation of axial leakage proposed by Brissenden and Green (1968). A fuller account of calculations performed by the candidate using this method is given in Doherty (1971A). The differential transport equation in annular geometry for the angular flux \( \phi(r, z, \Omega) \) along a direction \( \Omega \) can be written

\[
\eta \mu \frac{\partial \phi}{\partial r} - \frac{\eta \sqrt{1 - \mu^2}}{r} \frac{\partial \phi}{\partial \psi} + \gamma \frac{\partial \phi}{\partial z} + \Sigma \phi = S(r, z, \Omega) \tag{5.28}
\]

with \( \psi = \) angle in the horizontal plane between the projection of \( \Omega \) and the outward radius,

\( \Theta = \) angle between \( \Omega \) and the vertical cylinder axis,
\( \mu = \cos \psi, \)
\( \gamma = \cos \Theta, \)
\( \eta = \sin \Theta, \)
\( \Sigma = \) total (or transport corrected total) cross section, and
\( S = \) scattering (and possibly fission) source into direction \( \Omega. \)

Writing

\[
T_r = \eta \mu \frac{\partial \phi}{\partial r} - \frac{\eta \sqrt{1 - \mu^2}}{r} \frac{\partial \phi}{\partial \psi}
\]

equation 5.28 can be condensed to

\[
T_r \phi + \gamma \frac{\partial \phi}{\partial z} + \Sigma \phi = S \tag{5.30}
\]
A complex periodic solution of equation 5.29 is assumed to have the form

$$W(r, z, \Theta) = \exp(iBz) \left[ W_1(r, \Theta) + i W_2(r, \Theta) \right]$$  \hspace{1cm} \ldots \hspace{0.5cm} (5.31)$$

which enables equation 5.30 to be written

$$T_r(W_1 + i W_2) + (\Sigma + iBY)(W_1 + i W_2) = S$$  \hspace{1cm} \ldots \hspace{0.5cm} (5.32)$$

and in this form the $z$ dependence is eliminated and the original two dimensional equation is reduced to the one dimensional form which applies to axially infinite systems. From consideration of the properties of $W$, Brissenden and Green (1968) have identified $\phi$ with the real part of $W$.

$$\phi(r, z, \Theta) = \cos Bz W_1(r, \Theta) - \sin Bz W_2(r, \Theta)$$  \hspace{1cm} \ldots \hspace{0.5cm} (5.33)$$

The scalar flux $\phi$ is given by

$$\phi(r, z) = \int \phi(r, z, \Theta) \, d\Theta$$

$$= \cos Bz \int W_1(r, \Theta) \, d\Theta - \sin Bz \int W_2(r, \Theta) \, d\Theta.$$  \hspace{1cm} \ldots \hspace{0.5cm} (5.34)$$

If the finite cylinder is symmetrically located about the plane $z = 0$ the scalar flux must be symmetric in $z$. This implies

$$\int W_2(r, \Theta) \, d\Theta = 0$$  \hspace{1cm} \ldots \hspace{0.5cm} (5.35)$$

In the collision probability method, where only scalar fluxes are computed, it will be sufficient to evaluate the real part $W_1(r, \Theta)$, since the latter is the only term remaining in equation 5.34. The collision probability solution in the axially infinite case is equivalent to solving
the differential transport equation

\[ T_r \phi + \Sigma \phi = S \]  \hspace{1cm} \ldots (5.36)

Comparison with equation 5.32 shows us that the only modification needed is to replace \( \Sigma \) by \( \Sigma + iBY \). It is unfortunate that this small change results in a dramatic difference in the quality of the integrals which must be evaluated.

Equation 5.3 for the axially infinite problem can be written, with the integral over \( \theta \) undone, as

\[
Q_{j1} = \frac{1}{\pi r_1^2} \int_0^{r_1} dx \int_0^{\pi} d\theta \frac{\sin^2 \theta}{\Sigma_1 \Sigma_j} \left[ 1 - \exp(-2 \Sigma_1 y_1 / \sin \theta) \right] \exp(-\Sigma_2 y_2 / \sin \theta)
\]

\[
\exp(-\Sigma_{j-1} y_{j-1} / \sin \theta) \left[ 1 - \exp(-\Sigma_j y_j / \sin \theta) \right] \ldots (5.37)
\]

Replacing each \( \Sigma_k \) by \( \Sigma_k + iB \cos \theta \) gives

\[
Q_{j1} = \frac{1}{\pi r_1^2} \int_0^{r_1} dx \int_0^{\pi} d\theta \frac{\sin^2 \theta}{(\Sigma_1 + iB \cos \theta)(\Sigma_j + iB \cos \theta)}
\]

\[
\left[ 1 - \exp(-2 \Sigma_1 y_1 / \sin \theta) \exp(-2iB y_1 \cot \theta) \right] \exp(-\Sigma_2 y_2 / \sin \theta)
\]

\[
\exp(-iB y_2 \cot \theta) \ldots \exp(-\Sigma_{j-1} y_{j-1} / \sin \theta) \exp(-iB y_{j-1} \cot \theta)
\]

\[
\left[ 1 - \exp(-\Sigma_j y_j / \sin \theta) \exp(-iB y_j \cot \theta) \right]
\]

\[
= \frac{2}{\pi r_1^2} \int_0^{r_1} dx \left[ I(X_1, Y_1, B, \Sigma_1, \Sigma_j) - I(X_2, Y_2, B, \Sigma_1, \Sigma_j) \right.
\]

\[
- I(X_3, Y_3, B, \Sigma_1, \Sigma_j) + I(X_4, Y_4, B, \Sigma_1, \Sigma_j) \right] \ldots (5.38)
\]
where the \( X_i \) are as defined in equations 5.5 to 5.8,

\[
Y_1 = \sum_{k=2}^{j-1} y_k
\]

\[
Y_2 = Y_1 + 2y_1
\]

\[
Y_3 = Y_1 + y_j
\]

\[
Y_4 = Y_2 + y_j
\]

and

\[
I(X,Y,B,\Sigma_1,\Sigma_2) = \frac{1}{2} \int_{0}^{\pi} \sin^2 \theta \exp\left(-\frac{X}{\sin \theta}\right) \exp\left(-iBY \cot \theta\right) \frac{\exp\left(-iB \cos \theta\right)}{\Sigma_1 + iB \cos \theta} \frac{\exp\left(-iB \cos \theta\right)}{\Sigma_2 + iB \cos \theta} d\theta
\]

\[
(5.43)
\]

The extension to terms other than \( Q_{j1} \) is simply to replace \( K_{13} \) by the integral \( I \) with its appropriate arguments. Apart from the complication of evaluating \( I \), this part of the procedure is straightforward. However the boundary conditions which are used to reflect neutrons from the boundary are quite complicated and involve the computation of a number of terms not required in the axially infinite problem. A full discussion of this aspect is given by Doherty (1971A) and here we merely quote the relevant results.

For each region \( i \) from which neutrons start we compute the transfers to the boundary \( Q_{Bi} \). For the central region \( Q_{B1} \) is given by

\[
Q_{B1} = \frac{2}{\pi r_1^2} \int_{0}^{\pi} dx \left[ J(X_1,Y_1,B,\Sigma_1) - J(X_2,Y_2,B,\Sigma_1) \right]
\]

\[
(5.44)
\]
where

\[ X_1 = \sum_{k=2}^{N} \Sigma_k y_k \]  \hspace{1cm} \ldots(5.45) \\
\[ X_2 = X_1 + 2 \Sigma_1 y_1 \]  \hspace{1cm} \ldots(5.46) \\
\[ Y_1 = \sum_{k=2}^{N} y_k \]  \hspace{1cm} \ldots(5.47) \\
\[ Y_2 = Y_1 + 2 y_1 \]  \hspace{1cm} \ldots(5.48) \\

\[ J(X,Y,B,\Sigma) = \int_{0}^{\pi/2} d\theta \frac{\sin^2 \theta \exp(-X/\sin \theta) \exp(-iBY \cot \theta)}{\Sigma_1 + iB \cos \theta} \]  \hspace{1cm} \ldots(5.49) \\

and \( N \) is the number of annuli in the cell.

For neutrons arriving at the cell from region \( i \), we assume that the starting distribution after reflection is

\[ \frac{\Sigma_i \sin \theta \cos \psi}{\Sigma_i + iB \cos \theta} \]  instead of \( \sin \theta \cos \psi \)

as in the axially infinite problem.

Using this starting distribution we compute transfer elements \( Q_{jB}^i \) and \( Q_{BB}^i \), the superscript \( i \) identifying the starting distribution. The transfer elements \( T \) for the reflected cell are then given by

\[ T_{ji} = Q_{ji} + \frac{Q_{Bi} Q_{jB}^i}{1 - Q_{BB}^i} \]  \hspace{1cm} \ldots(5.50) \\

The justification for this procedure is that it correctly predicts the leakage from an infinite slab considered as a one region reflected cell. Experiments with simpler boundary conditions gave unsatisfactory numerical results. The extra work involved in these boundary conditions
is in computing a full set of \( Q_j^{1} \) instead of the one \( Q_j^B \) for each annulus that is required for the axially infinite problem.

The main difficulty in this method of calculation lies in the evaluation of the integrals \( I \) and \( J \). From comparison with numerical quadrature results we have established that an expansion to order \( B^4 \) is adequate for the range of \( B^2 \) normally encountered. The expression for \( J \) is

\[
J(X,Y,B,\Sigma) = \frac{1}{\Sigma} K_{13}(X) + \frac{B^2}{\Sigma} \left\{ K_{13}(X) \left[ \frac{3y}{8x} - \frac{3y}{x^2} - \frac{1}{\Sigma^2} \right] - K_{14}(X) \frac{y^2}{2x} + \right. \\
+ \left. K_{15}(X) \left[ \frac{1}{\Sigma^2} - \frac{4y}{8x} + \frac{4y^2}{x^2} \right] \right\} \\
+ \frac{B^4}{\Sigma} \left\{ K_{13}(X) \left[ -\frac{3y^4}{8x^2} + y^3 \left( \frac{2}{3\Sigma x} - \frac{1}{\Sigma^3} \right) + y^2 \left( \frac{3}{\Sigma^2 x^2} - \frac{1}{2\Sigma^2} \right) \right] \\
+ y \left( \frac{x}{5\Sigma^3} - \frac{3}{x\Sigma^3} \right) + \left( \frac{1}{\Sigma^4} - \frac{x^2}{30\Sigma^4} \right) \\
+ K_{14}(X) \left[ -\frac{y^3}{6\Sigma x^2} + \frac{y^2}{2\Sigma^2 x} - \frac{y}{5\Sigma^3} + \frac{x}{30\Sigma^4} \right] \\
+ K_{15}(X) \left[ \frac{y^4}{2x^2} + y^3 \left( \frac{4}{3\Sigma x^3} - \frac{2}{3\Sigma x} \right) + y^2 \left( \frac{1}{2\Sigma^2 x^2} - \frac{4}{\Sigma^2 x} \right) \right] + \\
+ y \left( \frac{4}{\Sigma^3 x^3} - \frac{x}{5\Sigma^3} \right) + \left( \frac{x^2}{30\Sigma^4} - \frac{7}{6\Sigma^4} \right) \} \\
\ldots (5.51)
\]
A similar expansion for $I$ can be obtained from the relation

$$I(X, Y, B, \Sigma_1, \Sigma_2) = \frac{1}{\Sigma_1 - \Sigma_2} \left[ J(X, Y, B, \Sigma_2) - J(X, Y, B, \Sigma_1) \right] \ldots (5.52)$$

These expressions involve only the Bickley functions which we have already discussed but instead of requiring only $K_{13}$ at each point we now require $K_{13}, K_{14}$ and $K_{15}$ and in addition there is considerable time required in the evaluation of the coefficients. Comparison with $S_n$ calculations show that the latter are more efficient than the collision probability solution discussed here.
Routines for the evaluation of collision probabilities in cluster geometry by direct integration along neutron paths have been described by Carlvik (1964), Beardwood et al. (1965), Amyot and Benoist (1963) and Doherty (1970). As in annular geometry the square outer boundary of the physical cell is replaced by a white reflecting circular one enclosing the same volume. Integrating lines are placed across the cluster at distances $x$ from the cluster centre. The integration over neutron paths which have their projection along each line gives rise to $K_{13}$ functions as in annular geometry.

Because the cluster is not invariant under arbitrary rotations a further integration must be performed over $\alpha$, the orientation of the integrating lines with respect to a fixed reference line in the cross section plane. Thus if ten values of $\alpha$ are considered, the time spent in evaluating the collision probabilities will be ten times that of an annular system containing the same number of regions. Cells of pressure tube reactors are physically quite large and a number of subdivisions (of the moderator in particular) must be made in order to reduce the error inherent in the flat source approximation. Thus cluster collision probability calculations using exact integration techniques are expensive to perform.

Possible alternatives are two dimensional $S_n$, smearing of fuel and coolant followed by one dimensional $S_n$ or collision probability, or the approximate methods we shall discuss below. Two dimensional $S_n$ solutions have so far been avoided and it is not clear that there could be any
saving in time over the exact collision probability solution. Smearing techniques are widely used, for example in the WIMS code described by Askew et al. (1966), but the smearing involves an approximation which restricts the accuracy to which the calculation can be performed. For multigroup calculations the accuracy of the smearing model is usually adequate but the model is unsuitable either for detailed check calculations or for the determination of resonance equivalence relations. For a detailed check calculation, which will not be performed too frequently, the computer time for an exact calculation can be spared. On the other hand for resonance equivalence relations we require a rapid solution technique and the method discussed below satisfies this requirement and at the same time avoids the difficulties of the conventional smearing approach.

Rapid approximate methods for clusters have been developed by Leslie and Jonsson (1964 and 1965), Bonalumi (1969), Doherty (1970), Bollacasa and Bonalumi (1970) and Yamamoto and Ishida (1971). We shall confine our attention to the last three, all of which make use of the method of Bonalumi (1961) for annular geometry. It is therefore appropriate to present the essential details of the latter approximation at this point.

The results for geometries so far discussed have been formulated in terms of $Q_{ij}$, the transfer element from region $j$ to region $i$ to preserve the suffix notation of matrix multiplication and to enable an easy description of void regions. In order to preserve the notation of Bonalumi from now on the conventional collision probabilities $P_{ij}$ will be used. $P_{ij}$ is the probability that a neutron born in region $i$ will collide in region $j$. In terms of our previous notation
The Bonalumi (1961) method for annular geometry consists of a series of steps. Firstly $P_{11}$ is the function $P_c(\sum r_1)$ tabulated by Case et al. (1953) for which rational polynomial approximations are available (Green 1964). A set of ring transmission probabilities $1 - G_{1j}$ are defined as follows:

$$1 - G_{1j} = \text{probability that a neutron born uniformly and isotropically in region 1, and arriving at the inner boundary of annulus j will be transmitted across it.}$$

Once the $G_{1j}$ have been calculated the probabilities $P_{1j}$ are simply

$$P_{12} = (1 - P_{11}) G_{12} \quad \cdots(6.3)$$

$$P_{13} = (1 - P_{11}) (1 - G_{12}) G_{13} \quad \cdots(6.4)$$

$$\vdots$$

$$P_{1j} = (1 - P_{11}) (1 - G_{12}) \cdots (1 - G_{1,j-1}) G_{1j} \quad \cdots(6.5)$$

The probabilities $P_{j1}$ can then be calculated from the reciprocity relation

$$V_1 \sum P_{ij} = V_j \sum P_{ji} \quad \cdots(6.6)$$

The transmission probabilities $1 - G_{1k}$ are calculated from the formulae

$$G_{1k} = 1 - \exp(-y_{1k}) \quad \cdots(6.7)$$

where
\[ y_{1k} = \sum_k r_k \frac{\pi \tau}{4} \left[ T \left( \frac{r_1}{r_k} \right) - \alpha_k T \left( \frac{r_1}{r_{k-1}} \right) \right] \] \hspace{1cm} \text{(6.8)}

with

\[ T(u) = \frac{2}{\pi} \left[ \frac{\sin^{-1} u}{u} + \sqrt{1 - u^2} \right] \] \hspace{1cm} \text{(6.9)}

\[ \alpha_k = \frac{r_{k-1}}{r_k} \] \hspace{1cm} \text{(6.10)}

\[ \tau = \frac{K_{i2}(x)}{K_{i3}(x)} \] \hspace{1cm} \text{(6.11)}

and

\[ x = \sum_2 (r_2 - r_1) + \sum_3 (r_3 - r_2) - \sum_{k-1} (r_{k-1} - r_{k-2}) + \frac{1}{2} \sum_k (r_k - r_{k-1}) \] \hspace{1cm} \text{(6.12)}

For the derivation of this result the reader is referred to Bonalumi (1961). The calculation of \( P_{ij} \) for \( i > 1 \) is complicated by the regions internal to \( i \) which are crossed by some of the neutron paths. Consider \( i = 2 \)

\[ P_{22} = \frac{P_{22}'}{2} + \left\{ P_{21}^\star - P_{21} \right\} G_{12} \] \hspace{1cm} \text{(6.13)}

where

\[ P_{22}' = \text{probability of collision in 2 without crossing region 1} \]

\[ P_{21}^\star = \text{probability that a neutron born in 2 will enter region 1} \]

\[ (P_{21}^\star - P_{21}) = \text{probability that such a neutron will re-emerge from region 1} \]

It is assumed in this equation that the angular distribution of neutrons re-emerging from region 1 is the same as if the neutrons were
born in region 1 (this allows the use of $G_{12}$).

$P_{21}^*$ is obtained from the limit of $P_{21}$ as $\Sigma_1 \to \infty$, where $P_{21}$ is calculated by reciprocity from $P_{12}$

$$P_{21} = \frac{\pi r_1}{2 \Sigma_2} \frac{1}{V_2} G_{12} \quad \ldots (6.14)$$

An expression for $P_{22}'$ has been given by Jonsson (1963)

$$P_{22}' = f_2 - P_{21}^* G_{12} \quad \ldots (6.15)$$

where

$$f_2 = P_c (R_2 \Sigma_2) \quad \ldots (6.16)$$

and $R_2$ is calculated from a prescription (based on unpublished work) of Schaefer.

To calculate $P_{2j}$ the probability is again divided into two parts depending on whether internal regions are crossed. $P_{21}^*$ enter region 1 and $P_{21}^* - P_{21}$ re-emerge. If we are calculating $P_{ij}$ then $P_{i,i-1}^* - \sum_{k=1}^{i-1} P_{ik}$ re-emerge. All the quantities $P_{ik}$ can be evaluated by reciprocity since $P_{ki}$ will already have been calculated. Hence the contribution to $P_{ij}$ of those making internal crossings is

$$\left[ P_{i,i-1}^* - \sum_{k=1}^{i-1} P_{ik} \right] \left[ 1 - G_{i-1,i} \right] \left[ 1 - G_{i-1,i+1} \right] \ldots \left[ 1 - G_{i-1,j-1} \right] G_{i-1,j}$$

The other contribution to $P_{ij}$ comes from neutrons leaving region $i$ without crossing internal regions. There are $(1 - P_{i,i-1}^* - P_{ii})$ of these per unit source in region $i$. 

Jonsson (1963) distinguishes a new set of ring transmission probabilities \( H_{ij} \) relating to neutrons born in the ring \( i \) rather than the solid rod with radius \( r_i \). Using these functions the second contribution to \( P_{ij} \) is

\[
(1 - P_{i,i-1}^* - P_{ii}) \cdot (1 - H_{i,i+1}) \cdot (1 - H_{i,i+2}) \ldots \cdot (1 - H_{i,j-1}) \cdot H_{ij}
\]

Since regions internal to \( i \) do not enter into the definition of the \( H \) functions, we may set \( \Sigma_k = 0 \) for \( k < i \) in order to establish an expression for \( H \) in terms of the Bonalumi \( G \) functions. This expression is given by Jonsson (1963) and the details will not concern us here.

As has already been mentioned, pressure tube cells usually contain a large moderator volume which must be subdivided in the collision probability calculation to avoid large errors from the flat source assumption. The moderator regions are annuli which can very well be treated by the Bonalumi approximation, whether the part of the cell containing the fuel pins is treated by direct integration or not.

Suppose that an annular boundary \( r_i \) is chosen so that all the rods are contained inside \( r_i \). The collision probabilities for regions internal to \( r_i \) must be computed by some means, for example by direct integration. At the end of this step we will have

\[
P_{jk} \quad \text{for } j, k \leq i
\]

and

\[
P_{j r_i} = 1 - \sum_{k \leq i} P_{jk} \quad \ldots (6.17)
\]

(the indices \( j \) and \( k \) are assumed to include all the fuel rods and their subdivisions, as well as the annuli internal to \( i \)).
P_{j,r_i} is the probability that a neutron born in j will arrive at the boundary r_i uncollided. From the definition of G_{j,i+1} in the Bonalumi approximation we can infer

\[ P_{j,i+1} = P_{j,r_i} G_{j,i+1} \quad \cdots (6.18) \]

\[ P_{j,i+2} = P_{j,r_i} (1 - G_{j,i+1}) G_{j,i+2} \quad \text{etc.} \quad \cdots (6.19) \]

If the internal probabilities \( P_{jk} \) have been computed by direct integration the Bonalumi transmission probabilities \( G_{jm} (m > i) \) will not be known. However these probabilities are relatively insensitive to details of the starting annulus j, as has been shown by the work of Hyslop (1963). The procedure used by Doherty (1970) is to smear the fuel rods into their surrounding coolant annuli using straight volume weighted cross sections for the smeared annuli. Then a complete Bonalumi calculation is performed for the whole cell and in the process the required values of \( G_{jm} \) for the smeared annuli are obtained. These \( G_{jm} \) are then used for both the coolant and moderator making up the smeared annulus.

This procedure results in a saving of about a factor of two when compared with full numerical integration across the moderator. The reaction rate distribution across the fuel pins is unaltered since these are essentially normalised through \( P_{j,r_i} \). Differences are observed in the ratio of moderator to fuel fluxes reported by Doherty (1970). A difference of up to 3 per cent in outer moderator flux was obtained for a 36 rod \( D_2O \) cooled Natural Uranium cluster on a 20 cm pitch. This difference is due more to the error in the Bonalumi approximation itself.
than to the smearing as can be seen from annular geometry results given by Doherty (1969).

The coupling of the Bonalumi approximation in the moderator with direct integration in the fuel was included in the PIJ code originally described by Beardwood et al. (1965). It represents an advance in sophistication over the earlier coupling of internal collision probabilities and diffusion theory in the moderator which have been used in the spectro work of Leslie (1963) and the G.F.G. approach of Schaefer and Allsopp (1965). The time spent in evaluation of moderator collision probabilities and fluxes is an insignificant portion of the total time in a calculation of this type.

The synthetic methods of Doherty (1970), Bollasca and Bonalumi (1970) and Yamamoto and Ishida (1971) are all very similar but differ in the important respect that each employs a different definition of the homogeneous cross section of a smeared annulus. The essence of the approach is to smear the fuel pins into the coolant annuli which enclose them and then perform an annular geometry calculation of the cell using the method of Bonalumi (1961) in the manner we have just outlined.

For each smeared annulus we construct a fictitious equivalent cylindrical subcell consisting of a central fuel pin, can, and a volume of coolant which is the total volume of coolant in the annulus divided by the number of fuel pins. An annular collision probability calculation is performed on the subcell again using the Bonalumi approximation. The individual probabilities for the fuel, can, and coolant in the smeared annulus are then apportioned in the following way.
Let $i$ be a simple annulus of the cell.

Let $j$ be a smeared annulus of the cell with fuel, can and coolant indexed by $m, n$.

Let $P^1_{ij}$ be the collision probabilities from the cell calculation, and $P^2_{mn}$ the collision probabilities from the subcell calculation.

Let $P^2_{mB}$ be the probability that a neutron born in region $m$ of the subcell will reach the boundary $B$ of the subcell.

\[
P^2_{mB} = 1 - \sum_n P^2_{mn} \quad \ldots(6.18)
\]

The probability $P^2_{Bm}$ is obtained from the reciprocity relation

\[
P^2_{Bm} = \frac{2}{\pi R} V_m \sum_m P^2_{mB} \quad \ldots(6.19)
\]

where $R$ is the outer radius of the subcell. Finally the probability $P^2_{BB}$ is obtained from

\[
P^2_{BB} = 1 - \sum_m P^2_{Bm} \quad \ldots(6.20)
\]

The individual probability $P_{im}$ is then defined to be

\[
P_{im} = P^1_{ij} P^2_{Bm} / (1 - P^2_{BB}) \quad \ldots(6.21)
\]

The physical assumption underlying equation 6.21 is simply that neutrons collide within the smeared annulus $j$ in the same proportion as they would if isotropically incident on the boundary $B$ of the subcell. The assignment of probabilities for neutrons leaving the smeared annulus $j$ can be established by reciprocity.
\[
P_{mi} = \frac{V_i \sum_i P_{im}}{V_m \sum_m}
\]
\[
= \frac{V_i \sum_i P_{ij}^l P_{BB}^m}{V_m \sum_m (1-P_{BB}^2)}
\]
\[
= \frac{V_j \sum_j P_{ji}^l P_{BB}^m}{V_m \sum_m (1-P_{BB}^2)}
\]

...(6.22)

From this point it is not too difficult to arrive at a self consistent value of \( \Sigma_j \) for the smeared annulus. From equation 6.22 it follows immediately that

\[
\sum_m V_m \sum_m P_{mi} = V_j \sum_j P_{ji}^l
\]

...(6.23)

Since equation 6.23 must be true for any annulus \( i \) distinct from \( j \) we deduce that

\[
\sum_m V_m \sum_m \left[ 1 - \sum_n P_{mn}^o \right] = V_j \sum_j (1 - P_{jj}^o)
\]

...(6.24)

where \( P_{mn}^o \) and \( P_{jj}^o \) are evaluated for neutron paths which do not cross regions internal to annulus \( j \). Equation 6.24 is the central equation in the treatment of Yamamoto and Ishida (1971). To evaluate \( \Sigma_j \) from this equation it is necessary to assume that \( P_{mn}^o \) can be written in the form

\[
P_{mn}^o = P_{mn}^2 + \frac{\gamma P_{mB}^2 P_{Bn}}{1-\gamma P_{BB}^2}
\]

...(6.25)
\( p_{mn}^2 \), as already defined, is the direct probability evaluated for the equivalent cylinder. \( \gamma \) is the fraction of neutrons reflected at the boundary by virtue of the fact that the annulus is viewed as a ring of neighbouring equivalent cylinders. Reflected neutrons are assumed to behave as though isotropically incident on the outer boundary of the equivalent cylinder. If \( N \) is the number of equivalent cylinders around the annulus, then combining equations 6.24 and 6.25 gives

\[
\begin{align*}
V \sum_j (1 - p_{jj}^0) &= \sum_m \Sigma_m \left[ 1 - \sum_n p_{mn}^2 - \sum_n \frac{\gamma p_{mn}^2 p_{Bn}}{1 - \gamma p_{BB}^2} \right] \\
&= \sum_m \Sigma_m p_{mB}^2 \left[ 1 - \frac{\gamma(1 - p_{BB}^2)}{1 - \gamma p_{BB}^2} \right] \\
&= \frac{1 - \gamma}{1 - \gamma p_{BB}^2} \sum_m \Sigma_m p_{mB}^2 \\
&= \frac{1 - \gamma}{1 - \gamma p_{BB}^2} \frac{N \pi R}{2} \sum_m p_{Bm}^2 \\
&= \frac{N \pi R}{2} \frac{(1 - \gamma)(1 - p_{BB}^2)}{1 - \gamma p_{BB}^2} \\
\end{align*}
\]

\( \ldots \) (6.26)
6.12

\( \gamma \) and \( \Sigma_j \) are both unknown and the procedure adopted by Yamamoto and Ishida is to demand

\[ \Sigma_j = \Sigma \quad \text{when all } \Sigma_m = \Sigma \quad \text{...(6.27)} \]

They have the simple volume weighted estimate for \( \Sigma \) and solved equation 6.26 for \( \gamma \). It is found that \( \gamma \) is not sensitive to the value of \( \Sigma \), so that when equation 6.26 is solved again for \( \Sigma_j \) the latter is obtained to good accuracy.

An alternative and somewhat simpler way to proceed, having established that \( \gamma \) is not sensitive to \( \Sigma \), is to use \( \Sigma = \Sigma_j \) in equation 6.27. This gives

\[
\frac{\pi R}{2} \left[ 1 - \gamma \right] \left[ 1 - p^2_{BB \left( \Sigma_j \right)} \right] = \frac{\pi R}{2} \left[ 1 - \gamma \right] \left[ 1 - p^2_{BB \left( \Sigma_m \right)} \right]
\]

i.e.

\[ p^2_{BB \left( \Sigma_j \right)} = p^2_{BB \left( \Sigma_m \right)} \quad \text{...(6.28)} \]

where \( p^2_{BB \left( \Sigma_j \right)} \) is evaluated with all cross sections in the equivalent cylinder set to \( \Sigma_j \) and \( p^2_{BB \left( \Sigma_m \right)} \) is evaluated with the real fuel, can and coolant cross sections. Equation 6.28 may be written in the form suitable for numerical solution

\[ 2 R \Sigma_j \left[ 1 - P_c \left( R \Sigma_j \right) \right] = \sum_{m} p^2_{Bm \left( \Sigma_m \right)} \quad \text{...(6.29)} \]

The corresponding equation in the treatment of Bollacasa and Bonalumi (1970) is
Equation 6.30 results from demanding that the transmission across the heterogeneous equivalent cylinder be the same as across a homogenised annulus. The preceding development shows that a consistent model can be obtained by demanding that the transmission across the heterogeneous cylinder be equated with the transmission across the homogenised cylinder. We therefore prefer equation 6.29 which, for practical purposes, is the same as that proposed by Yamamoto and Ishida.

The routine described by Doherty (1970) used simple volume weighting to define the smeared cross section. While the accuracy obtained on test calculations was adequate, volume weighting is clearly incorrect as the fuel cross section becomes large or the coolant density goes to zero. Using the definition of equation 6.29 the approximate method yields an accuracy comparable with that obtained from numerical quadrature in a fraction of the time. Because the quadrature method is time consuming there is a tendency to specify the quadrature mesh conservatively. The end result of a quadrature calculation with too few neutron paths may well be worse than could be obtained from the approximate method.
(a) **Review**

The accurate calculation of resonance absorption remains one of the difficult problems of reactor physics, despite the considerable effort already expended on this topic. Resonance calculation methods may be divided into three classes:

(i) equivalence relations

(ii) Monte Carlo

(iii) numerical solution of the slowing down equations.

Equivalence relations of varying degrees of sophistication have been developed and the common feature of all of them is computational speed. By contrast, the other two methods are slow and expensive and normally would be used only in checking new equivalence relations or for particular design calculations where high accuracy is demanded. Monte Carlo calculations are limited in accuracy by the number of neutron histories which can be accumulated in a reasonable amount of computer time. Special variance reduction techniques must be used to estimate the variation of absorption with fuel temperature or coolant density because the expected variation may be of the same order as the error in the primary estimate. This difficulty is avoided by numerical solution of the slowing down equations, but this method is limited by the error resulting from the flat source approximation. The latter error can be reduced by increasing the number of regions in the calculation but as the solution time varies somewhat faster than the square of the number of regions, the practical machine time limit is quickly reached.
The Australian Atomic Energy Commission has a slowing down code PEARLS (Chiarella 1971) for which the candidate supplied the collision probability routines used in the spatial solution at each energy point, and a Monte Carlo code MCRP written by the candidate. These programmes are very similar to the U.K.A.E.A. programmes SDR (Brissenden and Durston 1965) and MOCUP (Bannister et al. 1968). Resonance cross section for fuel nuclides are tabulated on a fine energy mesh ($10^5$ points from 20 keV down) using the GENEX programme (Brissenden and Durston 1968) which uses single level parameters for fertile nuclides and Vogt (1958) parameters for fissile nuclides. The assistance of U.K.A.E.A. staff in the preparation of these resonance tabulations is gratefully acknowledged.

A rationale for the multigroup type of resonance calculation has been given by Askew (1966) and a detailed proposal for equivalence relations based on numerical collision probabilities is set out in a further paper by Askew (1969). In broad outline the method we shall follow is similar to that proposed by Askew, though many of the details are quite different. As many of the codes in use at the A.A.E.C. were supplied by the U.K.A.E.A. Winfrith establishment, there are obvious advantages in maintaining compatibility with the Winfrith calculation scheme whenever possible. In details such as the resonance group structure we therefore have followed the WIMS code (Askew et al. 1966).

(b) Reaction rate in a two region cell with narrow resonance theory

The starting point for this development is the integral transport equation in the form solved by slowing down codes such as PEARLS

$$V_i \sum_j P_{ji} \left\{ \sum_k N_{jk} \int_E^{E/a_k} \sigma_{sk}(E') \phi_j(E')/[E'(1-\alpha_k)] \right\}$$

$$....(7.1)$$
Here i and j are indices which refer to regions of the cell and we have made the usual assumption that the spatial variation of the flux (or source) within a region can be ignored. $P_{ji}$ is the probability that a neutron starting in region j will collide in region i.

$$N_{jk} = \text{concentration of nuclide } k \text{ in region } j$$

$$\sigma_{sk}(E) = \text{microscopic elastic scattering cross section of nuclide } k \text{ at energy } E$$

$$\sigma_{k}(E) = \text{microscopic total cross section of nuclide } k \text{ at energy } E$$

$$\Sigma_{j}(E) = \text{macroscopic total cross section of the material in region } j$$

$$= \sum_{k} N_{jk} \sigma_{k}(E)$$

$$A_k = \text{atomic mass of nuclide } k, \text{ and}$$

$$\alpha_k = (A_k-1)^2/(A_k+1)^2$$

$$N_{jk} \int_{E}^{E/\alpha_k} dE' \sigma_{sk}(E') \phi_j(E')/\left[ E'(1-\alpha_k) \right]$$

is the source density of neutrons produced in region j by elastic scattering from nuclide k. The elastic scattering is assumed spherically symmetric in the centre of mass system and inelastic scattering has been ignored.

Following on from the early work of Wigner various approximate solutions to equation 7.1 were developed at Brookhaven (Chernick and Vernon 1958), Rothenstein 1960B). The simplest approximation which can be made is the narrow resonance approximation. Let us suppose that the fuel consists of a single isotope and that the moderator is non-absorbing.
Provided the flux recovers its asymptotic value between resonances, then in the absence of any absorption the fluxes above resonance in a two region cell will be given by

\[ \phi_1(E) = \phi_2(E) = \phi_0 / E \] ...(7.2)

where \( \phi_0 \) is a constant.

Ignoring interference scattering the fuel cross section \( \Sigma_1(E) \) can be written

\[ \Sigma_1(E) = \Sigma_1 = N_1 \left[ \sigma_p + \sigma_s(E) + \sigma_a(E) \right] \] ...(7.3)

where \( \sigma_p \) is the potential scattering cross section, \( \sigma_s(E) \) is the resonance scattering cross section and \( \sigma_a(E) \) is the absorption cross section. For a simple Breit-Wigner resonance the cross section depends on the following quantities:

\[ \Gamma_a, \text{ the absorption width of the resonance,} \]
\[ \Gamma_n, \text{ the scattering width of the resonance,} \]
\[ \Gamma, \text{ the total width of the resonance,} \]
\[ E_r, \text{ the energy of the resonance peak} \]
\[ g_s, \text{ the statistical spin factor,} \]
\[ \sigma_o, \text{ the peak height of the resonance at } 0^\circ K, \]
\[ \kappa_T, \text{ the mean temperature of the fuel,} \]
\[ A, \text{ the atomic mass of the fuel isotope.} \]

Thus

\[ \sigma_s(E) = \Gamma_n \sigma_o \psi(x, \theta) / \Gamma \] ...(7.4)
\[ \sigma_a(E) = \mathbf{r}_a \sigma_o \psi(x,\theta)/\Gamma \] ...

where \[ \theta = \Gamma (A/4kT_E) \] ...

\[ x = 2(E - E_r)/\Gamma \] ...

\[ \sigma_o = 2.6038 \times 10^6 g_s \Gamma_n / (\Gamma E_r) \] ...

and \[ \psi(x,\theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} dy \exp \left(-\frac{\theta^2(x-y)^2}{4}\right) / (1 + y^2) \] ...

The cross section of the moderator is simply

\[ \Sigma_2(E) = N_2 \sigma_m \] ...

If the resonance is assumed narrow compared to the scattering width of both fuel and moderator the source integral may be taken as coming only from the asymptotic flux above resonance. This gives

\[ \int_{E}^{E/\alpha_k} dE' \sigma_{ks}(E') \phi_j(E')/E'(1 - \alpha_k) \]

\[ = \int_{E}^{E/\alpha_k} dE' \sigma_{pk} \phi_o / \left[(E')^2 (1 - \alpha_k)\right] \]

\[ = \sigma_{pk} \phi_o / E \] ...

For the two region cell equation 7.1 can be rewritten as

\[ V_1 \Sigma_1(E) \phi_1(E) = V_1 P_{11} N_1 \sigma_p \phi_o / E + V_2 P_{21} N_2 \sigma_m \phi_o / E \] ...

\[ V_2 \Sigma_2(E) \phi_2(E) = V_1 P_{12} N_1 \sigma_p \phi_o / E + V_2 P_{22} N_2 \sigma_m \phi_o / E \] ...

Equation 7.12 gives \[ \phi_1(E) \] explicitly, thus enabling the resonance absorption \[ R \] to be evaluated:
\[ \phi_1(E) = \frac{(V_1 p_{11} N_1 \sigma_p + V_2 p_{21} N_2 \sigma_m)}{V_1 \Sigma_1(E)} \frac{\phi_o}{E} \quad \ldots(7.14) \]

\[ R = \int \phi_1(E) \sigma_a(E) \, dE \quad \ldots(7.15) \]

(c) Homogeneous theory using J functions

The expression corresponding to equation 7.14 in a homogeneous system would be

\[ \phi(E) = \frac{N_1 \sigma_p + N_2 \sigma_m}{N_1 \sigma_p + N_2 \sigma_m + N_1 (\sigma_s(E) + \sigma_a(E))} \frac{\phi_o}{E} \quad \ldots(7.16) \]

and correspondingly the resonance integral becomes

\[ R = \int \phi(E) \sigma_a(E) \, dE \]

\[ = \int \frac{dE(N_1 \sigma_p + N_2 \sigma_m) \sigma_a(E)}{(N_1 \sigma_p + N_2 \sigma_m) + N_1 [\sigma_s(E) + \sigma_1(E)]} \frac{\phi_o}{E} \]

\[ = \int \frac{dE}{s + \sigma_a(E) + \sigma_s(E)} \frac{\phi_o}{E} \quad \ldots(7.17) \]

where \( S = (N_1 \sigma_p + N_2 \sigma_m)/N_1 \) \ldots(7.18)

is the potential scattering per fuel atom and is independent of energy.

For the isolated resonance at \( E_r \)
Conventionally \( \frac{1}{E} \) is removed from the integral because its variation over the width of the resonance is negligible

\[
R = \phi_0 \int_{E_r^-}^{E_r^+} \frac{\sigma_a(E)}{s + \sigma_s(E) + \sigma_a(E)} \frac{dE}{E}
\]

\[
= \phi_0 \int_{E_r^-}^{E_r^+} \frac{\sigma_o \psi(x,\theta)}{s + \sigma_o \psi(x,\theta)} \frac{dE}{E}
\]

\[
= \phi_0 \left[ \int_0^\infty \frac{\sigma_o \psi(x,\theta)}{s + \sigma_o \psi(x,\theta)} \, dx \right]
\]

\[
= \phi_0 \left[ \int_0^\infty \frac{\psi(x,\theta)}{\beta + \psi(x,\theta)} \, dx \right]
\]

\[
= \phi_0 \left[ \frac{s}{\sigma_o} \right] \, J(\theta,\beta) \tag{7.19}
\]

where \( \beta = \frac{s}{\sigma_o} \tag{7.20} \)

Several methods of evaluating the integral \( J(\theta,\beta) \) have been devised for routine calculations, ranging from table look-up through empirical fitted approximations to rapid quadrature techniques. Thus it is possible to go through an energy group \( E_g \) and evaluate the contribution of each resonance to the total absorption. This has been the method previously
employed at the A.A.E.C. in programmes such as GYMEA (Pollard and Robinson 1966).

The alternative approach used in the WIMS programme (Askew et al. 1966) is to tabulate the integral

\[
I(\sigma_p) = \int_{E_g} \frac{\sigma_p \sigma_a(E)}{\sigma_p + \sigma_a(E) + \sigma_s(E)} \frac{dE}{E} \quad \ldots(7.21)
\]

and interpolate in the tables of \( I \) for the value corresponding to a particular \( \sigma_p \). Such tables could be prepared by summing the \( J(\Theta,\beta) \) contributions of individual resonances but in practice they are prepared from homogeneous slowing down calculations performed with the SDR code (Brissenden and Durston 1965). This has the advantage that effects which are ignored in the derivation of the \( J(\Theta,\beta) \) form, such as interference between potential and resonance scattering, will be reproduced correctly in the resonance integrals - at the tabular points at least. Interpolation in the tables of \( I \) is performed on the assumption that \( I \) is linear in \( \sqrt{\sigma_p} \).

(d) Homogeneous theory using the Russian subgroup method

An alternative method of interpolation is the Russian subgroup method (Nikolaev et al. 1971) which has interesting possibilities for numerical equivalence relations. Equation 7.21 can be rewritten

\[
I(\sigma_p) = \int_{E_g} \frac{\sigma_p \sigma_a(E)}{\sigma_p + \sigma_r(E)} \frac{dE}{E} \quad \ldots(7.22)
\]

where the resonance cross section \( \sigma_r(E) \) is simply

\[
\sigma_r(E) = \sigma_a(E) + \sigma_s(E) \quad \ldots(7.23)
\]
The integral of equation 7.22 can be approximated by the form

\[ I(\sigma_p) = \sum_i \frac{\sigma_{ai} \mu_i}{\sigma_{ri} + \sigma_p} \sigma \]  

...(7.24)

where \( \mu_i \) may be interpreted as the measure of the set of \( E \) for which \( \sigma_r(E) \approx \sigma_{ri} \) and \( \sigma_{ai} \) is the average of \( \sigma_a(E)/E \) on the same set. In the limit of large \( i \) equation 7.24 corresponds to an integration in measure so the approximation can be as accurate as one wishes. In practice very good approximations can be obtained from relatively small values of \( i \).

Test calculations have been performed on \(^{238}\text{U}\) using the WIMS group structure and 8 values of \( \sigma_r \) starting at 0.625 and proceeding in multiples of 4 to 1024. The integrals \( I(\sigma_p) \) were evaluated for 22 values of \( \sigma_p \) in the range \((10, 10^6)\) using the \( J(\theta, \beta) \) method outlined above. It is not expected that the use of \( I(\sigma_p) \) values obtained from slowing down calculations would alter the conclusions which can be drawn.

The numerical fits were made on the usual least squares basis, i.e. the minimisation of

\[ Q = \sum_j \left[ 1 - \sum_i \frac{a_i \sigma_{pj}}{(\sigma_{ri} + \sigma_{pj}) I(\sigma_{pj})} \right]^2 \]  

...(7.25)

This definition of \( Q \) gives equal weight to the error at each value \( \sigma_{pj} \).

The reader may wonder why the parameters \( \sigma_{ri} \) are specified and not obtained from the fit. A glance at the form of \( Q \) shows that unless the \( \sigma_{ri} \) are fixed no solution to the fitting problem will be found. It is also convenient to use the same set of \( \sigma_{ri} \) for each temperature because interpolation in temperature then reduces to interpolation of the \( a_i \).
For some groups the simple least squares solution gives a set of $a_i$ with alternating signs. Such a solution is not consistent with the measure theoretic interpretation

$$a_i = \mu_i \left< \frac{a}{E} \right> \quad \ldots(7.26)$$

and it is also inconvenient for our intended use of this interpolation scheme in equivalence relations. We have therefore imposed the additional constraints

$$a_i \geq 0 \quad \ldots(7.26)$$

These constraints make the fitting problem more difficult. One method used was to minimise

$$Q = \sum_j \left[ 1 - \sum_i \frac{b_i^2 \sigma_{pj}}{(\sigma_{ri} + \sigma_{pj}) I(\sigma_{pj})} \right]^2 \quad \ldots(7.28)$$

The problem is now non-linear and the VA06A routine described by Powell (1970) was employed. This method of solution is expensive, taking one hour of IBM 360/50 time to obtain fits at one temperature for thirteen resonance groups.

A more efficient method was developed by Trimble (1971) which reduces the computation time to about 5 minutes. $Q$ is written in matrix notation

$$Q = b^T a + a^T C a \quad \ldots(7.29)$$

and a direct search is conducted along the coordinate directions and along the eigenvectors of $C$ until a particular $a_k = 0$. This term is then excluded from the fit and the unconstrained solution for the remaining $a_i$
is obtained. If all are positive the solution is accepted otherwise the procedure repeats with the $Q$ of equation 7.29 modified to exclude $a_k$.

The constraints of equation 7.27 do not worsen the fits appreciably. The extreme error over the 13 groups was 1 per cent at one particular value of $\sigma_p$ and for many groups the error is less than 0.1 per cent for all values of $\sigma_p$. We therefore conclude that the subgroup method provides a reliable method of interpolation in $\sigma_p$. An investigation of temperature interpolation showed that linear interpolation in $\sqrt{T}$ was the best of the schemes tried. For $^{238}\text{U}$ the interpolation between 300$^\circ$K and 900$^\circ$K gave errors at 600$^\circ$K which were less than 1 per cent for all values of $\sigma_p$. It is therefore concluded that 300$^\circ$K intervals will be adequate for the temperature interpolation.

(e) Numerical equivalence relations

The aim of an equivalence relation is to express the integral for the heterogeneous cell in the same form as that arising in the homogeneous problem which can be evaluated by the methods just discussed. This means that we wish to equate the expressions of equations 7.15 and 7.17

$$\frac{S}{S + \sigma_a(E) + \sigma_s(E)} = \frac{V_1 P_{11} N_1 \sigma_p + V_2 P_{21} N_2 \sigma_m}{V_1 \Sigma_1(E)} \quad \ldots(7.30)$$

Solving for $S$ we obtain, after some manipulation,

$$S = \sigma_p + \frac{1}{N_1} \frac{\Sigma_1(E)(1-P_{11})}{P_{11}} \quad \ldots(7.31)$$

Using the collision probability methods discussed in the previous
sections, the cross section dependent portion of $S$ may be evaluated numerically for a range of values of $\Sigma_1$. Define

$$ F(\Sigma_1) = \frac{\Sigma_1(E) (1-P_{11})}{P_{11}} \quad \ldots (7.32) $$

In tables 7.1 and 7.2 values of $F(\Sigma_1)$ in annular geometry are presented for a range of rod sizes and pitches. For table 7.1 we have used 16 point Gauss quadrature integration to obtain the collision probabilities, while for table 7.2 the method of Bonalumi (1961) was employed. The outer boundary condition is white reflecting. The relevant number densities and cross sections are

$$ N_1 = 0.05 \quad N_2 = 0.025 \quad \sigma_p = 10 \quad \sigma_m = 10 $$
### TABLE 7.1

$F(\Sigma_1)$ for Single Rod Cells using Gauss Quadrature Probabilities

<table>
<thead>
<tr>
<th>Rod Radius</th>
<th>Moderator Radius</th>
<th>$F(N_1\sigma_p)$</th>
<th>$F(\infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>1.0</td>
<td>1.8946</td>
<td>1.4043</td>
</tr>
<tr>
<td>0.25</td>
<td>2.0</td>
<td>2.8010</td>
<td>1.8652</td>
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<tr>
<td>0.25</td>
<td>3.0</td>
<td>2.9931</td>
<td>1.9560</td>
</tr>
<tr>
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<td>4.0</td>
<td>3.0474</td>
<td>1.9793</td>
</tr>
<tr>
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<td>5.0</td>
<td>3.0663</td>
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</tr>
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<td>5.0</td>
<td>1.4287</td>
<td>0.9549</td>
</tr>
<tr>
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<td>4.0</td>
<td>1.4886</td>
<td>0.9830</td>
</tr>
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<td>5.0</td>
<td>1.5100</td>
<td>0.9931</td>
</tr>
<tr>
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<td>2.0</td>
<td>0.4291</td>
<td>0.3352</td>
</tr>
<tr>
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<td>4.0</td>
<td>0.6923</td>
<td>0.4781</td>
</tr>
<tr>
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<td>6.0</td>
<td>0.7289</td>
<td>0.4959</td>
</tr>
<tr>
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<td>8.0</td>
<td>0.7356</td>
<td>0.4992</td>
</tr>
<tr>
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<td>0.4999</td>
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<tr>
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<td>4.0</td>
<td>0.2776</td>
<td>0.2133</td>
</tr>
<tr>
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<td>6.0</td>
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<td>0.2430</td>
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<tr>
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<td>8.0</td>
<td>0.3404</td>
<td>0.2483</td>
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<tr>
<td>2.0</td>
<td>10.0</td>
<td>0.3427</td>
<td>0.2496</td>
</tr>
<tr>
<td>2.0</td>
<td>20.0</td>
<td>0.3434</td>
<td>0.2500</td>
</tr>
</tbody>
</table>
### TABLE 7.2

$F(\Sigma_1)$ for Single Rod Cells using Bonalumi Probabilities

<table>
<thead>
<tr>
<th>Rod Radius</th>
<th>Moderator Radius</th>
<th>$F(N_{1\Sigma_p})$</th>
<th>$F(\infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>1.0</td>
<td>1.8620</td>
<td>1.4020</td>
</tr>
<tr>
<td>0.25</td>
<td>2.0</td>
<td>2.7776</td>
<td>1.8638</td>
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<td>0.25</td>
<td>3.0</td>
<td>2.9815</td>
<td>1.9545</td>
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<td>4.0</td>
<td>3.0413</td>
<td>1.9789</td>
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<td>0.25</td>
<td>5.0</td>
<td>3.0627</td>
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<td>1.0</td>
<td>0.5499</td>
<td>0.4625</td>
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</tr>
<tr>
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<td>3.0</td>
<td>1.4209</td>
<td>0.9546</td>
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<td>4.0</td>
<td>1.4844</td>
<td>0.9829</td>
</tr>
<tr>
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<td>5.0</td>
<td>1.5077</td>
<td>0.9930</td>
</tr>
<tr>
<td>1.0</td>
<td>2.0</td>
<td>0.4260</td>
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<td>1.0</td>
<td>4.0</td>
<td>0.6901</td>
<td>0.4780</td>
</tr>
<tr>
<td>1.0</td>
<td>6.0</td>
<td>0.7281</td>
<td>0.4959</td>
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<tr>
<td>1.0</td>
<td>8.0</td>
<td>0.7353</td>
<td>0.4992</td>
</tr>
<tr>
<td>1.0</td>
<td>10.0</td>
<td>0.7369</td>
<td>0.4999</td>
</tr>
<tr>
<td>2.0</td>
<td>4.0</td>
<td>0.2775</td>
<td>0.2131</td>
</tr>
<tr>
<td>2.0</td>
<td>6.0</td>
<td>0.3302</td>
<td>0.2430</td>
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<tr>
<td>2.0</td>
<td>8.0</td>
<td>0.3403</td>
<td>0.2483</td>
</tr>
<tr>
<td>2.0</td>
<td>10.0</td>
<td>0.3426</td>
<td>0.2496</td>
</tr>
<tr>
<td>2.0</td>
<td>20.0</td>
<td>0.3434</td>
<td>0.2500</td>
</tr>
</tbody>
</table>
It can be seen from a comparison of $F(N_1 \sigma_p)$ with $F(\infty)$ that $F$ varies very little over the entire range of $\Sigma_1$. It is not surprising therefore that equivalence relations using an $S$ which does not depend on cross section have proved so successful. In the single rod case it is possible to fit $F$ to about 0.1 per cent over the range of interest with the rational approximation

$$F(\Sigma) = \frac{(A + B/\Sigma + C/\Sigma^2)/(D + E/\Sigma + 1./\Sigma^2)}{\ldots}(7.33)$$

The homogeneous resonance integral from the subgroup method is

$$I(\sigma_p) = \sum_i \frac{a_i \sigma_p}{\sigma_{ri} + \sigma_p} \ldots(7.34)$$

The corresponding heterogeneous resonance integral is

$$I = \sum_i \frac{a_i S(\sigma_{ri})}{\sigma_{ri} + S(\sigma_{ri})} \ldots(7.35)$$

where

$$S(\sigma_{ri}) = \sigma_p + \frac{1}{N_1} F(N_1(\sigma_p + \sigma_{ri})) \ldots(7.36)$$

The fact that we have a fit for $F$ is convenient but not essential to the development because the values of $S(\sigma_{ri})$ could be obtained directly from the defining equation 7.31 by performing the collision probability calculations with the appropriate $\Sigma_1$. A cross section dependent $S$ can also be incorporated in the $J(\theta, \beta)$ if $J$ is evaluated by quadrature, as in the routine described by Nicholson and Grasseschi (1969). In the homogeneous situation equation 7.19 gave
In the heterogeneous situation this becomes

\[ R = \frac{\phi_o}{E_r} S \int_0^\infty \frac{S(\psi) \psi(x, \theta)}{\sigma_o} \psi(x, \theta) \, dx \]  

\[ \sigma_o = \Gamma_n \]  

\[ \Gamma_n = 0.00152 \text{ eV} \]

The cells considered were those for which results have already been given in tables 7.1 and 7.2. The results of these calculations are set out in table 7.3. Those labelled Gauss were obtained with the fits to $F$ based on Gauss quadrature probabilities, and those labelled Bonalumi from the Bonalumi collision probabilities. The results labelled Chiarella were obtained by a procedure which is equivalent to that proposed by Chiarella (1969). The integral at $T = 0^\circ K$ has been evaluated using the Gaussian collision probability fit to $F$. An $S$ which does not depend on cross section is then obtained by equating the expressions of
equations 7.37 and 7.38 and iterating for the constant $S$. Chiarella's method involved analytic integration at $0^\circ K$ but the method we have adopted is more convenient for the comparison.

Two facts are obvious from table 7.3. The first is that the Bonalumi approximation gives adequate accuracy for $F(\Xi)$ and therefore for $S$. The second is that Chiarella's method leads to an overestimate of the absorption at temperatures above $T = 0^\circ K$ and to an overestimate of the change in absorption with temperature. The latter feature would be shared by all equivalence relations which employ a cross section independent $S$, though in view of the other errors inherent in resonance absorption calculations the practical importance of this particular error is almost certainly small.
### TABLE 7.3

R- Calculations using Different Approximations

<table>
<thead>
<tr>
<th>Rod radius</th>
<th>Moderator radius</th>
<th>Gauss T=300</th>
<th>Bonalumi T=300</th>
<th>Chiarella T=300</th>
<th>Gauss T=900</th>
<th>Bonalumi T=900</th>
<th>Chiarella T=900</th>
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<td>0.04795</td>
<td>0.04794</td>
<td>0.04802</td>
<td>0.04875</td>
<td>0.04875</td>
<td>0.04898</td>
</tr>
<tr>
<td>1.0</td>
<td>10.0</td>
<td>0.04797</td>
<td>0.04796</td>
<td>0.04805</td>
<td>0.04878</td>
<td>0.04877</td>
<td>0.04901</td>
</tr>
<tr>
<td>2.0</td>
<td>4.0</td>
<td>0.03964</td>
<td>0.03963</td>
<td>0.03965</td>
<td>0.04016</td>
<td>0.04016</td>
<td>0.04021</td>
</tr>
<tr>
<td>2.0</td>
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<td>0.04057</td>
<td>0.04057</td>
<td>0.04060</td>
<td>0.04113</td>
<td>0.04112</td>
<td>0.04119</td>
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<tr>
<td>2.0</td>
<td>8.0</td>
<td>0.04075</td>
<td>0.04074</td>
<td>0.04077</td>
<td>0.04130</td>
<td>0.04130</td>
<td>0.04137</td>
</tr>
<tr>
<td>2.0</td>
<td>10.0</td>
<td>0.04078</td>
<td>0.04078</td>
<td>0.04081</td>
<td>0.04134</td>
<td>0.04134</td>
<td>0.04141</td>
</tr>
<tr>
<td>2.0</td>
<td>20.0</td>
<td>0.04080</td>
<td>0.04080</td>
<td>0.04082</td>
<td>0.04135</td>
<td>0.04135</td>
<td>0.04143</td>
</tr>
</tbody>
</table>
Further numerical experiments have been performed to assess the accuracy of the subgroup equivalence relation of equation 7.35. $^{238}\text{U}$ was again the nuclide and resonance integrals were computed for the WIMS group structure given in table 7.4. Resolved resonance parameters were taken from Schmidt (1966) and a ladder of unresolved resonances was generated using the RESP programme of Brissenden and Durston (1968) from the average parameters given by Schmidt. Tables of resonance integral against $\sigma_p$ were generated using the $J(\theta,\beta)$ approach for each group. Subgroup fits to these tables were obtained in the manner previously described. Finally, the resonance integrals were computed from equation 7.35 for the same set of lattices as we have previously considered. The resulting resonance integrals were compared with those calculated directly from the original resonance parameters using the $\Sigma$-dependent $\beta$ in the numerical quadrature evaluation of $J(\theta,\beta)$.

Results are presented in table 7.5 for the last group which shows the worst errors and usually contributes a sizable proportion of the total resonance integral in $^{238}\text{U}$. The greatest error in table 5 is 0.5 per cent. In the other resonance groups the errors are often less than 0.1 per cent for all lattices so that the worst error in the total resonance integral should never exceed 0.25 per cent. In the fast energy groups the subgroup method always gives better than 0.1 per cent accuracy and the narrow resonance assumptions are adequate. We conclude that the simple method outlined here should suffice for fast reactor calculations. In the next chapter details are given of modifications required to compute resonance reactions in thermal reactors.
TABLE 7.4
Resonance Group Structure of WIMS

<table>
<thead>
<tr>
<th>Number</th>
<th>Upper Energy (eV)</th>
<th>Lower Energy (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9118</td>
<td>5530</td>
</tr>
<tr>
<td>2</td>
<td>5530</td>
<td>3519.1</td>
</tr>
<tr>
<td>3</td>
<td>3519.1</td>
<td>2239.45</td>
</tr>
<tr>
<td>4</td>
<td>2239.45</td>
<td>1425.1</td>
</tr>
<tr>
<td>5</td>
<td>1425.1</td>
<td>906.898</td>
</tr>
<tr>
<td>6</td>
<td>906.898</td>
<td>367.262</td>
</tr>
<tr>
<td>7</td>
<td>367.262</td>
<td>148.728</td>
</tr>
<tr>
<td>8</td>
<td>148.728</td>
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</tr>
<tr>
<td>9</td>
<td>75.5014</td>
<td>48.052</td>
</tr>
<tr>
<td>10</td>
<td>48.052</td>
<td>27.7</td>
</tr>
<tr>
<td>11</td>
<td>27.7</td>
<td>15.968</td>
</tr>
<tr>
<td>12</td>
<td>15.968</td>
<td>9.877</td>
</tr>
<tr>
<td>13</td>
<td>9.877</td>
<td>4.0</td>
</tr>
</tbody>
</table>
### TABLE 7.5

Narrow Resonance Subgroup Comparison for Group 13 in $^{238}$U

<table>
<thead>
<tr>
<th>Lattice</th>
<th>Exact RI</th>
<th>Subgroup RI</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.0307</td>
<td>6.0453</td>
<td>0.24</td>
</tr>
<tr>
<td>2</td>
<td>6.8424</td>
<td>6.8743</td>
<td>0.47</td>
</tr>
<tr>
<td>3</td>
<td>6.9930</td>
<td>7.0285</td>
<td>0.51</td>
</tr>
<tr>
<td>4</td>
<td>7.0349</td>
<td>7.0711</td>
<td>0.51</td>
</tr>
<tr>
<td>5</td>
<td>7.0497</td>
<td>7.0864</td>
<td>0.52</td>
</tr>
<tr>
<td>6</td>
<td>4.1512</td>
<td>4.1424</td>
<td>-0.21</td>
</tr>
<tr>
<td>7</td>
<td>5.0568</td>
<td>5.0520</td>
<td>-0.09</td>
</tr>
<tr>
<td>8</td>
<td>5.2604</td>
<td>5.2583</td>
<td>-0.04</td>
</tr>
<tr>
<td>9</td>
<td>5.3199</td>
<td>5.3188</td>
<td>-0.02</td>
</tr>
<tr>
<td>10</td>
<td>5.3410</td>
<td>5.3402</td>
<td>-0.01</td>
</tr>
<tr>
<td>11</td>
<td>3.8563</td>
<td>3.8463</td>
<td>-0.26</td>
</tr>
<tr>
<td>12</td>
<td>4.2257</td>
<td>4.2112</td>
<td>-0.34</td>
</tr>
<tr>
<td>13</td>
<td>4.2708</td>
<td>4.2559</td>
<td>-0.35</td>
</tr>
<tr>
<td>14</td>
<td>4.2791</td>
<td>4.2640</td>
<td>-0.35</td>
</tr>
<tr>
<td>15</td>
<td>4.2809</td>
<td>4.2659</td>
<td>-0.35</td>
</tr>
<tr>
<td>16</td>
<td>3.5409</td>
<td>3.5346</td>
<td>-0.18</td>
</tr>
<tr>
<td>17</td>
<td>3.6243</td>
<td>3.6165</td>
<td>-0.21</td>
</tr>
<tr>
<td>18</td>
<td>3.6395</td>
<td>3.6314</td>
<td>-0.22</td>
</tr>
<tr>
<td>19</td>
<td>3.6424</td>
<td>3.6347</td>
<td>-0.22</td>
</tr>
<tr>
<td>20</td>
<td>3.6440</td>
<td>3.6358</td>
<td>-0.22</td>
</tr>
</tbody>
</table>
CHAPTER 8
PRACTICAL RESONANCE CALCULATIONS

(a) Sources of error in the simple model

For a single rod cell the equivalence relation discussed in the previous section could at best be expected to reproduce the results of a two region slowing down calculation. Megier (1968) showed that the use of only two regions leads to a substantial overestimate of resonance absorption when compared with results obtained using more regions. Unfortunately his results are based on the approximation of Bonalumi (1961) which itself introduces errors when the fuel rod is subdivided. The true situation is not as bad as that indicated by the results of Megier, but the error in a two region calculation can still be significant. For example the two region estimate of absorption for a $^{238}$U rod of radius 0.5 cm surrounded by 5 cm of graphite will be about 1.5 per cent high (Robinson 1972). While it is possible to reduce the error in a slowing down calculation by increasing the number of regions, a similar improvement in the result obtained from the equivalence relation will only appear when the narrow resonance approximation is relaxed to allow a spatial variation of the scattering source. This is obvious from equations 7.12 and 7.13.

The other major error arises in attempting to condense to relatively few groups. The method of obtaining group cross sections from resonance integrals which we shall shortly discuss purports to preserve the simple flux weighted condensation which would be applied if a two region slowing down calculation had been performed. The end products of a two region slowing down calculation will be detailed fuel and moderator fluxes,
\( \phi^1(E) \) and \( \phi^2(E) \) respectively. Using the standard flux weighting condensation procedure the cross sections for the group \( (E_{g+1}, E_g) \) are given by the relations:

\[
\sigma_{iga} = \int_{E_{g+1}}^{E_g} \sigma_{ia}(E) \phi^1(E) dE / \int_{E_{g+1}}^{E_g} \phi^1(E) dE \quad \ldots(8.1)
\]

\[
\sigma_{igg'} = \int_{E_{g+1}}^{E_{g'}} dE' \int_{E_{g+1}}^{E_g} dE \phi^1(E) \sigma_{i}(E, E') / \int_{E_{g+1}}^{E_g} \phi^1(E) dE \quad \ldots(8.2)
\]

If the two region calculation were to be repeated using, say, the WIMS group structure of table 7.4 we would find that the few group calculation would give a higher estimate of absorption than the original slowing down result, and 1 per cent or 2 per cent errors would not be impossible.

Taken together these two effects may give rise to a significant overestimate of absorption from the simple equivalence relation. The error resulting from the narrow resonance approximation can be reduced by the use of a \( \lambda \)-method. It is difficult to see how the condensation procedure can be modified to give the desired result.

(b) \( \lambda \)-method

Using the narrow resonance approximation we have from equation 7.11

\[
\int_{E}^{E/\alpha_k} dE' \sigma_{sk}(E') \phi_j(E') / E'(1 - \alpha_k) = \sigma_{pk} \phi_0 / E \quad \ldots(8.3)
\]

If the mass of nuclide \( k \) is assumed infinite we obtain instead
The $\lambda$-method provides a means of interpolating between these two. The scattering source is assumed to be of the form

\[
\int E_{\alpha_k} \sigma_{sk}(E') \varphi_j(E')/ [E'(1 - \alpha_k)] = \lambda_k \sigma_{pk} \varphi_0/E + (1 - \lambda_k) \sigma_{sk}(E) \varphi_j(E) 
\]

...(8.5)

Thus equations 7.12 and 7.13 become instead

\[
V_1^2(E) \varphi_1(E) = V_1^1 P_{11} N_1 \left[ \lambda_1 \sigma_{p} \varphi_0/E + (1 - \lambda_1) \sigma_s(E) \varphi_1(E) \right] + V_1^2 P_{21} N_2 \sigma_m \left[ \lambda_2 \varphi_0/E + (1 - \lambda_2) \varphi_2(E) \right] 
\]

...(8.6)

\[
V_2^2(E) \varphi_2(E) = V_1^1 P_{12} N_1 \left[ \lambda_1 \sigma_{p} \varphi_0/E + (1 - \lambda_1) \sigma_s(E) \varphi_1(E) \right] + V_1^2 P_{22} N_2 \sigma_m \left[ \lambda_2 \varphi_0/E + (1 - \lambda_2) \varphi_2(E) \right] 
\]

...(8.7)

In the formulation of Sehgal and Goldstein (1966) the rational approximation is employed for $P_{11}$ and successive approximations for $\varphi_1(E)$ are obtained using the rational approximation for $P_{11}$ and the resonance cross section at 0°K. $\lambda_k$ are evaluated by equating successive iterants of the resonance integral. As our approach is based on tables of resonance integral for energy groups rather than resonance parameters, $\lambda_k$ cannot be obtained in this manner.
The method employed by Askew (1966) is to calculate homogeneous resonance integrals of $^{238}$U with admixtures of nuclide $k$ using the slowing down programme SDR and to choose $\lambda_k$ so that the result obtained from the $\lambda$-method is the same. This procedure allows a $\lambda_k$ for each group to be defined. $\lambda_k$ is specifically tuned to $^{238}$U resonances, but as the bulk of absorption takes place in $^{238}$U the error introduced in this way is probably not large.

The standard form of the equivalence relation can be recovered by solving equations 8.6 and 8.7 for $\phi_1(E)$ with $\phi_0/E = 1$ using the values of $\sigma_{ri}$ which appear in the subgroup tabulation. Instead of equation 7.36 we obtain

$$S(\sigma_{ri}) = \sigma_{ri} \phi_1(\sigma_{ri})/ [1 - \phi_1(\sigma_{ri})] \quad ... (8.8)$$

The difficulty with this procedure is the appearance of $\sigma_s(E)$ in equations 8.6 and 8.7. When $\sigma_{ri}$ is used in place of $\sigma_r(E)$ the appropriate $\sigma_{si}$ should accompany it. The method of obtaining $\sigma_{si}$ from the subgroup method is as follows.

Equation 7.24 is

$$\int_{E_g}^{E} \frac{\sigma p \sigma(E) dE}{(\sigma_p + \sigma_r(E)) E} = I(\sigma) = \sum_i \frac{\sigma_i \mu_i \sigma_p}{\sigma_{ri} + \sigma_p} \quad ... (8.9)$$

where $\mu_i$ is interpreted as the measure of the set of $E$ such that $\sigma_r(E) \approx \sigma_{ri}$. If we wish to obtain $\mu_i$ we can use a similar expression

$$\int_{E_g}^{E} \frac{\sigma p dE}{(\sigma_p + \sigma_r(E)) E} = \sum_i \frac{\mu_i \sigma_p}{\sigma_{ri} + \sigma_p} \quad ... (8.10)$$
If we are using the J-function method of constructing $I(\sigma_p)$ then the integral on the left of equation 8.10 is given by

$$
\int E_g \frac{\sigma_p dE}{(\sigma_p + \sigma_r(E)) E} = \tau_g - \sum_{\text{resonances}} \frac{\Gamma}{E_r} J(\Theta, \beta) \quad \ldots (8.11)
$$

where $\tau_g$ is the lethargy width of the group

and $\beta = \frac{\sigma_p}{\sigma_o}$ for each resonance.

$\mu_i$ can be obtained using the same fitting procedure as was previously applied to $I(\sigma_p)$. If slowing down calculations are used to generate $I(\sigma_p)$ then the integral of equation 8.11 is directly obtained from the group flux.

The appropriate scattering cross section $\sigma_{si}$ is obtained from the fit to the scattering integral

$$
\int E_g \frac{\sigma_p \sigma_s(E) dE}{(\sigma_p + \sigma_r(E)) E} = \sum_i \frac{\sigma_{si} \mu_i \sigma_p}{\sigma_{ri} + \sigma_p} \quad \ldots (8.12)
$$

$\sigma_{si}$ will also be of value in the correction for interaction between different resonance nuclides so the fact that the $\lambda$-method requires it is of little consequence.

(c) **Group cross sections from resonance integrals**

The method for obtaining group cross sections from resonance integrals is to follow the same procedure as if a slowing down calculation had been performed. Thus from equation 8.1
\[
\sigma_{\text{iga}} = \int_{E_{\text{g}+1}}^{E_{\text{g}}} \sigma_{i\alpha}(E) \phi_i(E) \, dE / \int_{E_{\text{g}+1}}^{E_{\text{g}}} \phi_i(E) \, dE \quad \ldots (8.13)
\]

The resonance integral \( I(\sigma_p) \) is computed from

\[
I(\sigma_p) = \int_{E_{\text{g}+1}}^{E_{\text{g}}} \frac{\sigma_p}{\sigma_p + \sigma_r(E)} \frac{1}{E} \sigma_a(E) \, dE \quad \ldots (8.14)
\]

\[
\frac{\sigma_p}{\sigma_p + \sigma_r(E)} \text{ represents the microscopic flux variation within the resonance and } 1/E \text{ is roughly the resonance to resonance flux variation.}
\]

We may therefore hope that, apart from flux depression within the group, \( I \) will be a reasonable approximation to the numerator of equation 8.13.

The corresponding denominator would be

\[
\phi_g = \int_{E_{\text{g}+1}}^{E_{\text{g}}} \frac{\sigma_p}{\sigma_p + \sigma_r(E)} \frac{dE}{E} \quad \ldots (8.15)
\]

which is precisely the quantity defined by equation 8.10 and 8.11. For \( \Gamma_n \ll \Gamma_\gamma \) this reduces to the form given by Askew (1966)

\[
\phi_g = \tau_g - I(\sigma_p) / \sigma_p \quad \ldots (8.16)
\]

\[
\sigma_{\text{iga}} = I(\sigma_p) / \left[ \tau_g - I(\sigma_p) / \sigma_p \right] \quad \ldots (8.17)
\]
Equation 8.17 is derived on the basis that flux depression within the group can be ignored. A more sensible approximation for $\phi(E)$ would be $p(E)/E$ but unfortunately there is no way of arriving at $p(E)$ in the preparation of tables. To minimize the effect of ignoring flux depression within the group the WIMS group structure (which we are also using) has been chosen so that the lower $^{238}\text{U}$ resonances are located at the lethargy centres of groups.

For the scattering term defined by equation 8.2 the flux depression within the group has an important effect which varies with the mass of the scattering nuclide. For $^{238}\text{U}$ with an $\alpha$ value of about 0.98 the whole contribution to the scattering integral comes from the interval $(E_{g+1}, 1.02 E_{g+1})$. $\sigma_{g\rightarrow g+1}$ computed with flux depression will therefore be smaller than if the depression is ignored. The holes in the flux at resonance will have an opposite effect because the numerator will be unchanged, but the denominator will be reduced. For lighter nuclides the scattering range is larger and the effect of flux depression is smaller. The effect of resonance holes is also reduced because the numerator and denominator are reduced simultaneously. To proceed further with this problem we make the following assumptions:

1. The depression takes place at the lethargy centre of the group so that for the top $\tau_g/2$ the flux is $1/E$ while for the bottom it is $p/E$. This is consistent with the siting of the $^{238}\text{U}$ resonances in the WIMS group structure.

2. The value of $p$ in each region can be obtained by performing a spatial calculation for the group without resonance absorption and a further calculation for the group with resonance absorption.
present. The ratio of the two estimates of flux for each region we take to be \( (1 + p)/2 \) for that region. This estimate cannot be exact, because it does not attempt to take account of the resonance holes, but it should be sufficiently accurate for the correction we shall apply.

For a nuclide with constant cross section \( \sigma_s \)

\[
\sigma_{g \rightarrow g+1} = \sigma_s \int_{E_g}^{E_{g+1}} \phi(E) \, dE \int_{E_g}^{E_{g+1}} P(E \rightarrow E') \, dE' / \int_{E_g}^{E_{g+1}} \phi(E) \, dE \quad \ldots(8.18)
\]

If the energy corresponding to the lethargy centre of group \( g \) is \( E_g \)

\[
\sigma_{g \rightarrow g+1} = \frac{2 \sigma_s}{(1+p) \tau_g} \left( p \, S + T \right) \quad \ldots(8.19)
\]

The terms \( S \) and \( T \) can be computed in advance from the usual form of \( P(E \rightarrow E') \)

\[
P(E \rightarrow E') = H(E - E')H(E' - \alpha E)/E(1 - \alpha) \quad \ldots(8.20)
\]

where \( H \) is the unit Heaviside function. The scatter matrix in the absence of flux depression is simply
Resonance interaction effects

A discussion of the method of incorporating the interaction between resonances of different fuel nuclides has been given by Askew (1966 and 1969) and essentially the same procedure is followed here. For each nuclide in turn we calculate $S(\sigma_{ri})$ of equation 7.36 ignoring both resonance scattering and resonance absorption in other fuel nuclides. Having computed

$$I = \sum_i \frac{a_i S(\sigma_{ri})}{\sigma_{ri} + S(\sigma_{ri})} \quad ... (8.22)$$

we can obtain an effective $\sigma_{pn}$ for this nuclide by equating

$$I = \sum_i \frac{a_i \sigma_{pn}}{\sigma_{ri} + \sigma_{pn}} \quad ... (8.23)$$

and solving for $\sigma_{pn}$. Using the fit of equation 8.12 we can also obtain a resonance scattering integral for the nuclide. From the absorption and scattering integrals we have a first estimate of $\sigma_{sn}$ and $\sigma_{an}$. Having completed one pass through the fuel nuclides we can define for each nuclide in turn a $\sigma_{so}$ and $\sigma_{ao}$ which are the mean scattering and absorption per fuel isotope of the other isotopes in the fuel. I can then be recomputed from

$$I_n = \sum_i \frac{a_i (\sigma_{pn} + \sigma_{so})}{\sigma_{ri} + \sigma_{pn} + \sigma_{so} + \sigma_{ao}} \quad ... (8.24)$$
Finally $\sigma_{an}$ for nuclide $n$ becomes

$$\sigma_{an} = \frac{I_n}{\tau_g - \sum_m \left( \frac{I_m}{\sigma_m} \right)}$$

...(8.25)

The computer code and libraries required to perform the sequence of calculation steps outlined in this chapter will not be complete for some time. It is therefore impossible to provide numerical evidence beyond that given in Chapter 7 in support of the approach adopted. However, from the similarities between this resonance treatment and that already used in the WIMS programme (Askew et al. 1966) we are confident that the results ultimately obtained from the model will be satisfactory. The main departure from the model proposed by Askew (1969) is the use of the subgroup method which allows numerical collision probabilities to be incorporated directly into the equivalence relation. In the earlier chapters we have described, for each geometry, a collision probability routine which is sufficiently fast and accurate for this purpose.
CHAPTER 9

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