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Calculation of resonance absorption in heterogeneous reactor systems

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CALCULATION OF RESONANCE ABSORPTION
IN HETEROGENEOUS REACTOR SYSTEMS

by

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SUMMARY

The problem of calculating the resonance escape probability in an isolated resonance in a two region heterogeneous reactor system at zero temperature is considered.

The first two chapters consist of background material most of which is quite well known but some originality in presentation is claimed in that the candidate has attempted to place the various different theories into a unified approach. One advantage in so doing is that the essential differences between the approaches of the Russian and Western workers are more clearly exhibited.

The checking of approximate theories requires the designing of a computer code which gives an 'exact' solution to the problem considered. To this end an algorithm is derived in chapter 3 upon which a computer code to give such exact solutions has been based.

Chapters 4 and 5 are concerned with the derivation of approximate theories.

In chapter 4 an equivalence relation between homogeneous and heterogeneous systems is derived and considerable discussion of the effect of the mutual screening of fuel elements on the equivalence relation is undertaken. It is in this latter investigation, when the better features of the Russian approach are incorporated into the equivalence relation, that the advantage of the earlier unified approach is seen.
In chapter 5 an approximate method of solving the slowing down equations is presented. The approximate solution is found by an application of the Galerkin method. The relation between this Galerkin method approximate solution and the well known $\lambda$ method approximate solution of Goldstein and Cohen is discussed.

Chapter 6 gives a discussion of the effectiveness of the equivalence relation derived in chapter 4 and it is shown that such error as there is arises mainly from the use of the narrow resonance approximation in the derivation of the equivalence relation.
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1. SLOWING DOWN AND ABSORPTION IN HETEROGENEOUS REACTOR SYSTEMS

1.1 Historical Review

The cross sections of fuel nuclides of interest in nuclear reactor theory (e.g. $^{235}\text{U}$, $^{238}\text{U}$) exhibit sharp peaks at various energies between fission and thermal in which the probability of radiative capture of neutrons undergoing the slowing down process is greatly increased. These sharp peaks in cross sections are known as resonances and the capture process as resonance absorption. [Weinberg and Wigner (1958)] It was realised by early workers in the field that reactor systems in which the fuel and moderator materials were physically separated (heterogeneous systems) were preferable to those in which the fuel and moderator were mixed homogeneously (homogeneous systems) since the amount of resonance absorption is reduced in the latter type of system.

The problem of finding reasonably simple and accurate expressions for the resonance absorption in both homogeneous and heterogeneous reactor systems has engaged the attention of research workers for many years. The most important theoretical work was done by Wigner (1955) in the U.S. and Gurevich and Pomeranchouk (1956) in the U.S.S.R., each approaching the problem of an isolated lump in an infinite sea of moderator from a slightly different point of view. The use of the narrow resonance approximation was fundamental to both of these works. By introducing a simple approximation to the neutron lump escape probability (the Wigner rational approximation), Wigner developed the notion of surface and volume absorption. The U.S.S.R. authors took more detailed account of the lump escape
probability but considered only purely absorbing fuel lumps.

A major step was taken by Chernick and Vernon (1958) who introduced the integral equations which govern the slowing down process (the slowing down equations) into the theory of both homogeneous and heterogeneous systems. These authors formalised the distinction between the narrow resonance and narrow resonance infinite absorber approximations and used these to obtain approximate solutions to the slowing down equations. They also discussed the problem of accounting for the screening of fuel lumps in regular heterogeneous lattices, elaborating on the work of Dancoff and Ginsburg (1944), who considered the screening of two neighbouring rods.

By using the Wigner rational and narrow resonance approximations Chernik and Vernon demonstrated an equivalence between homogeneous and heterogeneous systems. Obtaining more exact forms of this equivalence has been one of the major aims of recent research.

A significant advance was achieved by Goldstein and Cohen (1962), who in dealing with the homogeneous problem proposed a method of interpolating between the narrow resonance and narrow resonance infinite absorber approximations to obtain more accurate solutions to the slowing down equations. Higher order approximations of this type were investigated by Dyos and Keane (1966). This method was initially formulated for the case of the
narrow resonance approximation applied to the moderator nuclides but was subsequently extended to remove this restriction by Goldstein (1965). The manner in which temperature changes affect this method has been investigated by McKay and Pollard (1963). The method was extended to heterogeneous systems by Goldstein and Brooks (1964) and Sehgal and Goldstein (1966). This extension made use of an improved form of the Wigner rational approximation which had been developed by a number of authors; Bell (1959b), Rothenstein (1959) and Leslie, Hill and Jonsson (1965).

A problem fundamental to heterogeneous theory is that of finding simple and accurate approximations to the factor determining the screening of fuel lumps (The Dancoff factor). This depends on calculating the first flight collision probability in moderator. Case, de Hoffman and Placzek (1953) have shown that for fuel regions the calculation of first flight collision probabilities is facilitated through the use of chord distributions. Though well defined for convex fuel regions the chord distribution for concave moderator regions has remained a completely unknown, obscure and elusive function. Sauer (1963) has however, had some measure of success in approximating this function and from this obtained an approximation for the Dancoff factor. Sophisticated expressions for the Dancoff factor have been developed by Carlvik and Pershagen (1959) and Fukai (1961, 1963) but these are more complicated than the approximation of Sauer.
Hand in hand with these approximate analytical techniques, numerical methods have been developed to obtain accurate computer solutions to the slowing down equations. Nordheim (1961a) derived an algorithm for homogeneous systems. By applying the narrow resonance approximation to the external moderator Nordheim (1961b) extends this approach to heterogeneous systems. Slightly different numerical processes for the homogeneous equations were developed by Pollard (1964) and Mikhailus (1962). Various numerical techniques for dealing with the heterogeneous equations in all their complexity have been considered by Kier and Robba (1967) and Brissenden and Durston (1965).

The investigations in this thesis are concentrated on the following areas.

Firstly an algorithm using a sophisticated integration rule is developed for the numerical solution of the slowing down equations in heterogeneous systems. A particular feature of this algorithm is the use of a variable step length in order to deal with a wide energy range viz. 20Kev to 0.7ev.

An improved approximation to the first flight collision probability in the fuel is investigated and used to obtain a new equivalence relation between homogeneous and heterogeneous systems.

We then attempt to find an approximate solution to the slowing down equations in heterogeneous systems by use of the
Galerkin method. The approximation so derived is seen to be superior to ones currently in use. The relationship between the Galerkin method approximation and the \( \lambda \) method developed by Goldstein and others is also discussed.

Finally a numerical study is performed on a number of typical systems in order to give some estimate of the errors implicit in the approximation to the neutron collision probability in the fuel and also the error in the use of the narrow resonance approximation in the external moderator.

1.2 Basic Equations for Heterogeneous Systems

Chernik and Vernon (1958) derived the slowing down equations in heterogeneous systems on the basis of physical arguments. We shall demonstrate here how the slowing down equations may be obtained by integration of the Boltzmann transport equation.

We shall take as our model a two region heterogeneous system consisting of fuel lumps placed in a regular lattice arrangement in a sea of moderator. We shall consider a cell of such a system and seek the equations governing the neutron flux in the energy region in which resonance absorption occurs and from this the quantity of main interest, the probability that a neutron escapes capture while slowing down. To simplify the analysis we shall assume without loss of generality that there is only one nuclide in each region. We shall denote the fuel region with suffix 1 and the moderator region with suffix 2.
We let

\[ \phi_i(r, E) = \text{the flux at position } r \text{ and energy } E \text{ in the } i\text{th region} \]

\[ V_i = \text{the volume of region } i \]

\[ \sum_t (E) = \text{the total macroscopic cross section of the } i\text{th region} \]

\[ \sum_1 = \text{the macroscopic potential scattering cross section of the } i\text{th region} \]

\[ \sum_s (r', E' \rightarrow E) = \text{the differential cross section for a neutron having a scattering collision at } r' \text{ in region } i \text{ changing its energy from } E' \text{ to } E. \]

If we assume spherically symmetric isotropic scattering in the centre of mass system then

\[ \sum_s (r', E' \rightarrow E) = \frac{\sum_s (E')}{(1 - a_i) E'} \]

where

\[ \sum_s (E') = \text{the macroscopic scattering cross section of the } i\text{th region} \]

and \( a_i \) is the minimum fraction of a neutron's energy retained after an elastic collision with the nuclide in region \( i \).

Davison (1958) gives the integrated form of the Boltzmann transport equation

\[ \phi_i(r, E) = \int \frac{e^{-\tau_E(r; r')}}{4\pi |r-r'|^2} \left\{ \sum_{j=1}^{2} \phi_j(r', E') \sum_s (r', E' \rightarrow E)dE' \right\} dr' \quad (1.2.1) \]

for \( i = 1, 2 \)

where

\[ \tau_E(r; r') = \int_r^{r'} \sum_t (s, E) ds \quad (1.2.2) \]
and \( \sum_E (\sigma_E) \) = total macroscopic cross section at the point \( s \).

In the case of a uniform medium

\[
\tau_E (r;r') = \sum_t (E) |r-r'|^{-1}
\]

We shall concentrate our attention on the equation for the fuel flux, so that we put \( i = 1 \) in equation (1.2.1). Noting that

\[
\sum_E (E') = \sum_2 \text{ and assuming spherically symmetric isotropic scattering}
\]

in the centre of mass system we have

\[
\phi_1 (r,E) = \int_{V_1} \frac{d^3 r'}{4\pi |r-r'|^2} \frac{-\tau_E (r;r')}{E/\alpha_1} \phi_1 (r',E') \Sigma_1 (E') dE' + \int_{V_2} \frac{d^3 r'}{4\pi |r-r'|^2} \frac{-\tau_E (r;r')}{E/\alpha_2} \phi_2 (r',E') \Sigma_2 (E') dE' \]

A similar equation may be obtained for \( \phi_2 (r,E) \).

To solve these equations for the space and energy dependent fluxes would involve a great deal of effort. By expanding the spatial component in a series of Legendre polynomials Corngold (1957) and Takahashi (1960) have obtained expressions for the space and energy dependent fluxes for slab and cylindrical systems with hydrogenous moderators.

In this thesis we shall only concern ourselves with the spatially averaged, energy dependent fluxes,

\[
\phi_i (E) = \frac{1}{V_i} \int_{V_i} \phi_i (r,E) dr\quad i = 1,2
\]

Performing this space averaging integration on equation (1.2.4) we obtain
In order to remove the spatial dependence of the inner energy integrals in equation (1.2.5) we must assume that the flux is spatially flat in both the fuel and moderator regions. Ludewig (1967) has investigated the error in this assumption for slab systems. He shows that the error in the probability of escaping capture in an isolated resonance is positive and increases with slab thickness, also that for strongly absorbing systems the flat flux assumption is quite reasonable.

Now it is well known from the results of transport theory that

$$e^{-\tau_E(r,r')} = \frac{e^{-\tau_E(r,r')}}{4\pi|\mathbf{r}-\mathbf{r}'|^2}$$

is the probability density that a neutron born at \( r' \) arrives at \( r \) without a collision and thus

$$\frac{\Sigma_{t_1}(E)}{V_1} \int_{V_1} dr \int_{V_2} dr'e^{-\tau_E(r,r')} = \frac{\Sigma_{t_1}(E)}{V_1} \int_{V_1} dr \int_{V_2} dr'e^{-\tau_E(r,r')}$$

$$= \frac{V_j}{V_1} \Sigma_{t_1}(E) \int_{V_i} dr \int_{V_j} dr'e^{-\tau_E(r,r')}$$

$$= \frac{V_j}{V_1} \Sigma_{t_1}(E) \int_{V_i} dr \int_{V_j} dr'e^{-\tau_E(r,r')}$$

$$= \frac{V_j}{V_1} \Sigma_{t_1}(E) \int_{V_i} dr \int_{V_j} dr'e^{-\tau_E(r,r')}$$

$$= \frac{V_j}{V_1} \Sigma_{t_1}(E) \int_{V_i} dr \int_{V_j} dr'e^{-\tau_E(r,r')}$$

$$(1.2.6)$$

where
\[ P_{ji} = \text{the probability that a neutron born at energy } E \text{ in region } j \text{ will have its next collision in region } i. \quad (1.2.7) \]

We observe that these quantities are related to the coefficients of the energy integrals in equation (1.2.5).

Hence on multiplying throughout by \( \Sigma_i(E) \) in equation (1.2.5) and making the flat flux assumption we obtain

\[
V_1 \Sigma_{t_1} (E) \phi_1 (E) = V_1 P_{11} \int_E^{E/\alpha_1} \left[ \frac{\Sigma_s (E') \phi_1 (E') dE'}{(1-\alpha_1) E'} \right] \]

\[
+ V_2 (1-P_{22}) \int_E^{E/\alpha_2} \left[ \frac{\Sigma_2 \phi_2 (E') dE'}{(1-\alpha_2) E'} \right]
\]

\[ (1.2.8a) \]

A similar equation is obtained for \( \phi_2 (E) \)

\[
V_2 \Sigma_2 \phi_2 (E) = V_1 (1-P_{11}) \int_E^{E/\alpha_1} \left[ \frac{\Sigma_s (E') \phi_2 (E') dE'}{(1-\alpha_1) E'} \right] \]

\[
+ V_2 P_{22} \int_E^{E/\alpha_2} \left[ \frac{\Sigma_2 \phi_2 (E') dE'}{(1-\alpha_2) E'} \right]
\]

\[ (1.2.8b) \]

The integral equations (1.2.8) are those given by Chernik and Vernon (1958). The major part of our investigation shall be directed towards obtaining numerical and approximate analytic solutions to these equations. We shall henceforth refer to the set of equations (1.2.8) as the slowing down equations.

The above derivation is easily generalised to a system containing several regions and nuclides. For such a system the equations for the spatially flat flux are

\[
V_j \Sigma_j (E) \phi_j (E) = \sum_{i=1}^{M} V_i P_{ij} \int_{E/\alpha_{ik}}^{E} \left[ \frac{\Sigma_{ik} (E') \phi_i (E') dE'}{(1-\alpha_{ik}) E'} \right] \quad (j=1, \ldots M)
\]

\[ (1.2.9a) \]
where

\[ M = \text{the number of different regions} \]

\[ n_i = \text{the number of nuclides in region } i \]

and the subscript \( ik \) refers to the \( k^{th} \) nuclide in the \( i^{th} \) region.

e.g.

\[ \Sigma_{ik} = \text{macroscopic potential scattering cross section of} \]

the \( k^{th} \) nuclide in the \( i^{th} \) region.

It is quite often convenient to express the neutron balance in terms of the collision density,

\[ F_j(E) = \sum_{t_j} \Sigma_{t_j}(E) \phi_j(E) \]

in which case the slowing down equations assume the form

\[ V_j F_j(E) = \sum_{i=1}^{M} \sum_{p_{ij}} \int_{E}^{E/a_{ik}} \frac{E/a_{ik}}{\Sigma_{t_i}(E')} \frac{s_{ik}}{\Sigma_{t_i}(E')} \frac{F_i(E')}{(1-a_{ik})E'} dE' \]

The quantity of main interest however is not the flux but the resonance escape probability. We now outline the derivation of the expression for this quantity. We shall consider firstly the 2 region, 1 nuclide per region model.

Define

\[ q_i(r,E) = \text{Number of neutrons/unit time/unit volume which} \]

\[ \text{are scattered at } r \text{ from an energy above } E \text{ to an} \]

\[ \text{energy below } E \text{ in region } i. \]

Under the assumption of spherically symmetric isotropic scattering in the C of M system (Davison (1958))
Let us consider a cell of the regular heterogeneous system consisting of a fuel lump and moderator. We seek the average slowing down density in this cell. i.e. we seek

\[ q(E) = \text{the number of neutrons which slow down past energy} \]
\[ \frac{E}{\text{unit time/unit volume in the cell}}. \]

Obviously

\[ q(E) = \frac{1}{V_t} \int_{1}^{E} q_i(r, E) \text{dr} \tag{1.2.11} \]

where \( V_t = V_1 + V_2 = \text{total volume of cell.} \)

Hence, on performing the \( r \) integration we can express \( q(E) \) in terms of the spatially averaged fluxes. i.e.

\[ V_t q(E) = V_1 \int_{E}^{ \frac{E}{\alpha_1} } \frac{E}{\alpha_1} \Sigma_s (E')(E-\alpha_1 E')\phi_1(E')dE' \tag{1.2.12} \]

Generalising to the several nuclide, several region situation we obtain

\[ V_t q(E) = \sum_{i=1}^{M} \sum_{k=1}^{N_i} \frac{E/\alpha_{ik} \Sigma_s (E')(E-\alpha_{ik} E')\phi_1(E')dE'}{(l-\alpha_{ik})E'} \tag{1.2.13} \]

where

\[ V_t = \sum_{i=1}^{M} V_i = \text{total volume of cell.} \]
Since equations (1.2.9) and (1.2.13) shall be referred to constantly in this thesis we will find it convenient to make use of the following notation.

\[ S_{ik}(E) = \sum_{E} \frac{E/a_{ik} \sum \phi_i(E') dE'}{(E')^{(1-a_{ik})}} \]  

(1.2.14a)

\[ Q_i(E) = \sum_{k=1}^{n} Q_{ik}(E) \]  

(1.2.14b)

\[ Q_{ik}(E) = \sum_{E} \frac{E/a_{ik} \sum \phi_i(E') dE'}{(E')^{(1-a_{ik})}} \]  

(1.2.14c)

\[ Q_i(E) = \sum_{k=1}^{n} Q_{ik}(E) \]  

(1.2.14d)

In terms of this notation equations (1.2.9) and (1.2.13) have the form

\[ V_q = \sum_{j} \phi_j(E) = \sum_{i=1}^{M} V_i \sum_{j} p_{ij} s_j(E) \]  

(1.2.9)

\[ V_t q(E) = \sum_{i=1}^{M} V_i Q_i \]  

(1.2.13)

Differentiating (1.2.13) with respect to \( E \) and making use of (1.2.9)

\[ V_t \frac{dq(E)}{dE} = \sum_{i=1}^{M} V_i s_i(E) - \sum_{j=1}^{M} \frac{s_j(E)}{t_j} \sum_{i=1}^{M} V_i p_{ij} s_i \]

Making use of the relation \( \sum_{j=1}^{M} p_{ij} = 1 \) this equation may be rewritten
\begin{align*}
V_t \frac{dq(E)}{dE} &= \sum_{j=1}^{M} \frac{\Sigma_{a_j}(E)}{\Sigma_{t_j}(E)} \sum_{i=1}^{M} V_i P_{ij} S_i \\
&= \sum_{j=1}^{M} V_j (E) \phi_j(E) \\
\text{Integrating we obtain:} \\
q(E_s) - q(E) &= \sum_{j=1}^{M} \frac{V_i}{V_t} \int_{E}^{E_s} \Sigma_{a_j}(E') \phi_j(E') dE' \\
&= 1 - q(E) \\
\text{where } E_s = \text{source energy} \\
q(E_s) = \text{source distribution} = \text{slowing down density at } E_s. \\
\text{Normalising the source distribution to unity and defining} \\
p(E) = \text{probability that a source neutron will reach energy } E \text{ without being captured.} \\
\text{then } p(E) = 1 - q(E) \\
= \sum_{j=1}^{M} \frac{V_i}{V_t} \int_{E}^{E_s} \Sigma_{a_j}(E') \phi_j(E') dE' \\
\text{If } E_r \text{ is the peak energy of an isolated resonance} \\
\text{and } E^+_r, E^-_r \text{ are, respectively, the energies above and below } E_r \text{ at which the fluxes resume the asymptotic form, then} \\
p(E_r) = \sum_{j=1}^{M} \frac{V_i}{V_t} \int_{E^-_r}^{E^+_r} \Sigma_{a_j}(E') j(E') dE' \\
is the probability that a neutron escapes capture while slowing down through the resonance. The quantity } p(E_r) \text{ is known as the}
resonance escape probability and often just denoted by $p_r$. It is the calculation of $p_r$ with which we shall be concerned in this thesis.

1.3 The Effective Resonance Integral and Breit-Wigner Resonance Contours

It is conventional to express the resonance escape probability in terms of a quantity known as the effective resonance integral. Two definitions of this quantity have been proposed by Dresner (1960) and McKay (1964).

Dresner defines the effective resonance integral as "the lethargy integrated absorption cross section required to produce the same amount of absorption as actually takes place in a resonance, assuming that the flux has the same value it would have in the absence of the resonance".

This means that, in a cell of regular heterogeneous lattice, the probability of a neutron escaping capture in slowing down from energy $E_r^+$ above an isolated resonance to energy $E_r^-$ below the resonance is given by

$$p_r = 1 - V_1 I/\xi_n \sigma_a V_f$$  (1.3.1)

where $I$, the effective resonance integral is given by

$$I = \int_{E_r^-}^{E_r^+} \sigma_a(E) \phi(E) dE$$  (1.3.2)

Here $\phi(E)$ is the flux in the fuel region, $\sigma_a(E)$ is the microscopic absorption cross section of the fuel nuclide, $V_1$ is the volume of the fuel region,
\( \bar{\varepsilon}_h \) is the cell averaged neutron lethargy increment per collision and \( \sigma_h \) is the cell averaged microscopic potential scattering cross section. The neutron flux is assumed to have an asymptotic value above the resonance of \( 1/E \).

McKay has shown that a more useful expression for the resonance escape probability is given by

\[
p_r = \exp(-\frac{V_1 I}{\bar{\varepsilon}_h \sigma_h V})
\]  \hspace{1cm} (1.3.3)

He chooses this form since it compensates to some extent for the error due to the use of the narrow resonance and narrow resonance infinite absorber approximations in the case of strongly absorbing low energy resonances.

We shall use the form (1.3.3) in our work.

The resonance cross sections for an isolated resonance in absorbing material at \( 0^\circ A \) are well represented by the single level Breit-Wigner contour forms (Blatt and Weisskopf, 1952).

The appropriate expressions are

\[
\sigma_a(E) = \frac{\sigma_o \Gamma_n / \Gamma}{1 + x^2}
\]  \hspace{1cm} (1.3.4)

\[
\sigma_{sr}(E) = \frac{\sigma_o \Gamma_i / \Gamma}{1 + x^2}
\]  \hspace{1cm} (1.3.5)

where \( \sigma_a(E) \) is the microscopic resonance capture cross section of the fuel nuclide, \( \sigma_{sr}(E) \) is the microscopic resonance scattering cross section of the fuel nuclide, \( E_r \) is the resonance energy, \( \Gamma_n \), \( \Gamma_i \) and \( \Gamma \) are respectively the neutron, radiative capture and total widths of the resonance level, these quantities have
the dimensions of energy. \( \sigma_0 \) the peak total resonance cross section is given by

\[
\sigma_0 = \frac{4\pi}{k^2} g_J \frac{\Gamma_n}{\Gamma}
\]  \( \text{(1.3.6)} \)

where \( k \) is the wave number of the neutron in the neutron-nucleus centre of mass system and \( g_J \) is a statistical spin factor. After choosing the appropriate values of \( g_J \) and \( k \)

\[
\sigma_0 = 2.608 \times 10^6 \frac{\Gamma_n}{\Gamma E_r}
\]  \( \text{(1.3.7)} \)

In equations (1.3.4) and (1.3.5) \( \chi = \frac{2}{\Gamma} (E-E_r) \) \( \text{(1.3.8)} \)

Thus the total microscopic cross section of the fuel nuclide is given by

\[
\sigma_r(E) = \sigma_p + \frac{\sigma_0}{1+\chi^2}
\]  \( \text{(1.3.9)} \)

where \( \sigma_p \) is the microscopic potential scattering cross section of the fuel nuclide.

It is also convenient to define \( \sigma_r(E) \), the microscopic resonance cross section,

\[
\sigma_r(E) = \sigma_r(E) - \sigma_p
\]

The relations (1.3.4) and (1.3.5) apply at zero temperature when the nuclei are at rest in the laboratory frame of reference. At non-zero temperatures when the motion of the nuclei must be taken into account the resonance cross sections undergo Doppler broadening and the expressions become (see, for example, Dresner)
\[ \sigma_a(E) = \frac{\sigma_0 \Gamma}{\Gamma} \psi(x, \theta) \quad (1.3.10) \]

\[ \sigma_{sr}(E) = \frac{\sigma_0 \Gamma}{\Gamma} \psi(x, \theta) \quad (1.3.11) \]

where

\[ \Delta = \left( \frac{4mT}{M} \right)^{1/2}, \quad \theta = \frac{\Gamma}{\Delta} \]

\( T \) is the temperature in energy units, \( M \) is the mass of the nuclide, \( m \) is the neutron reduced mass and

\[ \psi(x, \theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\theta^2(x-y)^2/4} \frac{dy}{1+y^2} \quad (1.3.12) \]

In this thesis we shall concentrate on calculating the resonance integral for an isolated resonance in a regular two region lattice at \( 0^\circ A \).

1.4 Escape Probabilities

In this section we summarise some of the current approximations to the region escape probabilities introduced in equation (1.2.7).

The quantity we seek is in fact directly related to the fraction of uncollided neutrons reaching region \( i \) from region \( j \). The calculation of the flux of such neutrons can be regarded as a one velocity transport problem.

In a purely absorbing medium the one velocity flux at \( r \), in direction \( \Omega \) of neutrons having energy \( E \) viz. \( \phi(\mathbf{r'} \Omega, E) \) due to a unit isotropic point source at \( r' \) emitting neutrons at energy \( E \) is the solution of the one velocity transport equation,

(In what follows \( \Sigma_a(r, E) \) is the macroscopic absorption cross section at the point \( r \))
\[ \Omega \cdot \nabla \frac{\phi(r,\Omega,E)}{\Sigma_a(r,E)\phi(r,\Omega,E)} = \frac{\delta(r-r')}{4\pi} \]

The total flux at \( r \) of neutrons of energy \( E \) due to a unit isotropic point source at \( r' \) is given by

\[ \phi(r,r',E) = \int \phi(r,\Omega,E)d\Omega \]

and is found to be (Megrebian and Holmes, 1960)

\[ \phi(r,r',E) = \frac{e^{-\tau(r,r')}}{4\pi |r-r'|^2} \]

where

\[ \tau(r,r') = \int_0 |r-r'| \Sigma_a(r-R\Omega,E)dR \]

In regions in which both scattering and absorption are taken into account the energy dependent flux at \( r \), in direction \( \Omega \), at energy \( E \), \( \phi(r,\Omega,E) \), will be given by the Boltzmann transport equation

\[ \Omega \cdot \nabla \frac{\phi(r,\Omega,E)}{\Sigma_t(r,E)\phi(r,\Omega,E)} \neq \int \int \int \Sigma_a(r, \Omega')\phi(r, \Omega', E)dE'd\Omega' \]

\[ = \frac{\delta (r-r')}{4\pi} \]

Again the source term has been chosen for the case of an isotropic unit point source at \( r' \) emitting neutrons with energy \( E \).

If we ignore the scattering term in equation (1.4.4) the resulting equation would describe the flux at \( r \) due to un-collided neutrons born with energy \( E \) at the point source at \( r' \). We would in fact be dealing with a one velocity problem and our
new equation would have the same solution as equation (1.4.1) but with \( \tau(r,r') \) redefined as

\[
\tau(r;r') = \int_0^r (r-r') \Sigma_t(r-R, E) dR
\]

and now

\[
\phi(r;r') = \text{the total flux of energy } E \text{ at } r \text{ due to un-collided neutrons emanating from an isotropic unit point source at } r' \text{ with energy } E
\]

We are interested in finding the region escape probability in Multiregion systems. Hence we consider the situation in equation (1.4.6) where \( r \) and \( r' \) are in different regions.

We take \( r \) to be in region \( i \) having volume \( V_i \) and \( r' \) to be in region \( j \) having volume \( V_j \) (see figure 1.1)

![Fig. 1.1](image)

We define the quantity

\[
\pi(r') = \int_{V_i} \phi(r;r') dr
\]

(1.4.7)

= The average flux of energy \( E \) in region \( i \) due to uncollided neutrons emanating from an isotropic unit point source at \( r' \) with energy \( E \).
We can use $\pi(r')$ to derive an expression for the quantity in which we are interested. We define

$$P_i(r') = \sum_{t_i} \pi(E) \pi(r')$$

= The average number of collisions suffered in region $i$ by uncollided neutrons emanating from an isotropic unit point source at $r'$ with energy $E$.

= The probability that a neutron born at $r'$ in region $j$ will suffer its next collision somewhere in region $i$.

By averaging this function over region $j$ we obtain

$$P_{ji} = \frac{1}{V_j} \int_{V_j} P_i(r') dr' = \frac{\sum_{t_i} \pi(E)}{V_j} \int_{V_j} dr' \int_{V_i} dr \frac{e^{-\tau(r;r')}}{4\pi |r-r'|^2}$$

(1.4.9)

= The probability that a neutron born in region $j$ at energy $E$ will suffer its next collision in region $i$.

We observe that the expressions (1.2.7) and (1.4.9) are consistent.

By a change in the order of integration it is a simple matter to demonstrate the reciprocity theorem (Case, de Hoffman and Placzek, 1953) viz

$$V_i \sum_{t_i} \pi(E) P_{ij} = V_j \sum_{t_j} \pi(E) P_{ji}.$$ 

In particular we have from equation (1.4.9) a quantity which plays an important part in heterogeneous resonance theory

$$P_{jj} = \frac{\sum_{t_j} \pi(E)}{V_j} \int_{V_j} dr' \int_{V_j} dr \frac{e^{-\tau(r;r')}}{4\pi |r-r'|^2}$$

(1.4.10)
The probability that a neutron born in region \( j \) will suffer its next collision in region \( j \).

In the situation with which we shall be most concerned, that of a regular lattice, the path of integration of \( \tau(r;r') \) in equation (1.4.10) would traverse the regions separating the material of region \( j \). Consequently the expression for \( \tau(r;r') \) will be quite complicated and the integration in equation (1.4.10) invariably leads to special functions. Fayers (1966) reviews the methods of integrating equation (1.4.10) directly for slab and cylindrical systems. Bonalumi (1961) has derived expressions for cylindrical annuli.

The complicated nature of these expressions prohibits their use in approximate methods of solving the slowing down equations. For this reason rational type approximations have been developed for \( P_{jj} \).

In turns out to be most convenient to first of all express \( P_{jj} \) in terms of the lump escape probabilities (i.e. the probability that a neutron will reach the surface of the lump in which it was born). Then by developing rational type approximations for these lump escape probabilities we are able in turn to find rational type approximations for \( P_{jj} \).

We define

\[
P_{j}^{(esc)} = \text{The probability that a neutron born in a lump of the material of region } j \text{ will reach the surface of the lump without suffering a collision in transit.}
\]
By a direct application of the concepts introduced earlier in this section we find that

\[
p_j^{\text{esc}} = \frac{1}{V_j} \int_{S_j} dr' \int_{V_j} \frac{e^{-\Sigma t_j^E(r-r')}}{4\pi |r-r'|^2} \quad (1.4.11)
\]

In the integration (1.4.11) we consider \( r' \) to lie on the surface \( S_j \) of the volume \( V_j \) and \( r \) to be a general internal point.

For many geometries it is possible to perform the integration (1.4.11) directly. However it is also useful to introduce the concept of the chord distribution to calculate \( p_j^{\text{esc}} \) (Case, de Hoffman and Placzek (1953)).

Figure (1.2) illustrates a typical situation

\[
x = |r-r'|
\]

\[
dr = (n.\Omega) x^2 dx d\Omega
\]

Using the notation of figure (1.3) we have from equation (1.4.11)

\[
p_j^{\text{esc}} = \frac{1}{4\pi V_j} \int_{S_j} dr' \int_{V_j} e^{-\Sigma t_j^E} dx (n.\Omega) d\Omega
\]

\[
= \frac{1}{4\pi V_j \Sigma t_j^E} \int_{S_j} \int_{\Omega} \left( 1 - e^{-\Sigma t_j^E} \right) (n.\Omega) d\Omega dS
\]
At this point Case, de Hoffman and Placzek introduce the chord distribution function
\[
f_j(\ell) = \frac{1}{\pi S_j} \int_{S_j} dS \int_{\Omega=\Omega(\ell)} (\Omega.n) d\Omega \tag{1.4.13}
\]

= The probability that a chord in region j will have a length between \( \ell \) and \( \ell + d\ell \).

In terms of this function
\[
P_j^{\text{(esc)}} = \frac{S_j}{4V_j \Sigma t_j(E)} \left[ \left( 1 - e^{-\Sigma t_j(E)\ell} \right) \right] f_j(\ell) d\ell \tag{1.4.14}
\]

Hence the problem of finding \( P_j^{\text{(esc)}} \) can be reduced to that of finding the chord distribution function for the lump in question. This can however present just as much difficulty as the direct integration of equation (1.4.11), especially in the case of concave moderator regions for which the nature of the chord distribution function is very poorly understood.

An interesting approach which completely obviates the chord distribution has been proposed by Takahashi (1960). He solves equation (1.4.4) without the scattering term to find the uncollided flux in the moderator region. Then he uses this expression to perform the integrations (1.4.7) and (1.4.9) to find the lump escape probability.
There is a function closely related to $p_j^{(esc)}$ which plays an important part in the theory, it is defined as follows:

$$G_j = \text{the probability that a neutron incident on the surface } S_j \text{ of the region } j \text{ will suffer a collision in that region.}$$

An expression for this quantity is also found integrating the total flux of uncollided neutrons from an isotropic unit point source on the surface $S_j$. So that

$$G_j = \frac{4\Sigma t_j (E)}{S_j} \int_{S_j} dr' \int_{V_j} dr e^{-\Sigma t_j (E)|r-r'|} \frac{-\Sigma t_j (E)|r-r'|}{4\pi |r-r'|^2} \quad (1.4.15)$$

By comparing (1.4.15) with (1.4.11) we find that

$$G_j = \frac{4V_j \Sigma t_j (E)}{S_j} p_j^{(esc)} \quad (1.4.16)$$

which is the surface reciprocity theorem. (Fayers 1966).

An expression for $p_{jj}$ may be derived in terms of $p_j^{(esc)}$ and $G_j$. We shall consider a two region system. Let index 1 denote the fuel region and index 2 the moderator region. Henceforth we shall refer to $p_j^{(esc)}$ simply as $p_j$.

To obtain $p_{11}$ we consider a neutron born in a fuel lump and track it across fuel and moderator regions using the functions $p_1, G_1, p_2, G_2$ to describe the probability of crossing the various surfaces and regions without suffering a collision.
Referring to figure (1.3) we see that

\[ P_{11} = \text{the prob. that a neutron born in A collides in A} \]

+ \text{the prob. that a neutron born in A escapes A, passes through the mod, collides in B}

+ \text{the prob. that a neutron born in A escapes A, passes through the mod, passes through B, passes through mod, collides in C}

+ \text{etc.}

\[ = (1-P_1) + P_1(1-G_2)G_1 + P_1(1-G_2)(1-G_1)(1-G_2)G_1 + \ldots \]

i.e. \[ P_{11} = \frac{G_1 + G_2(1-P_1-G_1)}{1-(1-G_1)(1-G_2)} \] (1.4.17a)

Similarly

\[ P_{22} = \frac{G_2 + G_1(1-P_2-G_2)}{1-(1-G_1)(1-G_2)} \] (1.4.17b)

Since the derivation of the expressions (1.4.17) relied upon the average probabilities \( P_j \) and \( G_j \) it has been tacitly assumed that the neutrons fall isotropically onto each lump. Generally this assumption introduces small error. In fact the nature of this error has been investigated by Aisu and Minton (1964) who conclude that it is negligible except in the case of transparent slab absorbers.

These expressions for \( P_{11} \) and \( P_{22} \) were first
derived by Bell (1959a) and later by Rothenstein (1960) and Leslie, Hill and Jonsson (1965) under various other assumptions.

The quantity $G_2$ has become known in the literature as the Dancoff correction.

1.5 Approximations to the Lump Escape Probabilities

1.5.1 Rational Type Approximations

Rational type approximations to $p_i, G_1, p_2, G_2$ are found in terms of the mean chord length for a lump of the material of region $i$ viz.

$$\bar{\ell}_i = \int \ell f_i(\ell) d\ell$$

It is shown by Case, de Hoffman and Placzek that

$$\bar{\ell}_i = \frac{4V_i}{S_i} \quad (1.5.1)$$

where $V_i$ is the volume of the lump of material of region $i$ and $S_i$ its surface area.

So for two region lattices

$$V_1 \bar{\ell}_2 = V_2 \bar{\ell}_1$$

In terms of this quantity equation (1.4.14) may be written

$$p_j = \frac{1}{\bar{\ell}_j \sum_{\ell} t_j (E)} \int \left\{ (1-e^{-\tau_{ij}(E)}} \right\} f_j(\ell) d\ell \quad (1.5.2)$$

Wigner (1955) derived a rational approximation for $p_j$ on the basis of the following approximation
\[ \int \left( 1 - e^{-\sum t_j \ell} \right) f_j(\ell) d\ell = 1 - e^{-\sum t_j \ell} \approx \frac{\sum t_j \ell}{1 + \sum t_j \ell} \quad (1.5.3) \]

Hence, the approximation to \( P_j \) is

\[ P_j = \frac{1}{1 + \sum t_j \ell} \quad (1.5.4) \]

and the corresponding approximation to \( G_j \) is

\[ G_j = \frac{\sum t_j \ell}{1 + \sum t_j \ell} \quad (1.5.5) \]

Though it underestimates the actual escape probability the Wigner rational approximation (henceforth referred to as WRA) due to its simple form, allows us to cast the slowing down equations into a form amenable to analysis.

An interesting property of the WRA is that for fuel lumps it has the correct limiting behaviour in the case of \( \sum t_l \ell \) both large and small.

For example in the case of cylindrical fuel lumps (with which we shall be chiefly concerned in this thesis) the exact expression for \( P_1 \) is (Payers 1966)

\[ P_1 = \frac{1}{\sum t_l \ell} \{ 1 - \frac{4}{\pi} \int_{0}^{\pi/2} K_{1,3}(\sum t_l \ell \cos \psi) \cos \psi d\psi \} \quad (1.5.6) \]

where \( K_{i,n}(x) \), the Bickley function, is defined by
\[ K_{1,n}(x) = \int_0^\infty \frac{e^{-x \cosh u}}{\cosh^n u} \, du \quad (1.5.7) \]

From (1.5.6) we may derive the following limiting expressions for \( P_1 \):

\[ P_1 \to 1 - \frac{2}{3} \sum \frac{1}{t_1} \bar{l}_1 \quad \text{as} \quad \sum \frac{1}{t_1} \bar{l}_1 \to 0 \quad (1.5.8a) \]

\[ P_1 \to \frac{1}{\sum \frac{1}{t_1} \bar{l}_1} + \frac{3}{4(\sum \frac{1}{t_1} \bar{l}_1)^3} \quad \text{as} \quad \sum \frac{1}{t_1} \bar{l}_1 \to \infty \quad (1.5.8b) \]

From the WRA we obtain the following limiting expressions

\[ P_1 \to 1 - \sum \frac{1}{t_1} \bar{l}_1 \quad \text{as} \quad \sum \frac{1}{t_1} \bar{l}_1 \to 0 \quad (1.5.9a) \]

This is not exactly the same as (1.5.8a) but we see that both expressions exhibit the same behaviour.

Also

\[ P_1 \to \frac{1}{\sum \frac{1}{t_1} \bar{l}_1} + 0\left( \frac{1}{(\sum \frac{1}{t_1} \bar{l}_1)^2} \right) \quad \text{as} \quad \sum \frac{1}{t_1} \bar{l}_1 \to \infty \quad (1.5.9b) \]

The second terms of equations (1.5.8b) and (1.5.9b) are of different order.

Bell (1959b) suggested the following improvement to (1.5.4) for fuel lumps

\[ P_1 = \frac{1}{a + \sum \frac{1}{t_1} \bar{l}_1} \quad (1.5.10) \]
with $a$ having the following values

$$a = \begin{cases} 1.15 & \text{for slabs} \\ 1.30 & \text{for spheres and cylinders} \end{cases}$$

This approximation is superior to the WRA. The success of the introduction of this factor $a$ (the so-called Bell factor) has inspired attempts by Rothenstein (1959), and Leslie, Hill and Jonsson (1965) to find more refined estimates for it.

An approximation for cylindrical fuel lumps due to Booth (1965) played an important part in the work of Leslie, Hill and Jonsson. The approximation is

$$P_1 = 1 - \frac{\sum \frac{\ell}{t_1}(\sum \frac{\ell}{t_1} + c)}{(\sum \frac{\ell}{t_1} + b)^2}$$

(1.5.11)

where

$$b = \frac{1}{2} (3 + \sqrt{3}), \quad c = 2 + \sqrt{3}$$

This approximation does have the correct limits given by equation (1.5.8).

### 1.5.2 Approximate Chord Distributions

We see from equation (1.4.14) that a knowledge of the chord distribution function would enable us to calculate explicit expressions for the lump escape probabilities. The following chord distributions are derived by Case, de Hoffman and Placzek (1953):
(a) For a slab of thickness $a$
\[ f(l)dl = \frac{2a^2}{l^3} \, dl \quad (1.5.12) \]

(b) For an infinite cylinder of radius $a$
\[ f(l)dl = \frac{2d\ll_0}{\pi a l^3} \int_{z_0}^{l} \frac{(l^2-z^2)^{3/2}}{\sqrt{4a^2+z^2} - l^2} \, dz \quad (1.5.13) \]

where
\[ z_0 = \begin{cases} \sqrt{R^2-4a^2} & R > 2a \\ 0 & R < 2a \end{cases} \]

These exact expressions for the chord distribution functions have the disadvantage that they do not yield rational type approximations for $P_1$. Moreover for moderator regions the exact expression for the chord distribution function is difficult to find.

For these reasons Sauer (1963) developed approximate chord distribution functions for both fuel and moderator regions in a regular lattice of cylindrical fuel lumps.

Making the observation that the Wigner rational approximation may be obtained from the chord distribution
\[ f(l)dl = e^{-\ll_0 / \ll} d(\ll_0 / \ll) \]

he seeks a more accurate expression in the form
\[ f_{\text{app}}(l)dl = \frac{1}{n!} \left( \frac{(n+1)\ll}{\ll} \right)^n e^{-\frac{(n+1)\ll}{\ll_0}} d\left( \frac{(n+1)\ll}{\ll} \right) \quad (1.5.14) \]

and argues that the value of $n$ for which $f_{\text{app}}(l)$ exhibits the properties most important in the calculation of $P_1$ is obtained by equating $\ln l$ with $\int f_{\text{app}}(l) l n l dl$. The value of $n$ so obtained is $n = 3.58$. Substitution into equation (1.4.14) yields the following approximation to $P_1$. 


\[ P_n = \frac{1}{\Sigma t_1 l} \left[ 1 - \frac{1}{\left(1 + \Sigma t_1 l / (n+1)\right)^{n+1}} \right] \]  

(1.5.15)

Though quite a good approximation, equation (1.5.15) is difficult to apply in the solution of the slowing down equations because of its non linearity.

For the moderator region Sauer obtains the approximation

\[ f_2(\ell) d = \begin{cases} 0 & \ell < t \\ \exp\left[-(\ell-t)/(\bar{\ell}_2-t)\right] \left[\ell(\ell-t)/(\bar{\ell}_2-t)\right] & \ell \geq t \end{cases} \]  

(1.5.16)

where

\[ t = \tau \bar{\ell}_2 \]

and

\[ \tau = \left(\frac{\pi}{4}, \sqrt{1 + \frac{V_2}{V_1} - 1}\right) \frac{V_1}{V_2} - 0.08 \]

This leads to the approximation

\[ G_2 = 1 - e^{-\tau \Sigma t_1 \bar{\ell}_2} \]  

(1.5.17)

Bonalumi (1965) has further refined the approximation in equation (1.5.17) to obtain

\[ G_2 = 1 - e^{-t N \bar{\ell}_1 \sigma_m} \]  

(1.5.18)

where \( t_1 = t + \Delta t \)
Calculations performed by Carlvik (1967) indicate that the approximation (1.5.18) is quite accurate over a wide range of the parameters and we shall adopt it in our work.

1.6 Approximations for $P_{jj}$

We now use the rational approximations (1.5.4) and (1.5.5) in equations (1.4.17) to derive rational approximations for $P_{11}$ and $P_{22}$.

Thus into equation (1.4.17a) we substitute the rational approximation for the fuel lump escape probability

$$P_1 = \frac{1}{1 + \sum \frac{t_1}{\bar{\lambda}_1}}$$

and obtain

$$P_{11} = \frac{\sum \frac{t_1}{\bar{\lambda}_1}}{\sum \frac{t_1}{\bar{\lambda}_1 + G_2}} = \frac{\sigma_{t_1}}{\sigma_{t_1} + sG_2} \quad (1.6.1)$$

where $s = 1/N_1 \bar{\lambda}_1$ and $N_1$ is the number density of the fuel nuclide.

If we then substitute into equation (1.6.1) the
rational approximation for $G_2$ we obtain

$$P_{11} = \frac{\Sigma \frac{t_1}{t_1^2}}{\Sigma \frac{t_1}{t_1^2} + \Sigma \frac{t_2}{t_2^2}} = \frac{\sigma_{t_1}}{\sigma_{t_1} + s\sigma_m} \frac{s+\sigma_m}{s+\sigma_m} \quad (1.6.2)$$

where

$$\sigma_m = \frac{\Sigma \frac{t_2}{t_2^2}}{N_1 \cdot \frac{V_2}{V_1}} \quad (1.6.3)$$

It is a matter of simple algebra to demonstrate that with these approximations for $P_{11}$ and $P_{22}$ the reciprocity theorem is still satisfied.

A better estimate of $P_{11}$ is obtained by using the approximation to $P_1$ which includes the Bell factor (i.e. equation 1.5.10). From this

$$P_{11} = \frac{\Sigma \frac{t_1}{t_1^2}}{\Sigma \frac{t_1}{t_1^2} + \frac{aG_2}{a+(1-a)G_2}} = \frac{\sigma_{t_1}}{\sigma_{t_1} + s \sigma_e} \quad (1.6.4)$$

where

$$s = \frac{saG_2}{a+(1-a)G_2} \quad (1.6.5)$$

Equation (1.6.4) is the sought for rational approximation for $P_{11}$. Ultimately its effectiveness depends on the accuracy of $s_e$ which itself depends upon an accurate approximation for $G_2$ and an estimate of $a$ which takes account of the geometry and scattering of the fuel lump. It is clear that the values of $a$ given by Bell will be too crude for accurate work.
Leslie, Hill and Jonsson (1965) have proposed the following method of calculating a Bell factor. In essence they seek a factor $a$ so that $P_{11}$ has the form

$$P_{11} = \frac{\sigma t_1}{\sigma + a s G_2}$$

(1.6.6)

Using this approximation for $P_{11}$ and assuming that a scattering collision in the moderator region removes neutrons from the resonance energies (i.e. the narrow resonance approximation), the expression for the resonance integral will be a function of $a s G_2$ i.e.

$$I = F(a s G_2)$$

(1.6.7)

If, however, the more accurate approximation of Booth for $P_1$ (i.e. equation 1.5.11) is used in the calculation of $P_{11}$ then it may be shown that

$$I = d_1 F(r_1 s) - d_2 F(r_2 s)$$

(1.6.8)

where $r_1$, $r_2$, $d_1$ and $d_2$ are algebraic functions of $b$ and $G_2$.

The factor $a$ is then chosen by equating the expressions (1.6.7) and (1.6.8) and using for $F(s)$ the form derived empirically by Sumner (1963) viz

$$F(s) = A + B \sqrt{s}$$

(1.6.9)

where $A$ and $B$ are constants. This approach yields the following Bell factor
Leslie, Hill and Jonsson use for $G_2$ an expression derived by cylindricalising the outer boundary of the lattice cell.

Ishiguro and Takano (1968) have adopted a slightly different approach. They seek an approximation to $P_{11}$ in the form

$$P_{11} = \frac{d_1 \sigma t_1}{\sigma t_1 + r_1} + \frac{d_2 \sigma t_1}{\sigma t_1 + r_2}$$

(1.6.11)

Using the limiting expressions (1.5.8) in equation (1.4.17a) they show that $P_{11}$ has the following limits

$$P_{11} = 1 - \frac{1}{N_1 \overline{L}\sigma t_1} + 0 \left( \frac{1}{(N_1 \overline{L}\sigma t_1)^3} \right) \quad \text{as } N_1 \overline{L}\sigma t_1 \to \infty$$

(1.6.12)

$$P_{11} = N_1 \overline{D}\sigma t_1 + 0 [(N_1 \overline{D}\sigma t_1)^2 \ln(N_1 \overline{D}\sigma t_1)] \quad \text{as } N_1 \overline{L}\sigma t_1 \to 0$$

with $\overline{L} = \frac{\overline{L}_1}{G_2}$, $\overline{D} = (1/G_2 - 1/3)\overline{\lambda}_1$

They then choose $d_1, d_2, r_1, r_2$ by demanding that the expression (1.6.11) has the limiting values (1.6.12), so that

$$r_1 = [\omega_2 + (\omega_2^2 - 4\omega_3)^{1/2}] / 2$$

$$r_2 = [\omega_2 - (\omega_2^2 - 4\omega_3)^{1/2}] / 2$$

$$d_1 = (\omega_1 - r_2) / (r_1 - r_2)$$
\[ d_2 = \frac{(r_1 - \omega_1)}{(r_1 - r_2)} \]

where

\[ \omega_1 = \frac{G_2}{N_1 \bar{\ell}_1}, \quad \omega_2 = \frac{3}{N_1 \bar{\ell}_1} \quad \text{and} \quad \omega_3 = \frac{3G_2}{(N_1 \bar{\ell}_1)^2}. \]

This approximation is quite good for a wide range of \( N_1 \sigma_{t_1} \).
2. APPROXIMATE SOLUTION OF THE SLOWING DOWN EQUATIONS

2.1 Asymptotic Solution of the Slowing Down Equations

It is well known from basic slowing down theory (Glasstone and Edlund, 1952) that asymptotically the flux \( \phi_i(E) \) has the form

\[
\phi_i(E) = \frac{A}{E}
\]  

(2.1.1)

where A is a constant. We now seek the exact form of this constant for the equation (1.2.9) describing a general heterogeneous system. We substitute the asymptotic form (2.1.1) into the expression for the slowing down density (equation 1.2.13) and obtain

\[
VQ = A \sum_{i=1}^{M} \frac{n_i}{V_i} \Sigma_{ik} \xi_{ik}
\]

(2.1.2)

where \( Q \) is the asymptotic source.

From (2.1.2) we derive the result

\[
A = \frac{Q}{\bar{\Sigma}_h \Sigma_h}
\]

(2.1.3)

where \( \Sigma_h \), the cell averaged macroscopic potential scattering cross section, is given by

\[
\Sigma_h = \sum_{i=1}^{M} \frac{V_i}{V} \Sigma_i
\]

(2.1.4a)

and \( \bar{\xi}_h \), the cell averaged neutron lethargy increment per collision, is given by

\[
\bar{\xi}_h = \sum_{i=1}^{M} \frac{V_i}{V} \frac{n_i}{\Sigma_{ik}} \sum_{k=1}^{L} \frac{\Sigma_{ik}}{\Sigma_h} \xi_{ik}
\]

(2.1.4b)

In our work we shall assume an asymptotic source of 1 neutron/c.c/sec. and thus

\[
A = 1/\bar{\xi}_h \Sigma_h
\]

(2.1.5)
is the form of the asymptotic constant that we shall use.

In the definition of the resonance integral (section 1.3) we have assumed an asymptotic flux of $1/E$ since the asymptotic constant multiplies the resonance integral. In our approximate work we shall always include the asymptotic constant in this manner and hence assume a $1/E$ asymptotic flux. However when we come to consider the numerical solution of equations (1.2.9) and (1.2.16) we use the proper asymptotic flux (i.e. $1/\varepsilon_h E$) since the concept of the resonance integral does not occur in this exact approach.

2.2 Standard Approximations Employed in Resonance Theory.

2.2.1 The NR and WR Approximations to

$S_{ik}(E)$

There are two standard approximations to the quantity $S_{ik}(E)$ on the right hand side of equation (1.2.9). These have become known as the narrow resonance approximation (henceforth referred to as NR) and the wide resonance approximation (W.R.).

Recalling equation (1.2.14a) we have

$$S_{ik}(E) = \int_{E/\alpha_{ik}}^{E} \frac{\sum \phi_i(E')}{(1-\alpha_{ik})E'} dE' \quad (1.2.14a)$$

The NR approximation to this integral is based on the assumption that the width of the resonance is narrow compared to the energy change a neutron undergoes on
collision with the $i_k$th nuclide. So that $\phi'_1(E')$ may be replaced by its asymptotic value in equation (1.2.14a). Thus under the NR approximation

$$S_{ik}(E) = \frac{\Sigma_{ik}}{E} \quad (2.2.1)$$

In the case of the WR approximation it is assumed that the resonance width is wide compared to the energy change a neutron experiences on collision with the $i_k$th nuclide. This would imply that over the energy range $E, E/\alpha_{ik}$ the integrand $\Sigma_{ik}(E')\phi'_1(E')/E'$ would not vary a great deal and hence may be removed from beneath the integral sign to yield

$$S_{ik}(E) = \Sigma_{ik}(E)\phi'_1(E) \quad (2.2.2)$$

In deriving this last result we have used the fact that the WR approximation is only reasonably applied to those nuclides for which $\alpha_{ik} < 1$, that is, to heavy fuel nuclides.

2.2.2 Neglect of $1/E$ Variation

All approximate expressions for the resonance integral have the general form

$$I = \int_{E_r}^{E_r^+} \frac{\sigma_a \frac{\sigma_p}{\sigma_t}}{E} \frac{dE}{E} \quad (2.2.3)$$

where $\sigma_a(E)$ is the fuel microscopic absorption cross section, and the exact definition of $\sigma_p$ and $\sigma_t(E)$ would depend on the system being studied.
It has become standard practice to ignore the variation of $1/E$ in this integral and replace it by $1/E_r$ its value at the resonance peak. So equation (2.2.3) would become

$$I = \frac{1}{E_r} \int_{E_r}^{E_r^+} \sigma \sigma_p \, dE$$  \hspace{1cm} (2.2.4)

McKay (1964) has investigated the error involved in the use of this approximation and shows it to be negligible except for wide, low lying resonances. Transforming to the variable $x = 2(E - E_r)/\Gamma$ in equation (2.2.4) the expression for the resonance integral becomes

$$I = \frac{\Gamma}{2E_r} \int_{x_1}^{x_2} \sigma_a \sigma_p \, dx$$

where

$$x_2 = \frac{2}{\Gamma} (E_r^+ - E_r) \quad \text{and} \quad x_1 = \frac{2}{\Gamma} (E_r^- - E_r).$$

Since $(E_r^+ - E_r)$ and $(E_r^- - E_r)$ are finite and $\Gamma$ is usually small we take the limits $x_2$, $x_1$ to be respectively $\infty$, $-\infty$.

In extending the range of integration to infinity we tacitly assume that the wings of the resonance do not overlap into another resonance.

Another fundamental approximation involving the neglect of $1/E$ variation occurs in the transformation of $S_{1k}(E)$ to the variable $x = 2(E - E_r)/\Gamma$. The transformation is effected as follows.
Now for fuel nuclides $\alpha_{ik} = 1$, so for these nuclides we write

$$\frac{E/\alpha_{ik}}{\int_{E}^{41} \frac{\sum_{s_{ik}} (E') \phi_1(E') dE'}{(1-\alpha_{ik})E'} = \frac{\Gamma}{2E_r (1-\alpha_{ik})} \int_{x}^{r} \frac{\sum_{s_{ik}} (y) \phi_1(y) dy}{x}$$

with $\delta_{ik} = 2E_r (1-\alpha_{ik})/\Gamma$.

For simplicity we also retain the approximation in equation (2.2.5) for moderator nuclides even though $\alpha_{ik} < 1$. This should not introduce great error into the calculation of the resonance integral since the contribution to resonance flux by moderator scattering is largely dominated by off resonance conditions. As noted by Goldstein (1965) this transformation to the $x$ variable maintains the correct off resonance value of $S_{ik}(E)$.

Whenever we change to the $x$ variable in the calculation of flux we shall ignore the $1/E$ variation and replace $1/E$ by $1/E_r$. Since the flux is only required for the calculation of resonance absorption, when its main contribution is at energies near the resonance centre, such an approximation is consistent with equation (2.2.5).

2.3 The Slowing Down Equations for a Two Region Lattice

We shall henceforth consider only two region lattices. For this case the very general notation adopted in chapter 1 may be simplified somewhat.

We shall denote the fuel region by the suffix 1 and the moderator region by the suffix 2. For the fuel nuclide
we adopt the following notation

\[ \Sigma_s(E) = \text{the macroscopic scattering cross section of the fuel nuclide} \]
\[ \Sigma_p = \text{the macroscopic potential scattering cross section of the fuel nuclide} \]
\[ \Sigma_a(E) = \text{the macroscopic absorption cross section of the fuel nuclide} \]
\[ \Sigma_t(E) = \text{the macroscopic total cross section of the fuel nuclide} \]

and \( \sigma_s(E), \sigma_p, \sigma_a(E), \sigma_t(E) \) are the corresponding microscopic cross sections.

For moderator nuclides admixed in the fuel region we define

\[ \Sigma_{1i} = \text{the macroscopic scattering cross section of the } i^{\text{th}} \text{ moderator nuclide in the fuel region} \]

and for moderator nuclides in the external moderator region we define

\[ \Sigma_{2i} = \text{the macroscopic scattering cross section of the } i^{\text{th}} \text{ moderator nuclide in the moderator region.} \]

If \( n_1, n_2 \) are the number of moderator nuclides in the fuel and moderator regions respectively we define

\[ \Sigma_1 = \sum_{i=1}^{n_1} \Sigma_{1i} \text{ and } \Sigma_2 = \sum_{i=1}^{n_2} \Sigma_{2i} \]

we also define

\[ s_{1i} = \frac{\Sigma_{1i}}{N}, s_{2i} = \frac{\Sigma_{2i}}{N} \]
\[ s_1 = \frac{\Sigma_1}{N}, s_2 = \frac{\Sigma_2}{N} \text{ and } \sigma_m = \frac{s_2V_2}{V_1} \]
where \( N \) is the fuel nuclide concentration.

Finally we note that

\[
\Sigma_{t_1}(E) = \text{the macroscopic total cross section of the fuel region} = \Sigma_1 + \Sigma_{t}(E)
\]

and

\[
\Sigma_2 = \text{the macroscopic total cross section of the moderator region.}
\]

In terms of this notation the equations (1.2.9) assume the following form for a two region system

\[
V_1 \Sigma_{t_1}(E) \phi_1(E) = V_1 \phi_1 S_1(E) + V_2 (1-P_{22}) S_2(E) \tag{2.3.1a}
\]

\[
V_2 \Sigma_2 \phi_2(E) = V_1 (1-P_{11}) S_1(E) + V_2 P_{22} S_2(E) \tag{2.3.1b}
\]

where

\[
S_1(E) = \int_{E}^{E/\alpha} \frac{\Sigma (E') \phi_1(E')dE'}{(1-\alpha)E'} + \sum_{i=1}^{n_1} \int_{E}^{E/\alpha} \frac{\Sigma_{1i} \phi_1(E')dE'}{(1-\alpha_{1i})E'} \tag{2.3.2a}
\]

\[
S_2(E) = \sum_{i=1}^{n_2} \int_{E}^{E/\alpha} \frac{\Sigma_{2i} \phi_2(E')dE'}{(1-\alpha_{2i})E'} \tag{2.3.2b}
\]

with \( \alpha \) being the minimum fraction of a neutron's energy retained after an elastic collision with the fuel nuclide, and \( \alpha_{1i} \) and \( \alpha_{2i} \) the same quantity for collision with the \( i \)th moderator nuclide in the fuel and moderator regions respectively.

\section*{2.4 Approximations for an Isolated Lump}

We shall give an outline of the approximate solution of equations (2.3.1) in the case of an isolated fuel...
lump in an infinite sea of moderator. For this case the probability that a neutron entering the moderator from the fuel lump will have a collision in the moderator is 1 i.e. $G_2 = 1$ and hence the expressions for $P_{11}$ and $P_{22}$ given by equations (1.4.17) simplify to

$$P_{11} = 1 - P_1$$  \hspace{1cm} (2.4.1a)

$$P_{22} = 1 - \frac{G_1}{\Sigma_2}$$  \hspace{1cm} (2.4.1b)

It is clear that in this system the moderator flux will not deviate greatly from its asymptotic value, so we apply the NR approximation to the integral $S_2(E)$. Thus in accordance with equation (2.2.1)

$$S_2(E) = \frac{\Sigma_2}{E}$$  \hspace{1cm} (2.4.2)

Substituting equations (2.4.1) and (2.4.2) into equation (2.3.1), using the surface reciprocity theorem (equation 1.4.16) and the result $V_{1\overline{2}} = V_{2\overline{1}}$, the equation for the fuel flux becomes

$$\Sigma_{t_1}(E)\phi_1(E) = (1-P_1)S_1(E) + \Sigma_{t_1}(E)P_1/E$$  \hspace{1cm} (2.4.3)

This equation is the starting point for a number of theories.

2.4.1 The Gurevich-Pomeranchouk Theory

Gurevich and Pomeranchouk (1956) considered the fuel lump to be small and therefore made the plausible assumption that the neutrons do not experience scattering collisions in the lump. This means that the fuel lump is assumed
to have zero scattering cross section and hence the \( S_j(E) \) is ignored in equation (2.4.3). Thus

\[
\phi_j(E) = \frac{P_j}{E}
\]

Using the expression (1.4.14) for \( P_j \) and substituting into (1.3.2) we obtain the following expression for the resonance integral

\[
I = \frac{r}{2E} \frac{1}{F} \int \pi(\ell)f_1(\ell) d\ell \tag{2.4.4}
\]

where

\[
\pi(\ell) = \int_{-\infty}^{\infty} (1-e^{-\frac{a\ell}{1+x^2}}) dx
\]

\[
= \pi a e^{-a/2} \left( I_0 \left( \frac{a\ell}{2} \right) + I_1 \left( \frac{a\ell}{2} \right) \right) \tag{2.4.5}
\]

with \( a = \frac{N\sigma \Gamma}{\Gamma} \) and \( I_0 \) and \( I_1 \) are modified Bessel functions of zero and first order respectively.

In order to obtain some useful estimate from equation (2.4.5) Gurevich and Pomeranchouk considered the resonance integral to consist of the following two main contributions:

(i) The blockaded resonances for which \( a\ell_1 \gg 1 \)

(ii) The non-blockaded resonances for which \( a\ell_1 \ll 1 \)

Using standard expansions for the Bessel functions when \( a\ell \) is >> and << 1 (Whittaker and Watson, 1927)

\[
\pi(\ell) = 2\sqrt{\pi a\ell} \quad a\ell \gg 1
\]

\[
\pi(\ell) = \pi a\ell \quad a\ell \ll 1
\]
Using these and the approximation \[ \sqrt{\frac{\pi}{2}} f_1(l) d\ell = \sqrt{\frac{\pi}{2}} r \]
the following expression for the resonance integral is obtained

\[ I = \sum \alpha_r \quad + \quad \sum \beta_r \left( \frac{S}{M} \right)^{\frac{1}{2}} \]

non blockaded blockaded
resonances resonances

where \[ \alpha_r = \frac{\pi \sigma \gamma_r \gamma_r}{2E_r}, \quad \beta_r = \left( \frac{\rho}{4N} \right)^{\frac{1}{2}} \frac{\gamma_r}{E_r} \left( \frac{\pi \sigma \gamma_r \gamma_r}{\Gamma} \right). \]

\( \rho \) is the density of the fuel material and \( M \) is the mass of the fuel lump.

### 2.4.2 Wigner's Theory

Wigner (1955) developed a theory which takes account of the scattering in the fuel lump but does not take as detailed account of the escape probability as does the Gurevich-Pomeranchouk theory.

Wigner applies the NR approximation in the fuel region and so equation (2.4.3) yields the following expression for the fuel flux

\[ \phi_1(E) = \frac{1}{E} \left( \frac{s_1 \sigma \gamma_r + \rho \left( \frac{\sigma (E)}{\sigma (E)} - \frac{\sigma \gamma_r}{\gamma_r} \right)}{\sigma (E)} \right) \]

and hence the resonance integral is given by

\[ I = \frac{\pi \sigma \gamma_r \gamma_r}{2E_r} \left( \int_{-\infty}^{\infty} \frac{dx}{1 + \frac{\sigma \gamma_r}{s_1 + \sigma \gamma_r} + x^2} + \frac{\sigma \gamma_r}{\rho} \int_{-\infty}^{\infty} \frac{P_1 dx}{1 + x^2 (1 + \frac{\sigma \gamma_r}{s_1 + \sigma \gamma_r} + x^2)} \right) \]

Wigner proceeds from this expression by applying his rational approximation for \( P_1 \) (see equation 1.5.4)
where \( s = 1/Nl \)

Substituting into (2.4.8) and performing the integrations

\[
I = I_0 \left\{ (1 + \frac{\sigma_0}{s_1 + \sigma_p})^{-\frac{1}{2}} + \left(1 + \frac{\sigma_0}{s + s_1 + \sigma_p}\right)^{-\frac{1}{2}} - \left(1 + \frac{\sigma_0}{s_1 + \sigma_p}\right)^{-\frac{1}{2}} \right\}
\]

(2.4.10)

where

\[
I_0 = \frac{\pi \sigma_0 \Gamma / 2E_r}{2}
\]

2.4.3 An Intermediate Approach

A theory incorporating the best features of the Gurevich-Pomeranchouk and Wigner theories has been arrived at independently by a number of authors (Keane, 1958; Dresner, 1958 and Orlov, 1958). This theory takes account of the scattering in the fuel lump and detailed account of the escape probability.

As in Wigner's theory the NR approximation is applied in the fuel region and so equation (2.4.8) is obtained for the resonance integral. But now the exact expression for \( P_1 \) is substituted into the second integral. After a change in the order of integration

\[
\int_{-\infty}^{\infty} \frac{P_1 dx}{(1 + x^2)(1 + \frac{\sigma_0}{s_1 + \sigma_p} + x^2)} = \frac{s}{s_1 + \sigma_p} \int \pi(\ell) f_1(\ell) d\ell
\]

(2.4.11)
with
\[
\pi(\ell) = \int_{-\infty}^{\infty} \left\{1 - \exp \left[ -Nl(\sigma \omega_{1+p}) \left(1 + \frac{\sigma}{\sigma_{1+p}} \right)/ \left(1 + x^2 \right) \right] \right\} dx
\]
(2.4.12)

For \( \sigma_0 \ll (\sigma_{1+p}) \) the term \( \pi(\ell) \) is negligible while for \( \sigma_0 >> \sigma_{1+p} \)

\[
\pi(\ell) = \frac{\pi}{2} \left( \frac{\sigma_{1+p}}{\sigma_0} \right)^{3/2} \theta(\ell)
\]
(2.4.13)

where
\[
\theta(\ell) = \frac{4N(\sigma_{1+p})\ell^{1/2}}{\pi} - N(\sigma_{1+p})\ell - 2N(\sigma_{1+p}) \text{erfc}(N(\sigma_{1+p})\ell^{1/2})
\]

(2.4.14)

Substitution into equation (2.4.11) and then into equation (2.4.8) yields the result

\[
I = I_o \left[ \frac{\sigma}{\sigma_{1+p}} \right]^{1/2} + (\sigma_0)(\sigma_{1+p})^{1/2} \psi(\ell)/2N\ell
\]
(2.4.15)

where
\[
\psi(\ell) = \int f_1(\ell) \theta(\ell) d\ell.
\]
(2.4.16)

The function \( \psi(\ell) \) has been tabulated by McKay and Keane (1960) for slab, cylindrical and spherical fuel lumps.

Orlov (1958) arrives at this result from a different approach. It is instructive to give an account of his approach in our notation as it illustrates the essential difference of the Russian approach.

Orlov starts with the differential form of the Boltzmann transport equation, viz
where \( \phi_1(r, E, \Omega) \) is the fuel flux at \( r \), in direction \( \Omega \) at energy \( E \), and we have assumed no moderating nuclides to be present in the fuel region. Instead of integrating this equation to obtain equation (1.2.1), the starting point of Western theory, the Russians proceed directly to find an approximation to \( \phi_1(r, E, \Omega) \) from equation (2.4.17). They then integrate over volume \( (r) \) and direction \( (\Omega) \) to find the space averaged flux \( \phi_1(E) \). Because of this different approach the lump escape probabilities do not occur explicitly in the Russian formulation. In the Western approach the lump escape probabilities arise explicitly when, on integrating equation (1.2.5) we make the flat flux assumption and thus separate the spatial and energy integrations. The spatial integrations are in fact the lump escape probabilities.

Orlov applies the NR approximation to the scattering term on the RHS of equation (2.4.17) (i.e. puts \( \phi(r, E, \Omega) = 4 \pi / E \)). Equation (2.4.17) then reduces to

\[
\Omega \cdot \nabla \phi_1(r, E, \Omega) + \Sigma_t(E) \phi_1(r, E, \Omega) = \frac{\Sigma_p}{E} (2.4.18)
\]

This equation is then integrated to obtain \( \phi_1(r, E, \Omega) \),

\[
\phi_1(r, E, \Omega) = \phi_1(r_0, E, \Omega) e^{-\Sigma_t \theta + \frac{\Sigma_p}{\Sigma_t(E)E} (1 - e^{-\Sigma_t \theta})}
\]

where \( r_0 \) is on the surface of the lump and \( \theta = |r_0 - r| \)

(see fig. 2.1)
It is clear that a detailed knowledge of 
\( \phi(r_0, E, \Omega) \) would involve the transport equation for the moderator region. To overcome this complication Orlov assumes that the moderator flux has its asymptotic value (i.e. the NR approximation applied to moderator) and that it falls isotropically onto the surface of the fuel lump.

Hence

\[
\phi_1(r, E, \Omega) = \frac{1}{E} \left( e^{-\Sigma t \theta} + \frac{\Sigma p}{\Sigma t} (1-e^{-\Sigma t \theta}) \right).
\]

To find the spatially averaged flux we first integrate with respect to \( r \), so that

\[
\phi_1(E, \Omega) = \frac{1}{V_1} \int \phi(r, E, \Omega) dr = \frac{1}{V_1} \int \int \phi(r, E, \Omega)(n, \Omega) d\theta dS
\]

\[
= \frac{1}{V_1 E} \int \left( \frac{\Sigma p}{\Sigma t} l + \frac{(\Sigma - \Sigma p)}{\Sigma t} (1-e^{-\Sigma t \ell}) \right) (n, \Omega) dS
\]

then perform the \( \Omega \) integration

\[
\phi_1(E) = \frac{1}{4\pi} \int \phi_1(E, \Omega) d\Omega
\]
and using the result
\[ \int dS \int \frac{h(\varepsilon) (\Omega \cdot n) d\Omega}{\varepsilon} = \pi S \int h(\varepsilon) f_1(\varepsilon) d\varepsilon \] (2.4.19)
we obtain after a little manipulation
\[ \phi_1(E) = \frac{1}{E} \left( \frac{\Sigma P}{\Sigma_t(E)} + \frac{(\Sigma_t(E) - \Sigma_p)}{\Sigma_t(E)} P \right), \]
which is identical to equation (2.4.7) (with \( s_1 = 0 \)), from which Wigner's theory and the result (2.4.15) are derived.

### 2.5 Approximations for a Regular Two Region Lattice

We now direct our attention to a regular two region lattice system containing several nuclides per region. The slowing down equations for such a system are given by equations (2.3.1).

#### 2.5.1 The NR Approximation Applied to the Moderator Region

The equations (2.3.1) are greatly simplified if we apply the NR approximation to the \( S_2(E) \) term and also employ the reciprocity theorem. Under these approximations equation (2.3.1a) for the fuel flux reduces to
\[ \Sigma t_1(E) \phi_1(E) = (1-P_{11}) \Sigma t_1(E)/E + P_{11} S_1(E) \] (2.5.1)

We next introduce the rational approximation for \( P_{11} \) discussed in section (1.6) viz.
\[ P_{11} = \frac{\sigma_{t_1}}{\sigma_{t_1} + s_1 e} \] (1.6.4)
so that equation (2.5.1) becomes

\[
(s_e + \sigma_t) \phi_1(E) = \frac{s_e}{E} + \int_E^{E/\alpha} \frac{\sigma_s(E') \phi_1(E') dE'}{(1-\alpha)E'} + \sum_{i=1}^{n_L} \frac{s_{li} \phi_1(E') dE'}{(1-\alpha_{li})E'}
\]  

(2.5.2)

We note that equation (2.5.2) has the same form as the slowing down equation for the flux \( \phi(E) \), in an homogeneous system with the NR approximation applied to some moderator nuclides. More specifically for an homogeneous system, containing \( n_h \) heavy moderator nuclides to which the NR approximation is not applied (denoted by subscript 1) and \( n_L \) light moderator nuclides to which the NR approximation is applied (denoted by subscript L), the slowing down equation has the form (see e.g. McKay, 1964).

\[
(s_L + \sigma_t) \phi(E) = \frac{s_L}{E} + \int_E^{E/\alpha} \frac{\sigma_s(E') \phi(E') dE'}{(1-\alpha)E'} + \sum_{i=1}^{n_L} \frac{s_{li} \phi(E') dE'}{(1-\alpha_{li})E'}
\]  

(2.5.3)

with \( s_{li} \) the effective microscopic scattering cross section of the \( i^{\text{th}} \) heavy moderator nuclide, \( s_1 = \sum_{i=1}^{n_L} s_{li} \sigma_t (E) = s_1 + \sigma_t (E) \)

and \( s_L \) is the combined effective microscopic scattering cross section of the light moderator nuclides.

The similarity of equations (2.5.2) and (2.5.3) is the basis of the equivalence relation between homogeneous and heterogeneous systems (Chernik and Vernon, 1958). Through use of the rational approximation (1.6.4) we have replaced the heterogeneous system by an equivalent homogeneous system for which \( s_e \) is the effective microscopic scattering cross section of the narrow
resonance moderator. The advantage of this equivalence relation is that any method developed for solving the homogeneous equation may be immediately applied to the heterogeneous case simply by replacing the homogeneous $s_L$ by $s_e$. Unfortunately such an equivalence only exists when the NR and rational approximations are applied to the heterogeneous system.

2.5.2 The λ Method with the NR Approximation Applied to the External Moderator

We shall here give a brief outline of the more and more refined techniques which have been developed to solve the integral equation (2.5.2). Due to the equivalence mentioned above these results will of course apply equally to homogeneous and heterogeneous systems.

The earliest approximations involved application of the NR approximation to all moderator nuclides, so that equation (2.5.2) would reduce to

$$\left(s_e + s_1 + \sigma_{t_1}^E \right) \phi_1(E) = \frac{(s_e + s_1)}{E} + \int_{E}^{E/\alpha} \frac{\sigma_s(E') \phi_1(E') dE'}{(1-\alpha)E'} \tag{2.5.4}$$

Depending on whether the resonance is narrow or wide the fuel scattering integral may be treated with either the NR or WR approximations.

Firstly, applying the NR approximation to fuel scattering we obtain

$$\phi_1(E) = \frac{(s_e + s_1 + \sigma_p)}{(s_e + \sigma_{t_1}^E)E} \tag{2.5.5}$$
or, in terms of the $x$ variable

$$
\phi_1(x) = \frac{1}{E} \frac{1+x^2}{\beta_{11}^2 + x^2}
$$

(2.5.6)

where in anticipation of a general notation to be developed shortly, we define

$$
\beta_{11}^2 = 1 + \sigma_o / (s_e + s_1 + \sigma_p)
$$

(2.5.7)

On the other hand applying the WR approximation to the fuel scattering we obtain

$$
\phi_1(E) = \frac{(s_e + s_1)}{(s_e + s_1 + \sigma_a(E))E}
$$

(2.5.8)

i.e.

$$
\phi_1(x) = \frac{1}{E} \frac{1+x^2}{\beta_{10}^2 + x^2}
$$

(2.5.9)

where

$$
\beta_{10}^2 = 1 + \frac{\sigma_o \Gamma}{(s_e + s_1) \Gamma}
$$

(2.5.10)

The corresponding expressions for the resonance integrals are,

(i) for the NR approximation applied to the fuel nuclide

$$
I_{NR} = I_o / \beta_{11}
$$

(2.5.11)

(ii) for the WR approximation applied to the fuel nuclide

$$
I_{WR} = I_o / \beta_{10}
$$

(2.5.12)

Using the approximations (2.5.5) and (2.5.8) Chernick and Vernon (1958) iterate on the integral equation (2.5.4) to obtain second order approximations to $I_{NR}$ and $I_{WR}$.
The drawback of these approximations is that they are inadequate for those resonances which cannot properly be classified as wide or narrow. To handle these intermediate resonances, Goldstein and Cohen (1962) developed a method which interpolated between the NR and WR approximations. They developed the method under the assumption of the NR approximation to all moderator nuclides (i.e. they develop an approximate solution for equation 2.5.4). Hill and Schaeffer (1962) extended the method to the more general situation so that equation (2.5.2) could be handled without applying the NR approximation to all the moderator species. We give an outline of their method.

Parameters $\lambda_0$ (for the fuel nuclide) and $\lambda_1, \lambda_2, \ldots, \lambda_n$ (for the moderator nuclides) are introduced. These parameters are assumed to have values between 0 and 1. An approximate solution is then assumed, involving these parameters in such a way that when $\lambda_0, \lambda_1, \ldots, \lambda_n$ are all equal to 1, the NR approximation solution is retrieved and when $\lambda_0 = 0, \lambda_1, \ldots, \lambda_n$ all equal 1 the WR approximation solution is retrieved.

An approximation satisfying these conditions and which will be intermediate between the NR and WR extremes is,

$$\phi^{(1)}_\lambda (E) = \frac{1}{E} \frac{s e^{+s} + s + \lambda o \sigma p}{s e^{+s} + \lambda o \sigma p + \lambda o \sigma (E) + \sigma (E)}$$

or, in terms of the $x$ variable

$$\phi^{(1)}_\lambda (x) = \frac{1}{E} \frac{1+x^2}{r \beta^2 + x}$$
where
\[ s_\lambda = \sum_{i=1}^{n-1} \lambda_is_i \] and \[ \beta_{\lambda o}^2 = 1 + \frac{\sigma_o}{s + \lambda o} \frac{\Gamma + \delta \Gamma}{\gamma o \Gamma n} \]

We see that this definition of \( \beta_{\lambda o} \) is consistent with the \( \beta_{11} \) and \( \beta_{10} \) introduced earlier.

The expression (2.5.13) is used to iterate on the integral equation (2.5.2) to obtain \( \phi^{(2)}(E) \), a second order approximation to the flux. Using \( \phi^{(1)}(E) \) and \( \phi^{(2)}(E) \) the first and second order resonance integrals \( I^{(1)}_\lambda \) and \( I^{(2)}_\lambda \) are calculated.

The criteria for the selection of \( \lambda_o, \lambda_1, \ldots, \lambda_n \) is the equality of \( I^{(1)}_\lambda \) and \( I^{(2)}_\lambda \).

The second order flux is found to be
\[
\phi^{(2)}(x) = \frac{1}{E_x} \frac{(1+x^2)^{1/2}}{(\beta_{11}^2 + x^2)} \left( 1 + \frac{\sigma_o}{(s + 1 + \sigma_p) \delta} \frac{(\beta_{11}^2 - \beta_{10}^2)}{\beta_{\lambda o} \delta} \left\{ \tan^{-1} \frac{x+\delta}{\beta_{\lambda o}} - \tan^{-1} \frac{x}{\beta_{\lambda o}} \right\} \right.
\]
\[
+ \sum_{i=1}^{n-1} \frac{s_i}{i+1} \frac{1-\delta_{1i}}{(s + 1 + \sigma_p) \delta} \left\{ \tan^{-1} \frac{1+x+\delta_{1i}}{\beta_{\lambda o}} - \tan^{-1} \frac{x}{\beta_{\lambda o}} \right\} \right)
\]

The corresponding first and second order resonance integrals are
\[
I^{(1)}_\lambda = \frac{I_o}{\beta_{\lambda o}} \tag{2.5.15}
\]
\[
I^{(2)}_\lambda = \frac{I_o \left( 1 + \frac{\sigma_o}{(s + 1 + \sigma_p) \delta} \frac{(\beta_{11}^2 - \beta_{10}^2)}{\beta_{\lambda o} \delta} \tan^{-1} \frac{\delta}{\beta_{\lambda o} + \beta_{11}} \right)}{1 + \frac{\sigma_o}{(s + 1 + \sigma_p) \delta} \frac{(1-\delta_{1i})}{\beta_{\lambda o} \delta} \tan^{-1} \frac{\delta_{1i}}{\beta_{\lambda o} + \beta_{11}}} \]

Here we have used the result
\[\int_{-\infty}^{\infty} \tan^{-1} \frac{x+\delta}{a} \cdot \frac{b^2 + x^2}{b^2} \, dx = \frac{\pi}{b} \tan^{-1} \frac{\delta}{a+b}\]

This result was first given by Chernik and Vernon (1958) and we shall have occasion to use it often in the work of this thesis.

Putting \(I_{\lambda}^{(1)} = I_{\lambda}^{(2)}\) the following transcendental equation is obtained for the \(\lambda_0, \lambda_1, \ldots, \lambda_{n_1}\):

\[
\beta_{11} - \beta_{\lambda\lambda_0} = \frac{\sigma_p}{(s + s_{1+\sigma})_p} \beta_{1\infty} - \beta_{\lambda\lambda_0}^2 \tan^{-1} \frac{\delta}{\beta_{\lambda\lambda_0} + \beta_{11}} \]
\[
+ \sum_{i=1}^{n_1} \frac{s_{1i}}{(s + s_{1+\sigma})_p} (1-\beta_{\lambda\lambda_0}^2) \tan^{-1} \frac{\delta_{1i}}{\beta_{\lambda\lambda_0} + \beta_{11}} \quad (2.5.16)
\]

A suitable set of solutions to equation (2.5.16) is

\[
\lambda_i = 1 - \frac{\beta_{11} + \beta_{\lambda\lambda_0}}{\delta_{1i}} \tan^{-1} \frac{\delta_{1i}}{\beta_{11} + \beta_{\lambda\lambda_0}} \quad (i = 0,1,\ldots,n_1) \quad (2.5.17)
\]

(Note that \(\delta_{10} = \delta\))

Once the \(\lambda_i\)'s have been determined the resonance integral is calculated from equation (2.5.15). Goldstein (1965) extends this method to deal with homogeneous systems without applying the NR approximation to any nuclide. Sehgal and Goldstein (1966) apply the method to heterogeneous systems without applying the NR approximation to the external moderator. We shall now discuss this method.
2.5.3 The \( \lambda \) Method Without Applying the NR Approximation to the External Moderator

In this method Sehgal and Goldstein (1966) proceed directly from equations (2.3.1) to which the rational approximation for \( P_{11} \) (equation 1.6.4) is applied, reducing the equations to the form

\[
(s + \sigma)_{1}(E) = \frac{S_{1}(E)}{N} + \frac{s_{e}}{s_{2}} \frac{S_{2}(E)}{N} \tag{2.5.18a}
\]

\[
(s + \sigma)_{2}(E) = \frac{s_{e}}{\sigma_{m}} \frac{S_{1}(E)}{N} + \frac{(1-s_{e}/\sigma_{m})s}{s_{2}} \frac{S_{2}(E)}{N} \tag{2.5.18b}
\]

The following approximations to the fuel and moderator fluxes are obtained under the NR and WR approximations

(i) Applying the NR approximation to all nuclides in both fuel and moderator regions

\[
\phi_{1}(x) = \frac{1}{E} \frac{1+x^{2}}{E^{2}_{111}+x^{2}}, \quad \phi_{2}(x) = \frac{1}{E} \cdot \frac{1+(1-s_{e}/\sigma_{m})(\beta_{111}^{2}-1)+x^{2}}{\beta_{111}^{2}+x^{2}} \tag{2.5.19a}
\]

where, anticipating a more general notation than in the previous section

\[
\beta_{111}^{2} = 1 + \frac{\sigma_{o}}{s_{e}+s_{1}+\sigma_{p}}
\]

(ii) Applying the WR approximation to the fuel nuclide and the NR approximation to all other nuclides of the system

\[
\phi_{1}(x) = \frac{1}{E} \frac{1+x^{2}}{E^{2}_{110}+x^{2}}, \quad \phi_{2}(x) = \frac{1}{E} \cdot \frac{1+(1-s_{e}/\sigma_{m})(\beta_{110}^{2}-1)+x^{2}}{\beta_{110}^{2}+x^{2}} \tag{2.5.19b}
\]
where
\[
\beta^2_{110} = 1 + \frac{\sigma_0}{s_e + s_1} \frac{\Gamma \gamma}{\Gamma}
\]

As before the parameters, \( \lambda_0 \) for fuel, \( \lambda_1, \ldots, \lambda_{n_1} \) for admixed moderator in fuel and \( \mu \) for the external moderator scattering, are introduced. When a parameter equals 1 this means that NR is applied to the particular nuclide, and when equal to 0 WR is applied to the particular nuclide.

It is plausible from the form of equation (2.5.19) that an intermediate solution involving these parameters would be
\[
\phi_{11}^{(1)}(x) = \frac{1}{E} \frac{1 + x^2}{\mu \lambda_0 \lambda + x^2}, \quad \phi_{21}^{(2)}(x) = \frac{1}{E} \frac{a^2_{\mu \lambda_0} + x^2}{\mu \lambda_0 \lambda + x^2}
\]

where
\[
\beta^2_{\mu \lambda_0} = 1 + \frac{\sigma_0}{s_e + s_1 + \lambda_0 \sigma_p} \cdot \frac{\Gamma + \lambda_0 \Gamma}{\Gamma}
\]
\[
a^2_{\mu \lambda_0} = 1 + \mu (1 - s_e / s_m) (\beta^2_{\mu \lambda_0} - 1)
\]

and
\[
s_\lambda = \sum_{i=1}^{n_1} \lambda_i \cdot s_{1i}
\]

The method follows the same pattern as before i.e. substitute the approximations into equation (2.5.18) to find \( \phi_{11}^{(2)}(x) \) then use these to obtain \( I_{\lambda}^{(1)} \), \( I_{\lambda}^{(2)} \). After putting \( I_{\lambda}^{(1)} = I_{\lambda}^{(2)} \) the following transcendental equation is arrived at for the \( \lambda \)'s and \( \mu \),
\[(\beta_{111}^{\infty}-\beta_{\mu\lambda\sigma}^{\infty})(s_{e}+s_{1}+s_{p}) = s_{e}(a_{\mu\lambda\sigma}^{2}-\beta_{\mu\lambda\sigma}^{2})^{n}\sum_{i=1}^{\infty} \frac{1}{\delta_{2i}} \tan^{-1} \frac{\delta_{2i}}{\beta_{\mu\lambda\sigma}^{2}} + \frac{(\beta_{111}^{\infty}-\beta_{\mu\lambda\sigma}^{\infty})}{\delta_{11}} \tan^{-1} \frac{\delta_{11}}{\beta_{111}^{\infty}} \tan^{-1} \frac{\delta_{11}}{\beta_{\mu\lambda\sigma}^{\infty}} + \frac{(\beta_{111}^{\infty}-\beta_{\mu\lambda\sigma}^{\infty})}{\delta_{11}} \tan^{-1} \frac{\delta_{11}}{\beta_{111}^{\infty}} \tan^{-1} \frac{\delta_{11}}{\beta_{\mu\lambda\sigma}^{\infty}} \tag{2.5.21}\]

A suitable set of solutions is

\[\lambda_{i} = 1 - \frac{\delta_{11}}{\beta_{111}^{\infty} + \beta_{\mu\lambda\sigma}^{\infty}} \tan^{-1} \frac{\delta_{11}}{\beta_{111}^{\infty} + \beta_{\mu\lambda\sigma}^{\infty}} (i = 0, 1, ..., n_{1}) \tag{2.5.22}\]

\[\mu = 1 - \left(1 + \mu(s_{e}/\sigma_{m} - 1)\right) (\beta_{111}^{\infty} + \beta_{\mu\lambda\sigma}^{\infty})^{n} \sum_{i=1}^{\infty} \frac{1}{\delta_{2i}} \tan^{-1} \frac{\delta_{2i}}{\beta_{111}^{\infty} + \beta_{\mu\lambda\sigma}^{\infty}} \tan^{-1} \frac{\delta_{2i}}{\beta_{111}^{\infty} + \beta_{\mu\lambda\sigma}^{\infty}} \tag{2.5.22}\]

2.6 The Russian Approach for Lattice Systems

As we have just seen Western theory concentrates on using rational type approximations to the collision probabilities since only with these rational approximations is it possible to develop refined methods of solving the slowing down integral equations.

Russian theory has developed along different lines. The Russian workers have tackled directly the geometrical aspects of the problem but have crudely approximated the slowing down aspects. We have already had a glimpse of the Russian method when discussing the approaches of Orlov and Gurevich and Pomeranchouk for isolated lumps (section 2.4). We shall now give the main outline of extensions of these approaches to lattice systems developed by Marchuk (1958) and Petrov (1958).
2.6.1 Marchuk's Theory for a Slab Lattice System

Marchuk considers a regular lattice of fuel slabs of thickness \( d \), the distance between the centres of successive slabs being \( D \). Marchuk takes a cell of this system, as shown in figure (2.2), and tracks a neutron through the system by assuming perfect reflection at the cell walls.

No admixed moderator is considered in the fuel region.

We let \( \Sigma_2 \) = the macroscopic scattering cross section of the moderator

\[ \Sigma_t(E) = \text{the macroscopic total cross section of the fuel.} \]

Let us for the moment consider neutrons travelling in the direction \( \Omega \) and having energy \( E \).

If we let \( p_0(\Omega, E) \) = the fraction of neutrons absorbed in the fuel lump during the first traverse of the fuel lump
and

\[ p_k(\Omega, E) = \text{the fraction of neutrons absorbed in the fuel lump on the } k^{th} \text{ reflection from the boundary} \]

then the total fraction of neutrons of direction \( \Omega \) and energy \( E \), absorbed in the fuel lump is given by \( p(\Omega, E) \) where

\[ p(\Omega, E) = p_0(\Omega, E) + \sum_{k=1}^{\infty} p_k(\Omega, E) \quad (2.6.1) \]

The neutrons of energy \( E \) which are absorbed in the fuel lump of the cell in figure (2.2) come from three sources

(i) The neutrons slowed down to energy \( E \) in the moderator of the cell and then incident on the fuel lump. Marchuk assumes the flux of these neutrons, \( \phi_0(E) \), to be isotropic and equal to \( 1/4\pi E \). This is in fact the NR approximation applied to the external moderator.

(ii) The neutrons which are slowed down to energy \( E \) in the fuel lump itself.

(iii) The neutrons of energy \( E \) arriving from neighbouring cells.

The absorption of neutrons of groups (i) and (ii) is accounted for by the term \( p_0(\Omega, E) \) while the absorption of neutrons of group (iii) is accounted for by the term \( \sum_{k=1}^{\infty} p_k(\Omega, E) \).

Let

\[ \phi(M_1, \Omega, E) = \text{The incident flux falling onto the lump at } M_1 \text{ for the } i^{th} \text{ traverse of the lump} \]

\[ \phi(M'_1, \Omega, E) = \text{The exiting flux leaving the lump at } M'_1 \text{ after the } i^{th} \text{ traverse of the lump.} \]
Integrating along the line $M_0M_1$ we see that

$$\phi(M_1, \Omega, E) = \phi_o(E)(1 - e^{-\Sigma L})$$

(2.6.2)

Let us first take the evaluation of $\phi_o(\Omega, E)$ and consider initially the absorption of neutrons of group (i). By considering the fraction of neutrons absorbed at $N$ and then integrating along the line $M_1M_1'$ we see that

The fraction of neutrons absorbed in passing along $M_1M_1'$

$$\Omega_n \int ds(M_1, \Omega, E) \frac{a}{\Sigma t}(1 - e^{-\Sigma L})$$

(2.6.3)

(where $\Omega_n = \Omega \cdot n$ and $n$ is the normal to the lump surface), from which we also see that the fraction of neutrons absorbed on a traverse of the fuel lump is $\frac{\Sigma a}{\Sigma t}(1 - e^{-\Sigma L})$.

We now account for neutrons of group (ii) and in particular consider neutrons slowed down to energy $E$ at the point $P$ in the fuel lump. The fraction of such neutrons reaching $N$ from $P$ is given by

$$\Sigma_t \phi_o(E)e^{-\Sigma_t L}$$

Here Marchuk assumes that the flux of such neutrons is isotropic and equal to $l/4\pi E$ i.e. the NR approximation applied to scattering in the fuel.

Integrating all such contributions between $M_1$ and $N$ we obtain

Fraction of neutrons absorbed at $N$

$$\Omega_n \int ds(\phi_o(E) \frac{a}{\Sigma t}(1 - e^{-\Sigma L}))$$

after slowing down to energy $E$ in the fuel lump.
then integrating along $M_1$ and $M_1'$ we obtain

\[
\text{Fraction of neutrons absorbed after}\quad \text{slowing down to energy } E \text{ in the lump} = \Omega \frac{\Sigma}{\Sigma_t} \frac{a}{e} (1 - e^{-\frac{\Sigma}{\Sigma_t} E})
\]

We find $p_o(\Omega, E)$ by adding the expressions given by equations (2.6.3) and (2.6.4).

\[
p_o(\Omega, E) = \Omega \frac{d\phi_o(E)}{dE} \left( \frac{a}{\Sigma} + \frac{\Sigma}{\Sigma_t} \left( 1 - e^{-\frac{\Sigma}{\Sigma_t} E} \right) \right)
\]

It now remains to find an expression for $p_k(\Omega, E)$ for which we must first find an expression for $\phi(M_{k+1}, \Omega, E)$.

Now

\[
\phi(M_{k+1}, \Omega, E) = \phi(M_1, \Omega, E) \times \text{the fraction of neutrons that make } k \\
\text{traverses of the moderator and } (k-1) \\
\text{traverses of the fuel without collision} \\
\text{and } -k \Sigma \Sigma e^{-(k-1)\Sigma} E
\]

But

\[
\phi(M_1, \Omega, E) = \text{the flux at } M_1 \times \text{the fraction of neutrons that traverse} \\
\text{the lump without a collision} + \text{the flux due to neutrons} \\
\text{slowing down to energy } E \text{ in the lump and reaching } M_1' \\
\text{without collision.}
\]

\[
= \phi(M_1, \Omega, E) e^{-\Sigma \Sigma E e^{-(k-1)\Sigma} E} + \phi_o(E) \frac{\Sigma}{\Sigma_t} (1 - e^{-\Sigma \Sigma E})
\]

Using the fact that on each traverse the fraction $\frac{a}{\Sigma_t} (1 - e^{-\Sigma E})$ is captured, we see that
\[ p_k(\Omega, E) = \Omega \sum_n \frac{a}{\Sigma_t} (1-e^{-\Sigma_l t}) e^{-k \Sigma_2 L-(k-1) \Sigma_2 L} \phi(M'_1, \Omega, E) \]
\[ = e^{-\Sigma_2 L-\Sigma_l t} p_{k-1}(\Omega, E) \]

Thus substituting into equation (2.6.1)
\[ p(\Omega, E) = p_o(\Omega, E) + \frac{p_1(\Omega, E)}{1-e^{-\Sigma_2 L-\Sigma_l t}} \]  
(2.6.8)

which after substitution of the appropriate expressions for \( p_o(\Omega, E) \) and \( p_1(\Omega, E) \) and a considerable amount of algebraic manipulation becomes
\[ p(\Omega, E) = \Omega dS \phi_o(E) \left\{ \sum \Sigma \frac{a}{\Sigma_t} p_l + \frac{\Sigma a}{\Sigma^2_t} \right\} \frac{1-e^{-\Sigma_2 L}}{1-e^{-\Sigma_2 L-\Sigma_l t}} \]  
(2.6.9)

Marchuk then performs the energy integration over the resonance to obtain \( p(\Omega) \), the fraction of neutrons of direction \( \Omega \) suffering resonance absorption in the cell.
\[ p(\Omega) = \phi_o(E) \Omega dS \left\{ \sum \frac{a}{\Sigma_t} p_l + \frac{\Sigma a}{\Sigma^2_t} \frac{1}{1-e^{-\Sigma_2 L-\Sigma_l t}} \right\} \]  

In order that the ultimate expression for the resonance integral will have the same functional form as equation (2.4.5) Marchuk expresses \( p(\Omega) \) in the form
\[ p(\Omega) = \phi_o(E) \Omega dS \left\{ \sum \frac{a}{\Sigma_t} p_l + \phi(\Sigma p, \Sigma_2 L) \right\} \]  
(2.6.10)

where
\[ \phi(\Sigma p, \Sigma_2 L) = \left[ \frac{\Sigma a}{\Sigma^2_t} \frac{1-e^{-\Sigma_2 L}}{1-e^{-\Sigma_0 L-\Sigma_1 t}} \right] + \frac{\Sigma a}{\Sigma^2_t} dE \]  
(2.6.11)
It is clear that this function will play the same role in slab lattice theory as does the function $\pi(\ell)$ in isolated lump theory discussed in section (2.4.3). In fact the function $\phi(\Sigma_p \ell, \Sigma_0 L)$ is simplified in the same manner as $\pi(\ell)$.

Introducing the $x$ variable, assuming $\sigma_o \gg \sigma_p$ and putting $\beta = \Sigma_p \ell, \alpha = \Sigma_0 L$, $\phi$ reduces to

$$\phi(\beta, \alpha) = \frac{2\sqrt{\beta}}{\pi} \int_{-\infty}^{\infty} \frac{1-e^{-\beta+1/y^2}}{(1+\beta y^2)^2} \frac{1-e^{-\alpha}}{1-e^{-\alpha-(\beta+1/y^2)}} dy \quad (2.6.12)$$

Note that as $\alpha \to \infty$ (i.e. the case of an isolated lump)

$$\phi(\beta, \alpha) = \frac{2\sqrt{\beta}}{\pi} \int_{-\infty}^{\infty} \frac{1-e^{-\beta+1/y^2}}{(1+\beta y^2)^2} dy$$

which is easily shown to be a multiple of $\pi(\ell)$ (equation 2.4.12), so that the lattice theory has as a limiting case the approximate lump theory, as indeed it should.

Integrating over all $\Omega$ and using the result (2.4.19) the following expression for the resonance integral is eventually obtained

$$I = \frac{1}{E_r} \left[ \int \frac{\Sigma a_p}{E_t} + \frac{F(\alpha, \beta)}{f_1(\ell)} \right] dE \quad (2.6.13)$$

where

$$F(\alpha, \beta) = \int \phi(\Sigma_2 L, \Sigma_p \ell)f_1(\ell) d\ell$$

$$= \frac{4\sqrt{\beta}}{\pi} \int_{0}^{1} \sqrt{u} \ du \int_{-\infty}^{\infty} \frac{1-e^{-\beta}}{(1+\beta y^2)^2} \frac{1-e^{-\alpha/u}}{1-e^{-\alpha}} dy \quad (2.6.14)$$
where
\[ \beta = N\ell_1 \sigma_p / 2, \quad \alpha = N\ell_1 \sigma_m / 2 \quad \text{and} \quad \sigma_m = \Sigma_2 V_2 / N V_1. \]

Marchuk has tabulated the function \( F(\alpha, \beta) \) but differencing of his table indicates that some of the values might be in error. We have therefore recalculated \( F(\alpha, \beta) \) using a Gaussian integration rule. A table of our recalculated values, at the same values of \( \alpha \) and \( \beta \) as Marchuk's table, is given in appendix 2. Comparison with Marchuk's table shows that some of his values are in error, especially at lower values of \( \beta \).

2.6.2 Petrov's Method for Tight Lattices of Small Lumps

Petrov (1958) takes the concepts that Gurevick and Pomeranchouk developed for an isolated small lump and extends them to deal with the case of tightly packed lattices of small fuel lumps. With these assumptions Petrov employs the methods of gas kinetics to calculate the resonance escape probability, treating the fuel lumps as a nuclide species.

We shall here derive his result from the slowing down equations, this will allow us to demonstrate how the Dancoff correction may be incorporated into his final expression.

Applying the NR approximation to both fuel and moderator regions in equation (2.3.1a) and ignoring fuel scattering we obtain the following expression for the fuel flux
\[ \phi_1(E) = \frac{1}{E} (1-P_{11}) \quad (2.6.14) \]
For $P_{11}$ we use the expression derived in section (1.4) viz. equation (1.4.17a), so that

$$1 - P_{11} = \frac{1}{N\lambda_1 \sigma_a} \frac{G_1}{1 + rG_1}$$  \hspace{1cm} (2.6.15)$$

where

$$r = \frac{1 - G_2}{G_2}$$

Petrov approximates $G_2$, the probability that a neutron incident on moderator has its next collision in the moderator as equal to the mean free path in the moderator divided by the total mean free path in the fuel and moderator. This approximation is in fact equivalent to the Wigner rational approximation for $G_2$.

So Petrov takes the following approximate expression for $r$

$$r = \frac{1}{\Sigma_2 \bar{G}_2} = \frac{1}{N\lambda_1 \sigma_m}$$  \hspace{1cm} (2.6.16)$$

Substituting (2.6.15) into (2.4.16) we obtain the following expression for the resonance integral

$$I = \frac{1}{N\lambda_1} \cdot \frac{\Gamma}{2E} \int_{-\infty}^{\infty} \frac{G_1}{1 + rG_1} \, dx$$  \hspace{1cm} (2.6.17)$$

$$= \frac{1}{N\lambda_1} \cdot \frac{\Gamma}{2E} \frac{1}{1 + r} \int_{-\infty}^{\infty} \frac{f(1 - e^{-al})f_1(\ell)d\ell}{1 - \eta e^{-al}f_1(\ell)d\ell} \, dx$$  \hspace{1cm} (2.6.18)$$

where we put

$$\eta = \frac{r}{1 + r} = 1 - G_2 = \frac{1}{1 + N\lambda_1 \sigma_m}$$

de Petrov's work

and

$$a = N\sigma_o \frac{\Gamma}{\Gamma}$$
Petrov, by expanding the denominator, obtains an approximation to the integral in equation (2.6.18). Marchuk (1958) avoids any crude approximations and by assuming \( a \bar{\lambda}_1 \gg 1 \) (i.e. blockaded resonances) puts equation (2.6.18) into the form

\[
I = \frac{1}{\bar{\lambda}_1} \frac{1}{N} \left( \frac{1}{\sqrt{\bar{\lambda}_1}} \right) R(\eta)
\]

where

\[
R(\eta) = \frac{(1-\eta)}{\frac{1}{\bar{\lambda}_1}} \int_0^\infty \frac{1 - e^{-a\bar{\lambda}_1/\sqrt{x}}}{1 - \eta e^{-a\bar{\lambda}_1/\sqrt{x}}} f_1(x) \, dx.
\]

Marchuk tabulates \( R(\eta) \) and shows it to be a smooth function so that its table may easily be interpolated for practical work.

The main drawback of Petrov's approach is that fuel scattering is not taken into account.

The major restriction of all the Russian approaches is the application of the NR approximation to all nuclear species. Clearly to attempt directly to remove this crude approximation with a more refined slowing down model (such as the \( \lambda \) method) would lead to incredible complication.

In chapter 4 we shall demonstrate how to incorporate the Russian approach into more sophisticated slowing down models through the use of modified rational approximations for the collision probabilities.
3. AN ALGORITHM FOR THE NUMERICAL SOLUTION OF THE SLOWING DOWN EQUATIONS IN HETEROGENEOUS SYSTEMS - THE PROGRAMME PEARLS.

In this chapter we shall outline the derivation of an algorithm which allows the direct numerical solution of the slowing down equations in any type of heterogeneous system through the use of Simpson's rule. Unlike Nordheim (1961b) we shall not apply the NR to the external moderator.

A particular feature of our algorithm is its ability to change step length automatically at predetermined lethargies.

The direct solution of the slowing down equations will enable us to carry out a systematic investigation of the errors involved in the various approximations we shall employ viz. the rational approximations to the collision probabilities and the NR approximation to the external moderator, and also the errors involved in the approximate solution to the slowing down equations, such as the λ method discussed in chapter 2 and the Galerkin method to be developed in chapter 5.

3.1 General Description

We shall consider the slowing down equations in terms of the collision density, \( F_j(E) = \sum_{t_j} (E) \phi_j(E) \), so that the equations assume the form of equation (1.2.9b) viz.

\[
V_j F_j(E) = \sum_{i=1}^{M} V_i P_{ij} \sum_{k=1}^{n_i} \int \frac{E/\alpha_{ik}}{\Sigma s_{ik}(E')} \frac{F_i(E')dE'}{(1-\alpha_{ik})E'}
\]

(1.2.9b)
We transform from the energy variable $E$ to the lethargy variable $u$ where

$$u = \ln \frac{E^*}{E}$$

and $E^*$ is a reference energy which we shall take to be $10^7$ e.v.

In terms of this variable equation (1.2.9b) may be written in the form

$$V_j F_j (u) = \sum_{i=1}^{M} V_i P_{ij} \sum_{k=1}^{n_i} \int_{u-A_{ik}}^{u} C_{ik}(u')e^{u'-u}F_i(u')du' \quad (3.1.1)$$

where

$$\Delta_{ik} = \ln 1/\alpha_{ik}$$

and

$$C_{ik}(u) = \frac{\Sigma s_{ik}(u)}{\Sigma t_i(u)(1-\alpha_{ik})}$$

If we define the function

$$\overline{F}_j (u) = e^{u}F_j (u)$$

the exponentials will not occur explicitly in the equations and we hence avoid the awkwardness and labour of evaluating $e^u$ at each integration point. We see from equation (3.1.1) that the equation for $\overline{F}_j (u)$ will be

$$V_j \overline{F}_j (u) = \sum_{i=1}^{M} V_i P_{ij} \sum_{k=1}^{n_i} \int_{u-A_{ik}}^{u} C_{ik}(u')\overline{F}_i(u')du' \quad (3.1.2)$$

Applying the reciprocity theorem

$$\overline{F}_j (u) = \sum_{i=1}^{M} \overline{R}_{ji}(u) \sum_{k=1}^{n_i} \int_{u-A_{ik}}^{u} C_{ik}(u')\overline{F}_i(u')du' \quad (3.1.3)$$

Here $\overline{R}_{ji}(u) = P_{ji}(u) \Sigma_{t_j} (u)/\Sigma_{t_i}(u)$
From equation (1.2.16) the resonance escape probability will be given by

\[ p(u) = \frac{1}{\sum_{j=1}^{M} V_j} \int_{u}^{V_s} \frac{E_i}{\sum_{j=1}^{M} n_j} \sum_{j=1}^{M} n_j F_j(u') du' \]  

(3.1.4)

where \( u_s \) is the source lethargy.

For \( u < u_s \) we assume the asymptotic form (see section 2.1)

\[ F_i(u) = \sum_{j=1}^{M} E_j \eta_i \xi_j \]  

(3.1.5)

Following the notation of equation (1.2.14)

we put

\[ S_{ik}(u) = \int_{u-\Lambda_{ik}}^{u} C_{ik}(u') F_i(u') du' \]  

(3.1.6)

so that equation (3.1.3) may be written

\[ \bar{F}_j(u) = \sum_{i=1}^{M} Q_{ji}(u) \sum_{k=1}^{n_i} S_{ik}(u) \]  

(3.1.7)

The \( P_{ji}(u) \), the collision probabilities, have been evaluated for slab and cylindrical lattices by Doherty (1969) (using the method of Bonalumi) who has also written the FORTRAN subroutines to supply the functions \( Q_{ji}(u) \).

The \( C_{ik}(u) \), the functions of the cross sections, are in the case of fuel nuclides available from magnetic tapes containing the appropriate values at the 124,000 grid points (Doherty, 1968b). This has the obvious advantage of avoiding the lengthy recalculation of resonance cross sections for different
systems containing the same fuel nuclides.

We wish to derive an algorithm for the numerical solution of the integral equations (3.1.3) (which are of Volterra type) in the lethargy range \( u = 6.25 \) to \( u = 18.75 \) (i.e. \( E = 20 \) keV to \( E = 0.07 \) eV). The essence of the algorithm is the replacement of the integrals by their Simpson's rule sums.

We observe from the limits of the integrals in equation (3.1.3) \((u, u-\Delta_{ik})\) that this system of equations exhibits a peculiar delay behaviour in the \( u \) variable in that the values of the collision densities at \( u \) are directly affected by the values at all lethargies back to \( u-\Delta_{ik} \). It is this delay property which gives rise to some peculiar algorithmic difficulties which would not be encountered if the lower limit of the integral were fixed.

The major difficulty is the choice of an indexing system with which to refer to values of the collision densities at the previous lethargies. This indexing system must be economical in storage and time since for many moderator nuclides the range \( u, u-\Delta_{ik} \) covers a large number of grid points (the range for Deuterium, for example, covers 56,000 grid points for the smallest value of the step length).

The lethargy delay also creates some problems with the step length change since the collision densities being calculated at \( u \) on the new step length will depend on values
extending back to $u_{\Delta_{ik}}$, some of which will have been calculated with the old step length. So our indexing system must also be flexible enough to sort out, in an uncomplicated manner, those of the previously calculated values which are required in the calculation based on an integration rule with the new step length.

There is a wide choice of indexing systems to perform these tasks, however it is not a simple matter to find an indexing system which will perform these tasks with the minimum of logical decisions and data manipulations in the computer.

3.2 Choice of Grid

From the point of view of the neutron flux a constant step length in lethargy would be desirable as neutrons lose on average, the same amount of lethargy per collision. However from the point of view of the fuel nuclide cross section resonances occur at approximately constant energy spacings. For these reasons neither a constant lethargy nor a constant energy step length would give a satisfactory subdivision of the entire slowing down range.

From these considerations we choose a constant step length which changes at infrequent intervals. The lethargy variable was chosen since the interval for the integration rule remains fixed.

It would be inconvenient from programming considerations to have a collision range straddling two step
changes. Deutrium has a collision range of approximately 2.1 lethargy units and therefore it has been found convenient to change step length at every 2.5 lethargy units. Hydrogen of course has a much larger collision range (extending back to the source lethargy) but this nuclide will have the lower limit of the integral fixed and hence, as we have seen from the discussion in section 3.1, will be much simpler to handle.

The table below shows the step length and number of integration points in the various lethargy regions. The step length was chosen so as to enable the 6.68 eV resonance of U238, [in the 13.75 - (16.25-h₄) lethargy range] to be covered by 8,000 integration points.

<table>
<thead>
<tr>
<th>Lethargy Interval</th>
<th>Number of Points</th>
<th>Step Length</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.25-(8.75-h₁)</td>
<td>$2^4 \times 4000$</td>
<td>$h_1 = 3.90625 \times 10^{-5}$</td>
</tr>
<tr>
<td>8.75-(11.25-h₂)</td>
<td>$2^3 \times 3000$</td>
<td>$h_2 = 2h_1 = 7.81250 \times 10^{-5}$</td>
</tr>
<tr>
<td>11.25-(13.75-h₃)</td>
<td>$2^2 \times 4000$</td>
<td>$h_3 = 2h_2 = 1.56250 \times 10^{-4}$</td>
</tr>
<tr>
<td>13.75-(16.25-h₄)</td>
<td>$2 \times 4000$</td>
<td>$h_4 = 2h_3 = 3.12500 \times 10^{-4}$</td>
</tr>
<tr>
<td>16.25-(18.75-h₅)</td>
<td>4000</td>
<td>$h_5 = 2h_4 = 6.25000 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Table 3.1

3.3 Division of the Collision Range

In constructing a finite difference scheme based on Simpson’s rule we must bear in mind that an odd number of integration points are required for this integration rule.
Let $n_{ik}$ be the number of integration points for the integral in $S_{ik}(u)$. Suppose that $\ell_{ik}$ is the largest integer satisfying the equation

$$\Delta_{ik} = \ell_{ik} h + \delta'_{ik} \quad \delta'_{ik} > 0$$

(3.3.1)

where $h$ is the current step length, then the value of $n_{ik}$ appropriate for the application of Simpson's rule will be given by

$$n_{ik} = \begin{cases} 
\ell_{ik} & \text{for } \ell_{ik} \text{ odd} \\
\ell_{ik} + 1 & \text{for } \ell_{ik} \text{ even}
\end{cases}$$

(3.3.2)

In each case there will be some small segment $\delta_{ik}$ overlapping past the last integration point, given by

$$\delta_{ik} = \Delta_{ik} - (n_{ik}-1)h$$

(3.3.3)

In the following analysis we define

$$N = \text{the largest of all the } n_{ik}$$

$$u_1 = u_s - (N-1)h$$

and $$u_i = u_1 + i h,$$ where $h$ is the current step length.

It is difficult to grasp the analytical basis of the numerical algorithm without a clear picture of the manner in which the collision range $u_1, u_1 - \Delta_{ik}$ is split up. For this reason we give two simple examples of the division of the collision range in the two cases $\ell_{ik}$ odd and even, illustrating how the formulae (3.3.2) and (3.3.3) are applied in practice.
Example (i) \( l_{ik} \) odd

Suppose that \( \Delta_{ik} = 15h + \delta_{ik}' \), so that \( l_{ik} = 15 \) and \( \delta_{ik}' \) is the segment indicated in figure 3.1.

\[
\delta_{ik} u_{L-14} u_{L-13} u_{L-3} u_{L-2} u_{L-1} u_{L}
\]

Figure 3.1

Since Simpson's rule requires an odd number of points we rearrange the above equation thus

\[
\Delta_{ik} = 14h + (\delta_{ik}' + h)
\]

So finally

\[
l_{ik} = 15 = l_{ik} \]

\[
\delta_{ik} = \Delta_{ik} - 14h = \Delta_{ik} - (l_{ik} - 1)h = \delta_{ik}' + h
\]

and now Simpson's rule may be easily applied.

\[
\int_{u_{L} - \Delta_{ik}}^{u_{L}} f(u') du' = \int_{u_{L} - \Delta_{ik} - \delta_{ik}}^{u_{L} - \delta_{ik}} f(u') du' + \frac{h}{3} \left[ f(u_{L-14}) + 4f(u_{L-13}) + 2f(u_{L-12}) + \ldots + 2f(u_{L-2}) + 4f(u_{L-1}) + f(u_{L}) \right]
\]

Example (ii) \( l_{ik} \) even

Suppose that \( \Delta_{ik} = 10h + \delta_{ik}' \), so that \( l_{ik} = 10 \) and \( \delta_{ik}' \) is the segment indicated in figure 3.2.

\[
\delta_{ik} u_{L-10} u_{L-9} u_{L-8} u_{L-2} u_{L-1} u_{L}
\]

Figure 3.2.
Now we have an odd number of points (i.e. an even number of subdivisions) which is just exact for Simpson's rule, so that no rearrangement is necessary.

Hence

\[ n_{ik} = 11 = \ell_{ik} + 1 \]

\[ \delta_{ik} = \Delta_{ik} - 10h = \Delta_{ik} - (n_{ik} - 1)h = \delta'_{ik} \]

and Simpson's rule may be applied as follows

\[ \int_{u_{L-\Delta_{ik}}}^{u_{L}} f(u')du' = \int_{u_{L-10-\delta_{ik}}}^{u_{L-10}} f(u')du' + \frac{h}{3} \left( f(u_{L-10})+4f(u_{L-9})+2f(u_{L-8})+\ldots+4f(u_{L-1})+f(u_{L}) \right) \]

3.4 The Numerical Algorithm

3.4.1 The Algorithm for the Collision Densities

Using the subdivision described in section 3.3 we may in general write

\[ S_{ik}(u_L) = \int_{u_{L-n+1}}^{u_L} C_{ik}(u') \overline{F}_i(u')du' + E_{ik}(u_L) \quad (3.4.1) \]

where

\[ E_{ik}(u_L) = \int_{u_{L-n+1-\delta}}^{u_{L-n+1}} C_{ik}(u') \overline{F}_i(u')du' \quad (3.4.2) \]

Here, for simplicity of notation, we have dropped the subscript \( ik \) from \( n_{ik} \) and \( \delta_{ik} \) as double usage of this suffix would be redundant. We shall henceforth make free use of this convention when there is no danger of ambiguity.
We introduce the quantities

\[ g_{ik}^r = c_{ik}(u_r)\bar{F}_1(u_r) \]  
(3.4.3)

\[ j_{ik}^L = \sum_{\ell=1}^{n-1} g_{ik}^{L-n+2\ell} \quad k_{ik}^L = \sum_{\ell=1}^{n-3} g_{ik}^{L-n+2\ell+1} \]  
(3.4.4)

We also note that the identities

\[ j_{ik}^{L+1} = k_{ik}^L + g_{ik}^L \]  
(3.4.5)

\[ k_{ik}^{L+1} = j_{ik}^L - g_{ik}^{L-n+2} \]

Allow us to generate the functions recursively, so we avoid the lengthy recalculation of the sums in equation (3.4.4) at every point.

In terms of the above notation we can write, as follows, the Simpson's rule sum of the first integral in equation (3.4.4).

\[ \int_{u_{L-n+1}}^{u_L} c_{ik}(u')\bar{F}_1(u')du' = \frac{h}{3} \left( g_{ik}^{L-n+1} + 4j_{ik}^L + 2k_{ik}^L \right) + R_{ik}(u_L) \]  
(3.4.6)

where the remainder \( R_{ik}(u_L) \) can be put in the form [see e.g. Krylov, 1962]

\[ R_{ik}(u_L) = -\frac{nh}{180} \frac{d^4}{du^4} \left\{ c_{ik}(u)\bar{F}_1(u) \right\} \quad u=0 \]  
(3.4.7)

and \( u_{L-n+1} \leq \theta \leq u_L \)

For the step lengths which we propose to use
this remainder term should be negligible and we shall henceforth ignore it.

Thus on substituting (3.4.6) into (3.4.1) we obtain

\[ S_{ik}(u_L) = \frac{h}{3} \left[ g_{ik}^{L-n+1} + 4L_{ik} + 2K_{ik}^{L} + g_{ik}^{L} \right] + E_{ik}(u_L) \]  \hspace{1cm} (3.4.8)

We substitute this expression into equation (3.1.7) and obtain the finite difference equation

\[ \bar{F}_j(u_L) = \sum_{i=1}^{M} 0_{ji}(u_L) \sum_{k=1}^{\text{ni}} c_{ik}(u_L) \bar{F}_i(u_L) \]

We group all the unknowns \( \bar{F}_i(u_L) \{i=1,\ldots,M\} \) on the left hand side and obtain

\[ \bar{F}_j(u_L) - \frac{h}{3} \sum_{i=1}^{M} 0_{ji}(u_L) \sum_{k=1}^{\text{ni}} c_{ik}(u_L) \bar{F}_i(u_L) \]

\[ = \sum_{i=1}^{M} 0_{ji}(u_L) \sum_{k=1}^{\text{ni}} \left[ \frac{h}{3} \left( g_{ik}^{L-n+1} + 4L_{ik} + 2K_{ik}^{L} + g_{ik}^{L} \right) + E_{ik}(u_L) \right] \]  \hspace{1cm} (3.4.10)

We put

\[ \gamma_i = \sum_{k=1}^{\text{ni}} \frac{h}{3} \left( g_{ik}^{L-n+1} + 4L_{ik} + 2K_{ik}^{L} + g_{ik}^{L} \right) + E_{ik}(u_L) \]  \hspace{1cm} (3.4.11)

\[ \beta_{ji} = \begin{cases} 
- \frac{h}{3} 0_{ji}(u_L) \sum_{k=1}^{\text{ni}} c_{ik}(u_L) & \text{if } j \neq i \\
1 - \frac{h}{3} 0_{jj}(u_L) \sum_{k=1}^{\text{ni}} c_{ik}(u_L) & \text{if } j = i 
\end{cases} \]  \hspace{1cm} (3.4.12)

\[ \delta_j = \sum_{i=1}^{M} 0_{ji}(u_L) \gamma_i \]  \hspace{1cm} (3.4.13)
With this notation the set of finite difference equations (3.4.10) may be written in the concise form

$$\sum_{i=1}^{M} \beta_{ji} \overline{F}_i(u_L) = d_j \quad j = 1, \ldots, M \quad (3.4.14)$$

This set of linear equations may be solved by the Gauss-Jordan method to yield the unknowns $\overline{F}_i(u_L) \{i=1, \ldots, M\}$ at each point $u_L$.

### 3.4.2 The Evaluation of the Overlapping Integral $E_{ik}(u_L)$

Let

$$v_m = u_L - n_{ik} + m$$

for $m = 1, 2, 3, 4$

$$g_m = C_{ik}(v_m) \overline{F}_i(v_m)$$

$$r_m = e^{-v_m} g_m$$

then we may write the integral (3.4.2) as follows

$$E_{ik}(u_L) = \int_{v_1}^{v_1-\delta_{ik}} g_{ik}(u') du' \quad (3.4.15)$$

$$= \int_{v_1-\delta_{ik}}^{v_1} e^{u'} C_{ik}(u') F_i(u') du' \quad (3.4.16)$$

We evaluate $E_{ik}(u_L)$ by constructing an extrapolating polynomial. To be consistent with the accuracy of Simpson's rule we use a cubic extrapolating polynomial on the points
terms of the variable \( (u - v_2)/h \). On viewing equations (3.4.15) and (3.4.16) we observe two choices. We could construct the extrapolating polynomial either for \( g_{ik}(u) \) in equation (3.4.15) or for \( C^\alpha_{ik}(u) F^\alpha_i(u) \) in equation (3.4.16). It has been found that the former method gives rise to marked instabilities in the solution, probably because we are including the exponential function in the extrapolating polynomial. By constructing the cubic extrapolating polynomial for \( C^\alpha_{ik}(u) F^\alpha_i(u) \) we can avoid these instabilities.

It is nevertheless important to carry out the computation of \( E^\alpha_{ik}(u_L) \) in double precision arithmetic in order to avoid error build up. In fact slight inaccuracies in \( E^\alpha_{ik}(u_L) \) can, over a large number of points, magnify dramatically to considerably affect the accuracy of the solution. This might seem surprising when we consider that \( \delta^\alpha_{ik} \) is small. Certainly \( \delta^\alpha_{ik} \) forms only a small (practically negligible) fraction of the large scattering range of light moderator nuclides. For heavy fuel nuclides (which have a much smaller scattering range) this fraction is certainly not negligible (being for example about 1/50\(^{th}\) when the step length is \( h_4 \)) and therefore for fuel nuclides errors in \( E^\alpha_{ik}(u_L) \) would become important, especially since the fuel flux is varying so rapidly through resonances.

The extrapolating polynomial will have the form

\[
 r_{ik}(u) = C^\alpha_{ik}(u) F^\alpha_i(u) = d^\alpha_{ik} + a^\alpha_{ik} \left( \frac{u - v_2}{h} \right) + b^\alpha_{ik} \left( \frac{u - v_2}{h} \right)^2 + c^\alpha_{ik} \left( \frac{u - v_2}{h} \right)^3 \tag{3.4.17}
\]
Figure (3.3) illustrates the situation

Using results given by Todd (1958, p60) we find that

\[
\begin{align*}
    d_{ik} &= r_2 \\
    a_{ik} &= -\frac{1}{3} r_1 - \frac{1}{2} r_2 + r_3 - \frac{1}{6} r_4 \\
    b_{ik} &= \frac{1}{2} r_1 - r_2 + \frac{1}{2} r_3 \\
    e_{ik} &= -\frac{1}{6} r_1 + \frac{1}{2} r_2 - \frac{1}{2} r_3 + \frac{1}{6} r_4
\end{align*}
\]

The multiplication \( e^{-v_m} g_m \) at each point of the grid leads to round off error. We can avoid this by expressing the above coefficients in terms of the \( g_m \).

Thus by simple rearrangement we find that

\[
\begin{align*}
    d_{ik} &= e^{-v_1} d_{ik} \\
    a_{ik} &= e^{-v_1} a_{ik} \\
    b_{ik} &= e^{-v_1} b_{ik} \\
    e_{ik} &= e^{-v_1} e_{ik}
\end{align*}
\] (3.4.18)
where
\[
\begin{align*}
   d_{ik}^* &= e^{-\frac{h}{2} g_2} \\
   a_{ik}^* &= (-\frac{1}{3} g_1 - \frac{1}{2} e^{-\frac{h}{2} g_2} + e^{-2h} g_3 - \frac{1}{6} e^{-3h} g_4) \\
   b_{ik}^* &= (\frac{1}{2} g_1 - e^{-\frac{h}{2} g_2} + \frac{1}{2} e^{-2h} g_3) \\
   e_{ik}^* &= (-\frac{1}{6} g_1 + \frac{1}{2} e^{-\frac{h}{2} g_2} - \frac{1}{2} e^{-2h} g_3 + \frac{1}{6} e^{-3h} g_4)
\end{align*}
\]  

(3.4.19)

On substituting (3.4.17) into (3.4.16), integrating and making use of the expressions (3.4.18) and (3.4.19) we obtain
\[
E_{ik}(u_L) = d_{ik}^* t_1 - a_{ik}^* (t_2 + t_1/h) + b_{ik}^* (t_3 + 2t_2/h + t_1/h^2)
\]
\[
- e_{ik}^* (t_4 + 3t_3/h + 6t_2/h^2 + 6t_1/h^3) 
\]
\[ (3.4.20) \]

where
\[
\begin{align*}
   t_1 &= 1 - e^{-\delta_{ik}} \\
   t_2 &= 1 - (1 + \delta_{ik}/h) e^{-\delta_{ik}} \\
   t_3 &= 1 - (1 + \delta_{ik}/h)^2 e^{-\delta_{ik}} \\
   t_4 &= 1 - (1 + \delta_{ik}/h)^3 e^{-\delta_{ik}}
\end{align*}
\]  

(3.4.21)

Of the various possible ways of evaluating \( E_{ik}(u_L) \) we have found the one described here to be the quickest, the most stable and to involve the least round off error.

3.4.3 The Algorithm for the Resonance Escape Probability \( p(u) \).

Once having calculated the collision densities
from equation (3.4.21) we are able to calculate the quantity in which we are most interested, the resonance escape probability $p(u)$.

Putting

$$a_j(u) = \frac{\Sigma a_j}{t_j} (u)$$  \hspace{1cm} (3.4.22)$$

equation (3.1.4) for $p(u)$ may be written

$$p(u) = \sum_{j=1}^{M} \frac{V}{V_t} \int_{u_s}^{u} a_j(u')F_j(u')du'$$ \hspace{1cm} (3.4.23)$$

Let us suppose that the collision densities at $u_r$ have just been calculated, we would then turn to the calculation of $p(u_r)$ where

$$p(u_r) = \sum_{j=1}^{M} \frac{V}{V_t} \int_{u_s}^{u_r} a_j(u')F_j(u')du'$$

$$= \sum_{j=1}^{M} \int_{u_s}^{u_{r-2}} a_j(u')F_j(u')du' + \sum_{j=1}^{M} \frac{V}{V_t} \int_{u_{r-2}}^{u_r} a_j(u')F_j(u')du'$$ \hspace{1cm} (3.4.24)$$

The first integral in equation (3.4.24) is $p(u_{r-2})$ and is known from previous calculation. We replace the second integral in equation (3.4.24) by its Simpson's rule sum, so that

$$p(u_r) = p(u_{r-2}) + \frac{h}{3} \sum_{j=1}^{M} \frac{V}{V_t} \left[ a_j(u_{r-2})F_j(u_{r-2}) + a_j(u_{r-1})F_j(u_{r-1}) + a_j(u_r)F_j(u_r) \right]$$ \hspace{1cm} (3.4.25)$$
Hence we have a simple algorithm for the calculation of $p(u_r)$ in terms of the previously calculated $p(u_{r-2})$. This algorithm will of course only give us the resonance escape probability at every second grid point. To obtain $p(u)$ at every grid point it would be necessary to have two algorithms of the form (3.4.25), one for the even points and one for the odd points. In writing the computer programme PEARLS we have not bothered to do this since it is only the final resonance escape probability which we seek and this may be obtained with just the one algorithm. Figure (3.4) illustrates the basic ideas employed in deriving the algorithm for $p(u_r)$.

![Figure 3.4](image)

Since each lethargy range (i.e. those which are 2.5 lethargy units in width) is broken up into an even number of subdivisions (i.e. an odd number of points) we avoid the situation in which the point $u_{r-1}$ in the algorithm for $p(u_r)$ would be the lethargy at which the step length is doubled. The advantage in so doing is that we avoid the use of Simpson's rule for unequal step lengths when evaluating the second integral in equation (3.4.24) at this particular lethargy. Thus the
algorithm for $p(u_r)$ will proceed automatically across the step length change.

3.5 The Indexing System

In order to use the recurrence relations \((3.4.5)\) for $J_{ik}^L$ and $K_{ik}^L$ we will need to have stored the values of the array $g_{ik}^r$ at the $n_{ik}$ points $r = L-1, L-2, \ldots, L-n_{ik}+1$. However during the course of the calculation the index $L$ will run as high as 124,000 and hence to use the index $r$ to refer to the required value in the array would necessitate the use of a dimensioned array for $g_{ik}^r$, the size of which would be terribly wasteful in core storage area.

Consequently we define a special programme index which will cyclically assign the indices $1, 2, \ldots, n_{ik}$ to those $n_{ik}$ values of $g_{ik}^r$ required at any one time.

The basic concept is best clarified with a simple example. Consider a two nuclide system with $n_{11} = 11$, $n_{21} = 7$. We illustrate the storage indices in figure 3.5. The index above the grid line is the actual mathematical index (the index which runs to 124,000) that is the index $L$ in equation \((3.4.14)\). Below the grid line for each nuclide we have assigned, corresponding to each mathematical index, a storage index which runs repeatedly over the values $1, 2, \ldots, n_{ik}$. 
First point at which collision densities are calculated

Figure 3.5

Suppose that $F_1(u_{25})$, $F_2(u_{25})$ are to be next calculated, i.e. in equation (3.4.14) $L = 25$. In order to obtain the coefficients in equation (3.4.14) we must calculate the sums $J_{11}^{25}$, $K_{11}^{25}$, $J_{21}^{25}$, $K_{21}^{25}$ from the recurrence relations (3.4.5), which become here

$$J_{11}^{25} = K_{11}^{24} + g_{11}^{24}, \quad J_{21}^{25} = K_{21}^{24} + g_{21}^{24}$$

$$K_{11}^{25} = J_{11}^{24} - g_{11}^{15}, \quad K_{21}^{25} = J_{21}^{24} - g_{21}^{19}$$

Employing the indexing system shown in figure 3.5 we would find

$g_{11}^{24}$ stored as $g_{11}^{2}$, $g_{21}^{24}$ stored as $g_{21}^{6}$,

$g_{11}^{15}$ stored as $g_{11}^{4}$, $g_{21}^{19}$ stored as $g_{21}^{1}$.

Once $F_1(u_{25})$ and $F_2(u_{25})$ have been calculated we can compute $g_{11}^{25}$ and $g_{21}^{25}$, these would then be stored as $g_{11}^{3}$ and $g_{21}^{7}$ respectively.

Obviously with such a storage procedure we would never need to store more of the $g_{1k}^r$ than actually required at any one point.
We now require a formula which will enable us to reproduce this storage index in the general situation.

Consider the \( i_k \)th nuclide and let

\[
L_m = \text{the mathematical index} \\
s = \text{the storage index} \\
N = \text{the largest of all the } n_{ik}
\]  

We put

\[
L_s = L_m - 1 - N + n_{ik} \tag{3.5.2}
\]

\[
s = 1 + L_s - \left[ \frac{L_s}{n_{ik}} \right] n_{ik} \tag{3.5.3}
\]

where \( \left[ \frac{L_s}{n_{ik}} \right] \) represents the truncated integer result of the division \( L_s / n_{ik} \).

Obviously for the particular \( n_{ik} \) under consideration we can write

\[
L_m = (N - n_{ik} + 1) + \alpha n_{ik} + \beta \tag{3.5.4}
\]

where \( \alpha, \beta \) are integers and \( 0 \leq \beta \leq n_{ik} - 1, \alpha \geq 0 \).

Substituting into equation (3.5.2) we find that

\[
L_s = \alpha n_{ik} + \beta \tag{3.5.5}
\]

Now substitute (3.5.5) into (3.5.3) and we obtain

\[
s = 1 + \alpha n_{ik} + \beta - \left[ \frac{\alpha n_{ik} + \beta}{n_{ik}} \right] n_{ik} = 1 + \beta \tag{3.5.6}
\]
We see from equation (3.5.6) that as $\beta$ runs periodically over the integers 0, 1, 2, ..., $n_{ik}-1$, the index $s$ runs periodically over the integers 1, 2, ..., $n_{ik}$, which is in fact the required behaviour of the storage index as illustrated in figure 3.5.

In the programme PEARLS, all the indices $r$ in the array $g_{1k}^r$ are interpreted in terms of the index defined by equation (3.4.21).

### 3.6 The Step Length Change

We define

- $h_1 =$ the old step length
- $h_2 =$ the new step length $= 2h_1$.

Let $u_1$ be the very first lethargy at which the collision densities are to be calculated with the new step length $h_2$.

It is clear that use of the recurrence relations given in equation (3.4.5) over a range containing a step length change would require, as well as the indexing system discussed in section (3.5), a further indexing system to choose those values of the array $g_{1k}^r$ appropriate to the integration rule with step length $h_2$. This further indexing system would considerably complicate the situation and its use may be avoided if we first re-initialize the sums $J_{ik}^L$ and $K_{ik}^L$ on the basis of the new step length $h_2$. This in turn requires re-claculation (on the basis of the new step length)
of the $n_{1k}$ and $\delta_{1k}$ defined by equations (3.3.2) and (3.3.3).

The essence of the problem now is to define an algorithm which will retrieve and restore only those values of the array $g_{1k}^r$ (calculated with the previous step length $h_1$) which we need for the re-initialization of the sums $J_{ik}^L$, $K_{ik}^L$ and for the calculations with the new step length.

A particular example will help to clarify the general principles involved.

We consider again the two nuclide system given as an example in section (3.5). Let us suppose that $u_{65}$ is the changeover lethargy (i.e. $u_L$ in the above discussion).

We define the following quantities:

\[ \eta_{ik}^{(2)}, n_{ik}^{(2)} = \text{the values of } \eta_{ik}, n_{ik} \text{ respectively calculated with step length } h_2. \]

\[ N^{(2)} = \text{the largest of the } n_{ik}^{(2)}. \]

\[ L_m = \text{the new mathematical index.} \]

\[ L_m = \text{the old mathematical index} \]

and assume that

\[ n_{11}^{(2)} = 5, \quad n_{21}^{(2)} = 3. \]

The situation is illustrated in figure 3.6.
It is clear from figure (3.6) that of the previously calculated and stored values we shall need those at the points which are circled in order to calculate the collision densities at $u_{65}$. On the old mathematical index scale these points are two apart. But the functioning of the indexing system described in section (3.5) rests heavily upon the assumption that the required points are one apart on the mathematical index scale. Therefore before proceeding with the calculation of the collision densities with the step length $h_2$ we must define a new mathematical index which will scale the required previously stored values at points one apart. The upper line of figure 3.6 shows how, for this particular example, the points at which the required values are stored have been re-indexed one apart.

In general the new mathematical index can be found with the following algorithm: (In what follows L refers
to the changeover point i.e. the point 65 in figure 3.6).

(i) If $l_{ik}^{(2)}$ is even

$$L_m^{(2)} = L - n_{ik}^{(2)} + r$$

where $r = 2, \ldots, n_{ik} - 1$ in steps of 2.

(ii) If $l_{ik}^{(2)}$ is odd

$$L_m^{(2)} = L - n_{ik}^{(2)} + r$$

where $r = 4, \ldots, n_{ik} - 1$ in steps of 2.

Now with the required previously stored values appropriately re-indexed we are able to use equation (3.5.2) (with $L_m^{(2)}$ replacing $L_m^L$) and equation (3.5.3) to calculate the storage indices. We then recalculate $K_{ik}^{L-1}$ and $J_{ik}^{L-1}$ on the basis of the new step length and the algorithm follows the same steps as previously. When the next step length change is encountered the above procedure is repeated.

We demonstrate the re-initialization of $K_{ik}^L$ and $J_{ik}^L$ for the example in figure 3.6.

We first calculate, on the basis of the new step length, $J_{11}^{64}$, $K_{11}^{64}$, $J_{21}^{64}$ and $K_{21}^{64}$ (the 64 is on the new mathematical index scale).

$$J_{11}^{64} = g_{11}^2 + g_{11}^4, \quad K_{11}^{64} = g_{11}^3$$

$$J_{21}^{64} = g_{21}^2, \quad K_{21}^{64} = 0$$

Having re-initialized these quantities we
can then use the recurrence relations (3.4,5) to generate \( K_{ik}^{65} \) and \( J_{ik}^{65} \). Thus

\[
J_{11}^{65} = K_{11}^{64} + g_{11}^6 = g_{11}^3 + g_{11}^5 \\
K_{11}^{65} = J_{11}^{64} - g_{11}^2 = g_{11}^4 \\
J_{12}^{65} = K_{21}^{64} + g_{21}^6 = g_{21}^3 \\
K_{21}^{65} = J_{21}^{64} - g_{21}^2 = 0
\]

Note that in the above calculations the \( g_{ik} \) have been referred to with their new storage indices. (i.e. the indices in the lower two lines of figure 3.6).

From equation (3.4.8) we would then have

\[
S_{11}(u_{65}) = \frac{h_2}{3} \left[ g_{11}^2 + 4(g_{11}^3 + g_{11}^5) + 2g_{11}^4 + g_{11}^1 \right] + E_{11}(u_{65}) \\
S_{21}(u_{65}) = \frac{h_2}{3} \left[ g_{21}^2 + 4g_{21}^3 + 0 + g_{21}^1 \right] + E_{21}(u_{65})
\]

and the algorithm in section (3.4) would proceed automatically as before; we would arrive at equation (3.4.14) and solve for the collision densities at \( u_{65} \).

3.7 Operation of the Algorithm

The numerical algorithm discussed in the previous sections allows us to solve the slowing down equations in a step-by-step procedure. The basic steps in this procedure are

(i) We calculate the division of the collision interval
of each nuclide as per section (3.3).

(ii) We calculate the asymptotic collision density for a cell of the lattice and then compute the asymptotic value of the integrand of $S(u)$ at the points $1, 2, \ldots, n_{ik} - 1$.

(iii) We calculate the initial values of the sums $K_{ik}^L, J_{ik}^L$ from equation (3.4.4). (We use equation (3.4.5) to generate subsequent values of these quantities).

(iv) We calculate the co-efficients of $F_i(u_L)$ in equation (3.4.14) and solve for $F_i(u_L)$.

(v) Store (using the indexing system in section 3.5) the value of $g_{ik}^L$.

(vi) Calculate $p(u_L)$ at every second grid point from equation (3.4.18).

(vii) Proceed to the next grid point, calculate $K_{ik}^L, J_{ik}^L$ from the recurrence relations (3.4.5) and proceed through the algorithm as before.

(viii) At the step change lethargy the procedure outlined in section (3.6) is followed.

The computer programme PEARLS, based on this algorithm, has been written for the IBM 360/50H computer at the Australian Atomic Energy Commission. This programme can handle systems containing up to four regions. Homogeneous systems can be dealt with as a particular case by PEARLS, this has enabled us to carry out comparisons with the results obtained from the PEAS programme (Pollard, 1964) which solves only the homogeneous
system equations. Comparison of the results of PEAS and PEARLS for a range of homogeneous systems has yielded results in agreement to five decimal places, this in spite of the fact that PEAS uses a different grid and step length.

3.8 Asymptotic End Correction for Isolated Resonance Investigations

As so far developed the numerical algorithm will solve the slowing down equations over the entire slowing down range. The upper and lower limits of this range (i.e. at 6.25 and 18.75 lethargy units) have been chosen as the points within which all resonance absorption occurs.

For some theoretical investigations we may wish to solve the slowing down equations through an isolated resonance. For example, in the present thesis we have restricted our attention to isolated resonances and in particular the 6.68 eV resonance of U238 which occurs at a lethargy of about 14.2. To investigate this resonance we need only solve the slowing down equations in the lethargy interval 13.75 - (16.25-h₄) (see table 3.1). In so doing we tacitly assume that all the absorption due to this resonance occurs within these limits. While this is approximately true there is nevertheless a small amount of absorption which takes place in the wings of the resonance beyond these points.

To obtain an estimate of this absorption we shall assume that in the wings of the resonance the flux has
the form obtained from application of the NR approximation to all the nuclear species.

Let

\[ p_r = \text{the exact value of the resonance escape probability obtained by taking into account the absorption in the wings of the resonance} \]

\[ p_r' = \text{the value of the resonance escape probability obtained by using the numerical algorithm between 13.75 and 16.25-\(h\) lethargy units.} \]

Figure (3.7) illustrates the absorption cross section in the lethargy interval \(u_1, u_2\) (in the present argument \(u_1 = 16.25-\(h\), \(u_2 = 13.75\)). The variables \(x_1\) and \(x_2\) are the corresponding values of \(x = \frac{2}{\Gamma}(E-E_r)\), \(u_r\) is the lethargy corresponding to the resonance energy \(E_r\). The shaded portions represent the wings of the resonance in which we are currently attempting to estimate the absorption.
The exact value of the resonance escape probability, viz. $p_r$ is given by

$$1 - p_r = \frac{\Gamma}{2} \sum_{j=1}^{M} \frac{V}{V} \left( t \right) \int_{-\infty}^{\infty} \frac{\Sigma \alpha_j}{\Sigma t_j} F_j(x) dx$$

$$+ \frac{\Gamma}{2} \sum_{j=1}^{M} \frac{V}{V} \left( t \right) \int_{x_2}^{x_1} \frac{\Sigma \alpha_j}{\Sigma t_j} F_j(x) dx$$

(3.8.1)

Assuming NR flux in the wings of the resonance we have, in the range $(x_1, x_2)$

$$F_j(x) = \frac{\Sigma_i}{\bar{\Sigma}_h \Sigma E_r}$$

(3.8.2)

and in the range $(x_1, -\infty)$

$$F_j(x) = p_r \frac{\Sigma_i}{\bar{\Sigma}_h \Sigma E_r}$$

(3.8.3)

Assuming that there is only one absorbing species present in the system we drop the general notation of equation (3.8.1) and give the fuel region the subscript 1.

After some elementary integrations we find that

$$\frac{\Gamma}{2} \int_{x_2}^{\infty} \frac{\Sigma \alpha_i}{\Sigma t_i} F_i(x) dx = \frac{N \Sigma_o}{\bar{\Sigma}_h \Sigma E_r} \left( \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{x_2}{\beta} \right)$$
and
\[
\frac{1}{2} \Gamma \int_{-\infty}^{x_1} \frac{\sum a_1(x) F_1(x) dx}{\sum t_1(x)} = p_r \frac{NI_0}{\xi h \Sigma h} \left( \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \frac{x_1}{\beta} \right)
\]

where
\[
I_0 = \frac{\pi o \sigma \gamma}{2E r}, \quad \beta^2 = 1 + \frac{\sigma_o}{\sigma_I}
\]

and \(N\) is the absorber nuclide concentration.

Substituting these results into equation (3.8.1) and using the fact that
\[
1 - p_r' = \frac{\Gamma}{2} \sum_{j=1}^{M} \frac{V_j}{V} \int_{x_1}^{x_2} \frac{\sum a_j(x) F_j(x) dx}{\sum t_j(x)}
\]

we find after some manipulation
\[
p_r = \frac{p_r' - \frac{c}{\beta} \left( \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{x_2}{\beta} \right)}{1 + \frac{c}{\beta} \left( \frac{1}{2} + \frac{1}{\pi} \tan^{-1} \frac{x_1}{\beta} \right)}
\]  

(3.8.4)

where \(c = \frac{NI_0}{\xi h \Sigma h}\).

Using equation (3.8.4) the results of the PEARLS programme for an isolated resonance may be modified to account for absorption in the wings of the resonance.

For the systems we shall be studying in later chapters this modification increases the \(p_r'\) by about 0.5%.
We have already observed in section (2.5.1) the equivalence between heterogeneous and homogeneous systems when the NR approximation is applied to the external moderator. Our present aim is to introduce refinements into the calculation of $s_e$ (equation 1.6.4) which will take more accurate account of the geometry of the system.

We have discussed in sections (2.4.3) and (2.6.1) an approach to the calculation of resonance integrals (due mainly to Russian workers) which takes detailed account of the collision probabilities. This approach involved the application of the NR approximation to all nuclear species. It has not been possible to take advantage of the more sophisticated treatment of the collision probabilities of this approach in conjunction with any improved slowing down model such as the $\lambda$ method. This is so since to apply an improved slowing down model we must have a rational type approximation for the collision probabilities otherwise the analysis becomes unmanageable. In this chapter we shall introduce a method which will permit us to incorporate the more detailed method of handling collision probabilities into a rational approximation for the fuel region self collision probability.

In this chapter we shall consider the same system and assume the same notation as in section (2.3).
4.1 Corrected Rational Approximations

The basic aim of equivalence relation theory is to seek, for the quantity $P_{11}$ given by (see section 1.4),

$$P_{11} = \frac{G_1 + G_2 (1-P_1-G_1)}{1 - (1-G_1)(1-G_2)} \tag{1.4.17a}$$

an approximation in the form

$$P_{11} = \frac{\sigma_{t_1}}{s_e + \sigma_{t_1}} \tag{4.1.1}$$

where $s_e$ is a parameter dependent upon the scattering properties and the geometry of the system.

One method of obtaining $P_{11}$ in the required functional form equation (4.1.1) would be to seek the following types of rational approximations for $G_1$ and $G_2$,

$$G_1 = \frac{N\bar{\sigma}_t}{1+a_N\bar{\sigma}_t} \quad \text{and} \quad G_2 = \frac{N\bar{\sigma}_m}{1+a_mN\bar{\sigma}_m} \tag{4.1.2}$$

Here we have dropped the subscript 1 from $\bar{\alpha}_1$ and $\sigma_{t_1}$ since repeated use of this subscript in the current argument would be redundant. The constants $a_m, a_f$ are adopted in the spirit of the Bell factor discussed in section (1.6) and are chosen to give better approximations for $G_1$ and $G_2$ than the Wigner rational approximation while still retaining its convenient functional form. We shall henceforth refer to the approximations (4.1.2) as the corrected rational approximations.
Substituting the approximation for $G_j$ into equation (1.4.17a) we obtain

$$P_{11} = \frac{\sigma_t}{\sigma_t + s_e}$$  \hspace{1cm} (4.1.3)

where

$$s_e = \frac{G_2}{N \lambda [1 - (1 - a_f)G_1]}$$  \hspace{1cm} (4.1.4)

Using the approximation for $G_2$ this expression for $s_e$ reduces to

$$s_e = \frac{\sigma_m}{1 + a_K N \lambda \sigma_m}$$  \hspace{1cm} (4.1.5)

where

$$a_K = a_m + a_f - 1.$$  \hspace{1cm} (4.1.6)

We observe that this approach gives us a Bell type factor having a fuel contribution ($a_f$) and a moderator contribution ($a_m$), each of which is separable from the other. This allows us to consider separately the determination of each factor.

However we should bear in mind that assuming that the fuel and moderator contributions are separable in the above manner is the weak point of the approach using corrected approximations. We shall give deeper consideration to this point in sections (4.4) and (4.5).
4.2 Evaluation of the Fuel Factor $a_f$

4.2.1 The Resonance Integral Under the NR Approximation

Applying the NR approximation to both the fuel and moderator regions in equation (2.5.2) and performing the required integrations we obtain the following expression for the resonance integral

$$I = I_0 \left\{ (1 + \frac{\sigma_o}{\sigma_p})^{-\kappa} + \left[ (1 + \frac{\sigma_o}{s e + \sigma_p})^{-\kappa} - (1 + \frac{\sigma_o}{\sigma_p})^{-\kappa} \right] \right\}$$

Here, for the sake of simplicity, we assume that there is no admixed moderator in the fuel region. However the theory may be altered to account for such admixed moderator simply by replacing $\sigma_p$ with $s + \sigma_p$.

This expression may be simplified if we assume $\sigma_o >> s e + \sigma_p$. This assumption is quite reasonable for strongly absorbing resonances, such as the 6.68eV resonance of U238.

Under the approximation $\sigma_o >> s e + \sigma_p$ we have

$$(1 + \frac{\sigma_o}{s e + \sigma_p})^{-\kappa} - (1 + \frac{\sigma_o}{\sigma_p})^{-\kappa} = \sigma_o^{-\kappa} \left[ (s e + \sigma_p)^{\frac{1}{2}} - \sigma_p^{\frac{1}{2}} \right]$$

so that the expression for the resonance integral becomes

$$I = I_0 \left\{ \frac{\sigma_o}{\sigma_p}^{-\kappa} + \sigma_o^{-\kappa} \left[ (s e + \sigma_p)^{\frac{1}{2}} - \sigma_p^{\frac{1}{2}} \right] \right\}$$

(4.2.2)
In section (2.4.3) we have outlined the derivation of an expression for the resonance integral of an isolated lump. viz.

\[ I = I_o \left[ (\frac{\sigma_o}{\sigma_p})^{-\frac{1}{2}} + \frac{(\sigma_o \sigma_p)^{-\frac{1}{2}}}{2\eta} \psi(\bar{x}) \right] \]  

(2.4.15)

This expression was derived under the approximation \( \sigma_o \gg \sigma_p \) and \( \eta \sigma_o \gg 1 \) (i.e. for strongly absorbing resonances). Through the term \( \psi(\bar{x}) \) this expression takes detailed account of the geometry of the fuel lump.

4.2.2 Criterion for Selection of \( a_f \)

We choose \( a_f \) in such a manner that in the case of an isolated lump (i.e. \( G_2 = 1 \)) the expression for the resonance integral given by equation (4.2.2) becomes equal to the expression for an isolated lump given by equation (2.4.15). We will then have through equations (4.1.4) (for \( s_e \)) and (4.1.3) (for \( P_{11} \)), a rational approximation for \( P_{11} \) which in the calculation of resonance integrals (under whatever slowing down model we are using) will yield an expression taking detailed account of the lump escape probability.

Since the resonance integral given by equation (2.4.15) is derived under the NR approximation, resonance integrals calculated with the \( P_{11} \) obtained by the use of \( a_f \) can only be expected to yield exact results if we assume that all resonance absorption occurs close to the resonance peak. However
### Table 4.1 (facing page 105)

The Fuel Factor $a_f$

<table>
<thead>
<tr>
<th>$\Sigma_\infty$</th>
<th>Slab $a_f$</th>
<th>Cylinder $a_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.8830</td>
<td>0.0</td>
</tr>
<tr>
<td>0.1</td>
<td>0.7999</td>
<td>0.5198</td>
</tr>
<tr>
<td>0.5</td>
<td>0.8835</td>
<td>0.8236</td>
</tr>
<tr>
<td>1.0</td>
<td>0.8950</td>
<td>0.9203</td>
</tr>
<tr>
<td>2.0</td>
<td>0.9170</td>
<td>0.9741</td>
</tr>
<tr>
<td>3.0</td>
<td>0.9335</td>
<td>0.9884</td>
</tr>
<tr>
<td>6.0</td>
<td>0.9609</td>
<td>0.9973</td>
</tr>
</tbody>
</table>

### Table 4.2

The Moderator Factor $a_m$

<table>
<thead>
<tr>
<th>$\Sigma_\infty$</th>
<th>Slab $v_2/v_1=10.0$</th>
<th>Cylinder $v_2/v_1=20.0$</th>
<th>$v_2/v_1=100.0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>$\infty$</td>
<td>0.9677</td>
<td>1.0015</td>
</tr>
<tr>
<td>0.1</td>
<td>1.0865</td>
<td>0.9582</td>
<td>0.9118</td>
</tr>
<tr>
<td>0.5</td>
<td>0.8523</td>
<td>0.9309</td>
<td>0.9637</td>
</tr>
<tr>
<td>1.0</td>
<td>0.7960</td>
<td>0.9118</td>
<td>0.9430</td>
</tr>
<tr>
<td>2.0</td>
<td>0.7810</td>
<td>0.8955</td>
<td>0.9233</td>
</tr>
<tr>
<td>5.0</td>
<td>0.8337</td>
<td>0.8962</td>
<td>0.9145</td>
</tr>
<tr>
<td>$\infty$</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>
for many resonances such as assumption is not valid and we shall elaborate upon this point in chapter 6.

If \( G_2 = 1 \) then \( s_e = 1/a_f \bar{N} \bar{\Sigma} \) and equation (4.2.2) becomes

\[
I = I_0 \left( \frac{\sigma_o}{\sigma_p} \right)^{-\frac{1}{2}} + \sigma_o^{-\frac{1}{2}} \left( \frac{1}{a_f \bar{N} \bar{\Sigma}} + \sigma_p \right)^{\frac{1}{2}} - \sigma_p^{\frac{1}{2}} \right)
\]

(4.2.3)

The expressions (2.4.15) and (4.2.3) are equal if

\[
\sigma_o^{-\frac{1}{2}} \left( \frac{1}{a_f \bar{N} \bar{\Sigma}} + \sigma_p \right)^{\frac{1}{2}} - \sigma_p^{\frac{1}{2}} = \frac{\left( \sigma_o \sigma_p \right)^{-\frac{1}{2}}}{\psi(\bar{\Sigma})}
\]

which yields

\[
a_f = \frac{4 \bar{N} \bar{\Sigma} \sigma_p}{\psi^2(\bar{\Sigma}) + 4 \bar{N} \bar{\Sigma} \sigma_p \psi(\bar{\Sigma})}
\]

(4.2.4)

Table 4.1 shows \( a_f \) for slab and cylindrical fuel elements at various values of \( \bar{N} \bar{\Sigma} \sigma_p \). Let us find the limit of \( a_f \) as \( \sigma_p \to 0 \).

First we recall the definition of \( \psi(\bar{\Sigma}) \)

\[
\psi(\bar{\Sigma}) = \int \left( \frac{4y}{\pi} \right)^{\frac{1}{2}} e^{-y} - 2y \text{erfc} \sqrt{y} \text{erf} \sqrt{y} f(\bar{\Sigma}) d\bar{\Sigma}
\]

with \( y = \bar{N} \bar{\Sigma} \sigma_p \)

Expanding \( e^{-y} \) and \( \text{erf} \sqrt{y} \) for small \( y \) and then integrating we obtain

\[
\psi(\bar{\Sigma}) = \frac{4}{\sqrt{\pi}} \left( \bar{N} \sigma_p \right)^{\frac{1}{2}} \bar{\Sigma}^{-\frac{1}{2}} - 2 \bar{N} \sigma_p \bar{\Sigma} + \text{Higher order terms.}
\]

Substituting into (4.2.4) we have

\[
a_f = \frac{\bar{\Sigma}}{4} \left( \frac{1}{\bar{\Sigma}^2} \right)^2 \text{ as } \sigma_p \to 0
\]

(4.2.5)

But \( \bar{\Sigma} > \left( \frac{1}{\bar{\Sigma}^2} \right)^2 \) [see appendix 1 equation A1.2] and so in general

\( a_f > 0.785 \).
In particular, for cylindrical fuel elements we have from Appendix 1, equation (Al.7), that \( \ell^{1/2} = 0.973 \ell^{1/2} \) so that \( a_f \to 0.830 \).

For slab systems \( \ell^{1/2} = 0.943 \ell^{1/2} \) so \( a_f \to 0.883 \).

### 4.3 The Moderator Factor \( a_m \)

For a slab system the chord distribution is known and so \( G_2 \) may be found exactly as (Case, de Hoffmann and Placzek, 1953)

\[
G_2 = 1 - 2E_3\left(1\frac{\sqrt{N\sigma}}{m}\right) \tag{4.3.1}
\]

where

\[
E_3(z) = \int_1^\infty e^{-zy} \frac{dy}{y^3}
\]

Hence for a slab

\[
a_m = \frac{1}{1 - 2E_3\left(1\frac{\sqrt{N\sigma}}{m}\right)} - \frac{1}{N\sigma m} \tag{4.3.2}
\]

The function \( E_3(z) \) has been tabulated by Case, de Hoffmann and Placzek (1953) and for small \( z \) has the expansion

\[
E_3(z) = \frac{1}{2} - z - \frac{z^2}{2} (\ln z + \gamma - \frac{3}{2})
\]

so that as \( N\sqrt{\sigma m} \to 0 \)

\[
a_m \to -\frac{1}{4}(\ln \frac{N\sigma m}{2} + \gamma - \frac{3}{2}) \tag{4.3.3}
\]

For cylindrical fuel elements we make use of the excellent Sauer-Bonalumi approximation to the Dancoff factor (equation 1.5.18). Equating this approximation to the expression
for $G_2$ given in equation (4.1.2) we obtain

$$a_m = \frac{1 + (\tau_1 - t_1)N\sigma_m}{h(N\sigma_m)} - \frac{1}{N\sigma_m}$$

(4.3.4)

where

$$h(N\sigma_m) = 1 + (\tau_1 - t_1)N\sigma_m - e^{-tN\sigma_m}$$

and all other parameters are defined in equation (1.5.18)

As $N\sigma_m \to 0$

$$a_m = \frac{8}{7} - t + \frac{t^2}{2}$$

Table (4.2) shows $a_m$ for slabs and cylinders in a square lattice for various values of $N\sigma_m$.

4.4 The Correct Lattice Dependence of $s_e$

4.4.1 The Lattice Resonance Integral Under the NR Approximation

Applying the NR approximation to both fuel and moderator regions we have from equation (2.5.1)

$$\phi_1(E) = \frac{1}{E} \left( \frac{\sigma_p}{\sigma_t(E)} + \frac{\sigma_r(E)}{\sigma_t(E)} (1 - P_{11}) \right)$$

(4.4.1)

Here, for the sake of simplicity, we have dropped the subscript 1 from $\sigma_t$ and $\sigma_r$.

Bell's formula for $P_{11}$ (equation 1.4.17a)

may be cast into the form

$$1 - P_{11} = \frac{1}{N\sigma_t} \frac{G_1}{1 + rG_1}$$

(4.4.2)
where

\[ r = \frac{1-G_2}{G_2} \]

Substituting (4.4.2) into (4.4.1) we may obtain the following expression for the resonance integral

\[ I = \int \frac{\sigma_a \rho}{\sigma_t} \frac{dE}{E} + \frac{1}{N}\int \frac{\sigma_a \rho}{\sigma_t} \frac{G_1}{1+rG_1} \frac{dE}{E} \] (4.4.3)

In section (2.6.2) we outlined the method developed by Petrov (1958) for finding the resonance integral in tight lattices of purely absorbing fuel lumps under the NR approximation (i.e. when \( \sigma_p = 0 \) in equation 4.4.3). We shall now proceed to extend his method to lattices of any pitch in which scattering by the fuel lump is taken into account. This approach is a generalisation of the intermediate approach for isolated lumps (section 2.4.3) to lattices. The resulting expression for the resonance integral will take detailed account of the lattice arrangement and escape probabilities.

Consider the second term in equation (4.5.3) viz.

\[ \frac{1}{N}\int \frac{\sigma_a \rho}{\sigma_t} \frac{G_1}{1+rG_1} \frac{dE}{E} = \frac{\Gamma}{2\pi r} \frac{\Gamma}{2\pi} \frac{1}{N}\int \frac{\sigma_o}{\sigma_p} \frac{G_1}{1+rG_1} \frac{dx}{(1+\frac{\sigma_o}{\sigma_p} x^2)^2} \] (4.4.4)

Expressions for \( G_1 \) in slab and cylindrical geometries are well known, they are:-

(i) For cylindrical fuel elements we have from equation (1.5.6) that
\[ G_1 = 1 - \frac{4}{\pi} \int_0^{\pi/2} \cos \psi \, K_{1,3} \{N\bar{\sigma}_t \cos \psi\} d\psi \]
\[ = 1 - \frac{4}{\pi} \int_0^{\pi/2} \cos \psi \, K_{1,3} \{N\bar{\sigma}_t (1 + \frac{\sigma_o/\sigma_p}{1+z^2}) \cos \psi\} d\psi \]

(ii) For slab fuel elements we have from Case, de Hoffman and Placzek (1953) that
\[ G_1 = 1 - 2E_3(N\bar{\sigma}_t/2) \]
\[ = 1 - 2E_3\frac{N\bar{\sigma}_t}{2} (1 + \frac{\sigma_o/\sigma_p}{1+z^2}) \].

If we assume \( \sigma_o >> \sigma_p \) and make the change of variable \( z = (\sigma_o/\sigma_p)^{1/2}/x \) we obtain
\[ \int_{-\infty}^{\infty} \frac{G_1}{1+\rho G} \frac{dx}{(\frac{\sigma_o}{\sigma_p} + x^2)^2} = \frac{\pi}{2} (\frac{\sigma_p}{\sigma_o})^{3/2} \]
\[ K \] (4.4.5)

where
\[ K = \frac{4G_2}{\pi} \int_0^\infty \frac{1-\phi(N\bar{\sigma}z)}{1-(1-C_2)\phi(N\bar{\sigma})} \cdot \frac{z^2 dz}{(1+z^2)^2} \] (4.4.6)

with \( \phi(N\bar{\sigma}z) \) given by the following expressions:

(i) For cylindrical fuel elements
\[ \phi(N\bar{\sigma}z) = \frac{4}{\pi} \int_0^{\pi/2} K_{1,3} \{N\bar{\sigma}_o (1+z^2) \cos \psi\} \cos \psi d\psi \] (4.4.7a)

(ii) For slab fuel elements
\[ \phi(N\bar{\sigma}z) = 2E_3\frac{N\bar{\sigma}_t}{2} (1 + z^2) \] (4.4.7b)
In appendix 2 we give a tabulation of the function $K$. Substituting equation (4.4.5) into equation (4.4.4) and then this into equation (4.4.3) we find that the expression for the resonance integral becomes

$$I = I_0 \left\{ \left( \frac{\sigma_o}{\sigma_p} \right)^{\frac{1}{2}} + \frac{K}{2N_k} \left( \frac{\sigma_o}{\sigma_p} \right)^{\frac{1}{2}} \right\}$$

(4.4.8)

If we have an isolated lump system then $G_z = 1$, in which case

$$K(G_z = 1) = \frac{4}{\pi} \int_0^\infty \{1 - \phi(Nkz)\} \frac{z^2 dz}{(1 + z^2)^2}$$

(4.4.9)

It is not difficult to show that this latter integral is equal to the function $\psi(\overline{\lambda})$ defined by equation (2.4.16). So that for the isolated lump situation the resonance integral given by equation (4.4.8) reduces to the resonance integral given by equation (2.4.15) as it should. The $\psi(\overline{\lambda})$ of the isolated lump theory is replaced for lattice systems by the function $K$ (equation 4.4.6).

### 4.4.2 The Selection of $s_e$

In section (4.1) through use of the corrected rational approximations we obtained a rational approximation for $P_{11}$ in the form

$$P_{11} = \frac{\sigma_t}{\sigma_t + s_e}$$

(4.1.3)

where the factor $s_e$ depended on a fuel contribution $a_f$ and a moderator (or lattice configuration) contribution $a_m$, each
of these factors being determined separately. As we pointed out in section (4.1) this assumption of separability of fuel and moderator contributions is a weak point of the theory. We may remove this assumption if we demand from the outset an approximation of the form equation (4.1.3) for $P_{11}$ without assuming 'ab initio' the functional dependence of $s_e$ on the fuel and moderator contributions. We shall use the results of the previous section to find an expression for $s_e$.

We have already seen in section (4.2.1) that use of the approximation equation (4.1.3) in equation (4.4.1) leads to the following expression for the resonance integral

$$I = I_0 \left( (1 + \frac{\sigma_0}{\sigma_p})^{-\frac{1}{2}} + \left(1 + \frac{\sigma_0}{s_e + \sigma_p}\right)^{-\frac{1}{2}} - (1 + \frac{\sigma_0}{\sigma_p})^{-\frac{1}{2}} \right)$$

which under the approximation $\sigma_0 >> s_e + \sigma_p$ becomes

$$I = I_0 \left( \frac{\sigma_0}{\sigma_p}^{-\frac{1}{2}} + \sigma_0 \left\{ (s_e + \sigma_p)^{-\frac{1}{2}} - \sigma_p^{\frac{1}{2}} \right\} \right) \quad (4.2.2)$$

We choose $s_e$ by demanding that the two expressions for the resonance integral, equations (4.2.2) and (4.4.8), be always equal. The two expressions will be equal if

$$\sigma_0 \left\{ (s_e + \sigma_p)^{-\frac{1}{2}} - \sigma_p^{\frac{1}{2}} \right\} = \frac{K}{2N \bar{E}} (\sigma_0 \sigma_p)^{-\frac{1}{2}}$$

which yields

$$N \bar{E} s_e = \frac{K^2 + 4N \bar{E} \sigma K}{4N \bar{E} \sigma_p} \quad (4.4.10)$$
### TABLE 4.3

Calculated from equation (4.4.10)

<table>
<thead>
<tr>
<th>$G_2$</th>
<th>Slab System</th>
<th>Cylindrical System</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</tr>
<tr>
<td>$\bar{\sigma}_p$</td>
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<tr>
<td>6.0</td>
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<td>0.9330</td>
</tr>
</tbody>
</table>

### TABLE 4.4

Calculated from equation (4.4.11)

<table>
<thead>
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<th>Slab System</th>
<th>Cylindrical System</th>
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</thead>
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</tr>
<tr>
<td>$\bar{\sigma}_p$</td>
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<td></td>
</tr>
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<tr>
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Equation (4.4.10) gives the correct lattice dependence of $s_e$ (under the assumption of Bell's formula and use of the NR approximation).

Note that when $G_2=1$ in equation (4.4.10) we obtain $s_e$ for an isolated lump. Since in the notation of section (4.1) $s_e$ for an isolated lump is $1/a_f \overline{N} s$ and $K(G_2=1)$ is equal to $\psi(\overline{\lambda})$, we see that in this limit equation (4.4.10) yields the value of $a_f$ given by equation (4.2.4). Consideration of this limiting case gives up deeper insight into the difference between the present approach and that of the corrected rational approximations. Having obtained $a_f$, the fuel contribution, from equation (4.2.4) we then add $a_m$ the moderator contribution and obtain $s_e$ from equation (4.1.5). This expression for $s_e$ may be put into the form

$$\overline{N} s_e = \left( \frac{1-G_2}{G_2} + \frac{4N\bar{\sigma}_p}{\psi + 4N\bar{\sigma}_p \psi} \right)^{-1}$$

(4.4.11)

exhibiting clearly the separation of the fuel and moderator contributions. On the other hand equation (4.4.10) through the function $K$ involves the fuel and moderator contributions in such a manner that they are obviously inseparable.

In tables (4.3) and (4.4) we compare values of $\overline{N} s_e$ calculated by the two formulae equations (4.4.10) and (4.4.11) at various values of $G_2$. We see from these tables that the assumption of separability of the fuel and moderator contributions leads to an overestimate of $\overline{N} s_e$. 

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4.5 Comparison with the Theory of Marchuk for Slab Systems

In the theory of corrected rational approximations our criterion for selection of $s_e$ rested upon three major assumptions.

(i) We tacitly assumed that the fuel and moderator contributions to $s_e$ were separable

(ii) We have obtained $s_e$ through application of the NR approximation to all nuclear species

(iii) We have assumed Bell's formula (i.e. equation 1.4.17a) for $P_{11}$.

In the previous section we discussed how the first assumption may be removed. Assumption (ii) which is common to all the work in this chapter, will be discussed in chapter 6. Now we shall investigate the effect of assumption (iii) on the calculation of $s_e$ for slab systems.

We have outlined in section (2.6.1) the approach adopted by Marchuk in deriving, for a slab lattice under the NR approximation, an expression for the resonance integral which takes detailed account of the lattice arrangement. In particular we observed that since Marchuk's approach does not lead to the explicit introduction of $P_1, G_1, P_2, G_2$, his final result does not rely on Bell's formula nor does it involve one of the major assumptions of Bell's formula, namely that the resonance energy neutrons fall isotropically onto each fuel lump. It has already been pointed out by Aisu and Minton (1964) that for lattices of weakly absorbing...
transparent slabs Bell's formula for $P_{11}$ involves considerable error. This should not, however, affect our results since in the derivation of our expression for $s_e$ we have assumed $\sigma_o \gg \sigma_p$ and $N\bar{\sigma}_o \gg 1$ i.e. strongly absorbing systems to which the results of Aisu and Minton do not apply.

We shall use the result of Marchuk to derive an expression for $s_e$ which will not involve the assumption (iii) above. A comparison with the values of $s_e$ obtained from equation (4.4.10) for slab systems should give an indication of the error involved in the use of Bell's formula.

Marchuk's expression for the resonance integral can be put into the form (see equation 2.6.13)

$$I = I_o \left( \frac{\sigma_o}{\sigma_p} \right)^{-k_o} + \frac{F(\alpha, \beta)}{2N\bar{\sigma}} \frac{\sigma_o}{\sigma_p} (1 + \frac{\sigma_o^3}{\sigma_p^3}) \right)$$

(4.5.1)

But in Marchuk's derivation it is assumed that $\sigma_o \gg \sigma_p$ and so equation (4.5.1) becomes

$$I = I_o \left( \frac{\sigma_o}{\sigma_p} \right)^{-k_o} + \frac{F(\alpha, \beta)}{2N\bar{\sigma}} (\sigma_o \sigma_p)^{-k_o} \right)$$

(4.5.2)

We now choose $s_e$ by demanding that the expressions for the resonance integrals given by equations (4.2.2) and (4.5.2) be always equal. Note that in so doing we obtain a value for $s_e$ which does not involve the use of Bell's formula.
The two expressions will be equal if

\[ \sigma_0^{-\frac{1}{2}} \left( (s + \sigma_p)^{\frac{1}{2}} - \sigma_p^{\frac{1}{2}} \right) = (\sigma_0 \sigma_p)^{-\frac{1}{2}} \frac{F(\alpha, \beta)}{2N\lambda} \]  

(4.5.3)

which yields

\[ s_e = \frac{1}{N\lambda} \left( \frac{F^2(\alpha, \beta)}{4N\lambda \sigma_p} + F(\alpha, \beta) \right) \]  

(4.5.4)

We note that in the limiting case of an isolated lump (when \( F(\alpha, \beta) \rightarrow \psi(\lambda) \)) the value of \( s_e \) from equation (4.5.4) agrees with the value of \( s_e \) obtained from equation (4.1.4) when \( G_2 = 1 \). The two expressions are equivalent since in this situation Marchuk's derivation is equivalent to the intermediate approach for isolated lumps discussed in section (2.4.3).

For an isolated lump \( \alpha \rightarrow 0 \) (i.e. \( G_2 \rightarrow 1 \) or \( a_m \rightarrow 1 \)) and \( \lim_{\alpha \rightarrow \infty} F(\alpha, \beta) = \psi(\lambda) \) (see section 2.6.1) and so equation (4.5.4) becomes

\[ s_e = \frac{1}{N\lambda} \left( \frac{\psi^2(\lambda)}{4N\lambda \sigma_p} + \psi(\lambda) \right) \]  

(4.5.5)

On the other hand putting \( G_2 = 1 \) in equation (4.1.4) and using equation (4.2.4) for \( a_f \) we obtain

\[ s_e = \frac{1}{N\lambda a_f} = \frac{1}{N\lambda} \left( \frac{\psi^2(\lambda)}{4N\lambda \sigma_p} + \psi(\lambda) \right) \]

which is in agreement with equation (4.5.5).

In tables (4.5) and (4.6) values of \( N\lambda s_e \) are given for slab systems calculated by equations (4.4.10) and (4.5.4).
### TABLE 4.5 (facing page 116)

$
\bar{N}'(\sigma_e)$ for Slab Systems Using Marchuk's Theory

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<th>$\bar{N}'(\sigma_p)$</th>
<th>$\bar{N}'(\sigma_m)$</th>
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<th>1.5</th>
<th>5.0</th>
</tr>
</thead>
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</table>

The Dancoff Correction for Slabs at above values of $\bar{N}'(\sigma_m)$

<table>
<thead>
<tr>
<th>$\bar{N}'(\sigma_m)$</th>
<th>0.1</th>
<th>0.5</th>
<th>1.5</th>
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<tbody>
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<td>$G_2$</td>
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<td>0.6905</td>
<td>0.9674</td>
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</table>
at various values of $N\bar{\sigma}_p$ and $N\bar{\sigma}_m$. A comparison of the values in the two tables indicates that the error incurred through the use of Bell's formula is generally quite small and is most pronounced at smaller values of $N\bar{\sigma}_p$. 
5. APPROXIMATE SOLUTION OF THE SLOWING DOWN EQUATIONS
BY USE OF THE GALERKIN METHOD

5.1 General Discussion

For a two region lattice with the NR approximation applied to the external moderator the slowing down equation for the fuel flux assumes the form of equation (2.5.2) viz.

\[(s + \sigma_t) \phi(E) = \frac{s_E}{E} + \int \frac{E/\alpha}{E} \frac{\sigma_s(E')\phi(E')dE'}{(1-\alpha)E'} + \sum_{i=1}^{n_1} \int \frac{E/\alpha_{li}}{E} \frac{s_{li}\phi(E')dE'}{(1-\alpha_{li})E'}\]

(2.5.2)

We have dropped the subscript 1 from \(\phi_1(E)\), the fuel flux, and \(\sigma_{t1}(E)\) since use of this subscript would be redundant now that the moderator flux has been eliminated. Throughout the rest of this chapter, unless the contrary is stated, we shall assume the same notation as in section (2.5). Transforming to the \(x\) variable and performing a slight rearrangement, equation (2.5.2) becomes

\[(s + s_p + \sigma_p) \phi(x) = \frac{s_E}{E} + \frac{\sigma_p}{\delta} \int \frac{E/\alpha_{1\infty}}{1+y^2} \frac{\phi(\gamma)dy}{1+y^2} - \sum_{i=1}^{n_1} \frac{s_{li}}{\delta_{li}} \int \phi(\nu)dy\]

(5.1.1)

Equation (5.1.1) is a Volterra integral equation of the second kind, the standard form of which is

\[\phi(x) = f(x) + \lambda \int_a^x K(x,y)\phi(y)dy\]

(5.1.2)

where \(K\) and \(f\) are given functions, \(\lambda\) is a constant, \(\phi\) is the unknown and \(a \leq x \leq b\).
The solution of integral equations of the form of equation (5.1.2) has attracted continuing interest for almost a century. A summary of standard methods of solving integral equations is given by Berezin and Zhidkov (1965). The most obvious method of solution is to replace the integral by a quadrature rule sum and then solve the resulting finite difference equations. This, basically, was the procedure we adopted in chapter 3 where the quadrature rule employed was Simpson's rule.

Unfortunately this type of solution, involving as it does a large number of integration points, requires a considerable amount of computer time and consequently is unsuitable for day to day reactor design calculations. We must therefore seek some approximate analytic solution which will be the basis of a quick and reliable formula for the calculation of the resonance escape probability. Such formulae are required for computer codes like GYMEA (Pollard and Robinson, 1969) which is used frequently by Physicists and Engineers to study the feasibility of various reactor systems.

The most widely used method of solving Volterra integral equations of the form equation (5.1.2) is the method of successive approximations. An excellent classical account of this method is given by Goursat (1923). A more modern treatment involving the use of functional analysis is given by Stakgold (1967). Volterra (1913) has shown that the method of successive approximations is also applicable to integral equations with both limits variable (the slowing
down equation is of this type). He considered the integral equation

\[ \phi(x) = f(x) + \lambda \int_{x-d}^{x} K(x,y)\phi(y)dy \] (5.1.3) 

and went on to consider the more general case in which the lower limit of the integral is a function of \( x \).

The Goldstein \( \lambda \) method, discussed in chapter 2, is in fact an application of the method of successive approximations. However with this method applied to the slowing down equation it is not possible to obtain the third order, and higher, iterants in terms of elementary functions. Dyos and Keane (1966) were forced to resort to numerical integration to find the third order iterant of the flux.

In order to obtain mathematically tractable improvements on the \( \lambda \) method we shall turn to that class of direct approximate methods known as the method of weighted residuals (Becker, 1964) or the method of modal expansions (Stacey, 1967). A variety of well known methods are in fact particular cases of the method of weighted residuals e.g. the method of least squares, the variational method, the method of moments, the Galerkin method.

The essence of the method of weighted residuals is as follows. Suppose \( H \) is a linear operator, \( f(x) \) a given function and \( \phi(x) \) the unknown is given by the equation

\[ H\phi = f \] (5.1.4) 

in the range \( a \leq x \leq b \).
We assume an approximate solution, \( \tilde{\phi}(x) \), in the form

\[
\tilde{\phi}(x) = \sum_{i=1}^{n} \mu_i \phi_i(x)
\]  

(5.1.5)

where the \( \mu_i \) are to be determined and the \( \phi_i(x) \) are a set of \( n \) linearly independent trial functions considered to be capable of representing the solution and hence will be chosen from some prior knowledge of the behaviour of the solution. The \( \phi_i(x) \) constitute the basis of a linear vector subspace.

The exact solution of equation (5.1.4) may be written

\[
\phi(x) = \tilde{\phi}(x) + \delta \phi = \sum_{i=1}^{n} \mu_i \phi_i(x) + \delta \phi
\]  

(5.1.6)

For a given set of trial functions, \( \phi_i(x) \), the choice of \( \mu_i \) will affect the error, \( \delta \phi \). The basic aim of the method of weighted residuals is to choose the \( \mu_i \) in such a manner as to minimise the error term \( \delta \phi \) in some convenient "best" sense. The various particular cases of the method, mentioned above, arise from different selections of the "best" sense to be adopted for the minimisation of the error term.

For example by demanding that

\[
\int_{a}^{b} w(x) (H \delta \phi)^2 \, dx = \int_{a}^{b} w(x) \left( \sum_{i=1}^{n} \mu_i \phi_i - f \right)^2 \, dx
\]

(with \( w(x) \) a positive weighting function) be a minimum, we obtain the least squares method, which has been discussed at length by Mikhlin (1964).
The method of moments consists in seeking the $u_i$ so that $\delta \phi$ be orthogonal, in the sense indicated below, to some system of linearly independent functions $\psi_j(x)$.

i.e.

$$\int_a^b w(x) \delta \phi \psi_j(x) dx = 0$$

therefore

$$\int_a^b w(x) \left( \sum_{i=1}^n u_i \phi_i - f \right) \psi_j(x) dx = 0 \quad (j=1,\ldots,n)$$

(5.1.7)

This reduces to the Galerkin method when $\psi_j(x) = \phi_j(x)$, in which case we are in fact demanding that the first $n$ moments of $\delta \phi$ vanish in the vector subspace of the trial functions $\phi_i(x)$. Thus under application of the Galerkin method, equations (5.1.7) reduce to

$$\sum_{i=1}^n u_i m_{ji} = n_j \quad (j=1,\ldots,n)$$

(5.1.8a)

with

$$m_{ji} = \int_a^b w(x) \phi_j(x) \phi_i(x) dx$$

(5.1.8b)

$$n_j = \int_a^b w(x) \phi_j(x) f(x) dx$$

(5.1.8c)

Detailed discussion on questions of the convergence of the Galerkin method is given by Mikhlin.

The Galerkin method has been applied successfully in many areas of applied mathematics and many examples of its application (and also that of the associated Ritz method) to a wide
range of problems are given by Kantorovich and Krylov (1964). In the rest of this chapter we shall demonstrate how the method may be applied to obtain an approximate solution to the slowing down equation.

5.2 Choice of Trial Functions

The form of the solutions obtained under the application of the NR and WR approximations suggests a set of trial functions having the form

\[ \phi_1(x) = \frac{1}{E} \frac{1+x^2}{a_1^2+x^2} \]  

(5.2.1)

where in the NR and WR approximate solutions \( a_1 \) has the values \( \beta_{11} \) and \( \beta_{10} \) respectively. If we restrict ourselves (as indeed we shall) to an approximate solution involving only one trial function a problem which immediately presents itself is the determination of an appropriate value for \( a_1 \) to be used in our trial function. We might for example choose \( a_1 \) to be \( \beta_{11} \) or \( \beta_{10} \) or perhaps some linear combination of these two. Application of the Galerkin method based on trial functions using any of the values of \( a_1 \) just mentioned yields results which are all quite reasonable. However it would be preferable if our final result did not depend on the parameter \( a_1 \) being quite arbitrary. We shall in due course describe a procedure for the systematic determination of \( a_1 \) for any particular system.
For a two region lattice with the NR approximation applied to the external moderator we saw in section (5.1) that the equation for the fuel flux reduces to equation (5.1.1). If we define the operator $H$ by

$$H = \left( s + \frac{s}{1 + \frac{x^2}{1 + x^2}} \right) \phi(x) - \frac{\sigma p}{\delta} \int_{x}^{x+\delta} \frac{\beta^2 + y^2}{1 + y^2} \phi(y) dy - \sum_{i=1}^{n} \frac{s_i}{1 + \frac{x^2}{a^2 + x^2}} \phi(y) dy$$

then equation (5.1.1) may be written in the form

$$H\phi = \frac{s e}{E r}$$

In keeping with our discussion in the previous two sections we seek an approximate solution to equation (5.3.2) in the form

$$\bar{\phi}(x) = \mu \phi_1(x)$$

with

$$\phi_1(x) = \frac{1}{E r} \frac{1 + x^2}{a^2 + x^2}$$

and the factor $a$ occurring in the trial function $\phi_1(x)$ is as yet an undetermined parameter.

Applying the Galerkin procedure as outlined in section (5.1) we obtain the following equation for $\mu$,

$$m\mu = n$$
where

\[ m = \int_{-\infty}^{\infty} \sigma_a(x) \phi_1(x) H_\phi_1 \, dx \]  
(5.3.6a)

\[ n = \frac{se}{r} \int_{-\infty}^{\infty} \sigma_a(x) \phi_1(x) \, dx \]  
(5.3.6b)

We have chosen the fuel absorption cross section \( \sigma_a(x) \) as the weighting function which occurs in equations (5.1.8). This choice is not unreasonable since \( \sigma_a(x) \) is the weight associated with the fuel flux in the calculation of the resonance integral.

We first evaluate \( H_\phi_1 \),

\[
H_\phi_1 = \frac{1}{E} \left\{ \left( s_1 + \sigma \right) \frac{\beta^2}{2^1} + \frac{x^2}{a^2 + x^2} - \left( s_1 + \sigma \right) \frac{\beta^2 - a^2}{\delta} \frac{1}{a} \left( \tan \left( \frac{1x + \delta}{a} \right) - \tan \left( \frac{1x}{a} \right) \right) 
\right. \\
- \frac{1-a}{a} \sum_{i=1}^{n_1} s_{li} \left( \tan \left( \frac{1x + \delta}{a} \right) - \tan \left( \frac{1x}{a} \right) \right) \right\}
\]

some simple manipulation then gives us that

\[
\sigma_a(x) \phi_1(x) H_\phi_1 = \frac{\sigma_o \gamma}{E} \left\{ \left( s_1 + \sigma \right) \frac{\beta^2}{2^1} + \frac{x^2}{a^2 + x^2} - \left( s_1 + \sigma \right) \frac{\beta^2 - a^2}{\delta} \frac{1}{a} \left( \tan \left( \frac{1x + \delta}{a} \right) - \tan \left( \frac{1x}{a} \right) \right) 
\right. \\
- \frac{1-a}{a} \sum_{i=1}^{n_1} s_{li} \left( \tan \left( \frac{1x + \delta}{a} \right) - \tan \left( \frac{1x}{a} \right) \right) \right\}
\]
from which, after performing the integration from $\infty$ to $-\infty$, we finally obtain,

$$m = \frac{\sigma \Gamma_{y}}{\Gamma E^z} \pi \left\{ \left( \frac{\beta_{11}^2 + a^2}{e + 1 + p} \right) - \left( s + \sigma_{p} \right) - \frac{\sigma_{p} \beta_{11}^2 - a^2}{\delta} \tan \frac{-\delta}{2a} \right\} \right.$$  

$$- \frac{1 - a^2}{a} \sum_{i=1}^{n} \frac{s_{11} \tan \frac{-\delta_{i1}}{2a}}{\delta_{i1}}$$  

(5.3.7a)

The evaluation of $n$ is considerably simpler,

$$n = \frac{s e^{\sigma \Gamma_{y}}}{\Gamma E^z} \int_{-\infty}^{\infty} \frac{dx}{a^2+x^2} = \frac{\sigma \Gamma_{y}}{\Gamma E^z} \pi (s e)$$  

(5.3.7b)

and therefore by use of equation (5.3.5) $\mu$ becomes

$$\mu = s \left\{ \left( \frac{\beta_{11}^2 + a^2}{e + 1 + p} \right) - \left( s + \sigma_{p} \right) - \frac{\sigma_{p} \beta_{11}^2 - a^2}{\delta} \tan \frac{-\delta}{2a} \right\}^{-1}$$  

(5.3.8)

From the approximate expression for the flux given by equation (5.3.3) we obtain the following expression for the resonance integral

$$I = \mu \frac{I_{0}}{a}$$  

(5.3.9)

At this point the resonance integral is a function of the undetermined parameter $a$. We now turn to the problem of choosing an appropriate value for this parameter.

5.4 Selection of the Parameter $a$ Occuring in the Trial Function

If we choose $a$ equal to $\beta_{11}$, we find that, compared
with the exact results of the PEARLS programme, the resonance integral given by equation (5.3.9) will yield values considerably better than the λ method for the various heterogeneous systems displayed in table (5.1). On the other hand with a equal to β_{10} the Galerkin method (for the same systems) yields results similar to those obtained from the λ method. On these grounds it might at first sight seem plausible to argue that β_{11} is always the best choice for the parameter a. However we have no guarantee that in a different type of system and for a different resonance β_{10} (or perhaps the average of β_{11} and β_{10}) might not be a better choice for a than β_{11}. It is therefore clear that an empirical choice of the parameter a is not, in general, satisfactory.

Both the approximate flux \( \bar{\phi}(x) \) (equation 5.3.3) and the resulting resonance integral I (equation 5.3.9) which we have calculated by use of the Galerkin method, are functions of the free parameter a. We shall use \( \bar{\phi}(x) \) to iterate on the original equation (5.3.2) and so obtain \( \bar{\phi}^{(2)}(x) \), an iterated second order approximation to the flux. From \( \bar{\phi}^{(2)}(x) \) we shall obtain \( I^{(2)} \), a second order approximation to the resonance integral. We choose the parameter a by equating I and \( I^{(2)} \). This approach will yield us a transcendental equation for a (which will also involve μ).

Hence into the application of the Galerkin method we have incorporated the simultaneous use of the basic idea of the Cohen and Goldstein λ method, namely the equating of first
and second order approximations to the resonance integral in order to find an expression for a free parameter.

From a slight rearrangement of equation (5.3.2) and putting

\[ t = s \exp(s_1 + \sigma p) \]

we obtain for \( \phi^{(2)}(x) \) the following expression

\[
\phi^{(2)}(x) = \frac{(1 + x^2)}{t(\beta_{11}^2 + x^2)} \left\{ \frac{s e^r}{E} + \frac{\sigma}{\delta} \left( \frac{x + \delta}{1 + y^2} + \frac{\beta_{11}^2 y^2}{1 + y^2} \right) \phi(y) dy + \frac{n_1 s_1}{\delta} \sum_{i=1}^{\infty} \frac{x + \delta}{\delta} \phi(y) dy \right\}
\]

\[
= \frac{(1 + x^2)}{tE(\beta_{11}^2 + x^2)} \left\{ \frac{s + u(s_1 + \sigma p)}{t} + \frac{\sigma}{\delta} \frac{b_{11}^2 - a^2}{a} \left( \tan^{-1} \frac{x + \delta}{a} - \tan^{-1} \frac{x}{a} \right) \right\}
\]

\[ + \frac{u - (1 - a^2)}{a} \frac{n_1 s_1}{\delta} \sum_{i=1}^{\infty} \frac{x + \delta}{\delta} \left( \tan^{-1} \frac{x + \delta}{a} - \tan^{-1} \frac{x}{a} \right) \]

(5.4.1)

which yields the following expression for the second order approximation to the resonance integral,

\[
I^{(2)} = \frac{1}{2} \int_{-\infty}^{\infty} \sigma_a(x) \frac{\phi^{(2)}(x)}{\phi(x)} dx
\]

\[
= \frac{1}{\beta_{11}} \left\{ \frac{s + u(s_1 + \sigma p)}{t} + \frac{\sigma}{t} \frac{b_{11}^2 - a^2}{a} \tan^{-1} \frac{\delta}{\beta_{11}^2 + a} \right\}
\]

\[ + \frac{u - (1 - a^2)}{a} \frac{n_1 s_1}{\delta} \sum_{i=1}^{\infty} \frac{x + \delta}{\delta} \tan^{-1} \frac{\delta}{\beta_{11}^2 + a} \]

(5.4.2)

Equating the approximations (5.3.9) and (5.4.2) for the resonance integral we obtain the following transcendental
equation for $a$

$$
\frac{a}{b} = \frac{1}{\beta_{11}} \left( \frac{s + \mu(s + p)}{t^a} \right) + \frac{\mu}{t} \frac{\delta^2 - a^2}{a} \tan^{-1} \frac{\delta}{\beta_{11} + a} + \frac{1-a^2}{a} \sum_{i=1}^{\delta_1} \frac{s_{1i}}{\delta_{1i}} \tan^{-1} \frac{\delta_{1i}}{\beta_{11} + a}
$$

(5.4.3)

with $\mu$ given by equation (5.3.8), from which equation we see that $\mu$ is a function of $a$. Thus in essence the only unknown quantity in equation (5.4.3) is the parameter $a$.

Having solved equation (5.4.3) for $a$, we obtain $\mu$ from equation (5.3.8) and finally the resonance integral from equation (5.3.9).

5.5 *Connection with the $\lambda$ Method*

If in equation (5.4.3) we constrain $\mu$ to be always equal to 1 we obtain the following transcendental equation for $a$

$$
\beta_{11} - a = \frac{\sigma_p}{s + s_1 + \sigma_p} \frac{\delta^2 - a^2}{a} \tan^{-1} \frac{\delta}{a + \beta_{11}} + \frac{1-a^2}{a} \sum_{i=1}^{\delta_1} \frac{s_{1i}}{\delta_{1i}} \tan^{-1} \frac{\delta_{1i}}{a + \beta_{11}}
$$

(5.5.1)

On comparing this equation with equation (2.5.16) for the Cohen and Goldstein $\beta_{\lambda\lambda_0}$ we see that both equations are identical, with $a$ in equation (5.5.1) replacing $\beta_{\lambda\lambda_0}$ in equation (2.5.16). This occurrence is not as much of a coincidence as one might at first believe. The essence of the Cohen and Goldstein $\lambda$ method is to assume an approximate solution in the form

$$
\phi^{(1)}(x) = \frac{1}{E} \frac{1+x^2}{a^2+x^2}
$$
Table 5.1 Details of Data Used in Numerical Comparisons

(a) Saclay Systems. Cylindrical $^{238}$U fuel elements in square $D_2O$ moderator lattice. Data from Doherty (1968a).

<table>
<thead>
<tr>
<th></th>
<th>Conc. U</th>
<th>Conc. D</th>
<th>Conc. O</th>
<th>Inner radius</th>
<th>Outer radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>Saclay 1</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>1.459999</td>
<td>6.770269</td>
</tr>
<tr>
<td>Saclay 6</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>1.459999</td>
<td>11.848</td>
</tr>
<tr>
<td>Saclay 23</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>1.78</td>
<td>11.848</td>
</tr>
<tr>
<td>Saclay 7</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>2.2</td>
<td>7.334455</td>
</tr>
<tr>
<td>Saclay 16</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>2.2</td>
<td>16.9256</td>
</tr>
</tbody>
</table>

The data for the following systems has been taken from Megier, (1968). In all systems the cylindrical fuel lump is at the centre of a square moderator lattice.

(b) $U$ in fuel region, $D_2O$ in moderator region

<table>
<thead>
<tr>
<th></th>
<th>Conc. U</th>
<th>Conc. D</th>
<th>Conc. O</th>
<th>Inner radius</th>
<th>Outer radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>0.5</td>
<td>15.0</td>
</tr>
<tr>
<td>M2</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>1.0</td>
<td>15.0</td>
</tr>
<tr>
<td>M3</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>2.5</td>
<td>15.0</td>
</tr>
<tr>
<td>M4</td>
<td>0.047487</td>
<td>0.066554</td>
<td>0.033277</td>
<td>4.0</td>
<td>15.0</td>
</tr>
</tbody>
</table>

(c) $UO_2$ in fuel region, $D_2O$ in moderator region

<table>
<thead>
<tr>
<th></th>
<th>Conc. U</th>
<th>Conc. O</th>
<th>Conc. D</th>
<th>Conc. O</th>
<th>Inner radius</th>
<th>Outer radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>M5</td>
<td>0.022586</td>
<td>0.045497</td>
<td>0.066554</td>
<td>0.033277</td>
<td>0.5</td>
<td>15.0</td>
</tr>
<tr>
<td>M6</td>
<td>0.022586</td>
<td>0.045497</td>
<td>0.066554</td>
<td>0.033277</td>
<td>1.0</td>
<td>15.0</td>
</tr>
<tr>
<td>M7</td>
<td>0.022586</td>
<td>0.045497</td>
<td>0.066554</td>
<td>0.033277</td>
<td>2.5</td>
<td>15.0</td>
</tr>
<tr>
<td>M8</td>
<td>0.022586</td>
<td>0.045497</td>
<td>0.066554</td>
<td>0.033277</td>
<td>4.0</td>
<td>15.0</td>
</tr>
</tbody>
</table>
(facing page 129)

Table 5.1 (continued)

(d) U in fuel region, C in moderator region

<table>
<thead>
<tr>
<th></th>
<th>Conc. U</th>
<th>Conc. C</th>
<th>Inner radius</th>
<th>Outer radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>M9</td>
<td>0.047487</td>
<td>0.082770</td>
<td>0.5</td>
<td>15.0</td>
</tr>
<tr>
<td>M10</td>
<td>0.047487</td>
<td>0.082770</td>
<td>1.0</td>
<td>15.0</td>
</tr>
<tr>
<td>M11</td>
<td>0.047487</td>
<td>0.082770</td>
<td>2.5</td>
<td>15.0</td>
</tr>
<tr>
<td>M12</td>
<td>0.047487</td>
<td>0.082770</td>
<td>4.0</td>
<td>15.0</td>
</tr>
</tbody>
</table>

The units of the radii are cms. The units of the concentrations are Nuclides/(10^{-8} cms)^3.
(i.e. the Galerkin method approximate solution but with $\mu=1$) and then choose $a$ by equating the approximations to the resonance integral obtained from the first and second order flux iterants. Cohen and Goldstein put $a = \beta \lambda_o$ and pose the problem so as to seek the $\lambda_i$'s which will give a $\beta \lambda_o$ satisfying equation (2.5.16) (i.e. equation 5.5.1). It would seem preferable to solve directly for $a$ since we may then obviate the dubious step in going from equation (2.5.16) to (2.5.17) in order to obtain the equations for each of the $\lambda_i$. The doubtful nature of this step becomes pronounced when it is realised that in solving equation (5.4.3) for some systems we have observed more than one root to this equation and it would therefore not be unlikely that equation (5.5.1) might also have more than one root for some systems.

When the Cohen and Goldstein $\lambda$ method is posed in the manner outlined above we see that there is no necessity for the Cohen and Goldstein $\lambda$ to lie between 0 and 1, a fact which has already been noted in an entirely different argument by Ishiguro (1968).

5.6 Numerical Results

We have used the Galerkin procedure outlined in the previous sections to obtain approximations to the resonance integral for a variety of heterogeneous systems, the data for which is given in table (5.1). The resulting approximations to the capture probability are given in table (5.2) and are compared with the exact values computed by the PEARLS programme. We have restricted our
Table 5.2 Calculations of the Capture Probability

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>1-(p_r)</td>
<td>1-(p_r)</td>
<td></td>
<td>1-(p_r)</td>
<td></td>
<td>exact</td>
</tr>
<tr>
<td></td>
<td>(\mu)</td>
<td>Galerkin</td>
<td>% diff.</td>
<td>(\lambda)</td>
<td>% diff.</td>
<td>(1-p_r)</td>
<td></td>
</tr>
<tr>
<td>Saclay 1</td>
<td>0.6252</td>
<td>0.03133</td>
<td>5.4</td>
<td>0.033770</td>
<td>13.6</td>
<td>0.029733</td>
<td></td>
</tr>
<tr>
<td>Saclay 6</td>
<td>0.6260</td>
<td>0.010037</td>
<td>5.2</td>
<td>0.010830</td>
<td>13.5</td>
<td>0.009541</td>
<td></td>
</tr>
<tr>
<td>Saclay 23</td>
<td>0.5740</td>
<td>0.013192</td>
<td>4.3</td>
<td>0.014682</td>
<td>16.0</td>
<td>0.012648</td>
<td></td>
</tr>
<tr>
<td>Saclay 7</td>
<td>0.5159</td>
<td>0.047827</td>
<td>3.2</td>
<td>0.054865</td>
<td>18.4</td>
<td>0.046348</td>
<td></td>
</tr>
<tr>
<td>Saclay 16</td>
<td>0.5171</td>
<td>0.008525</td>
<td>2.9</td>
<td>0.009738</td>
<td>17.6</td>
<td>0.008282</td>
<td></td>
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<td>M1</td>
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<td>0.001356</td>
<td>6.2</td>
<td>0.001372</td>
<td>7.4</td>
<td>0.001277</td>
<td></td>
</tr>
<tr>
<td>M2</td>
<td>0.7180</td>
<td>0.003678</td>
<td>6.1</td>
<td>0.003835</td>
<td>10.7</td>
<td>0.003465</td>
<td></td>
</tr>
<tr>
<td>M3</td>
<td>0.4827</td>
<td>0.012920</td>
<td>2.0</td>
<td>0.01510</td>
<td>19.2</td>
<td>0.012667</td>
<td></td>
</tr>
<tr>
<td>M4</td>
<td>0.3613</td>
<td>0.024190</td>
<td>-2.4</td>
<td>0.031370</td>
<td>26.5</td>
<td>0.024791</td>
<td></td>
</tr>
<tr>
<td>M5</td>
<td>1.0428</td>
<td>0.000988</td>
<td>4.4</td>
<td>0.000988</td>
<td>4.4</td>
<td>0.000946</td>
<td></td>
</tr>
<tr>
<td>M6</td>
<td>0.8084</td>
<td>0.002738</td>
<td>2.1</td>
<td>0.002839</td>
<td>5.9</td>
<td>0.002682</td>
<td></td>
</tr>
<tr>
<td>M7</td>
<td>0.5902</td>
<td>0.010181</td>
<td>-5.9</td>
<td>0.011820</td>
<td>9.2</td>
<td>0.010821</td>
<td></td>
</tr>
<tr>
<td>M8</td>
<td>0.4608</td>
<td>0.019606</td>
<td>-14.3</td>
<td>0.025490</td>
<td>11.4</td>
<td>0.022881</td>
<td></td>
</tr>
<tr>
<td>M9</td>
<td>0.8500</td>
<td>0.003957</td>
<td>6.1</td>
<td>0.004003</td>
<td>7.4</td>
<td>0.003729</td>
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<tr>
<td>M10</td>
<td>0.7180</td>
<td>0.010705</td>
<td>6.0</td>
<td>0.011160</td>
<td>10.5</td>
<td>0.010101</td>
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<tr>
<td>M11</td>
<td>0.4827</td>
<td>0.037239</td>
<td>1.5</td>
<td>0.043410</td>
<td>18.3</td>
<td>0.036697</td>
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<tr>
<td>M12</td>
<td>0.3613</td>
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<td>-3.3</td>
<td>0.088610</td>
<td>24.5</td>
<td>0.071169</td>
<td></td>
</tr>
</tbody>
</table>
calculations to the 6.68 eV. resonance of U238 since, at the
time of the writing of the final draft of this thesis, preparation
for other fuels and resonances of data tapes for the PEARLS
programme had not been fully completed.

The names in column 1 of table (5.2) correspond
to the names given to the various heterogeneous systems in table (5.1).
Column 2 gives the value of \( \mu \) corresponding to that \( a \) which satisfies
equation (5.4.3). Columns 3 and 4 give, respectively, the capture
rate calculated by the Galerkin method and its percentage difference
from the exact result. Columns 5 and 6 give the corresponding
quantities obtained by use of the \( \lambda \) method. Column 7 gives the exact
result as obtained from the PEARLS programme.

The escape probability subroutines used by the
PEARLS programme for circular cylindrical fuel elements in a square
lattice circularise the square boundary of the cell in such a manner
as to retain the same moderator to fuel volume ratio. The radii
of the circularised cell are given in table (5.1). In the calculation
of the escape probabilities in the circularised cell the white
boundary condition has been used (Doherty, 1969a).

We observe that for those systems with \( \mu \) close
to 1 (such as M5) the Galerkin method is equivalent to the \( \lambda \) method.
This must be so in view of the discussion in section 5.5. For those
systems with \( \mu \) different from 1 we observe that in general the Galerkin
method is superior to the \( \lambda \) method (M8 seems to be the only exception).
Approximate flux (Eqn. 5.3.3.)
A more important observation is, that in contrast to the \( \lambda \) method, the percentage difference (from the exact result) of the Galerkin method result decreases as the system becomes more strongly absorbing. In particular let us consider the set of U/C systems M9, M10, M11, M12 which are successively more strongly absorbing due to the increasing radius of the uranium fuel element. For M9 (radius = 0.5 cms) the percentage difference is +6.1\%, as the radius increases (and consequently the system becomes more strongly absorbing) the percentage difference decreases steadily and for M12 (radius = 4 cms) the percentage difference is -3.3\%. On the other hand the percentage difference of the \( \lambda \) method result increases as the radius increases, for M12 the percentage difference is 24\%.

This behaviour of the percentage difference of the Galerkin method result is most fortuitous since, in the calculation of the criticality of the entire system a large percentage difference in the calculation of the resonance capture probability is more tolerable in less strongly absorbing systems than in more strongly absorbing systems.

Graphs of the Galerkin method and the exact (from the PEARLS programme) fuel fluxes for the systems M9 and M12 are displayed in figure (5.1).

In calculating the results set out in table (5.2) the value of \( s_e \) was calculated from equation (4.1.4), we have not used the more exact value of \( s_e \) obtained from equation (4.4.10) since for all the systems considered here \( G_2 \) is greater than 0.9.
5.7 Galerkin Method Solution of the Slowing Down Equations Without Application of the NR Approximation to External Moderator

Considering the successful application of the Galerkin method to the slowing down equations for a two region lattice with the NR approximation applied to the external moderator it would seem worthwhile extending the method to these same equations without applying the NR approximation to the external moderator. In other words we shall now attempt to take account of the variation of the moderator flux.

We shall take as our starting point the equations (2.3.1) for a two region lattice. In order to simplify the analysis we shall assume that there is only one nuclide in each of the fuel and moderator regions. This assumption is in no way restrictive and the method presented below is easily extended, in an obvious way, to the general situation of many nuclides per region.

With the above assumptions and employing the notation of section (2.3) equations (2.3.1) become

\[ V_1 \Sigma_t(E) \phi_1(E) = V_1 P_{11} \int \frac{E/\alpha \Sigma_s(E') \phi_1(E') dE'}{(1-\alpha)E'} + V_2 (1-P_{22}) \int \frac{E/\alpha_2 \Sigma_2 \phi_2(E') dE'}{(1-\alpha_2)E'} \]

\[ V_2 \Sigma_2 \phi_2(E) = V_1 (1-P_{11}) \int \frac{E/\alpha \Sigma_s(E') \phi_1(E') dE'}{(1-\alpha)E'} + V_2 P_{22} \int \frac{E/\alpha_2 \Sigma_2 \phi_2(E') dE'}{(1-\alpha_2)E'} \]
Here we have deviated slightly from the notation of section (2.3) in that since there is only one nuclide in the moderator region we write $\alpha_2$ for $\alpha_{21}$ and $\Sigma_2$ for $\Sigma_{21}$. We note also that since there is only the fuel nuclide present in the fuel region $\Sigma_{t1}(E)$ becomes simply $\Sigma_t(E)$.

After applying the rational approximation for $P_{11}$ (equation, 1.6.4) using the reciprocity theorem to obtain $P_{22}$ and performing some elementary operations, equation (5.6.1) becomes

$$\phi_1(E) = \frac{1}{(s + \sigma_t)} \int_E^{E/\alpha} \frac{s(E')\phi_1(E')dE'}{(1-\alpha)E'} + \frac{s_e}{s + \sigma_t} \int_E^{E/\alpha} \frac{\phi_2(E')dE'}{(1-\alpha_2)E'}$$

$$\phi_2(E) = \frac{s_e / \sigma_m}{s_e / \sigma_t} \int_E^{E/\alpha} \frac{s(E')\phi_1(E')dE'}{(1-\alpha)E'} + \frac{s_e + (1-s_e / \sigma_m)\sigma_t}{s_e / \sigma_t} \int_E^{E/\alpha} \frac{\phi_2(E')dE'}{(1-\alpha_2)E'}$$

The proper procedure at this point would be to solve equations (5.6.2) simultaneously for the fuel flux, however such a process would be very complicated and we shall instead use an approximation to the moderator flux suggested by the discussion in section (2.5.3). We see, from an inspection of the approximations given in equations (2.5.19a and b) for the moderator flux obtained under application of the NR and WR approximations to the fuel nuclides and the NR approximation to the moderator nuclide, that it would be plausible to assert that, with the approximation
for the fuel flux, is associated the approximation

\[
\frac{1}{E_r} \frac{1+x^2}{a^2+x^2}
\]

for the moderator flux.

Thus in equation (5.6.2a) we use the following approximation for \(\phi_2(x)\):

\[
\phi_2(x) = \frac{1}{E_r} \frac{d^2+x^2}{a^2+x^2}
\]  
(5.6.3)

with

\[
d^2 = 1+(1-s_e /\sigma_m)(a^2-1)
\]  
(5.6.4)

Thus, transforming to the \(x\) variable and performing some simple manipulations equation (5.6.2a) reduces to

\[
H\phi_1 = \frac{s_e}{E} \frac{d^2-a^2}{E} \left(\tan^{-1} \frac{x+\delta_2}{a} - \tan^{-1} \frac{x}{a}\right)
\]  
(5.6.5)

with the operator \(H\) defined by equation (5.3.1). (Note that in the present context \(s_1\) and all the \(s_{1i}\) are zero.) We observe that putting \(d\) equal to \(a\) in equation (5.6.5) reproduces equation (5.1.1). This must be so since putting \(d\) equal to \(a\) in equation (5.6.3) is equivalent to applying the NR approximation to the external moderator.

We now proceed to solve equation (5.6.5) with the Galerkin method using

\[
\psi_1(x) = \frac{1}{E} \frac{1+x^2}{a^2+x^2}
\]  
(5.6.6)

as the trial function for the fuel flux. Thus the approximate solution for the fuel flux will be
\[ \phi_1(x) = \mu \psi_1(x) \] (5.6.7)

with

\[ u = m/n \] (5.6.8a)

and

\[ m = \int_{-\infty}^{\infty} \sigma_a(x) \psi_1(x) H \psi_1 \, dx \] (5.6.8b)

\[ n = \frac{se}{E} \int_{-\infty}^{\infty} \sigma_a(x) \psi_1(x) \left( 1 + \frac{d^2 - a^2}{\delta^2 a} \left( \tan^2 \frac{11 + 1}{a} - \tan^2 \frac{-1}{a} \right) \right) \, dx \] (5.6.8c)

Obviously, the evaluation of \( m \) will be the same as in section (5.3) and we thus have

\[ m = \frac{s e \Gamma Y}{E Z} \frac{\pi}{a} \left\{ (s + \sigma_p) \frac{(\beta^2 + a^2)}{2a^2} - \sigma_p \frac{\beta^2 - a^2}{a} \tan \frac{1}{2a} \right\} \] (5.6.9a)

whilst

\[ n = \frac{s e \Gamma Y}{E Z} \frac{\pi}{a} \left\{ 1 + \frac{d^2 - a^2}{\delta^2 a} \left( \tan^2 \frac{11 + 1}{a} - \tan^2 \frac{-1}{a} \right) \right\} \, dx \] (5.6.9b)

Thus

\[ u = \frac{s e}{E Z} \left\{ 1 + \frac{d^2 - a^2}{\delta^2 a} \tan \frac{1}{2a} \right\} \left( (s + \sigma_p) \frac{(\beta^2 + a^2)}{2a^2} - \sigma_p \frac{\beta^2 - a^2}{a} \tan \frac{1}{2a} \right)^{-1} \] (5.6.10)
The approximate expression for the resonance integral is

\[ I = \frac{\Gamma}{2} \int_{-\infty}^{\infty} \sigma_a(x) \phi_1(x) \, dx \]

i.e.

\[ I = \mu \frac{I}{a} \quad (5.6.11) \]

To find the parameter \( a \) we proceed as in section (5.4) and find firstly \( \phi_1^{(2)}(x) \) an iterated second order approximation to the fuel flux and from this \( I^{(2)} \), a second order approximation to the resonance integral. By equation I to \( I^{(2)} \) we obtain a transcendental equation for \( a \).

From a rearrangement of equation (5.6.5) we obtain

\[ \phi_1^{(2)}(x) = \frac{1}{t} \frac{1+x^2}{\beta_1^2 + x^2} \left\{ \frac{s_e}{E_r} + \frac{s_e}{E_r} \frac{d^2-a}{\delta^2_a} \left\{ \tan^{-1} \frac{x+\delta}{a} - \tan^{-1} \frac{x}{a} \right\} + \frac{\sigma_p}{\delta} \int \frac{x+\delta}{1+y^2} \phi_1^{(1)}(y) \, dy \right\} \]

(5.6.12)

(2) We now obtain \( I^{(2)} \), the second order approximation to the resonance integral.
Asymptotic mod. flux.                Exact mod. flux. 
Approximate mod. flux.                Exact (Fuel) 
(Eqn. 5.6.3)                                  (Eqn. 5.6.7) 
Galerkin method (Fuel) 

M9

M12

Fig. 5.2 (facing page 137)
Thus equating equations (5.6.11) and (5.6.13) we obtain the following transcendental equation for \( a \),

\[
\frac{\beta}{a} = \left\{ \frac{e^{s+\mu \sigma}}{t} + \frac{(s / \mu) e^{d^2-a^2}}{t} \tan^{-1} \frac{\delta_2}{a+\beta} + \frac{\mu \sigma p}{t} \frac{\beta_2^2-a^2}{\delta a} \tan^{-1} \frac{\delta}{a+\beta} \right\}
\]

(5.6.14)

We see that if we put \( \mu \) equal to 1 in equation (5.6.14) then this equation is equivalent to equation (2.5.21), obtained by Sehgal and Goldstein (1966), if we identify \( d \) with \( \mu \lambda_0 \) and \( a \) with \( \frac{\beta}{\mu \lambda_0} \).

Table (5.3) gives the percentage differences in the resonance capture probability obtained by use of the method proposed in the present section for the four \( U/C \) systems M9, M10, M11, M12 (see table 5.1). In the first three columns of table (5.3) we give the values of \( \mu \), \( d \) and \( a \) which satisfy the transcendental equation (5.6.14), the fourth column gives the percentage error in the capture probability obtained by use of the Galerkin method, the last column gives the percentage error obtained by use of the \( \lambda \) method extended by Sehgal and Goldstein (1966) to remove application.
Table 5.3 (facing page 138)

Calculation of the Capture Probability Without Application
of the NR Approximation to External M derator

<table>
<thead>
<tr>
<th></th>
<th>$u$</th>
<th>$d$</th>
<th>$a$</th>
<th>Galerkin Method % error</th>
<th>Sehgal-Goldstein $\lambda$ Method % error</th>
</tr>
</thead>
<tbody>
<tr>
<td>M9</td>
<td>0.8494</td>
<td>24.33</td>
<td>24.37</td>
<td>6.0</td>
<td>7.0</td>
</tr>
<tr>
<td>M10</td>
<td>0.7168</td>
<td>30.33</td>
<td>30.43</td>
<td>5.8</td>
<td>9.7</td>
</tr>
<tr>
<td>M11</td>
<td>0.4805</td>
<td>36.78</td>
<td>37.08</td>
<td>1.0</td>
<td>15.6</td>
</tr>
<tr>
<td>M12</td>
<td>0.3584</td>
<td>38.92</td>
<td>39.44</td>
<td>-4.1</td>
<td>18.8</td>
</tr>
</tbody>
</table>
of the NR approximation to the external moderator. (The details of this method are outlined in section 2.5.3).

In figure (5.2) we give a plot of the approximate fuel and moderator fluxes for the least and most strongly absorbing of the U/C systems viz. M9 and M12.

From an inspection of table (5.3) we observe that the percentage errors of the Galerkin method results are reduced in comparison to the results obtained when the NR approximation was applied to the external moderator. This has the effect of giving a better result for those systems which previously had results with a positive percentage error but gives a worse result for those systems which previously had a negative percentage error. This trend is disappointing, since we might have hoped in all cases for an improvement over the results obtained when the NR approximation is applied to the external moderator, but it is probably due to the form we have assumed for the moderator flux. In actual fact to account properly for the variation of the moderator flux we would have to solve equations (5.6.2) simultaneously by the Galerkin method and introduce independent trial functions for \( \phi_1(x) \) and \( \phi_2(x) \). However this process involves many complications and we shall not attempt it in this thesis.
6. NUMERICAL COMPARISONS

We have discussed in section (1.6) the derivation of the equivalence relation of Leslie, Hill and Jonsson (1965) and we have also established in chapter 4 an equivalence relation based on an improved rational approximation. In estimating the errors in our approximate methods of calculating the resonance escape probability it would be most useful to have some idea of the magnitude of the error brought about by use of the various equivalence relations. By running the PEARLS programme with the exact formulae for the collision probabilities and then with the approximate formulae for the collision probabilities upon which the equivalence relation is based we can obtain the error involved in the use of the equivalence relation.

We shall consider the two region systems for which the data is given in table (5.1). In the notation of section (2.3) the slowing down equations for these systems have the form

\[ V_1 \frac{\Gamma_1}{t_1}(E) \phi_1(E) = V_1 P_{11} S_1(E) + V_2 (1-P_{22}) S_2(E) \]  
\[ V_2 \frac{\Gamma_2}{t_2}(E) = V_1 (1-P_{11}) S_1(E) + V_2 P_{22} S_2(E) \]

with the \( S_i(E) \) defined by equations (1.2.14).

We may approximate \( P_{11} \) and \( P_{22} \) by using one of the equivalence relations which we have discussed. So that

\[ P_{11} = \frac{\sigma_t}{s^{-\sigma} t_1}, \quad P_{22} = \frac{s^{-\sigma} (1-s/e/\sigma_m)}{s^{-\sigma} t_1} \]

where \( s_e \) may be calculated either from equation (1.6.5) or equation (4.1.4).
**TABLE 6.1 (facing page 140)**

Comparison of \((1-p_{_r})\) Using Various Equivalence Relations. \(6.68\mathrm{eV}\) resonance of \(^{238}\text{U}\)

<table>
<thead>
<tr>
<th>N(\bar{\jmath})σ (_p)</th>
<th>N(\bar{\jmath})σ (_m)</th>
<th>(s_e)</th>
<th>(1-p_{_r})</th>
<th>%diff</th>
<th>(s_e)</th>
<th>(1-p_{_r})</th>
<th>%diff</th>
<th>(s_e)</th>
<th>(1-p)</th>
<th>%diff</th>
<th>((1-p_{<em>r})</em>{\text{exact}})</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Wigner Rat. Approx.</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M1</td>
<td>0.5034</td>
<td>317.11</td>
<td>21.06</td>
<td>0.001169</td>
<td>-8.6</td>
<td>23.55</td>
<td>0.001242</td>
<td>-2.8</td>
<td>24.48</td>
<td>0.001269</td>
<td>-0.8</td>
</tr>
<tr>
<td>M2</td>
<td>1.0067</td>
<td>158.03</td>
<td>10.53</td>
<td>0.003189</td>
<td>-8.2</td>
<td>11.77</td>
<td>0.003396</td>
<td>-2.2</td>
<td>11.89</td>
<td>0.003415</td>
<td>-1.7</td>
</tr>
<tr>
<td>M3</td>
<td>2.5168</td>
<td>61.73</td>
<td>4.21</td>
<td>0.011858</td>
<td>-6.8</td>
<td>4.71</td>
<td>0.012682</td>
<td>-0.3</td>
<td>4.55</td>
<td>0.012421</td>
<td>-2.4</td>
</tr>
<tr>
<td>M4</td>
<td>4.0269</td>
<td>36.86</td>
<td>2.63</td>
<td>0.023538</td>
<td>-5.6</td>
<td>2.94</td>
<td>0.025234</td>
<td>1.2</td>
<td>2.79</td>
<td>0.024383</td>
<td>-2.2</td>
</tr>
<tr>
<td>M5</td>
<td>0.4123</td>
<td>317.11</td>
<td>44.28</td>
<td>0.000870</td>
<td>-8.0</td>
<td>49.51</td>
<td>0.000920</td>
<td>-2.8</td>
<td>51.83</td>
<td>0.000941</td>
<td>-0.5</td>
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<tr>
<td>M6</td>
<td>0.8246</td>
<td>158.03</td>
<td>22.14</td>
<td>0.002485</td>
<td>-7.4</td>
<td>24.76</td>
<td>0.002624</td>
<td>-2.2</td>
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</tr>
<tr>
<td>M7</td>
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<td>8.86</td>
<td>0.010203</td>
<td>-5.8</td>
<td>9.90</td>
<td>0.010747</td>
<td>-0.9</td>
<td>9.66</td>
<td>0.010622</td>
<td>-2.0</td>
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<tr>
<td>M8</td>
<td>3.2984</td>
<td>36.86</td>
<td>5.53</td>
<td>0.021897</td>
<td>-4.4</td>
<td>6.19</td>
<td>0.022993</td>
<td>0.4</td>
<td>5.91</td>
<td>0.022524</td>
<td>-1.7</td>
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<tr>
<td>M9</td>
<td>0.5034</td>
<td>349.73</td>
<td>21.06</td>
<td>0.003406</td>
<td>-8.8</td>
<td>23.55</td>
<td>0.003620</td>
<td>-3.1</td>
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<td><strong>L.H &amp; J. eqn(1.6.5)</strong></td>
<td></td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>M10</td>
<td>1.0067</td>
<td>174.28</td>
<td>10.53</td>
<td>0.009279</td>
<td>-8.4</td>
<td>11.77</td>
<td>0.009882</td>
<td>-2.4</td>
<td>11.89</td>
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<td>2.5168</td>
<td>68.08</td>
<td>4.21</td>
<td>0.034301</td>
<td>-6.9</td>
<td>4.71</td>
<td>0.036669</td>
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<td>4.0269</td>
<td>40.65</td>
<td>2.63</td>
<td>0.067510</td>
<td>-5.7</td>
<td>2.94</td>
<td>0.072307</td>
<td>1.0</td>
<td>2.79</td>
<td>0.069898</td>
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</tr>
<tr>
<td><strong>Eqn(4.1.4)</strong></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Saclay 1</td>
<td>1.4698</td>
<td>21.12</td>
<td>7.19</td>
<td>0.027550</td>
<td>-7.6</td>
<td>8.04</td>
<td>0.029355</td>
<td>-1.6</td>
<td>7.97</td>
<td>0.029214</td>
<td>-2.1</td>
</tr>
<tr>
<td>Saclay 6</td>
<td>1.4698</td>
<td>66.80</td>
<td>7.21</td>
<td>0.008830</td>
<td>-7.7</td>
<td>8.06</td>
<td>0.009418</td>
<td>-1.6</td>
<td>8.00</td>
<td>0.009372</td>
<td>-2.1</td>
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<tr>
<td>Saclay 23</td>
<td>1.7920</td>
<td>54.38</td>
<td>5.92</td>
<td>0.011751</td>
<td>-7.4</td>
<td>6.61</td>
<td>0.012543</td>
<td>-1.2</td>
<td>6.41</td>
<td>0.012413</td>
<td>-2.2</td>
</tr>
<tr>
<td>Saclay 7</td>
<td>2.2148</td>
<td>15.70</td>
<td>4.77</td>
<td>0.043319</td>
<td>-6.9</td>
<td>5.33</td>
<td>0.046216</td>
<td>-0.7</td>
<td>5.18</td>
<td>0.045459</td>
<td>-2.3</td>
</tr>
<tr>
<td>Saclay 16</td>
<td>2.2148</td>
<td>90.31</td>
<td>4.79</td>
<td>0.007727</td>
<td>-7.1</td>
<td>5.35</td>
<td>0.008259</td>
<td>-0.7</td>
<td>5.20</td>
<td>0.008120</td>
<td>-2.3</td>
</tr>
</tbody>
</table>
We have solved equations (6.1) with the PEARLS programme using for $P_{11}$ and $P_{22}$ first the exact expressions as given by Doherty (1969) and then the approximate expressions (6.2). In the latter instance $s_e$ was calculated in three different ways (i) Using the Leslie, Hill and Jonsson expression, equation (1.6.5) (ii) Using our expression, equation (4.1.4) (iii) Using the W.R.A. i.e. with $a_f = 1$ in equation (4.1.4).

The results of these calculations are displayed in table (6.1). For the purposes of these calculations we have not corrected the values of $p_r$ so as to account for the absorption in the extreme wings of the resonance. The values of $s_e$, $1-p_r$ and percentage differences of $1-p_r$ from the exact result are grouped under the appropriate headings for each of the three cases. The value of $G_2$ was obtained, as for the calculations in chapter 5, from the Sauer-Bonalumi expression, equation (1.5.18).

A survey of table (6.1) reveals the following points:

(i) The uncorrected Wigner rational approximation always causes an underestimate of the capture rate though the percentage difference decreases as the amount of absorption increases.

(ii) The Leslie, Hill and Jonsson equivalence relation gives negative percentage differences for weakly absorbing systems, but the percentage difference becomes positive as the amount of absorption increases.
TABLE 6.2 (Facing page 141)

'EXACT' VALUES OF $s_e$ AND $a_f$

<table>
<thead>
<tr>
<th></th>
<th>$s_e$ (exact)</th>
<th>$a_f$ (exact)</th>
<th>$a_f$ (eqn. 4.2.4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M1</td>
<td>24.86</td>
<td>0.8472</td>
<td>0.8601</td>
</tr>
<tr>
<td>M2</td>
<td>12.26</td>
<td>0.8586</td>
<td>0.8855</td>
</tr>
<tr>
<td>M3</td>
<td>4.73</td>
<td>0.8904</td>
<td>0.9258</td>
</tr>
<tr>
<td>M4</td>
<td>2.88</td>
<td>0.9139</td>
<td>0.9451</td>
</tr>
<tr>
<td>M5</td>
<td>52.39</td>
<td>0.8451</td>
<td>0.8543</td>
</tr>
<tr>
<td>M6</td>
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<td>Saclay 16</td>
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<td>0.9202</td>
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(iii) The equivalence relation equation (4.1.4) gives a low negative percentage difference for the weakly absorbing systems, however as the rate of absorption increases the percentage difference takes larger negative values but then decreases slightly for the most strongly absorbing systems.

By a process of interpolation on the values in table (6.1) we have found the values of $s_e$ which, when used in equations (6.2), will yield the exact values of $1-p_r$. These values and the corresponding values of $a_f$ are given in table (6.2).

A comparison of the values of $s_e$ in tables (6.1) and (6.2) indicates that the values of $s_e$ obtained from equation (4.1.4) always underestimate the correct value or, what amounts to the same thing, the value of $a_f$ given by equation (4.2.4) overestimates the correct value. It remains to explain the source of this overestimation of $a_f$.

We have already pointed out in chapter 4 that the corrected rational approximation approach involves three main assumptions (i) separability of the fuel and moderator contributions, (ii) use of Bell's formula for $P_{11}$, and (iii) application of the NR approximation to all nuclear species.

From the results obtained in section (4.4) and given that for all the systems considered in table (6.1) the value of $G_2$ is greater than 0.9 we see that assumption (i) introduces negligible error into the systems at present under consideration.
Assumption (ii) involving the use of Bell's formula for $P_{11}$ introduces negligible error for circular cylindrical systems as demonstrated by Aisu and Minton (1964). It would therefore seem that the underestimation of $s_e$ is due to the use of the NR approximation when obtaining the expression for $a_f$ in equation (4.2.4).

If we were to modify the derivation of $a_f$ to remove the NR approximation by applying the $\lambda$ method we would arrive at the equation

$$\frac{2\sqrt{\lambda N\xi\sigma}}{\sqrt{a_f}} \left(1 + a_f \lambda N\xi\sigma \right)^{\frac{1}{2}} - \left(a_f \lambda N\xi\sigma \right)^{\frac{1}{2}} = \psi(\lambda N\xi\sigma)$$

in place of the equation preceding equation (4.2.4). Hence in place of $a_f$ we obtain $a_f(\lambda)$ where

$$a_f(\lambda) = \frac{\lambda 4N\xi\sigma}{\psi^2(\lambda N\xi\sigma) + 4\lambda N\xi\sigma \psi(\lambda N\xi\sigma) p} \tag{6.3}$$

Thus since in general $\lambda$ lies between 0 and 1 the modified $a_f$ is evaluated at a smaller value of $\lambda N\xi\sigma_p$ than the $a_f$ of equation (4.2.4). Now we see from table (4.1) that, for circular cylindrical fuel elements, reducing the value of $\lambda N\xi\sigma_p$ reduces the value of $a_f$. This is the required trend for any improvement to $a_f$ as we have seen in table 6.2.

The above descriptive argument does not, of course, yield us an expression for $a_f$ which will correct for the application of the NR approximation but it does indicate the need and the direction of further investigations.
7. CONCLUSION

In the earlier survey chapters we saw the essential difference between the Russian and Western approaches. The Russian workers apply the NR approximation to the differential form of the Boltzmann transport equation and so obtain an approximation to the space, angle and energy dependent fuel flux. Integration of this quantity over space and angle then yields the spatially averaged fuel flux. In the Western approach the Boltzmann transport equation is integrated first of all to give the integral equations of the spatially averaged fluxes. The flat flux approximation is then made so that the spatial and energy integrations may be separated. The spatial integrations are the collision probabilities which are approximated with rational type approximations.

The desire to find improved rational type approximations to the collision probabilities, and hence at the same time obtain an equivalence between homogeneous and heterogeneous systems, stimulated the investigations in chapter 4. The equivalence relation derived there rested upon three main assumptions (i) the use of Bell's formula, (ii) the separability of the fuel and moderator contributions and (iii) the use of the NR approximation. The use of Bell's formula does not introduce significant error in circular cylindrical systems. It was found that the second assumption led to an overestimation of $s_e$ and formulae were derived which gave the correct dependence of $s_e$ on the Dancoff correction $G_2$. 
The third assumption, concerning the use of the NR approximation in the derivation of $s_e$, leads to underestimation of the capture rate by as much as 2.5% in some instances as was seen in chapter 6. Clearly it is toward refinement of this third assumption that further research must be directed. One possible approach would be to find a second expression for $s_e$ based on the use of the wide resonance approximation and then interpolate between the two values of $s_e$. But such further developments would require extensive research.

In chapter 5 an approximate solution to the slowing down equations based on the use of the Galerkin method was derived. The Goldstein and Cohen $\lambda$ method was seen to be a particular instance of this approach and indeed the Galerkin method solution was found to yield results in general superior to those given by the $\lambda$ method. An attempt was also made to account for the variation of the moderator flux but the results were a little disappointing due probably to the fact that the moderator flux can only properly be approximated by applying the Galerkin method directly to the coupled integral equations and assuming independent trial functions for the fuel and moderator fluxes. This would not be a simple task. Along with more refined estimates of the moderator flux further improvements could possibly be obtained by use of more than one trial function approximations. The relative success of the Galerkin method approximation indicates that the
problem of finding approximate solutions to the slowing down equations is by no means a closed issue and it seems to the candidate that the most profitable course lies in the use of direct approximate methods.

Finally, all the approximate theories developed in this thesis are only applicable to two region lattice systems. The task of extending these theories to multiregion lattice systems and to systems of cluster type geometries should provide many stimulating research problems.
Figure A1. (Facing page 147)
APPENDIX 1. THE AVERAGE VALUE OF POWERS OF THE CHORD LENGTH

From Schwarz's inequality in the form

\[ \int \ell^{2\alpha} f(\ell) d\ell > \left( \int \ell^{\alpha} f(\ell) d\ell \right)^2 \]

we see that

\[ \frac{\overline{\ell^{2\alpha}}}{\overline{\ell^\alpha}} > \left( \frac{\overline{\ell^\alpha}}{\overline{\ell}} \right)^2 \quad (A1.1) \]

from which we deduce the particular inequalities

\[ \frac{\overline{\ell^{2\alpha}}}{\overline{\ell^\alpha}} > \left( \frac{\overline{\ell^{2\alpha}}}{\overline{\ell^2}} \right)^2 \quad (A1.2) \]

and

\[ \frac{\overline{\ell^2}}{\overline{\ell}} > \left( \frac{\overline{\ell^2}}{\overline{\ell}} \right)^2 \quad (A1.3) \]

It is in fact possible to find the exact expression for \( \overline{\ell^\alpha} \) for cylindrical fuel elements by using the same co-ordinate system as used by Sauer (1963) to calculate \( \ln \ell \). This co-ordinate system is reproduced in figure A1 opposite.

Using the notation of figure A1 we have

\[ \left( \frac{\overline{\ell}}{\ell} \right)^\alpha = \frac{\int \frac{dS}{S} \int \frac{d\Omega}{4\pi} n_{\Omega} \frac{n}{\overline{\ell}} \left( \frac{n(\theta, \phi, \psi)}{\overline{\ell}} \right)^\alpha}{\int \frac{dS}{S} \int \frac{d\Omega}{4\pi} n_{\Omega} \frac{n}{\overline{\ell}}} \quad (A1.4) \]

Noting that \( d\Omega/S = d\psi/2\pi \), \( d\Omega = \sin \theta d\theta d\phi \), \( n_{\Omega} = \cos \psi \sin \theta \)

and \( n(\theta, \phi, \psi) = \ell_{\perp}/\sin \theta = \frac{\ell}{\ell} \cos \psi / \sin \theta \) we see that equation (A1.4) reduces to

\[ \left( \frac{\overline{\ell}}{\ell} \right)^\alpha = 2 \int_0^{\pi/2} \sin^{2-\alpha} \theta d\theta \int_0^{\pi/2} \cos^{1+\alpha} \psi d\psi \quad (A1.5) \]

The integrals in equation (A1.5) converge if \(-2 < \alpha < 3\) and are expressible in terms of the Gamma function as
\[
\left( \frac{x}{\ell} \right)^\alpha = \frac{\Gamma\left(\frac{3-\alpha}{2}\right) \Gamma\left(\frac{2+\alpha}{2}\right)}{\Gamma\left(\frac{4-\alpha}{2}\right) \Gamma\left(\frac{3+\alpha}{2}\right)} = F(\alpha) \tag{A1.6}
\]

By substituting \( \alpha = 1-n \) it can be seen that \( F(\alpha) \) is symmetrical about \( \alpha = \frac{1}{2} \).

The minimum value at \( \alpha = \frac{1}{2} \) can be obtained from (A1.6) in the form

\[
\left( \frac{x}{\ell} \right)^{\frac{1}{2}} = \frac{1}{9} \left( \frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} \right)^2
\]

i.e.

\[
\ell^{\frac{1}{2}} = 0.9726 \frac{x}{\ell}^{\frac{1}{2}} \tag{A1.7}
\]

which is in agreement with the value given by Galanin (1960).

To our knowledge the result (A1.6) has not appeared previously in the literature and is shown graphically in figure A2.
APPENDIX 2

TABULATION OF VARIOUS FUNCTIONS

(i) The function

\[ F(\alpha,\beta) = \frac{4\sqrt{\beta}}{\pi} \int_0^1 y \int_0^{\infty} \frac{-\left(\frac{1}{y^2} + \frac{\beta}{\mu}\right)}{-\left(1+\frac{\beta y^2}{\mu}\right)} \left(1-e^{-\frac{\alpha}{\mu}}\right) dy \]

where \( \alpha = \frac{N\bar{\sigma}_m}{2}, \beta = \frac{N\bar{\sigma}_p}{2} \) and \( \bar{\ell} \) is the mean chord length of the slab fuel element.

This function has been evaluated using a 32 point Gaussian integration rule and values are given in table A2.1.

\[ \begin{array}{|c|c|c|c|c|c|c|}
\hline
\bar{\sigma}_m & 0.1 & 0.3 & 0.5 & 1.5 & 5.0 & 12.0 \\
\hline
\bar{\sigma}_p & \phantom{0}0.0781 & 0.1753 & 0.2393 & 0.3927 & 0.4927 & 0.5029 \\
0.1 & 0.0841 & 0.2006 & 0.2816 & 0.4839 & 0.6199 & 0.6339 \\
0.2 & 0.0864 & 0.2122 & 0.3026 & 0.5354 & 0.6957 & 0.7125 \\
0.3 & 0.0876 & 0.2187 & 0.3152 & 0.5691 & 0.7476 & 0.7663 \\
0.4 & 0.0883 & 0.2229 & 0.3234 & 0.5929 & 0.7857 & 0.8061 \\
0.5 & 0.0896 & 0.2312 & 0.3408 & 0.6499 & 0.8840 & 0.9096 \\
1.0 & 0.0899 & 0.2335 & 0.3461 & 0.6703 & 0.9232 & 0.9514 \\
1.5 & 0.0900 & 0.2345 & 0.3482 & 0.6794 & 0.9421 & 0.9718 \\
2.0 & 0.0901 & 0.2351 & 0.3498 & 0.6866 & 0.9580 & 0.9891 \\
3.0 & 0.0902 & 0.2353 & 0.3504 & 0.6892 & 0.9645 & 0.9962 \\
6.0 & 0.0903 & 0.2355 & 0.3506 & 0.6905 & 0.9674 & 0.9995 \\
12.0 & 0.0903 & 0.2356 & 0.3507 & 0.6905 & 0.9674 & 0.9995 \\
20.0 & 0.0903 & 0.2356 & 0.3507 & 0.6905 & 0.9674 & 0.9995 \\
\hline
\end{array} \]
(ii) The function

\[ K = \frac{4G_2}{\pi} \int_0^{\infty} \frac{1 - \phi(N\ell z)}{1 - (1-G_2)\phi(N\ell z)} \cdot \frac{z^2 \, dz}{(1+z^2)^2} \]

where

\[ \phi(N\ell z) = \begin{cases} 
4 \int_0^{\pi/2} K_{1,3\{N\ell \sigma (1+z^2)\cos \psi\}} \cos \psi \, d\psi & \text{for cyl.} \\
2E_3\{\frac{N\ell \sigma}{2} (1+z^2)\} & \text{for slab fuel elements} 
\end{cases} \]

We make the transformation \( z = \tan \theta \) so that

\[ K = \frac{4G_2}{\pi} \int_0^{\pi/2} \frac{1 - \phi(N\ell \theta)}{1 - (1-G_2)\phi(N\ell \theta)} \cdot \sin^2 \theta \, d\theta \]

and

\[ \phi(N\ell \theta) = \begin{cases} 
4 \int_0^{\pi/2} K_{1,3\{\frac{N\ell \sigma \cos \psi}{\cos^2 \theta}\}} \cos \psi \, d\psi & \text{(cylinder)} \\
2E_3\{\frac{N\ell \sigma}{2\cos^2 \theta}\} & \text{(slab)} 
\end{cases} \]

The function \( K \) has been evaluated using a 16 point Gaussian integration rule and values are given in tables A2.2 and A2.3 for regular lattices of slab and cylindrical elements.
TABLE A2.2

K for slab lattices

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<th>N\bar{\pi}</th>
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TABLE A2.3

K for Cylindrical Lattices

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