Formulation and calculation of resonance overlap effects

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FORMULATION AND CALCULATION OF RESONANCE OVERLAP EFFECTS

P. J. O'Halloran

M.Sc. THESIS

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SUMMARY

Resonance absorption calculations are particularly important in a study of a reactor breeding fuel. For a breeding reactor new problems arise in resonance calculations as resonances of different nuclide species compete for neutrons. The reaction rate of one species is lowered by the presence of another species as neighbouring resonances may no longer be considered to be isolated from each other. The purpose of the thesis is to study the effect of a resonance of one absorber overlapping a resonance of another absorber.

The study of resonance overlap involves an extension of well developed resonance calculational methods. Two approaches are possible (i) a (large) computer is used to solve the slowing down equation or (ii) an approximate analytic technique is pursued. Under (i) a study of a few selected problems is feasible. However, computer time becomes excessive in routine resonance calculations. Under (ii) accuracy of the approximation is important. Methods (i) and (ii) thus complement each other with method (ii) being the routine computational tool.

In this work various aspects of resonance theory which are important in overlap calculations are discussed. The material is developed from simple slowing down theory. Mathematical properties of various functions which arise in the thesis are studied in order to present a logical development of resonance theory. The main work is the temperature dependence of the overlap correction. As a check on the validity of the proposed overlap correction, a comparison is made with the work of other authors.
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1. Historical Review of the Slowing Down Equation

1.1 General Introduction

In a nuclear reactor the slowing down of fission neutrons is caused by elastic collisions of the fast neutrons from fission with the nuclei of reactor material. During the course of slowing down the neutrons are subject to capture (absorption) by reacting with any material which does not yield neutrons. This important process of absorption during slowing down is called resonance absorption – resonance because historically the radiative capture in the sharp nuclear resonance lines of $^{238}U$ was the first such absorption reaction considered. (Dresner 1960).

In the early development of nuclear reactors, interest in resonance absorption centred mainly in the $(n,\gamma)$ reaction of $^{238}U$, absorption in which was found to prevent the use of natural uranium as a fuel except when mixed with heavy water or separated into lumps. Besides its importance from the point of view of neutron economy, resonance capture of neutrons by 'fertile' nuclei such as $^{238}U$ and $^{232}Th$ leading to the formation of fissile nuclei like $^{239}Pu$ and $^{233}U$ in breeder reactors is also of interest. The fissile nuclei also exhibit resonance behaviour in their cross sections for both radiative capture and fission, a fact which assumes prime importance in non-thermal reactors. Thus, as McKay (1964) has stated, the phenomenon of resonance absorption is worthy of close study, especially when account is taken of the fact that resonance cross sections are sensitive to temperature variations.

1.2 Analytic Solutions of the Slowing Down Equation

It was Fermi and Szilard in the late 30's who made the historic
decision to explore the possibility of using thermal neutrons as chain carriers. Little was known of absorption at this time though the above scientists recognised that resonance absorption could be diminished by placing the uranium in the form of lumps, rather than mixing it homogeneously with the moderator. According to Creutz (1955) this idea of lumping the uranium also was made independently in the early 40's by many investigators throughout the world. Notable among these researchers were Harteck in Germany, Halban, Kowarski and Joliot in France. Gurevich and Pomeranchouk (1955) in Russia also did original work in this period.

The first published results of slowing down theory was by Amaldi and Fermi (1936) and Bethe (1937) who studied the energy distribution of neutrons slowing down in hydrogen. Early in the 40's, Placzek (1946a) obtained an explicit expression for the collision density of neutrons slowing down in a non-absorbing medium. Later Placzek (1946b) published the first account of an approximate expression for the collision density of neutrons slowing down in an absorbing medium. It is this work which is the basis of later slowing down theory although Placzek here considered only a weak absorption medium for neutrons well below the source. Marshak (1947) published an extensive study of neutron slowing down including capture, time and space dependence.

In the early 50's Goertzel and Greuling obtained an approximate solution to the slowing down equation by making the restriction that the second derivative of the slowing down density with respect to lethargy was negligible when the absorption varied slowly with lethargy. In the presence of weak absorption Keane (1961) obtained the results of Goertzel and Greuling by solving the integral equation via Laplace transforms.
Further studies on slowing down in a non-absorbing medium were made by de Marcus (1959) who determined the number of elastic collisions required to thermalize neutrons emitted from fission; Dyos (1964) who showed that the solution to the slowing down equation was a constant under certain conditions, and Wilkins (1962) who applied Renewal theory to the problem.

In general the class of problems for which analytic solutions of the slowing down equation have been obtained, does not appear to have much practical application. Therefore there has been a great deal of research into approximate solutions of the slowing down equation.

1.3 Approximate Solutions of the Slowing Down Equation

The solution of the slowing down integral equation through each resonance is possible using direct numerical techniques. For example see Nordheim (1961), Collins (1963) and Pollard (1964). However, as the machine time becomes prohibitive for routine calculations there has been much investigation into approximate analytic techniques.

Early approaches consisted of using either Wigner's (1955) narrow resonance (NR) or Spinney's (1957) infinite mass (IM) approximations. These approximations depended on whether the practical width of the resonance (the energy span between the two points where the resonance and potential scattering cross sections become equal) was small or large compared with the maximum loss of neutron energy on collision with the resonance absorber.
A major step in the study of absorption was made by Goldstein and Cohen (1962) who developed a method for determining approximate solutions intermediate between the IM and NR extremes and which they called the intermediate resonance (IR) approximation. Their technique consisted in iterating on the basic slowing down equation using as a first iterant an interpolation between the IM and NR approximations. This new approach, overcoming the weakness of the earlier approximations by not having to decide arbitrarily whether scattering by the absorber was included (NR) or excluded (IM), initiated many research papers.

McKay and Pollard (1963) showed that the interpolation formula was insensitive to temperature and so extended the IR method to Doppler broadened resonances. McKay (1964) developed an improved form applicable to low lying resonances. McKay's ideas were further extended by McKay, et.al. (1965). Keane and Dyos (1966), Keane and Forner (1966) found solutions to the slowing down equation using Goldstein and Cohen's method.

1.4 The Overlap Problem

A further complicating factor to resonance theory was discovered by Codd and Collins (1963) who obtained results which, at the time, were most unexpected. They showed that the Doppler coefficient for Pu$^{239}$ resonances could be considerably affected by the presence of U$^{238}$ resonances. As overlap effects would have ramifications for the design and safety of reactors, a rush of computations were made by many researchers to investigate Codd and Collins results.

Hutchins (1964) investigating the overlap of unlike fuel isotopes
and the temperature dependence of the average flux over an energy interval containing resonances, found that these two above effects approximately cancelled. Stevens and Smith (1965) developed one of the first codes to include resonance overlap in absorption calculations. Froelich and Ott (1965) showed that the net Doppler coefficient of fast reactors is unaffected by the interaction effect between resonances.

Earlier Hwang (1965), using an original and apparently useful procedure for the overlap problem, obtained results inferring that the resonance interference would substantially increase the Doppler effect of the system. However, Nicholson (1965) pointed out an important error in Hwang's paper which could have invalidated Hwang's results.

The complex problem of overlap has necessitated the development of large computer codes and an increasing departure from the original simple correction proposed by Rowlands and used in Codd and Collins' paper (ibid.). Keane (1966) has reverted to the use of a simple correction by modifying Rowlands' formula (unpublished) used by Codd and Collins (ibid.). Keane obtained his correction by analytical methods after assuming the temperature to be zero. Keane and O'Halloran (1966) further modified the formula mainly by numerical methods so to include the temperature parameters in the formula.

The main purpose of this work is the presentation of a logical development of resonance theory leading to overlap studies and the derivation of the approximate formula of Keane and O'Halloran (ibid.) (chapters 2,3) and a numerical study both to show the magnitude of the overlap effects and to check the accuracy of the approximate expressions derived (chapters 4,5).
2. Background Theory

2.1 Slowing Down of Neutrons in an Infinite Homogeneous Medium

2.1.1 Introduction

Considering the energy range of approximately $10^4$eV. to 4eV., it is reasonable to assume that the slowing down of neutrons is due almost entirely to elastic scattering suffered by the neutrons upon collision with nuclei of the moderator (Glasstone and Edlund, chapter 6). Such collisions can be discussed by the methods of classical mechanics, assuming the neutron and the scattering nucleus to behave as perfectly elastic spheres.

It is also assumed that the neutrons are so sparse that they don't collide with one another, an assumption which is not valid for gas mixtures and which makes the transport theory of gas mixtures more complicated.

2.1.2 Dynamics of Collisions

By applying the principles of conservation of momentum and of energy and using the centre of mass coordinate system, it can be shown that

$$\frac{E'}{E} = \frac{m^2 + M^2}{(m+M)^2} + \frac{2mM}{(m+M)^2} \cos \theta,$$

(2.1)

where $m$ and $M$ are, respectively, the mass of a neutron and a particular nucleus, $E$, $E'$ are the energies of the neutron before and after the collision, and $\theta$ is the angle of scattering. Defining the mass ratio, $A$, as $M/m$ and $\alpha$ as $\left(\frac{A-1}{A+1}\right)^2$, we have
\[
\frac{E'}{E} = \frac{1+A^2}{(1+A)^2} + \frac{2A}{(1+A)^2} \cos \theta 
\]  

(2.2)

\[
\text{i.e., } \frac{E'}{E} = \frac{1+\alpha}{2} + \frac{1-\alpha}{2} \cos \theta 
\]  

(2.3)

Evidently, \( E'=E \) for \( \theta=0 \) (glancing collision), that is, the neutron energy remains unchanged; while, for \( \theta=\pi \), (head-on collision) \( E'=\alpha E \), the neutron energy undergoes the greatest possible change.

\[
\text{That is, } \begin{cases} 
\frac{dE'}{(1-\alpha)E} , & \alpha E \leq E' \leq E \\
0 , & E' < \alpha E 
\end{cases} 
\]  

(2.5)

2.1.3 Basic Equations

Consider the slowing down and resonance absorption of neutrons in an infinite homogeneous mixture of \( n \) different nuclides. Let
α_i E ≤ E′ ≤ E be the energy range attainable by a neutron of initial energy E after a collision with a nucleus of the i-th kind. As it is evident that the number of neutrons colliding in dE equals the number of neutrons arriving in dE after scattering from above plus the number of neutrons that are born in dE, then the integral equation for the slowing down of neutrons in a homogeneous medium becomes

\[ \Sigma_t(E)\phi(E)dE = \sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \frac{\Sigma s_i(E')\phi(E')dE'}{(1-\alpha_i)E'} + S(E)dE \]

that is,

\[ \Sigma_t(E)\phi(E) = \sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \frac{\Sigma s_i(E')\phi(E')dE'}{(1-\alpha_i)E'} + S(E) \tag{2.6} \]

where \(\phi(E)\) = the flux of neutrons per unit energy at energy E,
\(S(E)\) = the number of source neutrons per unit energy at energy E,
\(\Sigma_t(E)\) = the macroscopic total cross section at energy E,
\(\Sigma s_i(E)\) = the macroscopic scattering cross section of the i-th kind of nuclide at energy E.

The slowing down density equation is derived by noting that the fraction of neutrons having a collision in dE' with the i-th kind of nuclide and which have a final energy less than E is \((E-\alpha_i E')/(1-\alpha_i)E'\). Thus

\[ q(E) = \sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \Sigma s_i(E')\phi(E') \frac{E-\alpha_i E'}{(1-\alpha_i)E'} dE' , \tag{2.7} \]

where \(q(E)\) is the number of neutrons that get past E.

Differenting (2.6) and using (2.7) we have

\[ \frac{dq(E)}{dE} = \Sigma_t(E)\phi(E) - S(E) , \tag{2.8} \]
where \( \Sigma_a(E) \) is the total macroscopic absorption cross section of the mixture at energy \( E \). Note that \( \Sigma_t(E) = \Sigma_a(E) + \Sigma_s(E) \), the \( \Sigma_s(E) \) being the total macroscopic scattering cross section of the mixture.

### 2.1.4 Lethargy

The slowing down process can be expressed as a strict renewal process by a simple change of variable. We introduce lethargy as

\[
u = \ln E^/E, \quad \text{where } E^ \text{ is a given energy usually taken above the neutron source.}
\]

\[
\therefore \quad du = -\frac{dE}{E}.
\]

The flux and source neutrons are also defined in lethargy respectively as

\[
\phi(u)du = -\phi(E)dE
\]

and

\[
S(u)du = -S(E)dE.
\]

\[
\therefore \quad \phi(u) = E \phi(E) \tag{2.9}
\]

and

\[
S(u) = E S(E) \tag{2.10}
\]

Equations (2.6) and (2.8) now become

\[
\Sigma_t(u)\phi(u) = \sum_{i=1}^{n} \int_{u-\ln \alpha_i}^{u} \Sigma_s_i(u') \frac{\phi(u')e^{-(u-u')}}{1-\alpha_i} du' + S(u) \tag{2.11}
\]

and

\[
\frac{dq(u)}{du} = -\Sigma_a(u)\phi(u) + S(u) \tag{2.12}
\]

From equation (2.11) it is seen that the lethargy range attainable by a neutron after a collision with a nucleus of the \( i \)th kind is

\[
u - \ln \frac{1}{\alpha_i} \leq u' \leq u, \quad \text{that is, } 0 \leq u-u' \leq \ln \frac{1}{\alpha_i}.
\]

The range is thus independent of the pre-collision lethargy and the kernel of the slowing down
equation is

\[
    k_i(u) = \begin{cases} 
        \frac{1}{1-\alpha_i} e^{-u}, & 0 \leq u \leq \ln \frac{1}{\alpha_i} \\
        0, & u > \ln \frac{1}{\alpha_i}
    \end{cases}
\] (2.13)

We define \( \xi_i \) to be the average change in lethargy of a neutron per collision with the \( i \)-th nuclide, and so

\[
    \xi_i = \frac{1}{1-\alpha_i} \int_0^{\ln \frac{1}{\alpha_i}} u e^{-u} du
\]

\[
    \therefore \quad \xi_i = 1 - \frac{\alpha_i}{1-\alpha_i} \ln \frac{1}{\alpha_i}
\] (2.14)

An analytical solution has not been found for the general slowing down equation because of the complicated energy behaviour of the cross section. However, an asymptotic solution can be derived for zero absorption and an exact solution can be obtained when the material is Hydrogen. These two special situations will be discussed in sections 2.1.6 and 2.1.7.

2.1.5 Resonance Escape Probability

If the absorption region is situated at an energy well below the source, equation (2.12) becomes

\[
    \frac{dq(u)}{du} = - \Gamma_a(u) \phi(u),
\] (2.15)

or

\[
    \frac{dq(u)}{q(u)} = - \frac{\Sigma_a(u) \phi(u) du}{q(u)}.
\]

Integrating between the limits \( 0(=q(u_o)) \) and \( q(=q(u)) \), where \( u_o \) is the lethargy well before the occurrence of the resonances, we have

\[
    \left[ \ln q(u) \right]_0^q = - \int_{u_o}^u \frac{\Sigma_a(u') \phi(u') du'}{q(u')} - \int_u^{u_o} \frac{\Sigma_a(u') \phi(u') du'}{q(u')}
\]

i.e.

\[
    \frac{q}{q_0} = e^{-\int_{u_o}^u \frac{\Sigma_a(u') \phi(u') du'}{q(u')}}
\] (2.16)
If \( u \) is after the resonances, the fraction \( \frac{q}{0} \) is the probability, \( p \), that a neutron will escape capture as it is slowed down through the resonances. It is called the resonance escape probability.

\[
\therefore \quad p = e^{-\int_{u_0}^{u} \frac{\Sigma_a(u')\phi(u')}{q(u')} du'}
\]

which is a measure of the number of neutrons surviving absorption to lethargy \( u \). If an isolated resonance is considered,

\[
\frac{q(u^*)}{across \quad \text{resonance}}
\]

For a number of isolated resonances with resonance escape probabilities, given by \( p_1, p_2, \ldots, p_n \), it can be seen from equation (2.18) that

\[
P = \prod_{i=1}^{n} p_i .
\]

2.1.6 Slowing Down Equation...an asymptotic solution

As mentioned in section (2.1.4), an asymptotic solution can be obtained from the slowing down equation in the special case of zero absorption. Equation (2.11) thus becomes

\[
\Sigma_s(u)\phi(u) = \sum_{i=1}^{n} \int_{1-u-\ln \frac{1}{\alpha_i}}^{u} \Sigma_{s_i}(u') \phi(u') \frac{e^{-(u-u')}}{1-\alpha_i} du' + S(u). \tag{2.19}
\]

Taking Laplace transforms, we have

\[
\mathcal{L}\{\Sigma_s(u)\phi(u)\} = \sum_{i=1}^{n} \mathcal{L}\{\Sigma_{s_i}(u)\phi(u)\}K_i(p) + \overline{S(p)}
\]

and assuming the \( \Sigma_{s_i} \) all vary the same way in energy the above equation becomes

\[
\mathcal{L}\{\Sigma_s(u)\phi(u)\} = \sum_{i=1}^{n} \frac{\Sigma_{s_i}}{\Sigma_s} \mathcal{L}\{\Sigma_s(u)\phi(u)\}K_i(p) + \overline{S(p)} \tag{2.20}
\]
where \( K_i(p) = \int_0^\infty \frac{\ln \frac{1}{\alpha_i} e^{-(p+1)u}}{1-\alpha_i} \, du \)

\[
= \frac{1-\alpha_i}{(1-\alpha_i)(p+1)}
\]

that is,

\[
\mathcal{L} \{ \sum_s (u) \phi(u) \} = \frac{1}{S(p)} (2.21)
\]

Since \( K_i(0) = 1 \), the denominator of (2.21) has a zero at \( p=0 \).

Therefore using L'Hospital's Rule we have

\[
\lim_{p \to 0} \frac{p}{1-\sum_i \sum_s \frac{s_i}{\xi_s} K_i(p)} = \frac{1}{1-\sum_i \sum_s \frac{s_i}{\xi_s} K_i(0)}
\]

However

\[
K_i'(p) = \frac{1}{1-\alpha_i} \frac{-(p+1)\alpha_i}{(p+1)^2} (1-\alpha_i)^{p+1}
\]

\[
\therefore K_i'(0) = -1 + \alpha_i \frac{\ln \alpha_i}{1-\alpha_i}
\]

\[
= -\xi_i, \text{ using (2.14).}
\]

Therefore the first term in the Laurent expansion of \( \frac{1}{1-\sum_i \sum_s \frac{s_i}{\xi_s} K_i(p)} \)

is \( \frac{1}{\xi_p} \), where \( \xi_p \), defined as \( \sum_i \sum_s \frac{s_i}{\xi_s} \xi_i \), is called the mean value of the average change in lethargy. Equation (2.21) becomes

\[
\mathcal{L} \{ \sum_s (u) \phi(u) \} = \frac{1}{p \xi} S(u).
\]
Inverting, we thus obtain the first term of the asymptotic expansion as
\[ \Sigma_s(u)\phi(u) = \frac{1}{\xi} \int_{\infty}^{u} S(u) \, du . \]

Therefore below the source the asymptotic solution is
\[ \Sigma_s(u)\phi(u) = \frac{Q}{\xi} , \]

(2.22)

Q being the number of source neutrons. In terms of energy, (2.22) becomes
\[ \Sigma_s(E)\phi(E) = \frac{Q}{\xi E} . \]

(2.23)

2.1.7 Exact Solution for Slowing Down in Hydrogen

To obtain an exact solution of the slowing down equation, we consider the situation when the material is Hydrogen. As \( A(=m/M) \) equals 1 for Hydrogen, equations (2.6) and (2.7) degenerate respectively to
\[ \Sigma_t(E)\phi(E) = \int_{E}^{\infty} \frac{\Sigma_s(E')dE'}{E'} \]

and
\[ q(E) = \int_{E}^{\infty} \frac{\Sigma_s(E')\phi(E')E \, dE'}{E'} \]

\[ \therefore \frac{dq(E)}{q(E)} = \frac{\Sigma_a(E)dE}{\Sigma_t(E)E} . \]

(2.24)

Integrating (2.24) between the limits \( Q(=q(E_o)) \) and \( q(=q(E)) \), where \( E_o \) is the energy at the source, we have
\[ \frac{q}{Q} = e^{-\int_{E_o}^{E} \frac{\Sigma_a(E')dE'}{\Sigma_t(E')E'}} \]

(2.25)

The fraction is the probability of a neutron in Hydrogen reaching an energy \( E \).
2.2 The Effective Resonance Integral

2.2.1 Introduction

Three well known approximations for the calculation of the resonance escape probability, namely the narrow resonance, the narrow resonance infinite absorber and the intermediate resonance approximations, will be discussed later in section 2.2. Although different assumptions are made, the effective resonance integral in each of the three approximations is proportional to an expression of the form $J(\beta, t)$. Therefore, applications of the resonance overlap results, discussed in section 3, could be made to the above three approximations.

2.2.2 Doppler Broadened Breit Wigner Contours

A resonance is defined by the energy $E_r$ at which it occurs, and by the widths $\Gamma_\gamma$ and $\Gamma_n$ which are the probability of radiative capture and neutron emission respectively. The Breit-Wigner single level cross-sections of a nucleus for the absorption and scattering of a neutron at energy $E$ are given by (Huria, 1964)

$$\sigma_a = \sigma_o \frac{\Gamma_\gamma}{\Gamma} \sqrt{\frac{E_r}{E}} \frac{1}{1 + \frac{4}{\Gamma^2}(E-E_r)^2}$$

and

$$\sigma_s = \sigma_o \frac{\Gamma_n}{\Gamma} \frac{1}{1 + \frac{4}{\Gamma^2}(E-E_r)^2} + \frac{(\sigma_o \sigma_{po} \Gamma_n)^{1/2}(E-E_r)/\Gamma}{1 + \frac{4}{\Gamma^2}(E-E_r)^2} + \sigma_{po} \quad (2.26)$$

where

- $\sigma_a$ = absorption cross-section,
- $\sigma_s$ = total scattering cross section,
- $E_r$ = Resonance energy,
- $E = \text{neutron energy relative to that of the nucleus},$
- $\sigma_o = \text{total cross section at } E=E_r \left(\approx 2.6 \times 10^6 \frac{\Gamma_r}{\Gamma_n}\right),$
- $\Gamma_\gamma = \text{radiation width},$
\( \Gamma_n \) = neutron width,
\( \Gamma \) = total width of resonance,
\( \sigma_{po} \) = energy independent potential scattering cross section,
\( g \) = statistical factor depending upon the spin quantum numbers of the target nucleus and the compound nucleus.

The three terms on the R.H.S. of (2.26) represent the resonance scattering, the interference scattering effect between resonance and potential scatterings and the potential scattering respectively. For many resonances the second term gives very little contribution to the total absorption, especially at working temperatures. Hence we will neglect the interference term in order to simplify the formulae. Also we will assume that \( \sqrt{\frac{E_r}{E}} \) equals 1 in subsequent calculations.

The above equations are those for stationary target nuclei. However, the motion of these nuclei become relatively important when the temperature of the absorber increases. This motion leads to a broadening of the resonance line with a drop in the maximum cross section. It is found that the rise of temperature distorts the natural line shape into one which is Gaussian at and near the resonance energy but reverts to the natural line shape off the resonance. This phenomenon is known as the Doppler broadening of the resonance.

The simple approach to the Doppler broadening assumes that the velocity of the nucleus is small compared to the neutron velocity and that the relative velocity, \( v' \), can be taken as \( v'^2 \approx V^2 - 2vV \) where \( V \) is the velocity of the neutron and \( v \) the velocity of the atom. Averaging \( v \) over a Maxwellian spectrum and assuming the Breit-Wigner form for the
resonance cross section, viz

\[ \sigma_r = \frac{\sigma_0}{1 + \left( \frac{mv'}{\Gamma} - \frac{2E_r}{\Gamma} \right)^2} \]

then

\[ \sigma_r = \sigma_o \psi(x,t) \]

where \( \sigma_r = \) the microscopic resonance cross section, \( = \sigma_a + \sigma_s \)

\( t = 4kT E_r / \Gamma^2 A, \quad x = \frac{2}{\Gamma} (E - E_r) \)

\( k = \) Boltzmann's constant,

\( A = \) the mass of the nucleus in units of the mass of a neutron,

\( T = \) the temperature in degrees absolute,

and

\[ \psi(x,t) = \frac{1}{(4\pi t)^2} \int_{-\infty}^{\infty} e^{- (x-y)^2 / 4t} \frac{dy}{1+y^2} \]  \[(2.27)\]

with \(-\infty < x < +\infty\) and \( t > 0 \). The \( \psi(x,t) \) function is known as the Doppler broadened or Voigt function. It was originally obtained by Bethe and Placzek (1937).

Recently, Cook (1965) has obtained the accurate form of the Doppler broadened Breit-Wigner resonance contour without employing the above approximations. He has shown that the correction is important for low energy resonances but can be neglected over the major part of the resonance region.

2.2.3 Narrow Resonance (N.R.) approximation

In the narrow resonance approximation the assumptions made are that (i) the absorption is large only in an energy interval which is small compared with \((1-\alpha)E\); (ii) the resonances are widely spaced so that, as there is little absorption between the resonances, the asymptotic value
(equation (2.23)) would hold. Therefore, equation (2.6) would become, well below the source,

\[
\sum_t(E)\phi(E) = \sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \sum_{i}^{} \left( \phi(E') \frac{dE'}{\left(1-\alpha_i\right)E'} \right)
\]

\[
= \sum_{i=1}^{n} \frac{Q}{\xi(1-\alpha_i)} \int_{E}^{E/\alpha_i} \frac{dE'}{E'}^2
\]

\[
\implies \phi(E) = \frac{Q}{\xi \sum_t(E)E}
\]

Also equation (2.8) becomes

\[
\frac{dq(E)}{dE} = \sum_a(E)\phi(E)
\]

which, on integration, becomes

\[
[q(E)]^0_q = \int_E^{E_0} \sum_a(E')\phi(E')dE'
\]

\[
Q - q = \frac{Q}{\xi} \int_E^{E_0} \frac{\sum_a(E')dE'}{\sum_t(E')E'}
\]

\[
\therefore \quad p = 1 - \frac{1}{\xi} \int_E^{E_0} \frac{\sum_a(E')dE'}{\sum_t(E')E'}
\]

If the integral is small compared to unity, we can write

\[
- \frac{1}{\xi} \int_E^{E_0} \frac{\sum_a(E')dE'}{\sum_t(E')E'}
\]

\[
\implies p \approx e^{-\frac{1}{\xi} \int_E^{E_0} \frac{\sum_a(E')dE'}{\sum_t(E')E'}}
\]

which is called the narrow resonance approximation to the resonance escape probability.

An alternative derivation of equation (2.31) will now be given, which does not rely on the above assumptions (i) and (ii), and the exponential approximation in equation (2.31).
Working in terms of lethargy a neutron would make, on the average, \( \frac{\text{du}}{\xi} \) collisions in \( \text{du} \). Assuming that \( q(u) \) does not vary in a \( \text{du} \) interval, the total number of collisions occurring in \( \text{du} \) would be \( \frac{q(u)}{\xi} \text{du} \). However, the total number of collisions would also equal \( \Sigma_t(u) \phi(u) \text{du} \). That is,

\[
\frac{q(u)}{\xi} \text{du} = \Sigma_t(u) \phi(u) \text{du}
\]

\[
\therefore \quad \frac{\phi(u)}{q(u)} = \frac{1}{\xi \Sigma_t(u)}
\]

(2.32)

Thus the escape probability equation (2.18) becomes

\[
p = e \int_{\text{Exacr.}} \frac{\Sigma}{\xi \Sigma_t(u')} \text{du}
\]

\[
\quad \text{across } \text{resonance } \quad \text{or, in terms of energy, is}
\]

\[
\int_{\text{res.}} \frac{\Sigma}{\xi \Sigma_t(E')E'} \text{dE}'
\]

(2.33)

\[
p = e
\]

(2.34)

which agrees with the former N.R. approximation (2.31) and which helps to explain why the approximation is far better than that which would be expected on the basis of the usual assumptions. Therefore,

\[
\frac{N}{\xi} \frac{I}{\Sigma_p} = e
\]

(2.35)

where \( \Sigma_p \) = macroscopic potential cross section of the mixture,

\( N = \) the number of resonant absorbing nuclei per \( \text{cm} \),

and

\[
I = \frac{1}{N} \int_{\text{res.}} \frac{\Sigma \Sigma (E')}{\xi \Sigma_t(E')} \text{dE}'
\]

(2.36)

I is called the effective resonance integral.

\[
i.e. \quad I = \int_{\text{res.}} \frac{\sigma_a}{\sigma_a + \sigma \Sigma_p} \frac{\text{dE}}{E}
\]

(2.37)

where \( \sigma_p \) = potential cross section per absorber atom.
\[ p = \frac{1}{\xi \sigma_p} \int \frac{\sigma a}{1 + \left( \frac{\sigma a + \sigma_s}{\sigma_p} \right)^E} \, dE \]

When the mixture is very dilute, that is when the potential scattering cross section of the moderator is high \((\sigma_p \gg \sigma_r)\), equation (2.36) becomes

\[ I = \lim_{\sigma_p \to \infty} \int \frac{\sigma a}{1 + \left( \frac{\sigma a + \sigma_s}{\sigma_p} \right)^E} \, dE \]

i.e.

\[ I = I_\infty = \int \frac{\sigma a \, dE}{E} \] (2.39)

which is known as the infinitely dilute resonance integral.

However, if the resonances are assumed to be narrow, the \(1/E\) factor in (2.36) varies little across the resonance centred at \(E_r\), so that \(1/E\) can be replaced by \(1/E_r\). Keane (unpublished) has shown that the error involved here is of the order of a maximum error of a few percent. Changing the variable from \(E\) to \(x\), where \(x = 2(E-E_r)/\Gamma\), and extending \(x\) from \(-\infty\) to \(+\infty\), we have from (2.37)

\[ I = \frac{\Gamma}{2E_r} \int_{-\infty}^{\infty} \frac{\sigma a}{1 + \left( \frac{\sigma a + \sigma_s}{\sigma_p} \right)^x} \, dx \] .

Using the Breit-Wigner contour,

\[ I = \frac{\Gamma \sigma_p}{2E_r} \int_{-\infty}^{\infty} \frac{\psi(x,t)}{\psi(x,t) + \beta_1} \, dx \] (2.40)
letting $\beta_1 = \frac{\sigma_p}{\sigma_0}$. Equation (2.40) is often written as

$$I = \frac{\Gamma}{E_r} \frac{\sigma_p}{\sigma_r} J(\beta_1, t)$$  \hspace{1cm} (2.41)

where

$$J(\beta_1, t) = \int_0^\infty \frac{\psi(x, t)}{\psi(x, t) + \beta_1} \, dx$$  \hspace{1cm} (2.42)

The alternative derivation of the effective resonance integral, which is not based on the usual N.R. assumption enables us to consider resonances which are not necessarily isolated. Therefore, we have used equation (2.36) in the study of overlapping resonances in section 4.

2.2.4 Narrow Resonance Infinite Absorber (N.R.I.A.) Approximation

The usual assumption that the resonances are narrow compared with the energy lost by a neutron on collision with any of the nuclei in the system, is certainly not valid for the low energy resonances of the absorber. The maximum energy lost by a neutron on collision with an atom of the absorber is in many cases considerably less than the energy range of the resonance.

In the N.R.I.A. approximation it is assumed that a collision with an absorber nucleus does not modify the energy of the neutron (i.e. $\alpha = 1$). This occurs only if the absorber mass is infinite. However, it is assumed that the resonances are narrow in comparison with the energy lost on collision with a moderator atom.
Thus the resonance escape probability in equation (2.31) can be obtained as

\[ P = e^{-\frac{1}{\xi \sigma_m} \int_{res} \frac{\sigma_a}{\sigma_m} \frac{dE}{1 + \frac{\sigma_a}{\sigma_m} E}}, \]  

(2.43)

where the subscript \( m \) refers to the non-resonant moderator. That is

\[ P = e^{-\frac{I}{\xi \sigma_m}}. \]

I, the effective resonance integral for the N.R.I.A. approximation, is

\[ I = \int \frac{\sigma_a}{1 + \frac{\sigma_a}{\sigma_m} E} \, dE. \]  

(2.44)

Following the derivation of equation (2.40),

\[ I = \frac{\sigma_m \Gamma}{2 E_r} \int_{-\infty}^{\infty} \frac{\psi(x, t)}{\psi(x, t) + \beta_2} \, dx \]  

(2.45)

where \( \beta_2 = \frac{\sigma_m \Gamma}{\sigma_0 \Gamma G} \). Hence, in the case of the N.R.I.A.

\[ I = \frac{\Gamma \sigma_m}{E_r} J(\beta_2, t). \]  

(2.46)

### 2.2.5 The Intermediate Resonance (I.R.) Approximations

Because of the difficulty in choosing one of the two earlier approximations to the effective resonance integral, Goldstein and Cohen (1962) proposed an intermediate (I.R.) approximation. This interpolates between the N.R. and the N.R.I.A. approximations by partially neglecting the scattering of the absorber rather than completely including or completely excluding such scattering. This is achieved by determining the value of a parameter \( \lambda \) between 0 and 1 instead of letting it be zero or unity.
Solutions to the slowing down equation for a 2 nuclide system under N.R. and N.R.I.A. are initially made, and then the first approximation to the flux is made in the form

\[ \phi^{(1)}_\lambda(E) = \frac{A}{(\sigma_a + \lambda \sigma_s + \lambda \sigma_{pf} + \sigma_{pm})} \frac{1}{E} \]

where \( f \) and \( m \) are subscripts used to identify fuel and moderator and \( A \) is a constant.

This value of \( \phi^{(1)}_\lambda(E) \) is put in the R.H.S. of equation (2.6), and, upon integrating, a second approximation for the flux, \( \phi^{(2)}_\lambda(E) \), is found. Goldstein and Cohen then submit that the best \( \lambda \) is given by

\[ \int_{E'} (E') \phi^{(2)}_\lambda(E') dE' = \int_{E'} (E') \phi^{(1)}_\lambda(E') dE' . \]

So that the resonance escape probability equation will now be of the form

\[ p = e^{\frac{1}{\xi \sigma_{pm}}} \int \frac{\sigma_a}{1 + \frac{\sigma_s}{\lambda \sigma_{pf} + \sigma_{pm}}} \frac{dE}{E} \]

\[ = \frac{1}{\xi \sigma_{pm}} \text{ e} \]

that is, \( p = e^{\frac{1}{\xi \sigma_{pm}}} \),

and \( I \), the effective resonance integral for the I.R. approximation, is now

\[ I = \int \frac{\sigma_a}{1 + \frac{\sigma_s}{\lambda \sigma_{pf} + \sigma_{pm}}} \frac{dE}{E} \]

i.e. \[ I = \frac{\Gamma}{2E \Gamma} \frac{1}{\psi(x,t) + \beta_3} \int_{-\infty}^{\infty} \psi(x,t) \psi(x,t) dx \]
where \( \beta_3 = \frac{G \Gamma}{\sigma} \) and \( G = \frac{\Gamma + \lambda \Gamma}{\lambda \sigma + \sigma} \). Hence

\[
I = \frac{\Gamma}{2E_r G} J(\beta_3, t) \tag{2.49}
\]

In particular, Goldstein and Cohen considered the 192eV resonance of \( \text{U}_{238} \) in a 1:1 mixture of \( \text{U}_{238} \) and hydrogen obtaining \( \lambda = 0.264 \).

Dyos and Keane (1966) have shown that the iterative process converges and, in doing so, obtained a value of \( \lambda = 0.31 \) after equating the first and third approximation. Keane and Horner (1966) have obtained the limiting value of \( \lambda = 0.33 \) from an exact solution of the integral equation.

2.3 The Doppler Contour (Voigt) Functions

Associated with the Doppler broadened line shape function (see equation (2.27)) is the Doppler broadened interference line shape function

\[
\psi(x,t) = \frac{1}{(4\pi t)^2} \int_{-\infty}^{\infty} ye^{-(x-y)^2/4t} dy . \tag{2.50}
\]

Although it has been assumed that the interference term is to be negligible for the purpose of this work, both functions will now be discussed as some of their important properties are similar and inter-related.

2.3.1 Alternative Forms

It is well known that all of the common properties of the Voigt functions may be obtained readily from a consideration of the Fourier cosine transform of \( \psi(x,t) \) and the Fourier sine transform of \( \phi(x,t) \).
These transforms, \( F_c \{\psi(x,t)\} = (\frac{\pi}{2})^\frac{1}{2} e^{-pt} \) and 

\( F_s \{\phi(x,t)\} = (\frac{\pi}{2})^\frac{1}{2} e^{-pt} \), when inverted become

\[
\psi(x,t) = \int_0^\infty e^{-p^2t-p} \cos px \, dp 
\]  

(2.51a)

and

\[
\phi(x,t) = \int_0^\infty e^{-p^2t-p} \sin px \, dp .
\]  

(2.51b)

Born (1933) considered the function \( \chi(x,t) \) defined as

\[
\chi(x,t) = \psi(x,t) + i\phi(x,t) 
\]  

(2.52)

i.e.

\[
\chi(x,t) = \int_0^\infty e^{-p^2t-p(1-ix)} \, dp ,
\]  

(2.53)

and investigated some of the properties of \( \chi(x,t) \) as a complex function of the real variable \( x \). He expressed equation (2.53) as

\[
\chi(x,t) = \frac{1}{(4\pi t)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \frac{e^{-u^2}}{w+iu} \, du ,
\]

by a change of variable and letting \( w = (1-ix)/2t^{\frac{1}{2}} \). Rationalizing the denominator and neglecting the odd function in the integrand, we obtain

\[
\chi(x,t) = \frac{w}{(4\pi t)^{\frac{1}{2}}} \int_{-\infty}^{\infty} \frac{e^{-u^2}}{w^2+u^2} \, du 
\]  

(2.54)

Recent studies of this and related functions have been by Bell, Buckler and Pull (1963), Keane and Clancy (1964), and Reichel (1964).

By studying some of the properties of the \( \chi(x,t) \) function we are led, by equating real and imaginary parts of equation (2.52) to the properties of the Voigt functions.
2.3.2 Some Properties of the $\chi(x,t)$ function

From equation (2.53) we have

$$\chi(x,t) = \frac{1}{1-ix} \psi(0, \frac{t}{(1-ix)z})$$

$$= \left(\frac{\pi}{4t}\right)^{1/2} \text{er}c \left(\frac{1-ix}{2\sqrt{t}}\right) ,$$

(2.55)

where $\text{er}c \, u = \frac{2}{\sqrt{\pi}} e^{u^2} \int_0^\infty e^{-y^2} dy$. Putting $t = 0$ in (2.53),

$$\chi(x,0) = \frac{1}{1-ix}$$

(2.56)

and $x = 0$ in equation (2.55)

$$\chi(0,t) = \left(\frac{\pi}{4t}\right)^{1/2} \text{er}c \left(\frac{1}{2\sqrt{t}}\right)$$

(2.57)

The following integrals can be evaluated using contours by following Keane and Clancy (1964). An alternative approach is given which eliminates the need to extend to the complex plane.

(i) $\int_{-\infty}^{\infty} \chi(x,t) dx = \pi$. 

(2.58)

Using the result in equation (2.53),

$$\int_{-\infty}^{\infty} \chi(x,t) dx = \int_{-\infty}^{\infty} e^{-p-p^2t} \delta(p) \int_{-\infty}^{\infty} e^{ips} dx .$$

But $\int_{-\infty}^{\infty} e^{ips} dx = 2\pi \delta(p) ,

(2.59)$

because the Fourier transform of the delta function is 1, namely

$$\int_{-\infty}^{\infty} \delta(x) e^{-isx} dx = 1 ,$$

and, inverting we have $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{isx} ds .$

$$\therefore \int_{-\infty}^{\infty} \chi(x,t) dx = 2\pi \int_{0}^{\infty} e^{-p-p^2t} \delta(p) dp$$

$$= \pi .$$
\[(ii) \int_{-\infty}^{\infty} \chi(x,t) dx = 0, \quad n > 1 \quad (2.60)\]

\[
\int_{-\infty}^{\infty} \chi(x,t) dx = \frac{n}{\pi} \int_{0}^{\infty} e^{-p_j - p_j^2 t} dp_j \int_{-\infty}^{\infty} e^{i(p_1 + \ldots + p_n)x} dx
\]

\[
= \frac{n}{\pi} \int_{0}^{\infty} e^{-p_j - p_j^2 t} 2\pi \delta(p_1 + \ldots + p_n) dp_j.
\]

But as the \(p_j\)'s are never negative and are different, \(p_1 + \ldots + p_n \neq 0\), for \(n > 1\). Therefore the result in equation (2.60) follows.

\[(iii) \int_{-\infty}^{\infty} \frac{\chi(x,t)}{x-a} dx = \pi i \chi(a,t) \quad (2.61)\]

\[
\int_{-\infty}^{\infty} \frac{\chi(x,t)}{x-a} dx = \int_{0}^{\infty} e^{-p - p^2 t} dp \int_{-\infty}^{\infty} \frac{e^{ipx}}{x-a} dx.
\]

The right hand integral can be found as a Cauchy Principal value by integrating \(\int \frac{e^{ipz}}{z-a} dz\) round the semicircle in the upper half plane. As the only pole is \(z = a\) and as the integral vanishes round the semicircle, we have, assuming \(a\) is real,

\[
\int_{-\infty}^{\infty} \frac{e^{ipx}}{x-a} dx = \pi e^{ipa}.
\]

\[
\therefore \int_{-\infty}^{\infty} \frac{\chi(x,t)}{x-a} dx = \pi i \chi(a,t).
\]

\[(iv) \int_{-\infty}^{\infty} \frac{\chi(x,t)}{x^2 + a^2} dx = \frac{\pi}{a(1+a)} \psi(0, \frac{t}{(1+a)^2}) = \frac{\pi \sqrt{\pi}}{2at} \text{erfc}\left(\frac{1+a}{\sqrt{2t}}\right) \quad (2.62)\]

\[
\int_{-\infty}^{\infty} \frac{\chi(x,t)}{x^2 + a^2} dx = \int_{0}^{\infty} e^{-p - p^2 t} \int_{-\infty}^{\infty} \frac{e^{ipx}}{x^2 + a^2} dx.
\]
The right hand integral can be found by integrating \[ \int_{-\infty}^{\infty} e^{\frac{ipx}{x^2+a^2}} \, dx \] round the semicircle in the upper half plane. The only pole inside the contour is \( z = ia \).

\[ \therefore \int_{-\infty}^{\infty} e^{\frac{ipx}{x^2+a^2}} \, dx = \frac{\pi}{a} e^{-pa} \]

Hence

\[ \int_{-\infty}^{\infty} \frac{x(x,t)}{x^2+a^2} \, dx = \frac{\pi}{a} \int_{0}^{\infty} e^{-p^2 t - p(1+a)} \, dp \]

\[ = \frac{\pi}{a(1+a)} \psi(0, \frac{t}{(1+a)^2}) \]

\[ = \frac{\pi/\pi}{2a\sqrt{t}} \text{erf} \left( \frac{1+a}{2\sqrt{t}} \right) \]

2.3.3 Some Properties of the Voigt Functions

(i) Asymptotic series

When \( t \) is small, or \( x \) is large, it follows from expanding the \( e^{-p^2 t} \) factor in equations (2.51a) and (2.51b) that

\[ \psi(x,t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^{2n}}{dx^{2n}} \frac{1}{1+x^2} \]  \hspace{1cm} (2.63a)

and

\[ \phi(x,t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^{2n}}{dx^{2n}} \frac{x}{1+x^2} \]  \hspace{1cm} (2.63b)

(ii) \( \psi(x,0) \) and \( \phi(x,0) \).

In particular when \( t = 0 \) in equations (2.63a), (2.63b)

\[ \psi(x,0) = \frac{1}{1+x^2} \]  \hspace{1cm} (2.64a)

and

\[ \phi(x,0) = \frac{x}{1+x^2} \]  \hspace{1cm} (2.64b)

which agrees with equation (2.56).
From equation (2.58), we have
\[
\int_{-\infty}^{\infty} \psi(x,t) \, dx = \pi, \quad (2.65a)
\]
and
\[
\int_{-\infty}^{\infty} \phi(x,t) \, dx = 0. \quad (2.65b)
\]

It is to be noted that \( \int_{-\infty}^{\infty} \psi(x,t) \, dx \) is independent of \( t \).

(iv) \( \psi(0,t) \) and \( \phi(0,t) \)

From equation (2.57)
\[
\psi(0,t) = \left( \frac{\pi}{4t} \right)^{\frac{1}{2}} \text{erfc} \left( \frac{1}{2\sqrt{t}} \right) \quad (2.66a)
\]
and
\[
\phi(0,t) = 0 \quad (2.66b)
\]

(v) \( \int_{0}^{\infty} \psi(x,t_1)\psi(x,t_2) \, dx \) and \( \int_{0}^{\infty} \phi(x,t_1)\phi(x,t_2) \, dx \).

Using the Paresval theorem for Fourier transforms, it can be seen that
\[
\int_{0}^{\infty} \psi(x,t_1)\psi(x,t_2) \, dx = \frac{\pi}{2} \int_{0}^{\infty} e^{-2p}\psi^2(t_1+t_2) \, dp
\]
\[
= \frac{\pi}{4} \psi(0, \frac{t_1+t_2}{4}). \quad (2.67a)
\]

Similarly it can be shown that
\[
\int_{0}^{\infty} \phi(x,t_1)\phi(x,t_2) \, dx = \frac{\pi}{4} \phi(0, \frac{t_1+t_2}{4}) \quad (2.67b)
\]
(vi) Differential Equations

It follows immediately from equations (2.51a) and (2.51b) that \( \psi(x,t) \) and \( \phi(x,t) \) both satisfy the heat equation

\[
\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial \psi}{\partial t}.
\]  

(2.68)

By differentiating (2.51a) with respect to \( x \),

\[
\psi'(x,t) = \frac{1}{2t} \phi(x,t) - \frac{x}{2t} \psi(x,t)
\]

and from (2.51b)

\[
\phi'(x,t) = \frac{1}{2t} - \frac{1}{2t} \psi(x,t) - \frac{x}{2t} \phi(x,t)
\]

are obtained. Combining these, the Voigt functions are found to satisfy the second order differential equations

\[
4t^2 \psi'' + 4tx\psi' + (1+x^2+2t)\psi = 1 \tag{2.69a}
\]

and

\[
4t^2 \phi'' + 4tx\phi' + (1+x^2+2t)\phi = x. \tag{2.69b}
\]

(vii) Special Integral Results

As special results, required in the numerical analysis in later sections, we have from equation (2.61)

\[
\int_{-\infty}^{\infty} \frac{\psi(x,t)}{x-a} \, dx = -\pi \phi(a,t) \tag{2.70a}
\]

and

\[
\int_{-\infty}^{\infty} \frac{\phi(x,t)}{x-a} \, dx = \pi \psi(a,t) \tag{2.70b}
\]

which is the well known Hilbert transform property (Keane and Clancy 1964).

From equation (2.62), we have

\[
\int_{0}^{\infty} \frac{\psi(x,t)}{1+x^2} \, dx = \frac{\pi}{4} \psi\left(0, \frac{t}{4}\right) \tag{2.71}
\]
and from equation (2.67a)
\[ \int_0^\infty \psi^2(x,t) \, dx = \frac{\pi}{4} \psi_0, \frac{t}{2} \]  (2.72)

2.3.4 Numerical Evaluation of the Voigt Functions

The numerical evaluations of the \( \psi(x,t) \) and \( \phi(x,t) \) functions are best performed by a Taylor's expansion as used by Doherty (1964) in his PSICHI code. The derivatives above the first in the Taylor's expansion are expressed in terms of \( \psi(x,t) \), \( \psi'(x,t) \), \( \phi(x,t) \) and \( \phi'(x,t) \) using the differential equations (2.69a) and (2.69b).

For large \( x \), the asymptotic expansions (2.63a) and (2.63b) may be used. These series converge quite rapidly if the quotient \( x/\sqrt{t} \) is large giving

\[ \psi(x,t) \approx \frac{1}{1+x^2} \left[ 1 + \frac{(6x^2-2)t}{(1+x^2)^2} \right] \]  (2.73a)

and

\[ \phi(x,t) \approx \frac{x}{1+x^2} \left[ 1 + \frac{(2x^2-6)t}{(1+x^2)^2} \right]. \]  (2.73b)

In the wings of a resonance, where \( x \gg \sqrt{t} \),

\[ \psi(x,t) \approx \frac{1}{1+x^2} \left( = \psi(x,0) \right) \]  (2.74a)

and

\[ \phi(x,t) \approx \frac{x}{1+x^2} \left( = \phi(x,0) \right). \]  (2.74b)

If \( x \gg 100 \), the function may be further simplified by letting

\[ \psi(x,t) \approx \frac{1}{x} \]  (2.75a)

and

\[ \phi(x,t) \approx \frac{1}{x}. \]  (2.75b)

Chiarella (1966) in his investigation of methods for the numerical evaluation of the Voigt functions obtained further useful results in their behaviour.
2.4 The J(β,t) function

The J(β,t) function, mentioned in equations (2.42), (2.46) and 2.49), has been extensively tabulated in the form J(β,0) by Dresner (1956), and by Adler et al. (1958), where \( \theta = \frac{1}{2} \sqrt{M/kT} \). Some of the properties of J(β,t), used in later sections, will now be discussed.

(i) \( J(β,0) \)

If \( t=0 \), so that \( \psi(x,0) = \frac{1}{1+x^2} \), then

\[
J(β,0) = -\frac{\pi}{2\sqrt{β}(1+β)}
\]  

(ii) \( J(β,t) \) for large \( β \).

For large \( β \), the integrand can be expanded in powers of \( 1/β \) to obtain

\[
J(β,t) \approx \frac{1}{β} \int_0^\infty \psi(x,t)dx - \frac{1}{β^2} \int_0^\infty \psi^2(x,t)dx
\]
i.e.

\[
J(β,t) \approx \frac{π}{2β} - \frac{π}{4β^2} \psi(0,\frac{t}{2})
\]  

after using equations (2.65a) and (2.67a). If \( β \) is very large,

\[
J(β,t) \approx \frac{π}{2β}.
\]  

(iii) Differentiation of \( J(β,t) \) with respect to \( t \).

Differentiation of the \( J(β,t) \) function with respect to \( t \), gives

\[
\frac{∂J}{∂t} = \int_0^∞ \frac{β}{(ψ+β)^2} \frac{∂ψ}{∂t} dx
\]

\[
= β \int_0^∞ \frac{1}{(ψ+β)^2} \frac{∂^2ψ}{∂x^2} dx,
\]

upon using the heat equation (2.68). Then, after integrating by parts

\[
\frac{∂J}{∂t} = 2β \int_0^∞ \frac{1}{(ψ+β)^3} \left( \frac{∂ψ}{∂x} \right)^2 dx
\]

(2.79)
3 J is obtained showing that $\frac{\partial J}{\partial t}$ is always positive. It can also be seen from this equation that $\frac{\partial J}{\partial t} \to 0$ both for $\beta \to 0$ and $\beta \to \infty$ and therefore a maximum exists for some value of $\beta$. It was shown by Horner and Keane (1967) that this maximum value occurs at approximately $\beta = 0.1$ when $t = 0$.

(iv) $J(\beta, t)$ approximations for small $\beta$.

As $\beta \to 0$ the integrand in $J(\beta, t)$ is approximately unity until $x$ is so large that $\psi(x, t)$ may be replaced by $1/x^2$. Thus we may replace $\psi(x, t)$ by $1/x^2$ for all $x$ in (2.76) and obtain

$$J(\beta, t) = \frac{\pi}{2\sqrt{\beta}}$$

(2.80)

2.5 The Asymptotic Value of $\int_0^\infty \frac{\psi}{(\psi + \beta)^n} \, dx$ for small $\beta$

The asymptotic expansion of the above integral is used in the tabulation of the $F(\beta_1, \beta_2, t_1, t_2)$ tables in section 3.

We wish to show that as $\beta \to 0$ the dominant term for $\int_0^\infty \frac{\psi(x, t)}{[\psi(x, t) + \beta]^n} \, dx$ is the same as that for $\int_0^\infty \frac{\psi(x, 0)}{[\psi(x, 0) + \beta]^n} \, dx$ which is $O\left(\frac{1}{\beta^{n-2}}\right)$.

To verify this assumption we only have to show that

$$\beta^{n-\frac{1}{2}} \int_0^\infty \left[ \frac{\psi(x, t)}{[\psi(x, t) + \beta]^n} - \frac{\psi(x, 0)}{[\psi(x, 0) + \beta]^n} \right] \, dx \to 0$$

as $\beta \to 0$.

But

$$\int_0^N \left[ \frac{\psi}{(\psi + \beta)^n} - \frac{\psi_0}{(\psi_0 + \beta)^n} \right] \, dx$$

is finite for finite $N$ even with $\beta = 0$.

so we need only show that

$$\lim_{\beta \to 0} \beta^{n-\frac{1}{2}} \int_0^\infty \left[ \frac{\psi(x, t)}{N[\psi(x, t) + \beta]^n} - \frac{\psi(x, 0)}{[\psi(x, 0) + \beta]^n} \right] \, dx = 0$$

where we may choose $N$ large but finite.
For sufficiently large $N$ it is allowable to replace $\psi(x,t)$ by the first two terms in its asymptotic expansion, viz

$$\psi(x,t) = \frac{1}{x^2} + \frac{6t}{x^4}.$$  

Thus since $\psi(x,0) = \frac{1}{1+x^2} = \frac{1}{x^2}$ for large $x$ we obtain

$$I = \int_0^\infty \frac{\psi(\psi+\beta)^n - \psi(\psi+\beta)^n}{N (\psi+\beta)^n (\psi+\beta)^n} \, dx$$

$$= \int_0^\infty \frac{\left(\frac{1}{x^2} + \frac{6t}{x^4}\right)\left(\frac{1}{x^2} + \beta\right)^n - \frac{1}{x^2}\left(\frac{1}{x^2} + \frac{6t}{x^4} + \beta\right)^n}{N \left(\frac{1}{x^2} + \frac{6t}{x^4} + \beta\right)^n \left(\frac{1}{x^2} + \beta\right)^n} \, dx.$$  

Changing the variable to $u=x/\beta$ we obtain after some manipulation

$$I = \frac{1}{\beta^{n-2}} \int_{N/\beta}^\infty \frac{u^{2n-2}\left((1+\frac{6t}{u^2})\left(1+u^2\right)^n - (1+\frac{6t}{u^2} + u^2)^n\right)}{(1+\frac{6t}{u^2} + u^2)^n (1+u^2)^n} \, du$$

or retaining only terms $O(\beta)$ in the integrand

$$I = \frac{6t}{\beta^{n-2}} \int_{N/\beta}^\infty u^{2n-4} \frac{(1 - \frac{n}{1+u^2})}{(1+u^2)^n} \, du$$

Thus

$$\lim_{\beta \to 0} \beta^{n-1} I = \lim_{\beta \to 0} 6t \beta \int_{0}^\infty \frac{u^{2n-4}}{(1+u^2)^n} \left(1 - \frac{n}{1+u^2}\right) \, du = 0$$

as required.

Hence, as $\beta \to 0$

$$\int_0^\infty \frac{\psi}{(\psi+\beta)^n} \, dx = \int_0^\infty \frac{x^{2n-2}}{(1+\beta x^2)^n} \, dx$$

$$= \frac{\sqrt{\pi}}{2} \frac{\Gamma(n-\frac{1}{2})}{\Gamma(n)} \frac{1}{\beta^{n-2}}.$$  

(2.81)
3. Temperature Dependence of Resonance Overlap

3.1 Introduction

Codd and Collins (1963) presented a paper giving preliminary results of a study of the effect of U-238 - Pu-239 resonance overlap on the Doppler coefficient in a dilute fast reactor. The authors concluded at the time that the Pu-239 contribution to the Doppler coefficient could be rendered negative by the presence of the U-238. Previously this Pu-239 contribution had been computed to be positive by as much as 40% of the negative Doppler coefficient contributed by U-238.

Consequently the overlap problem has been discussed by a number of authors including Hutchins (1964) and Hwang (1965) who both investigated the problem of the effects of resonance overlap on the Doppler coefficient. Keane (1966) examined the range of validity of a simple correction formula proposed by Rowlands (unpublished) which was used in the original Codd and Collins paper.

3.2 Keane's Model

Keane (1966) developed a simple model in order to investigate analytically the range of validity of, and the correction necessary to Rowlands' formula and also to provide an alternative expression for those concentrations where Rowlands' formula has its greatest error, viz. for concentrated systems (small β).

His model first neglected the small correction due to overlapping of resonances belonging to the same isotope. This seems reasonable as the investigations of the spacing of resonance levels by Wigner (1957),
Nicholson (1960) and Gilks and Wilkins (1966) suggest that small values of $D/D$ are unlikely, where $D$ and $\overline{D}$ are resonance and mean resonance spacings respectively. Wigner came to his conclusion using perturbation theory whereas the others have used statistical methods.

An ideal resonance absorber now was assumed, in which the resonance spacing, the capture width and the reduced neutron width are constant (in practice, the appropriate average spacing and resonance parameters could be used here). Since only the resonances over a small energy range are important in estimating the effect of overlap, the neglect of the energy dependence of the neutron width and the peak heights of the resonances in a sequence was assumed not to lead to a significant error.

The model thus considered the effective resonance integral of a resonance of one absorber in the presence of a sequence of resonances belonging to a second absorber.

The resonance under consideration was taken to be at energy $E_1$ with a total width of $\Gamma_1$. It was assumed that the nearest resonance of the second absorber was at energy $E_2$ with total width $\Gamma_2$ and that the spacing of the sequence was $D_2$. The Breit-Wigner contours for the $E_1$ resonance and the contours of the sequence were assumed to be $\psi(x,t_1)$ and $\psi(px+q+n\gamma,t_2)$ respectively, where $p=\Gamma_1/\Gamma_2$, $q=2(E_1-E_2)/\Gamma_2$ and $\gamma=2D_2/\Gamma_2$.

\[
\therefore \quad I = \frac{\Gamma_1 E}{2E_1} \int_{-\infty}^{\infty} \frac{\psi(x,t_1)}{\psi(x,t_1)+\varepsilon \sum_{n=-\infty}^{\infty} \psi(px+q+n\gamma,t_2)+\beta_1} \ dx \quad (3.1)
\]
where \( \varepsilon = \frac{N_2 \sigma_{02}}{N_1 \sigma_{01}} \),

\( \sigma_{01} \) = the peak heights of the resonance with total width \( \Gamma_1 \),

\( N_1 \) = the number of \( i \)th nuclei per c.c. of the mixture,

\( \beta_1 = \frac{\sigma_p}{\sigma_{01}} \),

\( \sigma_p = \frac{\Sigma_p}{N_1} \).

It was then assumed that the spacing of the resonances of the first absorber was not a multiple (or fraction) of the spacing of the sequence due to the second absorber. Therefore \( q \) would vary uniformly between \(-\gamma/2\) and \( \gamma/2\), depending on the particular resonance of the first absorber that was being considered. The average effect of the sequence on a resonance of the first absorber is thus

\[
I = \frac{\Gamma_1 \Sigma_p}{2E_1} \int_{-\infty}^{\infty} \frac{\psi_1}{\psi_1 + \beta_1} \, dx \cdot \frac{1}{\gamma} \int_{-\gamma/2}^{\gamma/2} \frac{\psi_1 + \beta_1}{\psi_1 + \varepsilon + \sum_{n=-\infty}^{\infty} \psi_2 + \beta_1} \, dq
\]

(3.2)

where

\( \psi_1 = \psi(x, t_1) \)

\( \psi_2 = \psi(px + q + n\gamma, t_2) \)

\[
\therefore \quad I = \frac{\Gamma_1 \Sigma_p}{2E_1} \left[ 2J(\beta_1, t_1) - \frac{1}{\gamma} \int_{-\infty}^{\infty} \frac{\psi_1}{\psi_1 + \beta_1} \, dx \int_{px-\gamma/2}^{px+\gamma/2} \sum_{n=-\infty}^{\infty} \frac{\psi(u+n\gamma, t_2)}{\psi(u+n\gamma, t_2) + \varepsilon + \sum_{n=-\infty}^{\infty} \psi_2 + \beta_1} \, du \right]
\]

(3.3)

As the integral from \( px-\gamma/2 \) to \( px+\gamma/2 \) was effectively over the range of one complete resonance of the second absorber, Keane again neglected the small effect due to overlap of members of the same sequence. Hence equation (3.3) becomes
In order to evaluate equation (3.4) analytically it was now assumed that $t_2=0$ so that $\psi(u,t_2)=1/(1+u^2)$. If $I_1$ is the double integral in (3.4)

$$I_1 = \int_{-\infty}^{\infty} \frac{\psi_1}{\psi_1 + \beta_1} \, dx \int_{-\infty}^{\infty} \frac{\psi_2}{\psi_1 + \beta_1} \, du$$

$$= \pi \varepsilon \int_{-\infty}^{\infty} \frac{\psi_1}{\psi_1 + \beta_1} \, dx \frac{\psi_2}{(\psi_1 + \beta_1)(\psi_1 + \beta_1 + \varepsilon)}$$

Now $t_1$ was assumed equal to $0$. Therefore (3.5) can be evaluated in terms of the complete elliptic integrals $K$ and $E$ to give

$$I_1 = 4J(\beta_1,0) \, J(\beta_2,0) \, F(\beta_1,\beta_2)$$

where $F(\beta_1,\beta_2) = (2/\pi) [E-\beta_2(K-E)]$ and the modulus of the elliptic integrals is

$$k = [(1+\beta_1)(1+\beta_2)]^{-\frac{1}{2}}.$$ 

Thus

$$I = \frac{\Gamma \Sigma P}{E_1} \, J(\beta_1,0) \left[1-F(\beta_1,\beta_2) \, \frac{\Gamma_2}{D_2} \, J(\beta_2,0)\right]$$

which includes a correction factor $F(\beta_1,\beta_2)$ to Rowlands' simple formula, viz:

$$I = \frac{\Gamma \Sigma P}{E_1} \, J(\beta_1,t_1) \left[1 - \frac{\Gamma_2}{D_2} \, J(\beta_2,t_2)\right].$$

After evaluating the $F(\beta_1,\beta_2)$ function for various values of $\beta$ it was concluded that the correction for resonance overlap is greatest in concentrated systems since it is for small $\beta$ that the function $J(\beta,t)$ has its greatest value.
3.3 Temperature Dependence of the Correction Factor

The modified form of Rowlands' formula, equation (3.6), was obtained by assuming that \( t_1 = t_2 = 0 \) for the system, so that equation (3.4) could be solved analytically. However, it is more realistic to consider a correction factor of the form \( F(\beta_1, \beta_2, t_1, t_2) \).

Following the approach of Keane and O'Halloran (1966), we obtain from equation (3.4),

\[
I = \frac{\Gamma y_1 \Sigma}{E_1} J(\beta_1, t_1) [1 - \frac{\Gamma 2}{D_2} J(\beta_2, t_2) F(\beta_1, \beta_2, t_1, t_2)] \tag{3.8}
\]

where

\[
F(\beta_1, \beta_2, t_1, t_2) = \frac{\int_0^\infty \frac{\psi_1}{\psi_1 + \beta_1} \, dx \int_0^\infty \frac{\psi_2}{\psi_2 + (\psi_1 + \beta_1)/\epsilon} \, dy}{\int_0^\infty \frac{\psi_1}{\psi_1 + \beta_1} \, dx \int_0^\infty \frac{\psi_2}{\psi_2 + \beta_2} \, dy} \tag{3.9}
\]

The double integral in the numerator of (3.9) can be simplified if we assume that either \( t_1 \) or \( t_2 \) is zero. We obtain

\[
F(\beta_1, \beta_2, t_1, 0) = \frac{\epsilon \sqrt{\beta_2 (1 + \beta_2)} \int_0^\infty \frac{\psi_1}{\psi_1 + \beta_1} \frac{dx}{\sqrt{\psi_1 + \beta_1} (\psi_1 + \beta_1 + \epsilon)}}{\int_0^\infty \frac{\psi_1}{\psi_1 + \beta_1} \, dx} \tag{3.10}
\]

and

\[
F(\beta_1, \beta_2, 0, t_2) = \frac{\int_0^\infty [1 - \frac{\sqrt{\beta_2 (\psi_2 + 1/\epsilon)}}{\sqrt{(\psi_2 + \beta_2) (\psi_2 + \beta_2 + 1/\epsilon)}}] \, dy}{\int_0^\infty \frac{\psi_2}{\psi_2 + \beta_2} \, dy} \tag{3.11}
\]
Equations (3.10) and (3.11) are suitable for numerical integration and allow us to study independently the Doppler Broadening of the resonances of the two sequences. The double integral in (3.9) is far more difficult to evaluate but, in view of the fact shown later in 3.4, that the variation of \( F(\beta_1, \beta_2, 0, t_2) \) with \( t_2 \) is quite small, sufficient information about the temperature variation of \( F(\beta_1, \beta_2, t_1, t_2) \) can be found by considering (3.10) and (3.11).

When \( t_1 \to \infty \) the function \( \psi_1 \) is negligible compared to \( \beta_1 \) and so equation (3.9) gives

\[
F(\beta_1, \beta_2, \infty, t_2) = 1
\]  

(3.12)

If on the other hand \( t_2 \to \infty \) then \( \psi_2 \) in the denominators of the integrals in equation (3.9) can be neglected to give

\[
F(\beta_1, \beta_2, t_1, \infty) = \frac{\int_0^\infty \frac{\psi_1}{(\psi + \beta_1)^2} \, dx}{\int_0^\infty \frac{\psi_1}{\psi_1 + \beta_1} \, dx}
\]  

(3.13)

3.4 The Correction for Limiting Concentrations

Difficulties arise in the numerical evaluation of equations (3.10) and (3.11) where either \( \beta_1 \) or \( \beta_2 \) tend to zero or infinity. For such concentrations the function \( F(\beta_1, \beta_2, t_1, t_2) \) can be simplified analytically.
3.4.1 \( F(\infty, \beta_2, t_1, t_2) \)

Since \( \varepsilon = \frac{\beta_1}{\beta_2} \) we see that the term \( (\psi + \beta_1) / \varepsilon \) in equation (3.9) tends to \( \beta_2 \) as \( \beta_1 \to \infty \).

Thus \( \lim_{\beta_1 \to \infty} F(\beta_1, \beta_2, t_1, t_2) = 1 \) \( \quad (3.14) \)

This shows that \( \beta_1 \to \infty \) leads to the same result as \( t_1 \to \infty \).

3.4.2 \( F(\beta_1, \infty, t_1, t_2) \)

For \( \beta_2 \to \infty \) it follows from equation (3.9) that

\[
\lim_{\beta_2 \to \infty} F(\beta_1, \beta_2, t_1, t_2) = -\frac{\beta_1}{\int_0^\infty \frac{\psi_1}{(\psi + \beta_1)^2} \, dx} \quad \int_0^\infty \frac{\psi_1}{\psi_1 + \beta_1} \, dx \quad (3.15)
\]

This result is the same as obtained in equation (3.13) for \( t_2 \to \infty \) and reflects the fact that infinite dilution and infinite temperature both give maximum resonance absorption (i.e. there is no shielding).

The integrals in (3.15) have to be evaluated numerically except that for \( t_1 = 0 \) we can obtain analytically that

\[
F(\beta_1, \infty, 0, t_2) = 1 - \frac{1}{2(1 + \beta_1)} \quad (3.16)
\]

3.4.3 \( F(\beta_1, 0, t_1, t_2) \)

When \( \beta_2 \to 0 \) then the function \( \psi_2 = \psi(y, t_2) \) in equation (3.9) can be replaced by its asymptotic value \( \frac{1}{1 + y^2} \). (See equation 2.64). Thus the right hand side of (3.9) reduces to that of equation (3.10), which as
\[ \beta_2 \to 0 \] becomes

\[
\sqrt{\beta_1} \int_0^\infty \frac{\psi_1}{(\psi_1+\beta_1)^{3/2}} \, dx
\]

\[ F(\beta_1, 0, t_1, t_2) = \frac{\int_0^\infty \psi_1}{\int_0^\infty \psi_1 + \beta_1} \, dx \quad (3.17) \]

### 3.4.4 \( F(0, \beta_2, t_1, t_2) \)

When \( \beta_1 \to 0 \) then by expressing equation (3.9) in the form

\[
\int_0^\infty \psi_1 \left[ \frac{1}{\psi_1 + \beta_1} - \frac{\beta_1}{\psi_1 + \beta_1} \right] \, dx
\]

\[ F(\beta_1, \beta_2, t_1, t_2) = \frac{\int_0^\infty \psi_1}{\int_0^\infty \psi_1 + \beta_1} \, dx \int_0^\infty \psi_2 \, dy \]

we see that in each integral, \( \psi_1 \) can be replaced by its asymptotic value \( \frac{1}{1+x^2} \) (See equation 2.64.) Thus

\[
\lim_{\beta_1 \to 0} F(\beta_1, \beta_2, t_1, t_2) = \int_0^\infty \frac{1-\sqrt{\frac{\beta_2}{\psi_2+\beta_2}}}{\psi_2+\beta_2} \, dy \quad (3.18)
\]

which is the same as equation (3.11) with \( \epsilon \to 0 \).

### 3.4.5 \( F(0, 0, t_1, t_2) \)

In view of the result established in chapter 2 it follows from either equation (3.17) or (3.18) that

\[ F(0, 0, t_1, t_2) = \frac{2}{\pi} . \quad (3.19) \]
3.5 Numerical Results

3.5.1 Numerical Methods

The integrals in equations (3.10), (3.11), (3.13), (3.15), (3.16) were evaluated numerically on the IBM 1620 computer at Wollongong University College. The numerical integration was extended to $x=200$ and corrections obtained analytically to extend the range in the asymptotic region. Computer time was saved by dividing the range into four intervals so that the contribution to the integration was approximately equal.

Simpson's rule was used, the intervals being halved until the required accuracy was obtained. Computer time was saved here by using a method suggested by B. Noble (1964) for storing the ordinates used in Simpson's rule. The PSICHI block (Doherty 1964) for the evaluation of $\psi(x,0)$ was changed slightly so that input values of $t$ were possible instead of $T$ (absolute temperature).

3.5.2 Results

The results obtained are shown in Tables I to VI. As anticipated in section 3.2, it can be seen that the variation with $t_2$ is small.

Tables were evaluated for $t=1, 10, 100$ and $\beta$ values of .25, .667, 1.5 and 4. These are to be compared with the table of values for $t=0$ obtained earlier (Keane 1965).
### TABLE I

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\(F(\beta_1, \beta_2, 10, 0)\)

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### TABLE IV

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### TABLE VI

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<td>.70</td>
<td>.80</td>
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</table>
3.5.3 Approximate Algebraic Fit from Results

The limiting values in equations (3.12), (3.13), (3.14) and (3.16) together with the results that

(i) $F$ varies only slightly with $\beta_2$;
(ii) $\beta_1=0$ gives the same result as $t_1=0$;
and (iii) $\beta_2=0$ gives the same result as $t_2=0$, suggest a simple expression of the form

$$F(\beta_1, \beta_2, t_1, t_2) = 1 - \frac{1}{2[1+\beta_1 G(t_1)]} + \frac{R}{[1+\beta_1 G(t_1)][1+\beta_2 H(t_2)]}$$

where $G(t_1)$ and $H(t_2)\to 1$, as $t_1$ and $t_2\to 0$,
$G(t_1)$ and $H(t_2)\to \infty$, as $t_1$ and $t_2\to \infty$.

For simplicity we further assume that

$G(t) = H(t) = 1+t^2$.

By trial and error, it was found that all the results fit the expression

$$F(\beta_1, \beta_2, t_1, t_2) = 1 - \frac{1}{2[1+\beta_1 (1+t_1^3)]} + \frac{1}{6[1+\beta_1 (1+t_1^3)][1+\beta_2 (1+t_2^3)]}$$

(3.20)

The greatest error occurs for $\beta_1=\beta_2=0$ when the fitted expression (3.20) gives .6667 instead of being .6366 ($= \frac{2}{\pi}$) which is a 5% error.

It is felt that in view of the assumptions in the model and the unlikelihood of calculations being of interest at this extreme limit, the fit for equation (3.20) is quite satisfactory.
4. Separation Dependence of Resonance Overlap

4.1 Introduction

To obtain some insight into the magnitude of the mutual shielding of two resonances, a simple model has been used to find the percentage decrease in absorption as a function of separation.

The model assumes that the effective resonance integral of the two resonances is given by the usual theory with the cross sections given as the sum of the two line shape functions. The theory is given in the next section and the results are presented in table form in section 4.5.

4.2 The Model

Consider two neighbouring resonances belonging to the same or different absorber atoms. In the following analysis we will neglect the macroscopic flux variation in the vicinity of the resonances under study. This variation would be due to the non-recovery of the flux to the asymptotic form (1/E) from disturbances due to the resonances at the higher energies. The inclusion of the flux non-recovery effect in resonance overlap calculations is discussed by McKeegan (1967).

Assuming narrow resonance theory to be adequate for the resonance overlap calculation, equation (2.34) namely,

\[- \frac{1}{\xi} \int_{\Sigma_a \text{res}} \frac{\Sigma_t}{E} \, dE\]

applied to calculating the resonance escape probability of one of the resonances gives
\[
\begin{aligned}
P &= e^{-\frac{1}{\xi} \int \frac{\Sigma a_l}{\Sigma r_i + \Sigma p} \frac{dE}{E}} \\
&= e^{-\frac{1}{\xi} \int \frac{N_1 \sigma a_l}{N_1 \sigma r_1 + N_2 \sigma r_2 + \Sigma p} \frac{dE}{E}} 
\end{aligned}
\]

(4.1)

where the parameters are defined as in earlier sections and the integration extends over the particular resonance under study. The subscripts \(i=1,2\) refer to the particular resonance in which we are interested and the overlapping resonance respectively. Equation (4.2) is written as

\[
P = e^{-\frac{1}{\xi} M_1} 
\]

(4.3)

where \(M_1\) is defined as the macroscopic resonance integral of the selected resonance. Thus

\[
M_1 = \Sigma_p \int \frac{N_1 \sigma a_l}{N_1 \sigma r_1 + N_2 \sigma r_2 + \Sigma p} \frac{dE}{E} .
\]

(4.4)

If the Breit-Wigner resonance forms are assumed and the energies are measured from \(E_{r1}\), the centre of the particular resonance in which we are interested, we obtain its macroscopic resonance integral, namely,

\[
M_1 = \Sigma_p \int_{-\infty}^{\infty} \frac{\Gamma y_{r1}}{\Gamma_{r1}} \frac{N_1 \sigma o_1 \psi(x,t_1)}{\psi(x,t_1) + N_2 \sigma o_2 \psi(ax+b,t_2) + \Sigma p} \frac{dE}{E} 
\]

(4.5)

where \(x = 2(E-E_{r1})/\Gamma_{r1}\)

and

\[
ax+b = 2(E-E_{r2})/\Gamma_{r2} .
\]
Therefore \( a = \Gamma_1 / \Gamma_2 \)
and \( b = 2 (E_{r1} - E_{r2}) / \Gamma_2 \).

We are interested in the change of a resonance integral due to the presence of another resonance at various separations. The second resonance can be of the same species or of a different species. That is, we are interested in integrals of the form

\[
\int \frac{\Sigma a_1}{\Sigma r_1 + \Sigma p} \frac{dE}{E} \quad \text{and} \quad \int \frac{\Sigma a_1}{\Sigma r_1 + \Sigma r_2 + \Sigma p} \frac{dE}{E}
\]

where the former would represent an isolated resonance integral and the latter a resonance under the influence of a neighbouring resonance.

The effect of separation of the resonances on overlap is measured in terms of percentage change, for not only is \( b \) dependent on \( E_{r2} \) but also the \( \sigma_{02} \) factor in \( \Sigma r_2 \) (the \( \sigma_{02} \) decreases as \( E_{r2} \) increases). Hence \( d \), the decrease of the resonance integral due to the presence of a neighbouring resonance is

\[
d\% = \frac{N_1 I_1 - M_1}{N_1 I_1} \times 100\%, \quad (4.6)
\]

where \( I_1 \) and \( M_1 \) are the isolated and the macroscopic resonance integrals of the resonance in which we are interested. The term \( N_1 I_1 \) is used instead of just \( I_1 \) (the effective resonance integral) because we wish to compare it with the macroscopic resonance integral and this last integral involves the number of atoms of the species per cc. of the mixture.

4.3 Bounds of Percentage Decrease in the Model

4.3.1 Two resonances at the same energy and \( nN_1 = N_2 \)

Consider two identical resonances at the same energy but with
\[ nN_1 = N_2. \] We have from equation (4.4)

\[ M_1 = \sum_p \left( \frac{N_1 \sigma_{al}}{(n+1)N_1 \sigma_{rl}} + \frac{\Sigma_p}{E} \right) \]  \hspace{1cm} \text{(4.7)}

\[ = \frac{\Gamma \Sigma_p}{2(n+1)E r_1} \int_{-\infty}^{\infty} \frac{\psi(x,t)}{\psi(x,t) + \frac{\sigma_p}{(n+1)\sigma_o}} \text{dx} \]  \hspace{1cm} \text{(4.8)}

\[ = \frac{\Gamma \Sigma_p}{(n+1)E r_1} J(t, \frac{\sigma_p}{(n+1)\sigma_o}) \]  \hspace{1cm} \text{(4.9)}

However, regarding the resonance as isolated, we have

\[ N_1 I_1 = \sum_p \left( \frac{N_1 \sigma_{al}}{N_1 \sigma_{rl}} + \frac{\Sigma_p}{E} \right) \]  \hspace{1cm} \text{(4.10)}

\[ = \frac{\Gamma \Sigma_p}{E r_1} J(t, \frac{\sigma_p}{\sigma_o}) \]  \hspace{1cm} \text{(4.11)}

Therefore from equation (4.6), we have

\[ J(t, \frac{\sigma_p}{\sigma_o}) - \frac{1}{n+1} J(t, \frac{\sigma_p}{(n+1)\sigma_o}) \]  \hspace{1cm} \text{(4.12)}

\[ \frac{d\%}{J(t, \frac{\sigma_p}{\sigma_o})} = \frac{100\%}{J(t, \frac{\sigma_p}{\sigma_o})} \times 100\% \]

From equation (2.78) we had that if \( \beta \) is large, \( J(t, \beta) \approx \pi / 2 \beta \).

\[ \therefore \quad d\% = 0\% \]

as would be expected since the mixture here would be very dilute and there would be no effect from overlap.

If \( \beta \) is small, we have, from equation (2.80) that \( J(t, \beta) \approx \pi / 2 \sqrt{\beta} \), and so equation (4.12) becomes
\[
\frac{\frac{\pi \sqrt{\sigma_0}}{2 \sigma_p} - \frac{1}{n+1}}{\frac{\pi \sqrt{(n+1)\sigma_0}}{2 \sigma_p}} \times 100%
\]

i.e. \( d\% = \left(1 - \frac{1}{\sqrt{n+1}}\right) \times 100\% \) (4.13)

### 4.3.2 Special Cases \((n=1 \text{ and } \frac{1}{2})\)

Taking \( n=1 \), that is, \( N_1 = N_2 \) we have from (4.13)

\[d\% = \left(1 - \frac{1}{\sqrt{2}}\right) \times 100\%
\]

i.e. \( d\% = 29.29\% \),

which is the upper limit for the percentage decrease when \( N_1 = N_2 \).

Similarly if \( n = \frac{1}{2} \), that is, \( N_1 = 2N_2 \), the upper limit becomes

\[d\% = 18.3\% \]

### 4.4 The code EROS

EROS (Effective Resonance Overlap with respect to Shielding) has been coded to evaluate numerically integrals of the form \( M_1 \) and \( N_1 I_1 \) (see equation (4.7) and (4.10)), so that the percentage changes due to overlap can be calculated. The output also includes \( J(\beta, t) \) values for the resonances treated as if they were isolated so that comparison can be made with the simple formulae discussed in chapter 3. Values of the overlapped macroscopic resonance integrals have been normalised to unity just above the resonances so that results can be compared directly with those of Codd and Collins (1963).

The input involves the data for two independent resonances, namely their energy levels \( E_i \); neutron widths \( \Gamma_{ni} \); radiative widths \( \gamma_i \);
total widths $\Gamma_i$: statistical spin factor $g_{J_i}$; potential scattering $\sigma_{pi}$; the number of the resonance species per unit volume $N_i$; the temperature of each species $T_i$ and their atomic weights. The moderator parameters imputed are its potential scattering and the number of moderator species per unit volume.

The integrals were evaluated on the IBM 1620 Computer at the Wollongong University College using Simpson's Rule and computer time was saved by techniques similar to those used in chapter 3. Added accuracy was obtained by using the Richardson's extrapolation formula (Pollard, 1967). Computer time was also saved by taking advantage of the 'smoothness' of the integrals in the wings of the resonances. The total range of the integration was subdivided into a number of intervals and the value of the integral stored when the required accuracy was obtained.

The upper and lower limits of the integration were also imputed as data. Throughout the programming both these limits were taken as 200 units (in terms of half widths of the resonance in which we are interested). Where one resonance dominated its neighbouring resonance, provision was made in the programme to calculate new upper and lower limits so that, at all times, the limits would be at least 200 units (in terms of the half widths of the dominating resonance) from the nearest resonance. Hence the lower limit, LL, is

$$LL = \text{minimum} \left(-200, S - 200 \frac{\Gamma_2}{\Gamma_1}\right),$$

and the upper limit, UL, is

$$UL = \text{maximum} \left(200, S + 200 \frac{\Gamma_2}{\Gamma_1}\right),$$

where $S$ is the separation of the resonances in units of $\Gamma_1/2$. 
The $M^1$ integral needed values of the $\psi(x,t)$ function for both resonances, and so after storing the value for the lower resonance, the higher resonance values were obtained using the change of variable $y = (x\Gamma_1 - 2S)/\Gamma_2$. The IBM 1620 PSICHI block (Doherty 1964) was again used to evaluate the $\psi(x,\theta)$ function.

The programmes were run at an accuracy of 0.5% in general with an added accuracy of 0.1% near the resonance peaks.

4.5 Numerical Results

4.5.1 Table I

The percentage decrease in the macroscopic resonance integrals have been evaluated at temperature $T = 0^\circ A$ and for combinations of various resonance parameters so as to give an idea of the overlap effect. The computations were performed for various resonance separation levels where $E_{r1} = 100eV$, $\Gamma_n = 0.03eV$ for both resonances and $\Gamma_2 = 0.05eV$ in the three sets of calculations.

For the first set of calculations, the two resonances were identical in all respects except for the varying of the energy of the second resonance.

For the second problem the number of nuclei with the first resonance was double the number with the second resonance (that is, $N_1 = 2N_2$). All other parameters were as for the first problem.

In the third set of calculations, the parameters were the same
as in the first problem except that the total width of the first resonance was double that of the second resonance.

4.5.2 Table II

The temperature effect on the percentage decrease of the macroscopic resonance integral has been shown for temperatures of T=0°A and 300°A. The computations were performed for identical resonance parameters and for a potential cross section of 2,000 barns.

4.5.3 Tables III and IV

The effect of spacing on overlap was measured for different energy levels of the interested resonance, namely at 100eV, 1,000eV and 10,000eV. The data used for this table was the mean s-wave resonance parameters used by Codd and Collins (1964), namely

\[ ^{238}U \]
\[ \langle \Gamma \rangle = 0.025\text{eV} ; \quad \langle \Gamma^0 \rangle = 0.002\text{eV} ; \quad <D> = 18.3\text{eV} \]

\[ ^{239}Pu \]
\[ \langle \Gamma \rangle = 0.038\text{eV} ; \quad <\Gamma_f> = 0.076\text{eV} ; \]
\[ \langle\Gamma^0\rangle_n = 0.00072\text{eV} ; \quad <D> = 7.2\text{eV for } J=0 \]
\[ \langle\Gamma^0\rangle_n = 0.00024\text{eV} ; \quad <D> = 2.4\text{eV for } J=1, \]

where J is the spin quantum number of the compound nucleus formed by the target nucleus and the neutron (the resonance parameters are as defined earlier and the bracketed parameters are their statistical mean values). Also the background nonresonant scattering cross section was taken to be 75b per \(^{238}U\) atom and 525b per \(^{239}Pu\) atom.
The results from this table are also used in chapter 5 to investigate the accuracy of the correction to Rowland's formula. The code EROS was used for calculating the decrease in effective resonances of a plutonium 239 resonance by the overlapping of uranium 238 resonances. An indication of the accuracy of the EROS code is also given by comparing Codd and Collins (ibid.) and EROS results.

**TABLE I**

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<th>T=0°A</th>
<th>SEPARATION (eV)</th>
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<tr>
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<td>0.0 0.2 0.4 0.6 0.8 1.0 2.0</td>
</tr>
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<td>26.6 8.5 3.0 1.2 0.6 0.4 0.0</td>
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<tr>
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<tr>
<td>Γ₁=2Γ₂ \ N₁=N₂</td>
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**TABLE II**

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<tr>
<td>0°A</td>
<td>28.2 4.1 1.2 0.5 0.3 0.2 0</td>
</tr>
<tr>
<td>300°A</td>
<td>25.6 19.3 8.3 2.2 0.5 0.3 0</td>
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TABLE III

| ENERGY LEVEL (eV) | SEPARATION (eV) | Percentage Decrease \( d_q(E_g,E_g) \)% *
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<tr>
<td>100</td>
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<td>68.6</td>
</tr>
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<td>1,000</td>
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<td>56.6</td>
</tr>
<tr>
<td>10,000</td>
<td>16.2</td>
<td>16.1</td>
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</tbody>
</table>

* \( d_q(E_g,E_g) \) = fractional decrease of Pu\(^{239}\) resonance integral due to the presence of a neighbouring U\(^{238}\) resonance.

TABLE IV

| ENERGY LEVEL (eV) | SEPARATION (eV) | Percentage Decrease \( d_q(E_g,E_g) \)%
<table>
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<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
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<td>100</td>
<td>81.7</td>
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</tr>
<tr>
<td>10,000</td>
<td>12.4</td>
<td>12.3</td>
</tr>
</tbody>
</table>

It is to be noted that the fractional decrease becomes negligible as the separation approaches half the U\(^{238}\) sequence spacing of 9.15eV. This is made use of in chapter 5 for the deviation of averaged absorption values.
5. Numerical Comparison of Overlap Formulae

5.1 Introduction

The main purpose of this chapter is to compare the accuracy of various resonance formulae which include a compensating factor for the overlap effect. We will use the numerical results from the code EROS (see chapter 4) as the basis for comparison.

The reliability of the EROS results is shown by comparing them in section 5.3 with results given in a paper by Codd and Collins (1963). Hence it is first necessary to give a brief outline of Codd and Collins' paper.

5.2 Codd and Collins' Paper

Defining $A_9(E_9, E_8)$ as the macroscopic absorption in Pu$^{239}$ for one resonance of Pu$^{239}$ with a resonance energy of $E_9$ influenced by one resonance of U$^{238}$ with a resonance energy of $E_8$, the above authors considered the absorption in a single Pu$^{239}$ s-wave resonance with spin $J=1$ as a function of separation from a U$^{238}$ resonance at 1 KeV for two temperatures 300°K and 600°K. The resonances were assumed to have a Doppler-broadened single-level Breit-Wigner shape. The plutonium and uranium were assumed to be intimately mixed so that both resonances broadened when the temperature rose.

They assumed that the collision density was constant through the resonances so that the absorption $A_9(E_9, E_8)$ was given by an integral similar to the one derived for $M_1$ in equation (4.4) apart
from a normalisation constant which depends on the absolute level of the flux. The Doppler change in $A_9(E_g,E_8)$ was then given by

$$\Delta A_9 = A_9(E_g,E_8)_{600^\circ K} - A_9(E_g,E_8)_{300^\circ K}$$  \hspace{1cm} (5.1)$$

The results for $A_9(E_g,E_8)$ and $\Delta A_9$ were graphed after both were normalised to unity at large separation, i.e., for an isolated Pu$_{239}$ resonance. They found that $A_9(E_g,E_8)$ was appreciably reduced when the resonances were close together. The Doppler change $\Delta A_9$ was large and positive for very closely spaced resonances, but large and negative for separations between about 1eV and 3eV.

A mean value for $\Delta A_9$, denoted by $\overline{\Delta A_9}$, was also estimated by assuming a constant level density of Pu$_{239}$ resonances, and averaging the $\Delta A_9$ values over the range $D_8 = -9.15eV$ to $D_8 = 9.15eV$, i.e., over a range equal to the mean U$_{238}$ level spacing. They obtained a result

$$\overline{\Delta A_9} = -0.062$$  \hspace{1cm} (5.2)$$

after normalising to unit flux just above the resonances. A corresponding value for an isolated Pu$_{239}$ resonance was found to be

$$\overline{\Delta A_9} = +0.053.$$  \hspace{1cm} (5.3)$$

The (5.2) result was found to agree within 1% of that obtained by an approximate analytical formula of Rowlands. He developed the following formulae for the mean Pu-239 and U-238 absorptions per atom per unit energy interval, allowing for overlapping of Pu-239 and U-238 resonances.
\[
\bar{A}_9 = \sigma_{b9} \Gamma_a \, J_9(1 - g \, J_g/D_9)/D_9\]  
\[
\bar{A}_8 = \sigma_{b8} \Gamma_a \, J_8(1 - g \, J_g/D_8)/D_8, \]  

where the suffices 8 and 9 refer to \textsuperscript{238}U and \textsuperscript{239}Pu. The quantity \(\sigma_b\) denotes the non-resonant scattering cross section of the medium per absorber nucleus. Also, \(J\) is the usual \(J(\beta,t)\) function and \(\Gamma, \Gamma\) and \(D\) denote the mean absorption and total widths and level spacing, respectively. Rowlands obtained the above expressions by assuming the following approximation to the macroscopic total cross section

\[
\Sigma_t = \Sigma_b + \Sigma_{t8} + \Sigma_{t9}
\]

\[= (\Sigma_b + \Sigma_{t8})(\Sigma_b + \Sigma_{t9})/\Sigma_b \]  

provided \(\Sigma_{t8} \Sigma_{t9}/\Sigma_b \Sigma_t \ll 1\). Here \(\Sigma_b, \Sigma_{t8}\) and \(\Sigma_{t9}\) denote, respectively, the macroscopic total non-resonant cross section of the medium, and the macroscopic total resonant cross section of \textsuperscript{238}U and \textsuperscript{239}Pu.

### 5.3 Comparison of EROS and Codd and Collins' Results

In Codd and Collins' paper (ibid.) \(A_9(E_g,E_g)\) results were graphed showing the dependence of the macroscopic absorption in a \textsuperscript{239}Pu resonance at 1 KeV on the separations from a neighbouring \textsuperscript{238}U resonance for a temperature of 300\textsuperscript{°}A. Table I gives these values of \(A_9(E_g,E_g)\), estimated from the graph, together with the EROS calculation for \(A_9(E_g,E_g)\). It is to be noted that Codd & Collins' normalised value for \(A_9(E_g,E_g)\) is related to the d\% of chapter 4 by the relationship

\[
A_9(E_g,E_g) = 1 - d(E_g,E_g)/100 \]  

(5.7)
Tables II, III and IV give the dependence of the absorption $A_9(E_8,E_g)$ and the Doppler change, $\Delta A_9(E_9,E_8)$, in absorption for a Pu$^{239}$ resonance of the $J=1$ sequence (with mean parameters as given in chapter 4) on separations from a neighbouring U$^{238}$ resonance for a temperature change of $300^\circ$K to $600^\circ$K. Following Codd and Collins, the $\Delta A_9(E_9,E_8)$ values have been normalised to unit flux above the resonances and are designated by $\Delta A_9(E_9,E_8)$ in the Tables. The Pu$^{239}$ resonance was taken at $100\text{eV}$, $1,000\text{eV}$ and $10,000\text{eV}$ respectively.

In Table III an extra column, $\Delta A_9^*(\text{Codd and Collins})$ has been added. Throughout the tables the $\Delta A_9^*(E_9,E_8)$ values have been normalised to unity for large separations as was done in Codd and Collins' paper. The accuracy in the EROS code was .5% and each run took approximately 25 minutes on the IBM 1620 at Wollongong University College.

<table>
<thead>
<tr>
<th>Separation (eV)</th>
<th>0</th>
<th>.25</th>
<th>.50</th>
<th>.75</th>
<th>1.0</th>
<th>1.5</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>4.0</th>
<th>6.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>EROS</td>
<td>.41</td>
<td>.43</td>
<td>.50</td>
<td>.60</td>
<td>.71</td>
<td>.88</td>
<td>.96</td>
<td>.98</td>
<td>.99</td>
<td>.995</td>
<td>1</td>
</tr>
<tr>
<td>Codd &amp; Collins</td>
<td>.41</td>
<td>.43</td>
<td>.50</td>
<td>.60</td>
<td>.71</td>
<td>.88</td>
<td>.97</td>
<td>.98</td>
<td>.99</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>
### TABLE II

Pu$^{239}$ at 100eV

<table>
<thead>
<tr>
<th>SEPARATION (eV)</th>
<th>$A_9(E_g,E_g) \text{ (cm}^{-1}\text{)}$</th>
<th>$\Delta A_9*(E_g,E_g)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>600$^\circ$K</td>
<td>300$^\circ$K</td>
</tr>
<tr>
<td>0.0</td>
<td>1.29E-1</td>
<td>1.24E-1</td>
</tr>
<tr>
<td>0.25</td>
<td>1.81E-1</td>
<td>2.00E-1</td>
</tr>
<tr>
<td>0.5</td>
<td>3.16E-1</td>
<td>3.80E-1</td>
</tr>
<tr>
<td>0.75</td>
<td>4.63E-1</td>
<td>5.17E-1</td>
</tr>
<tr>
<td>1.0</td>
<td>5.23E-1</td>
<td>5.73E-1</td>
</tr>
<tr>
<td>1.5</td>
<td>6.21E-1</td>
<td>6.13E-1</td>
</tr>
<tr>
<td>2.0</td>
<td>6.41E-1</td>
<td>6.22E-1</td>
</tr>
<tr>
<td>2.5</td>
<td>6.42E-1</td>
<td>6.23E-1</td>
</tr>
<tr>
<td>3.0</td>
<td>6.50E-1</td>
<td>6.31E-1</td>
</tr>
<tr>
<td>4.0</td>
<td>6.54E-1</td>
<td>6.34E-1</td>
</tr>
<tr>
<td>6.0</td>
<td>6.54E-1</td>
<td>6.34E-1</td>
</tr>
</tbody>
</table>

### TABLE III

Pu$^{239}$ at 1,000eV

<table>
<thead>
<tr>
<th>SEPARATION (eV)</th>
<th>$A_9(E_g,E_g) \text{ (cm}^{-1}\text{)}$</th>
<th>$\Delta A_9*(E_g,E_g)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>600$^\circ$K</td>
<td>300$^\circ$K</td>
</tr>
<tr>
<td>0.0</td>
<td>1.03E-2</td>
<td>8.89E-3</td>
</tr>
<tr>
<td>0.25</td>
<td>1.05E-2</td>
<td>9.36E-3</td>
</tr>
<tr>
<td>0.5</td>
<td>1.13E-2</td>
<td>1.09E-2</td>
</tr>
<tr>
<td>0.75</td>
<td>1.24E-2</td>
<td>1.28E-2</td>
</tr>
<tr>
<td>1.0</td>
<td>1.38E-2</td>
<td>1.50E-2</td>
</tr>
<tr>
<td>1.5</td>
<td>1.68E-2</td>
<td>1.85E-2</td>
</tr>
<tr>
<td>2.0</td>
<td>1.91E-2</td>
<td>2.06E-2</td>
</tr>
<tr>
<td>2.5</td>
<td>2.03E-2</td>
<td>2.08E-2</td>
</tr>
<tr>
<td>3.0</td>
<td>2.12E-2</td>
<td>2.13E-2</td>
</tr>
<tr>
<td>4.0</td>
<td>2.15E-2</td>
<td>2.14E-2</td>
</tr>
<tr>
<td>6.0</td>
<td>2.15E-2</td>
<td>2.14E-2</td>
</tr>
</tbody>
</table>
The accuracy of the $\Delta A_9(E_9, E_8)$ values is somewhat limited due to its derivation by subtraction and this would explain the slight discrepancy in Table III of the EROS and Codd and Collins results.

### 5.4 Average Effect of Overlap on Resonance Absorption

In the derivation of Rowland's formula and in the corrections to it (see chapter 3), it was assumed that the peak of the nearest member of the overlapping sequence could, with equal probability, lie anywhere between a distance of 0 and $\frac{1}{2}D_2$ eV from the fixed resonance under consideration. On the other side of the resonance under consideration there will be another member of the overlapping sequence.
lying between $-D_2$ and $-\frac{1}{2}D_2eV$.

If the resonance under consideration overlaps with $2n+1$ resonances of the sequence then the members of the sequence will lie in ranges $\frac{2r-1}{2}D_2$ to $\frac{2r+1}{2}D_2$ from the peak of the fixed resonance. If $I$ is the value of the resonance integral of the fixed resonance in the presence of one member of the overlapping sequence when the spacing is $S$ then the average value of $I$ in the presence of $2n+1$ overlapping resonances is

$$I = \sum_{r=-n}^{n} \frac{2r+1}{2} \cdot D_2 \int_{\frac{2r-1}{2}D_2}^{\frac{2r+1}{2}D_2} I dS$$

$$= 2 \int_{0}^{\infty} I dS \quad (5.8)$$

since, by assumption, there is overlap with only $2n+1$ resonances and so

$$\int_{\frac{2n+1}{2}D_2}^{\infty} I dS = 0.$$ 

In the derivation of equation (5.8) we have assumed that the spacing $D_2$ between the resonances of the overlapping sequence is constant and we have neglected any statistical variation in resonance spacing.
In particular, taking the parameter $d_g(E_9, E_8)$ which is negligible for spacings of less than half the spacing of the overlapping sequence of $^{238}U$ (see Tables III and IV of chapter 4) we have

$$\bar{d}_g(E_8) = \frac{2 \int_0^\infty d_g(E_9, E_8) dS}{D_8}$$

(5.9)

where $\bar{d}_g(E_8)$ is the average decrease in the Plutonium 239 resonance integral due to the presence of a sequence of overlapping Uranium 238 resonance.

As $d_g(E_9, E_8)$, defined as the fractional decrease of the Plutonium 239 resonance integral due to the presence of a neighbouring Uranium 238 resonance, is such that

$$A_g(F_9, E_8) = (1 - d_g(E_9, E_8)) A_g(E_8)$$

(5.10)

where $A_g(E_8)$ is the isolated macroscopic resonance integral of Plutonium, it is reasonable to take

$$\bar{A}_g(E_8) = (1 - \bar{d}_g(E_8)) A_g(E_8)$$

(5.11)

where $\bar{A}_g(E_8)$ is the averaged Plutonium 239 absorptions per atom per unit energy interval.

For the overlap of the $J=1$ resonances of Plutonium 239 (see parameters given in chapter 4) with Uranium 238 it would not be valid to average over a spacing of 2.4eV since the effect is still marked outside this range. Codd and Collins obtained their averaged results here directly by using Rowlands' approximation formula.
5.5 Comparison of Overlap Formulae with EROS

For the system considered by Codd and Collins the value of $\beta$ for Pu$^{239}$ at 1,000eV is of the order of unity so that no significant correction is expected to Rowlands' formula. To obtain a smaller value of $\beta$ we will consider overlap between U$^{238}$ and Pu$^{239}$ at 100eV and assume a system for which the background scattering cross section is 25 barns per U$^{238}$ atom and 175 barns per Pu$^{239}$ atom. Otherwise the parameters are the same as for Codd and Collins.

Such values of scattering cross section are likely to be met in calculations for heterogeneous systems where the U$^{238}$ and Pu$^{239}$ are lumped into fuel rods.

The values of $\bar{A}_9(E_8)$ and $\bar{A}_8(E_9)$ for this system have been calculated via EROS and equation (5.11).

Table V gives these EROS $\bar{A}_9(E_8)$ and $\bar{A}_8(E_9)$ values and those calculated by Rowlands', Keane's, Keane and O'Halloran's Formulae. Isolated value for $A_9$ are also included. Reiterating, for convenience, these overlap formula we have Rowlands' formula

$$\bar{A}_1(E_2) = \frac{\Gamma_1 \Sigma}{E_1} J(\beta_1, t_1) \left[ 1 - \frac{\Gamma_2}{D_2} J(\beta_2, t_2) \right], \quad (5.12)$$

Keane's formula

$$\bar{A}_1(E_2) = \frac{\Gamma_1 \Sigma}{E_1} J(\beta_1, t_1) \left[ 1 - \frac{\Gamma_2}{D_2} J(\beta_2, t_2) F(\beta_1, \beta_2) \right] \quad (5.13)$$

where the correcting factor $F(\beta_1, \beta_2)$ was obtained using zero
temperatures and finally Keane and O'Halloran's formula

\[ \overline{A}_1(E_2) = \frac{\Gamma \overline{\Sigma} \beta_1}{E_1} J(\beta_1, t_1) [1 - \frac{\Gamma}{D_2} J(\beta_2, t_2) F(\beta_1, \beta_2, t_1, t_2)] \]  

(5.14)

where the parameters are those as defined in chapter 3. The correcting factor \( F(\beta_1, \beta_2, t_1, t_2) \) was obtained using equation (3.20).

### TABLE V

<table>
<thead>
<tr>
<th>FORMULA</th>
<th>( \overline{A}_9(E_8) )</th>
<th>( \overline{A}_8(E_9) )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>300°K</td>
<td>600°K</td>
</tr>
<tr>
<td>EROS</td>
<td>.456</td>
<td>.484</td>
</tr>
<tr>
<td>Rowlands</td>
<td>.448</td>
<td>.476</td>
</tr>
<tr>
<td>Keane</td>
<td>.458</td>
<td>.488</td>
</tr>
<tr>
<td>Keane and O'Halloran</td>
<td>.455</td>
<td>.484</td>
</tr>
<tr>
<td>Isolated Value</td>
<td>.494</td>
<td>.529</td>
</tr>
</tbody>
</table>

\( \beta_9 = .437 ; \; \beta_8 = .00215 \)

\( E_9 = 100\text{eV} \)

It should be appreciated that as we are using the EROS results as the basis of our comparison and as the EROS calculations had an accuracy of 0.5%, the comparison is somewhat limited. However, it is to be noted that Rowlands' and Keane's approximation formulae give lower and upper bounds to the \( \overline{A} \) values and that Keane and O'Halloran's formula agrees with EROS to the third significant figure. Incidentally, the above formulae all gave identical values to 3 significant values for the original Codd and Collins data.
5.6 Conclusion

The code EROS and the corrected form of Rowlands' formula are based on the same model and the agreement of the results in Table V is a verification of the accuracy of the EROS code.

The model discussed in this thesis has neglected the flux perturbations due to the non-recovery of flux outside the resonances. This could be significant and would lead to different values of the overlap correction for members of the overlapping sequence at the same distance below and above the resonance. The aim of this thesis has been to remove the assumption in Rowlands' analysis that \[ \frac{\sum t_8}{\sum b} \frac{\sum t_9}{\sum t} \ll 1 \] and at the same time to allow for Doppler broadening which was neglected in Keane's treatment. The effect of flux perturbations, while it may be as large as the effect investigated herein, will still be small and should be able to be taken into account with a further correction to Rowlands' simple formula.

Based on our model which assumes a constant collision density, it has been shown that in a heterogeneous system the effect of overlap of resonances at low energies is not well represented by Rowlands' formula and should be estimated by the corrected formula derived in chapter 3 of this thesis. However, for homogeneous systems where the value of \( \beta \) is likely to be large in the energy regions of interest, Rowlands' formula will give quite accurate results.
6. ACKNOWLEDGMENTS

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