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RESONANCE OVERLAP - EFFECT OF NEIGHBOURING RESONANCES

by

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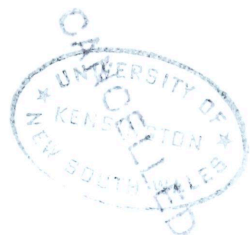

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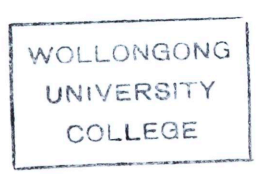

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ABSTRACT

The neutron flux in the region of, and below a resonance is considered. The results of Goldstein which give an asymetric flux shape in the region of a resonance are adjusted to allow for neutron absorption in the resonance, and gives reasonable agreement with the computed results. A simple formula for the calculation of the absorption in a resonance is developed, and it is found that it satisfactorily expresses the dependence of absorption on the total scattering cross section, and the energy of resonance, but gives a greater variation with temperature than is so. The approximation is found to be suitable for estimating the flux perturbation effects caused by neutron absorption. Maximum flux depression occurs at about .9 of a moderator collision range above the resonance lethargy. Flux perturbations from a resonance cause slight variations in the absorption by a lower resonance, when the separation lethargy is about one moderator lethargy interval. This effect is estimated and compared with calculated values. A value of about 1 per cent increase in the reduction of absorption is found to occur for predominantly absorbing resonances.

SUMMARY

The introductory chapter is devoted to the historical development of the resonance overlap problem, and the next chapter deals with the theory of the slowing down of neutrons, the properties of the Breit Wigner resonance profile, and theory of resonance absorption.

In the third chapter, the approximation for the flux in the region of a narrow resonance at zero temperature, which was obtained by Goldstein, is modified in order to allow for the decrease in the neutron concentration because of absorption. The result gives the correct form of the below resonance flux, which was the fault in the approximation of Goldstein.

Perturbation in the flux because of resonance absorption is discussed at length. An expression is obtained for the shape of a resonance which would give no flux perturbation, and which gives a single discontinuous reduction in the flux at the energy of resonance. The resonance shape is found to be hyperbolic in form. A comparison is made between the absorption rate for the 'no perturbation' resonance profile, and for the Breit Wigner profile.

The predominant interest is in the interference of two resonances when the separation of the resonances is about one moderator collision interval. A parabolic approximation is obtained for the absorption rate in a resonance, for zero temperature, and the approximation is extended

so as to be applicable to any temperature. The approximation is used to estimate the amount of flux perturbation caused by absorption in the central region of a resonance, and this estimate is used to evaluate the resulting change in the absorption by a second resonance at a lower energy. The estimates take into account the amount of neutron absorption in the upper resonance, and also the resulting flux perturbations. The results are applicable only when the resonances are separated by about one moderator collision interval.

To verify the analytical work, a programme EXPEAS was designed to solve the slowing down equation through two resonances. Each problem requires a large amount of computer time, and the number of calculations had to be restricted. The calculations show that the estimate of absorption in the central resonance region gave a rough estimate of the absorption in the whole resonance, but the approximation suffers from an excessive temperature variation. The numerical calculations show that the flux perturbations from a resonance are successfully predicted by the method adopted, and the change in the absorption by the lower resonance is also estimated satisfactorily.

An appendix is devoted to the development of a more general form of the Placzek function. The method used is similar to that of Teichmann, but allows for the presence of more than one nuclear species.

CONTENTS

1. HISTORICAL REVIEW

1.1 Introduction

When the possibility of a sustained nuclear reaction was first suggested by Turner (1940), which was based on the experimental work of Anderson, Fermi and Szilard (1939), it was considered that the unknown amount of resonance absorption could well prevent such a sustained reaction. It was also thought that even though such a reaction could possibly be initiated, the resulting temperature rise could cause the reaction to cease because of increased resonance absorption. Thus it was imperative that adequate information on the resonances of fertile material be obtained.

Earlier work had laid the groundwork for investigations into the effects of the resonances of fertile material, on the behaviour of possible reactors. Breit and Wigner (1936) had obtained approximate analytical expressions for the 'shape' of a resonance, by extending the work of Voigt (1912) to nuclear structures. The amount of resonance absorption of a fertile species is dependent upon the energy distribution of the neutrons present, and Amaldi and Fermi (1936) and Bethe (1937) had considered the problem of the energy distribution of neutrons when slowing down in a hydrogen medium.

Considerable work, both theoretical and experimental, was accomplished in the United States during the period 1939-45, most of which was not published except in later review articles. The first experimental results on nuclear resonances were obtained by the Princeton University group by use of a cyclotron. One of the fundamental results

obtained during the period was that of Placzek (1946). In 1940 he was able to obtain an analytical expression for the energy distribution of neutrons slowing down from a mono-energetic source in a homogeneous medium other than hydrogen. Though the derivation has been improved subsequently by Teichmann (1960), little use has been made of Placzek's result, which, several authors have suggested, ought to be taken into consideration. Placzek (1946b) extended his solution to include the slowing down of neutrons in a weakly absorbing medium.

1.2 Early Work on Resonance Absorption

It was realised in the early stages of development that a lattice arrangement of fuel elements would significantly reduce the amount of resonance absorption, but would also shield the fissile material. Much work was done to determine the optimum spatial distribution of fuel elements, during the years prior to the First Geneva Conference on the Peaceful Uses of Atomic Energy (1955). The self-shielding effect of resonances had also been investigated. The reports delivered during the Conference by workers from the U.S.S.R. indicated that work similar to that of workers in the United States, had been carried out by the Russians. Wigner (1955) was the first to distinguish between the so-called narrow resonances and wide resonances, the distinction being based primarily on whether a neutron could lose enough energy in one collision to 'jump' across the resonance. Independent work by Gurevich and Pomeranchouk (1955) was fundamentally similar to the work of Wigner (1955). Early work done by the American, British and Russian workers established that natural uranium was not a practical fuel unless it were 'lumped', or else mixed with heavy water.

In the years immediately following 1955, resonance effects in heterogeneous media were extensively studied by several workers. Dresner (1956) was the first to achieve reasonable results in the calculation of resonance absorption, by evaluating the resonance integrals for homogeneous media. Independent results, which were essentially similar, were published by Nordheim (1958), Dresner (1958) and Chernick and Vernon (1958), and were obtained for resonance absorption in heterogeneous media. The calculations were based on the infinite mass (IM) approximation for wide resonances, and on the narrow resonance approximation of Wigner, when the resonances were narrow. Allowance was made for the unresolved resonance region by means of statistical estimation.

Further development was obtained by Spinney (1957) and Chernick and Vernon (1958), who introduced iterative procedures based on both the NR and IM approximations, and were able to improve the resonance absorption estimates considerably. Rothenstein developed Spinney's method still further, and obtained results which involve a method of extensively correcting simpler approximations.

Also subsequent to the First Geneva Conference, was the development of the Monte Carlo method of studying neutron behaviour during moderation. The method is essentially one of tracing neutrons from birth till they reach thermal energy, allowing for possible modes of collision. It is a statistical method and requires time consuming computer codes to evaluate the probabilities of neutron behaviour.

Another development after 1955 was the formulation of approximate

analytical expressions for the spatial diffusion (Transport Theory) in homogeneous and heterogeneous media. From this were developed certain equivalence theorems, relating neutron behaviour in heterogeneous media, to the behaviour of neutrons in homogeneous media. Many of the results were obtained from consideration of Thermodynamic Principles, and have a wide range of applicability.

1.3 Recent Work on Resonance Absorption

A major development in the study of Resonance Absorption was initiated by the work of Cohen and Goldstein (1962). They took as a first approximation, an interpolation between the IM, and NR approximations, which are extreme cases. An iterative procedure was then applied to the slowing down equation to determine the constants of the interpolation. Though their work was restricted to Breit-Wigner single level, zero temperature resonance profiles, the restriction was subsequently removed by the work of McKay and Pollard (1963), and was further modified by Pollard (1964). Goldstein and Brooks (1964) extended the interpolation method to heterogeneous media. Goldstein (1964) and Keane and Dyos (1965) have done similar independent work on the flux in the region of a resonance, which is ultimately concerned with the amount of absorption in a resonance.

1.4 Resonance Overlap

Corngold and Schermer (1959) considered the resonance overlap effect of two resonances. They found that the interference was greatest for a resonance which was predominantly a scattering resonance, at the higher energy, and least for an absorption resonance at the higher energy. No account was taken in their work of any perturbation effects in the neutron

distribution.

In August 1963, Codd and Collins presented a paper on their investigation of the resonance overlap effect of U_{238} and Pu_{239}, using the method A of Nicholson (1960). They found that the resonance overlap formula of Rowlands (unpublished) to which they refer, to give a reasonably semi-quantitative estimate of such effects. They also reported on the numerical evaluation, by the computer code "Reslow", of the slowing down equation through a single U_{238} resonance. The perturbation in the neutron flux at energies below the energy of resonance, so obtained was suggestive of the Placzek function. Hwang (1963) also presented a paper relating to work done on the resonance overlap effect for energies greater than 1 Kev.

The papers of Codd and Collins, and Hwang, which were presented at a conference sponsored by the Argonne National Laboratory, gave impetus to the study of resonance overlap, which was considered important because it modified the previous estimates of the absorption by all the resonances of a resonant species.

Keane (1965) analysed the formula of Rowlands in order to correct it in the region of greatest error, but at the same time, to maintain its simplicity. Estimates of the overlap effect were obtained in terms of Jacobian Elliptic Functions, by Keane when the temperature was taken as zero. This work has been extended by O'Halloran and Keane (1966).

Though work has been done on the problem of resonance overlap, no consideration has been given to flux perturbation effects and to the effect of the decrease in the neutron population (because of absorption). This thesis is concerned primarily with the development of an approximation for the absorption in the central region of a resonance which is used to obtain an estimate of the perturbation in the neutron flux below a resonance, and to estimate the effect of flux perturbation on the absorption by a resonance of lower energy.

2. BACKGROUND THEORY

2.1 Basic Assumptions

A neutron does not possess an electric charge and is not subject to the inverse square coulomb force. So, for even small velocities, a neutron can approach a nucleus to within the range of influence of the nuclear forces, and react with the nucleus. The reaction of a nucleus and a neutron can result in the production of a new nuclear species, or merely the scattering of the neutron accompanied by degradation of the neutron energy, or fission of the nucleus.

The production of a new nuclear species may involve the absorption of the neutron into the structure of the former nucleus to form a compound nucleus.

If scattering of the neutron occurs, and the nucleus is left in its ground state, the total kinetic energy of the particles is conserved during the collision and the collision is elastic.

When the nucleus is left in an excited state, corresponding to one of the quantum energy states of the nucleus, and the neutron is scattered, the kinetic energy of the particles is not conserved in the laboratory and centre of mass frames and the scattering is inelastic. For inelastic scattering to occur, the colliding particles must have a kinetic energy in excess of the energy corresponding to the first excited state of the nucleus, which is large. The inelastic scattering of a neutron degrades the energy of the neutron in large amounts, of the order 10^5 ev.

Only elastic scattering and absorption are to be considered, and it is assumed that the scattering is isotropic in the centre of mass frame of reference. The probability, $p(E')$ that a neutron of energy, E, before collision will have an energy in the range $(E', E'+dE')$ after the collision is given by Glasstone and Edlund (1952) as

$$p(E')dE' = \frac{dE'}{(1-\alpha)E} \quad \text{for } \alpha E \leq E' \leq E$$

and $$p(E')dE' = 0 \qquad \text{for } E' < \alpha E,\ E' > E$$

where α is the maximum fractional energy loss in such a collision and is given by

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 ,$$

where A is the mass number of the target nucleus.

2.1.1 Cross Section

The rate of a particular reaction between nuclei and monoenergetic neutrons of velocity v, is given by

$$\frac{\text{No. of reactions}}{\text{cm}^3\ \text{sec}} = \sigma \times \frac{\text{No. of Target Nuclei}}{\text{cm}^3} \times \frac{\text{No. of neutrons}}{\text{cm}^3} \times v .$$

where σ is the proportionality constant and is termed the microscopic cross section for the reaction being considered and has dimension of cm^2. Cross sections are usually given in barns instead of cm^2, where

$$1 \text{ barn} = 10^{-24} \text{ cm}^2.$$

An equivalent expression for the cross section is given by

$$\sigma = \frac{\text{Fraction of target nuclei reacting per second}}{n\ v}$$

where n is the number of neutrons of velocity v per cm^3.

2.1.2 Slowing Down Equation

In an infinite homogeneous medium, under slowing down equilibrium, the rate of removal of neutrons from an energy interval (E,E+dE) is equal to the rate of neutron replacement. Thus

$$\Sigma_t \phi(E)dE = \sum_{i=1}^{n} \int_E^{E/\alpha_i} \frac{\Sigma_{si}\phi(E')dE'}{(1-\alpha_i)E'} dE + S(E)dE \ , \qquad 2.1$$

where

(i) $\Sigma_t \ \phi(E)dE$ is the rate of removal of neutrons per unit volume, from the energy interval (E,E+dE), Σ_t being the total of all macroscopic cross sections of the n nuclear species present and is given by

$$\Sigma_t = \sum_{i=1}^{n} (\Sigma_{ai}+\Sigma_{si}) \ ,$$

(ii) $\int_E^{E/\alpha_i} \Sigma_{si} \ \phi(E') \ \frac{dE' \ dE}{(1-\alpha_i)E'}$ is the rate per unit volume at which neutrons enter the energy interval (E,F+dE) after having had the last collision with a nucleus of the i^{th} nuclear species,

(iii) S(E)dE is the rate per unit volume at which neutrons are produced, with an initial energy in the interval (E,E+dE),

(iv) Σ_{si} and Σ_{ai} are respectively, the macroscopic scattering and absorption cross sections of the i^{th} nuclear species (which may be functions of neutron energy), and

(v) $\phi(E)$ is the neutron flux.

Equation 2.1 is often more conveniently expressed in terms of the lethargy, u, defined by

$$u = \ell n(E_o/E) \ ,$$

where E_o is any specified energy usually taken to be 10 MeV. In terms of the lethargy equation 2.1 becomes

$$\Sigma_t \phi(u)du = \sum_{i=1}^{n} \int_{u-\ell n\ 1/\alpha_i}^{u} \frac{\Sigma_{si}\phi(u')}{1-\alpha_i} e^{-(u-u')}\, du'du + S(u)du \ . \qquad 2.2$$

2.1.3 Slowing Down Density, q(E)

The slowing down density is defined to be the number of neutrons slowing down to below an energy E, per unit volume and time, and is shown by Glasstone and Edlund (1952) to be

$$q(E) = \sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \Sigma_{si}\phi(E') \frac{E-\alpha_i E'}{(1-\alpha_i)E'}\, dE' \qquad 2.3$$

By differentiating equation 2.3 and using equation 2.1, we get

$$\frac{d}{dE} q(E) = \sum_{i=1}^{n} \Sigma_{ai}\phi(E) - S(E) \qquad 2.4$$

or, in terms of lethargy

$$\frac{d}{du} q(u) = - \sum_{i=1}^{n} \Sigma_{ai}\phi(u) + S(u) \qquad 2.5$$

2.1.4 The Average Logarithmic Energy Decrement, ξ

The average logarithmic energy decrement (or average gain in lethargy per collision), for the i^{th} nuclear species, ξ_i, is expressed by

$$\xi_i = \int_{u}^{u+\ell n\ 1/\alpha_i} \frac{u'-u}{1-\alpha_i} e^{-(u'-u)} du'$$

and so,

$$\xi_i = 1 - \frac{\alpha_i}{1-\alpha_i} \ln 1/\alpha_i \ . \qquad 2.6$$

An alternative expression for ξ_i is given by

$$\xi_i = \int_E^{E/\alpha_i} \frac{E-\alpha_i E'}{(1-\alpha_i)E'^2} dE' \ . \qquad 2.7$$

2.2 Asymptotic Solution of Slowing Down Equation

In a non-absorbing medium, equation 2.1 reduces to

$$\sum_{i=1}^{n} \Sigma_{si}\phi = \sum_{i=1}^{n} \int_{u-\ln 1/\alpha_i}^{u} \Sigma_{si}\phi \frac{e^{-(u-u')}}{1-\alpha_i} du' + S(u) \ . \qquad 2.8$$

Application of the one-sided Laplace Convolution Theorem, gives

$$\mathcal{L}\{\phi \sum_{i=1}^{n} \Sigma_{si}\} = \sum_{i=1}^{n} \kappa_i(p) \mathcal{L}\{\phi \Sigma_{si}\} + \bar{S}(p)$$

where

$$\mathcal{L}\{y(u)\} = \bar{y}(p) = \int_0^{\infty} e^{-pu} y(u) du$$

and $$\kappa_i(p) = \frac{1-\alpha_i^{p+1}}{(1-\alpha_i)(p+1)} \ .$$

On the assumption that the scattering cross sections are constant, equation 2.8 can be rearranged to give

$$\Sigma_s \mathcal{L}\{\phi\} = \bar{S}(p) + \frac{\bar{S}(p) \sum_{i=1}^{n} \frac{1-\alpha_i^{p+1}}{(1-\alpha_i)(p+1)} \Sigma_{si}}{1 - \sum_{i=1}^{n} \frac{\Sigma_{si}}{\Sigma_s} \frac{1-\alpha_i^{p+1}}{(1-\alpha_i)(p+1)}} \qquad 2.9$$

where $$\Sigma_s = \sum_{i=1}^{n} \Sigma_{si} \ .$$

The second term on the right hand side of equation 2.9 has a simple pole at p=0, and is the pole with the largest real part, and gives the dominant term for large u. The residue at p=0, is by L'Hopital's Rule,

$$\frac{2\pi i}{\sum_{i=1}^{n} \xi_i \frac{\Sigma_{si}}{\Sigma_s}} = \frac{2\pi i}{\bar{\xi}\,\Sigma_s} ,$$

where

$$\Sigma_s \bar{\xi} = \sum_{i=1}^{n} \xi_i \Sigma_{si} . \qquad 2.10$$

The inversion of equation 2.8 for large u is

$$\Sigma_s \phi(u) = S(u) + \int_o^u \frac{S(u)}{\bar{\xi}}\, du . \qquad 2.11$$

If u_f is the largest lethargy at which neutrons are produced, then when $u>u_f$, equation 2.11 can be expressed as

$$\Sigma_s \phi(u) = \frac{Q}{\bar{\xi}} , \qquad 2.12$$

where

$$Q = \int_{source} S(u)du .$$

The full inversion of equation 2.9 is discussed in Appendix A.

2.3 Resonances

For the reactions of interest when a nucleus absorbs a neutron, a compound nucleus is formed, which may not be in its energy ground state, depending on the energies and momenta of the colliding particles. If the energy of the incident neutron is such that the compound nucleus would have an excited energy near one of its quantum states, the reaction

rate, and hence the cross section of the nucleus is large. A resonance occurs where the cross section is large corresponding to some quantum state of the compound nucleus. The large value of the cross section does not occur at a precise neutron energy, but is spread over a finite width of neutron energies because of Heisenberg's Uncertainty Principle, and also because of the spread of the thermal energies of the nuclei.

The compound nucleus will decay to a more stable form by the emission of energy. Three possible modes of decay are considered:-

Channel 1: A neutron is ejected, the resulting nucleus being of the same nuclear species as the original nucleus. If the incident neutron energy was not large, the final nucleus would be in its ground state (because the inelastic scattering threshold is high), and the overall effect would be an elastic collision. This resonance scattering is distinct from the normal collision or potential scattering, and the two types are here denoted by the subscripts s, and p, respectively.

Channel 2: Some particle, other than a neutron is ejected, resulting in the formation of a more stable nucleus, which may undergo further disintegration subsequently. The effect is to remove the neutron from the neutron population.

Channel 3: The compound nucleus disintegrates by fission which produces neutrons at source energies.

If $\lambda_i (i=1,2,3)$ is the disintegration constant for the i^{th} disintegration channel, the partial width Γ_i is defined as

$$\Gamma_i = \hbar \lambda_i$$

where $\hbar$ is Planck's constant.

The standard symbols used are:-

$$\Gamma_n = \Gamma_1 \; ; \quad \Gamma_\gamma = \Gamma_2 \; ; \quad \Gamma_f = \Gamma_3 \; .$$

The total width of the resonance is defined as

$$\Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f$$

and has the dimension of energy. The absorption width Γ_a, is

$$\Gamma_a = \Gamma_\gamma + \Gamma_f$$

since both channels 2 and 3 remove the neutron. The probability that the compound nucleus will decay via the i^{th} channel is

$$\frac{\Gamma_i}{\Gamma} \quad (i=1,2,3) \; .$$

Weinberg and Wigner (1958) and Dresner (1960) discuss the preceding ideas in greater length.

2.4 Flux in the Region of a Narrow Resonance

Following Horner (1966) and combining equations 2.3, 2.7 and 2.8, we get

$$\begin{aligned} q(E) - \bar{\xi}\,\Sigma_r E\phi &= \sum_{i=1}^{n} \int_E^{E/\alpha_i} \left\{ \frac{\Sigma_{si}(E')\phi(E')(E-\alpha_i E')}{(1-\alpha_i)E'} - \frac{\Sigma_{pi}}{\Sigma_p} \frac{\Sigma_t(E)\phi(E)(E-\alpha_i E')E}{(1-\alpha_i)E'^2} \right\} dE' \\ &= \sum_{i=1}^{n} \int_E^{E/\alpha_i} \left\{ \Sigma_{si}(E')\phi(E')E' - \frac{\Sigma_{pi}}{\Sigma_p} \Sigma_t(E)\phi(E)E \right\} \frac{E\,dE'}{(1-\alpha_i)E'^2} \\ &\quad - \sum_{i=1}^{n} \alpha_i \int_E^{E/\alpha_i} \left\{ \Sigma_{si}(E')\phi(E')E' - \frac{\Sigma_{pi}}{\Sigma_p} \Sigma_t(E)\phi(E)E \right\} \frac{dE'}{(1-\alpha_i)E'} \end{aligned}$$

2.13

Except for a factor E the first summation on the R.H.S. of equation 2.13 may be written as

$$\sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \frac{\Sigma_{si}(E')\phi(E')dE'}{(1-\alpha_i)E'} - \sum_{i=1}^{n} \frac{\Sigma_{pi}}{\Sigma_p} \frac{\Sigma_t E\phi}{(1-\alpha_i)} \int_{E}^{E/\alpha_i} \frac{dE'}{E'^2}$$

$$= \sum_{i=1}^{n} \int_{E}^{E/\alpha_i} \frac{\Sigma_{si}(E')\phi(E')dE'}{(1-\alpha_i)E'} - \Sigma_t \phi(E)$$

$$= 0$$

by virtue of equation 2.1, since S(E) may be taken to be zero in the resonance region.

The integrands of the second summation of equation 2.13 differ from the integrands of the first summation by a factor E'. Consequently if the values of Σ_{si} and Σ_{ai} are appreciable over only small ranges of E', that is, the resonance is narrow and remote from other resonances, or if E' is large, the second set of integrals do not differ appreciably from the first set, and the second summation of integrals must be close to zero, and to small error can be put to zero. Hence

$$q(E) \simeq \bar{\xi}\, \Sigma_t E\phi \qquad 2.14$$

which is the narrow resonance approximation.

2.5 Resonance Escape Probability

On dividing equation 2.5 by q(u) and integrating we get

$$q(u) = Q\, e^{-\sum_{i=1}^{n} \sum_{j} \int_{o}^{u} \frac{\Sigma_{aij}\, \phi}{q}\, du'} \qquad 2.15$$

where Q is the strength of the neutron source, Σ_{aij} is the absorption cross section of the j^{th} resonance of the i^{th} nuclear species and the

summation over j covers all resonances which have absorption in the range $0 \leq u' \leq u$.

If $p_{ij}(u)$ denotes the probability that a neutron reaches lethargy u, without absorption by the ij^{th} resonance, and if p(u) denotes the combined probabilities for all the resonances, then

$$\frac{q(u)}{0} = p(u) = e^{-\sum_{i=1}^{n} \sum_{j} \int_{o}^{u} \frac{\Sigma_{aij}(u)\phi(u)}{q(u)} du}$$

$$= \prod_{i=1}^{n} \prod_{j} e^{-\int_{o}^{u} \frac{\Sigma_{aij}(u)\phi(u)}{q(u)} du}$$

$$= \prod_{i=1}^{n} \prod_{j} p_{ij} \quad . \qquad 2.16$$

For regions where the neutron lethargy is well below lethargies of resonance, Σ_{aij} and Σ_{sij} are small, and using equation 2.14 in the form

$$\frac{\phi(u)}{q(u)} \simeq \frac{1}{\bar{\xi}\ \Sigma_t}$$

we get

$$p_{ij} \simeq \exp\left\{-\int_{o}^{u} \frac{\Sigma_{aij}\ du}{\bar{\xi}[\Sigma_p + \sum_{i=1}^{n} \sum_{j} (\Sigma_{aij}+\Sigma_{sij})]}\right\} \qquad 2.17$$

and

$$\phi(u) \simeq \frac{0\ p(u)}{\bar{\xi}[\Sigma_p + \sum_{i=1}^{n} \sum_{j} (\Sigma_{aij}+\Sigma_{sij})]} \quad . \qquad 2.18$$

The values of $\phi(u)$ are, at extreme values of u, given by

$$\phi(o) = \frac{O}{\xi\ \Sigma_p}$$

$$\phi(\infty) = \frac{Op}{\xi\ \Sigma_p} \quad ,$$

which are the correct asymptotic values.

2.6 Breit Wigner Line Shape Function

The profile of a resonance about the resonance energy E_r is assumed to be the Doppler Broadened line shape function of Breit Wigner:

$$\psi(x,\theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\frac{1}{4}\theta^2(x-y)^2}}{1+y^2}\, dy \quad , \qquad 2.19$$

where (i) $\theta = \frac{\Gamma}{2}\sqrt{\frac{A}{E_r kT}}$

(ii) T is the absolute temperature of the mixture

(iii) $x = (E-E_r)/\ \Gamma/2$

(iv) k is Boltzman's constant.

The resonance absorption and scattering profiles are given by:

$$\sigma_a = \frac{\Gamma_a}{\Gamma}\, \sigma_o\, \psi(x,\theta) \qquad 2.20$$

$$\sigma_s = \frac{\Gamma_n}{\Gamma}\, \sigma_o\, \psi(x,\theta) \quad , \qquad 2.21$$

where σ_o is the peak height of the resonance profile and is

$$\sigma_o = \frac{2.608 \times 10^6\ g\ \Gamma_n}{\Gamma\ E_r} \qquad 2.22$$

g being the spin factor of the target nucleus.

2.6.1 Some Properties of the Function $\psi(x,\theta)$

The integral $\int_{-\infty}^{\infty} \psi(x,\theta)dx$

can be evaluated by using 2.19, and by reversing the order of integration. Thus

$$\int_{-\infty}^{\infty} \psi(x,\theta)dx = \pi \ .$$

If the auxiliary function

$$\phi(x,\theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{y\ e^{-\frac{1}{4}\theta^2(x-y)^2}}{1+y^2}\ dy \qquad 2.23$$

is defined, then as $\psi(x,\theta)$ is an even function of x, while $\phi(x,\theta)$ is an odd function of x, the Fourier Cosine, and Sine transforms give, respectively

$$\mathcal{F}_c\{\psi(x,\theta)\} = \sqrt{\pi}/2\ e^{-s-s^2/\theta^2} \qquad 2.24$$

$$\mathcal{F}_s\{\phi(x,\theta)\} = \sqrt{\pi}/2\ e^{-s-s^2/\theta^2}\ , \qquad 2.25$$

Inversion of the equations 2.24 and 2.25 give the alternative expressions

$$\psi(x,\theta) = \int_0^{\infty} e^{-s-s^2/\theta^2} \cos sx\ ds \qquad 2.26$$

and

$$\phi(x,\theta) = \int_0^{\infty} e^{-s-s^2/\theta^2} \sin sx\ ds\ . \qquad 2.27$$

When x = 0,

$$\psi(0,\theta) = e^{\theta^2/4} \int_0^{\infty} e^{-(s+\frac{1}{2}\theta^2)^2/\theta^2}$$

$$= \tfrac{1}{2}\sqrt{\pi}\ \theta\ e^{\theta^2/4}\ \text{erfc}\ \theta/2 \qquad 2.28$$

and

$$\phi(0,\theta) = 0 \quad . \qquad 2.29$$

Corresponding to zero temperature, $\theta = \infty$, we have

$$\psi(x,\infty)+i\ \phi(x,\infty) = \int_0^\infty e^{-s}\ e^{isx}\ ds$$

$$= \frac{1+ix}{1+x^2}$$

so that

$$\psi(x,\infty) = \frac{1}{1+x^2} \qquad 2.30$$

and

$$\phi(x,\infty) = \frac{x}{1+x^2} \quad . \qquad 2.31$$

2.6.2 Differential Equation for $\psi(x,\theta)$

If the equations 2.19 and 2.23 are integrated by parts we get,

$$x\ \psi(x,\theta) = \phi(x,\theta) - \frac{2}{\theta^2}\frac{\partial}{\partial x}\psi(x,\theta) \qquad 2.32$$

and

$$x\ \phi(x,\theta) = 1 - \psi(x,\theta) - \frac{2}{\theta^2}\frac{\partial}{\partial x}\phi(x,\theta) \qquad 2.33$$

Differentiation of equation 2.32 yields

$$x\frac{\partial}{\partial x}\psi(x,\theta) + \psi(x,\theta) = \frac{\partial}{\partial x}\phi(x,\theta) - \frac{2}{\theta^2}\frac{\partial^2}{\partial x^2}\psi(x,\theta) \qquad 2.34$$

The quantity $\frac{\partial}{\partial x}\phi(x,\theta)$ can be eliminated from equation 2.34 by use of equation 2.33, and from the resulting equation, the quantity $\phi(x,\theta)$ can be eliminated by use of equation 2.32. The end result is

$$\psi'' = +\tfrac{1}{4}\theta^4 - \theta^2 x\psi' - (2+\theta^2+\theta^2x^2)\psi \qquad 2.35$$

where the primes denote differentiation with respect to x.

A similar differential equation can be obtained for the function $\phi(x,\theta)$ using a similar method.

By differentiating equation 2.35 the third derivative of $\psi(x,\theta)$ is expressed in terms of the lower derivatives, and is by virtue of equation 2.35 expressible in terms of ψ and ψ'. This argument can be extended to the n^{th} order derivative. Thus all derivatives of $\psi(x,\theta)$ at any point x_o, can be evaluated if $\psi(x_o,\theta)$ and $\psi'(x_o,\theta)$ are known. The value of ψ at x=0 is known by equation 2.28 and $\psi'=0$ at x=0 since the function ψ is an even function. By use of a Taylor's series, values of ψ and its x-derivatives can be calculated for all x.

The numerical procedure for calculating ψ adopted by Pollard (1964) is to obtain values for ψ, ψ', ψ'', ψ''' by using a truncated Taylor expansion by stepping out from x=0 and evaluating the derivatives (up to the third) at each point.

2.6.3 Asymptotic Series for $\psi(x,\theta)$

Though a numerical technique was discussed in section 2.6.2 for the evaluation of $\psi(x,\theta)$ for all x, the stability and accuracy of the method depends on the choice of step length and the number of derivatives used. For high accuracy for large x, the method becomes cumbersome, and use is made of asymptotic series.

By expanding the term e^{-s^2/θ^2} in equations 2.26 and 2.27 we get

$$\psi(x,\theta) \simeq \sum_{n=0}^{\infty} \int_o^{\infty} (-\frac{1}{\theta^2})^n \frac{1}{n!} s^{2n} e^{-s} \cos sx \, ds$$

and $$\phi(x,\theta) \simeq \sum_{n=0}^{\infty} \int_o^{\infty} (-\frac{1}{\theta^2})^n \frac{1}{n!} s^{2n} e^{-s} \sin sx \, ds \ .$$

Hence we have

$$\psi(x,\theta) - i\phi(x,\theta) \simeq \sum_{n=0}^{\infty} \int_{o}^{\infty} \left(-\frac{1}{\theta^2}\right)^n \frac{1}{n!} s^{2n} e^{-s} e^{-isx} dx$$

which is a Fourier transform giving

$$\psi(x,\theta) - i\phi(x,\theta) \simeq \sum_{n=0}^{\infty} \frac{(-1)^n}{\theta^{2n}} \frac{1}{n!} \frac{d^{2n}}{dx^{2n}} \frac{1}{1+ix} \qquad 2.36$$

and

$$\psi(x,\theta) \simeq \sum_{o}^{\infty} \frac{(-1)^n}{\theta^{2n}} \frac{1}{n!} \frac{d^{2n}}{dx^{2n}} \frac{1}{1+x^2} \qquad 2.37$$

However, the asymptotic series for both $\psi(x,\theta)$ and $\phi(x,\theta)$ are best obtained using equation 2.36, the general result being for $\psi(x,\theta)$

$$\psi(x,\theta) \simeq \sum_{o}^{\infty} \frac{(-1)^n}{\theta^{2n}} \frac{(2n)!}{n!} \left\{ \sum_{k=0}^{2n} (-1)^k \, {}^{2n+1}C_k \, x^{2k} \right\} \qquad 2.38$$

and the first three terms of the series are

$$\psi(x,\theta) \simeq \frac{1}{1+x^2} \{1+[(3x^2-1)+(15x^2(x^2-2)+3)V]\} \qquad 2.39$$

where $V = \frac{1}{(1+x^2)^2} \frac{2}{\theta^2}$.

When x is sufficiently large, further truncation is possible to give

$$\psi(x,\theta) \simeq \frac{1}{1+x^2} \qquad 2.40$$

2.7 Effective Resonance Integral

On the assumption that, in parts of the analysis for an isolated resonance, p(u) is close to unity, q(u) does not change appreciably over the resonance; then to first order of approximation, using equation 2.14, we have

$$\phi(E) = 0/\bar{\xi}E\Sigma_t$$

for a single resonant species mixed with a moderator.

The absorption per unit volume would be

$$\int_o^{E_o} \Sigma_a \, \phi(E)dE = \frac{Q}{\xi} \int_o^{E_o} \frac{\Sigma_a}{\Sigma_p+\Sigma_a+\Sigma_s} \frac{dE}{E} .$$

After dividing both top and bottom of the right hand side by N, the number of resonant nuclei per unit volume, an equivalent equation is obtained in terms of the microscopic cross sections. For σ_a and σ_s, their values from equations 2.20 and 2.21 are used to give

$$N \int_o^{E} \sigma_a \, \phi(E)dE = \frac{Q}{\xi} \int_o^{E_o} \frac{\frac{\Gamma_a}{\Gamma} \sigma_o \, \psi(x,\theta)}{\sigma_p+\sigma_o \, \psi(x,\theta)} \frac{dE}{E}$$

$$= \frac{Q}{\xi} \int_o^{E_o} \frac{\Gamma_a}{\Gamma} \frac{\psi(x,\theta)}{\beta+\psi(x,\theta)} \frac{dE}{E}$$

where $\beta = \frac{\sigma_p}{\sigma_o}$ and σ_p is the scattering cross section of the mixture per resonant atom. The absorption in the resonance is taken to be

$$\frac{Q}{\xi} \frac{\Gamma_a}{2E_r} \int_{-\infty}^{\infty} \frac{\psi(x,\theta)}{\beta+\psi(x,\theta)} dx \qquad 2.41$$

where the limits of x have been extended to $\pm \infty$ because the limits $0, E_o$ correspond to such large values of x, that extension of the limits to $\pm \infty$ gives negligible contribution to the integral, and $\frac{1}{E}$ in its explicit form is put equal to $\frac{1}{E_r}$, since $\frac{1}{E}$ varies little through the part of the resonance providing the major contribution to the integral.

The quantity

$$I = \frac{\Gamma_g \sigma_p}{E_r} \int_0^\infty \frac{\psi(x,\theta)}{\beta+\psi(x,\theta)}\, dx \qquad 2.42$$

is termed the Effective Resonance Integral. The function

$$J(\theta,\beta) = \int_0^\infty \frac{\psi(x,\theta)}{\beta+\psi(x,\theta)}\, dx \qquad 2.43$$

has been tabulated by Dresner (1960) and others.

2.7.1 Some Extreme Values for $J(\theta,\beta)$

(i) When T=0,

$$\psi(x,\infty) = \frac{1}{1+x^2}$$

and substitution in equation 2.43 yields

$$J(\infty,\beta) = \int_0^\infty \frac{1}{\beta\left(\frac{1+\beta}{\beta}+x^2\right)}\, dx$$

$$= \pi/2\sqrt{\{\beta(1+\beta)\}} \; . \qquad 2.44$$

(ii) When β is large, or when T is large we have

$$\beta >> \psi(x,\theta)$$

since $\psi(x,\theta) \leq 1$

and for large T,

$$\psi(x,\theta) \simeq 0 \qquad 2.45$$

hence $$J(\theta,\beta) \simeq \int_0^\infty \frac{\psi(x,\theta)}{\beta}\, dx$$

$$\simeq \pi/2\beta \; . \qquad 2.46$$

(iii) When β is small, over the central region of a resonance the integrand becomes

$$\frac{\psi}{\psi+\beta} \simeq 1$$

and can be replaced by

$$\frac{\frac{1}{1+x^2}}{\frac{1}{1+x^2}+\beta} \simeq 1$$

and when x becomes large in the wings of the resonance

$$\psi \simeq \frac{1}{1+x^2}$$

hence the integral is approximately equal to

$$\int_0^\infty \frac{\frac{1}{1+x^2}}{\beta+\frac{1}{1+x^2}}\,dx = \pi/2\{\beta(1+\beta)\}$$

and as β is small

$$J(\theta,\beta) \simeq \pi/2\sqrt{\beta}\ . \qquad 2.47$$

3. FLUX DISTURBANCE DUE TO A RESONANCE

3.1 Introduction

The Narrow Resonance (NR) approximation assumes that the flux in the region of a resonance is given by the relation

$$\Sigma_t \phi(E) = \Sigma_p \phi_o(E) = \frac{\cap}{\xi E}$$

where ϕ_o is the flux in the absence of any resonances. As the total cross section, $\Sigma_t(E)$, is symmetrical about $E=E_r$, so also is $E\phi(E)$ for the NR approximation, but $E\phi(E)$ cannot be symmetrical because of neutron depletion due to absorption. Further, any absorption and any change in the ratio of the scattering cross sections of the nuclear species present give rise to perturbation effects. So, for a resonance, apart from the asymmetry in $E\phi(E)$ caused by the reduction in the neutron population, asymmetry is also present because of perturbation effects.

Goldstein (1964) and Keane and Dyos (1965) independently obtained expressions which give an asymmetric flux in the resonance region. For the expressions obtained, the below resonance flux, considered as a functio of u, returned to the above resonance value, indicating that the expression do not take neutron absorption into account. Goldstein showed that a flux shape which would approach the correct below-resonance value could be obtained by considering the resonance as a negative source.

3.2 A Resonance as a δ-sink

If the width Γ, of a resonance is reduced in such a way that the

resonance absorption probability remains constant, the resonance becomes a δ-sink of magnitude (1-p)Q, p being the resonance escape probability which also remains constant during the limiting process.

The flux resulting from a δ-source of magnitude S, located at u_r is given by

$$\frac{S}{\Sigma_p} P_2(u-u_r)$$

and so the flux in the region of a δ-sink is

$$\Sigma_t \phi = \frac{Q}{\xi} \{1 - \overline{\xi}(1-p)\ P_2(u-u_r)\} \qquad 3.1$$

The general expression for the Placzek Function, $P_n(u)$ is derived in Appendix A and is expressed by equation A4. It is to be noted that the subscript denotes the number of different nuclear species which are considered in the slowing down of neutrons. In section 2.2, an expression, equation 2.12, was derived for the asymptotic value of $P_n(u)$, namely

$$P_n(\infty) = \frac{1}{\xi} \quad .$$

In the region

$$0 < u < 3\ \ell n \frac{1}{\alpha_1} \quad ,$$

where the subscript 1 refers to the moderating species, the function $P_n(u)$ fluctuates about its ultimate value. When $u >> u_r$, equation 3.1 reduces to

$$\Sigma_t \phi(u) = \frac{Q}{\xi} p \, , \qquad 3.2$$

and also, as $\Sigma_a = \Sigma_s = 0$ when $u \gg u_r$,

$$\Sigma_t = \Sigma_p ,$$

giving

$$\Sigma_p \phi = \frac{Q}{\xi} p \qquad 3.3$$

which is the correct limiting form of the below resonance flux.

3.3 A Resonance as a Negative Source

The infinite mass (IM) approximation assumes that a resonant nucleus is of infinite mass, and so, the collision of a neutron and a resonant nucleus does not degrade the energy of the neutron and the resonant nuclei do not contribute to the slowing down of neutrons. Equation 2.1 could be written using the IM approximation,

$$\Sigma_{p_1} \phi = \int_{u-\ell n\ 1/\alpha_1}^{u} \Sigma_{p_1} \phi \frac{e^{-(u-u')}}{1-\alpha_1} du' + S(u) - \Sigma_a \phi$$

where the subscript 1 refers to the moderator. On rearranging the Laplace transform of this equation

$$\mathcal{L}\{\Sigma_{p_1} \phi\} = \bar{S}(p) + \frac{K(p)}{1-K(p)} \bar{S}(p) - \{\Sigma_a \phi\} - \frac{K(p)}{1-K(p)} \{\Sigma_a \phi\} .$$

Inversion gives,

$$\Sigma_t \phi = S(u) + \int_0^u P_1(u-u')\ S(u')\ du' - \int_0^u P_1(u-u')\ \Sigma_a \phi\ du' ,$$

and for regions well below the source,

$$S(u) = 0,\ P_1(u-u') = \frac{1}{\xi} ,$$

and so,

$$\Sigma_t \phi = \frac{Q}{\xi} - \int_0^u P_1(u-u')\ \Sigma_a \phi\ du' \qquad 3.4$$

Equation 3.4 includes flux perturbations caused by the moderator, and if $P_1(u)$ is replaced by $P_2(u)$ some of the flux perturbation effect caused by the resonant species will also be present. Thus

$$\Sigma_t\phi = \frac{Q}{\xi} - \int_o^u P_2(u-u')\Sigma_a\phi \, du' \qquad 3.5$$

This equation is not exact. Consideration of the more general form of the slowing down equation (equation 2.1) with the two integrals on the right hand side, corresponding to the two nuclear species present, leads to a transform which is not amenable to inversion to a suitable form.

When $u >> u_r$, $P_2(u-u')$ can be replaced by its asymptotic value $\frac{1}{\xi}$, using equation 2.12, since $P_2(u-u')$ will be near its asymptotic value in the region where Σ_a and Σ_s differ appreciably from zero. Hence

$$\Sigma_t\phi \simeq \frac{Q}{\xi} - \frac{1}{\xi}\int_o^u \Sigma_a\phi \, du' \qquad 3.6$$

which gives the correct form of the below resonance flux, namely

$$\Sigma_p\phi = \frac{Q}{\xi} p$$

in agreement with equation 3.3.

3.4 Resonance Profile for no Flux Perturbations

Computer codes which calculate the absorption by a species over the whole range of lethargy take into account only the coarse structure of the flux and allow in essence for discontinuous reductions in the flux at the energies of resonance. It is of interest to obtain an expression for the profile of a resonance, so that the fine structure, as well as the coarse structure, of the flux is to consist of a discontinuous reduction at the energies of resonance with no resulting flux perturbations. We now do this.

If $(\Sigma_p+\Sigma_s)\phi$ is to change only at $u=u_r$, by an amount $(1-p)\phi_o$, where ϕ_o is the flux above a particular resonance and p is once again the resonance escape probability, then

$$(\Sigma_s+\Sigma_p)\phi = \Sigma_p\ \phi_o(1-(1-p)\ H(u-u_r)) \qquad 3.7$$

Assuming the presence of only one species of nuclei, and combining equation 3.7 with the equation

$$(\Sigma_a+\Sigma_s+\Sigma_p)\phi = \int_{u-\ell n\ 1/\alpha}^{u} (\Sigma_s+\Sigma_p)\phi\ \frac{e^{-(u-u')}}{1-\alpha}\ du' + S(u)$$

we get

$$\Sigma_a\phi = \frac{1-p}{1-\alpha}\ \Sigma_p\ \phi_o\ \{\left(e^{-(u-u_r)}-\alpha\right)\ H(u-u_r)+\alpha\ \left(1-e^{-(u-u_r-\ell n\ 1/\alpha)}\right)H(u-u_r-\ell n\ 1/\alpha)\} \qquad 3.8$$

The right hand side of the above equation is a non-zero function over the range $(u_r, u_r+\ell n\ 1/\alpha)$, and zero elsewhere, and equation 3.8 can be modified to read

$$\Sigma_a\phi = \frac{\Sigma_p(1-p)}{1-\alpha}\ \phi_o\left(e^{-(u-u_r)}-\alpha\right)\ H(u-u_r)\ H(u_r+\ell n\ 1/\alpha-u) \qquad 3.9$$

In view of the remarks of section 2.3, it is assumed that

$$\Sigma_s = \frac{\Gamma_n}{\Gamma_a}\ \Sigma_a$$

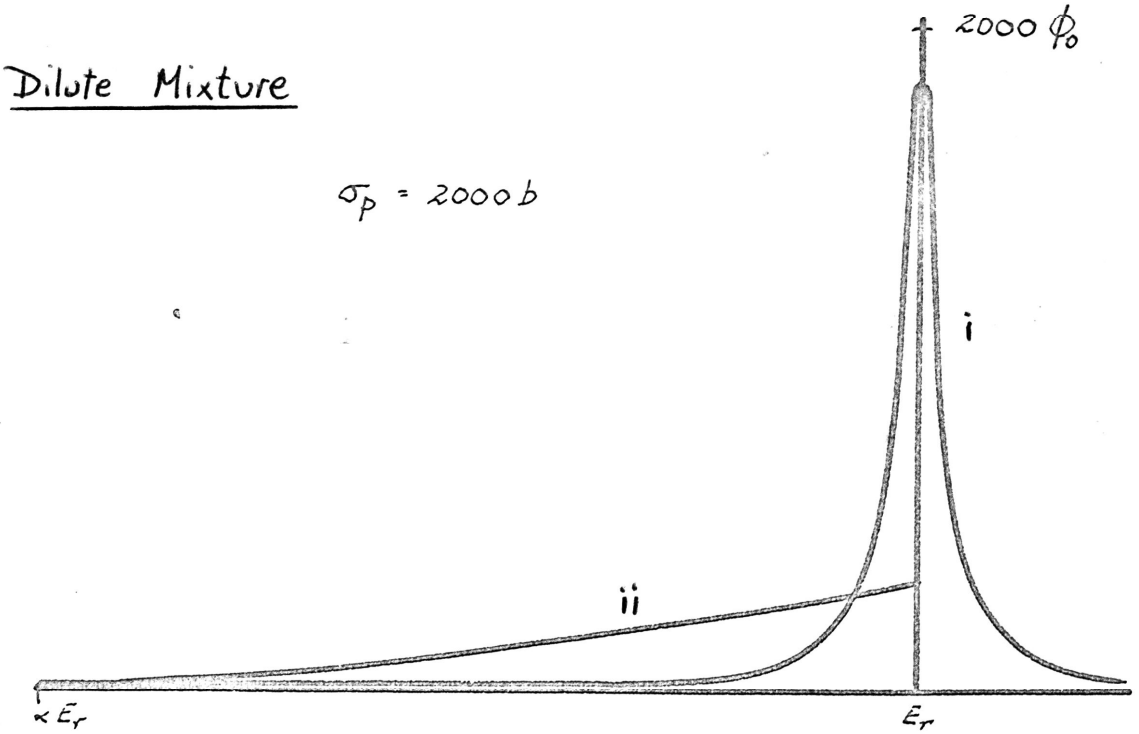
and combining equations 3.7 and 3.9 gives

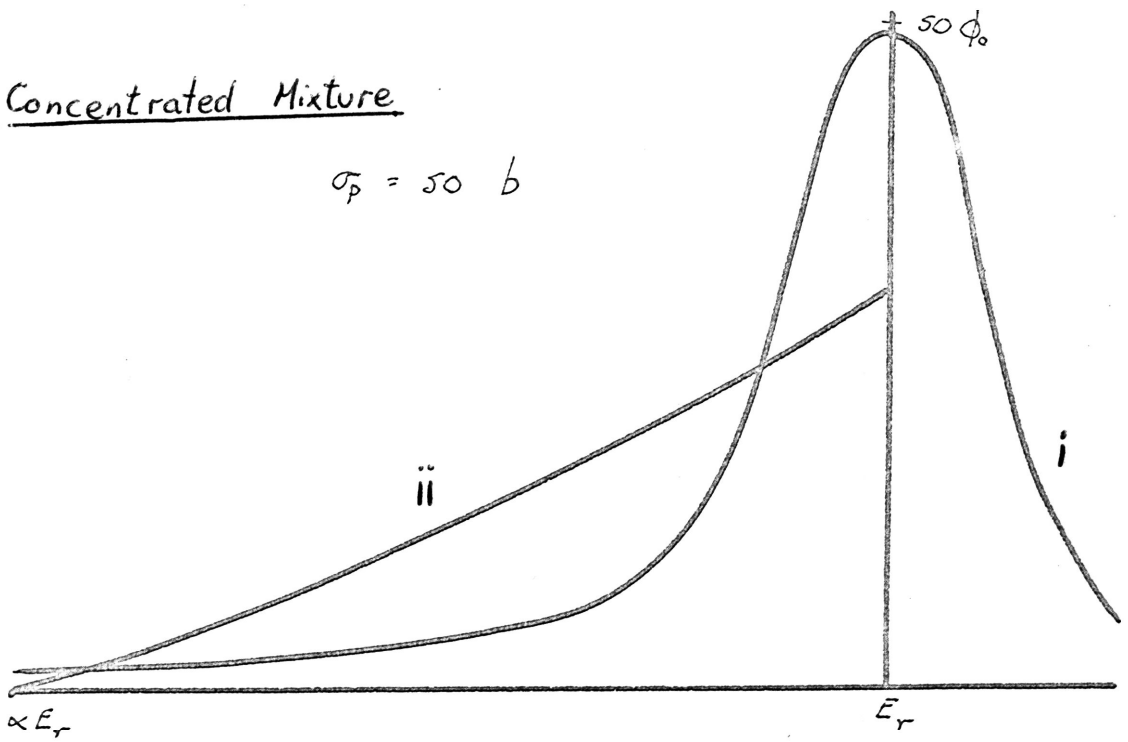
$$\Sigma_a = \frac{\Sigma_p\left(e^{-(u-u_r)}-\alpha\right)}{\frac{(1-\alpha)p}{1-p} - \frac{\Gamma_n}{\Gamma_a}\left(e^{-(u-u_r)}-\alpha\right)}\ H(u-u_r)\ H(u_r+\ell n\ 1/\alpha-u)\ . \qquad 3.10$$

It is to be noted that the absorption cross section is a function of α and Σ_p, which are parameters relating to the moderating species.

Fig I Comparison of $\sigma_a \phi$ for (i) Breit-Wigner Profile

(ii) "No perturbation" Profile





If we make the substitution

$$x = \frac{2(E-E_r)}{\Gamma}$$

then

$$\Sigma_a = \frac{\Sigma_p\left(\frac{x\Gamma}{2E_r} + (1-\alpha)\right)}{\frac{(1-\alpha)p}{1-p} - \frac{\Gamma_n}{\Gamma_a}\left(\frac{x\Gamma}{2E_r} + (1-\alpha)\right)} H_1 H_2 \quad . \tag{3.11}$$

where H_1, H_2 are the Heaviside functions of equation 3.10.

The function defined by equation 3.11 is a section of a rectangular hyperbola, whose asymptotes are

$$x = \left(\frac{p}{1-p} - \frac{\Gamma_n}{\Gamma_a}\right) \frac{(1-\alpha)\ 2E_r\ \Gamma_a}{\Gamma\ \Gamma_n} \tag{3.12}$$

$$\Sigma_a = \frac{-\Sigma_p\ \Gamma_a}{\Gamma_n} \quad . \tag{3.13}$$

The largest value of Σ_a is when $x = 0$, and is

$$\Sigma_{a\ max} = \frac{\Sigma_p}{\frac{p}{1-p} - \frac{\Gamma_n}{\Gamma_\gamma}} \quad . \tag{3.14}$$

In Fig. 1, a comparison is made between $\sigma_a\phi$ given by equation 3.9 and $\sigma_a\phi$ for the Breit Wigner profile for zero temperature and resonance parameters corresponding to the 6.7 ev resonance of U_{238}. The value of 1-p is taken as

$$1-p = \frac{\Gamma_a}{2E_r\ \bar{\xi}}\ \frac{\pi}{\sqrt{\{\beta(1+\beta)\}}}$$

and the expression for $\sigma_a\phi$ for the Breit Wigner profile is

$$\sigma_a\phi = \frac{\Gamma_a}{\Gamma}\ \frac{\sigma_o\sigma_p}{\sigma_o+\sigma_p+x^2\sigma_p}\ \phi_o \quad .$$

The parameters used for the two sets of curves were

$\bar{\xi} = .207$ $\quad E_r = 6.7$ ev

$\alpha = .64$ $\quad \Gamma_\gamma = 25 \times 10^{-3}$ ev

$T = 0^oK$ $\quad \Gamma_n = 1.6 \times 10^{-3}$ ev

The curves indicate that, for a concentrated mixture, the profile of equation 3.9, and the Breit Wigner profile have similar peak values, and both give appreciable absorption over a wide range of energy. However, for a dilute mixture, the peak values of absorption are quite different. The Breit Wigner profile gives appreciable absorption over only a small section of its infinite range, while the 'no perturbation' profile gives appreciable absorption over all of its finite range.

3.5 Flux Through a Resonance

Goldstein (1964) derived an expression for the flux in the region of a resonance. The expression gives the same value for the flux below, as above, the resonance and this obviously does not allow for the depletion of the flux due to absorption. An alternative expression which allows for flux depletion is derived in this section.

Briefly, Goldstein's method is an iterative procedure based on a modified form of equation 2.1

$$\Sigma_t \phi = \Sigma_{p1}\, \phi_o + \int_{u-\ell n\ 1/\alpha_2}^{u} \frac{(\Sigma_{p2}+\Sigma_s)\phi\ e^{-(u-u')}\, du'}{(1-\alpha_2)} \qquad 3.15$$

Equation 3.15 is a NR approximation with respect to the moderator, and is based on the result

$$\int_{u-\ell n\ 1/\alpha_1}^{u} \frac{\Sigma_{p1}\ e^{-(u-u')}\phi_o\ du'}{1-\alpha_1} \simeq \Sigma_{p1}\, \phi_o$$

which is so, because over most of the range of integration, the flux

$$\phi(u') \simeq \phi_o$$

(being off resonance).

On the assumption of a Breit Wigner single level resonance profile for zero temperature, Goldstein took the first iterant as the NR approximation

$$\phi_1 = \frac{\Sigma_p \phi_o}{\Sigma_t} = \frac{\phi_o(1+x^2)}{\beta_1^2 + x^2} \qquad 3.16$$

where,

$$\beta_1^2 = 1 + \frac{\sigma_o}{\sigma_p} . \qquad 3.17$$

The second iterant became

$$\Sigma_t \phi = \Sigma_{p1} \phi_o + \int_{u-\ell n\ 1/\alpha_2}^{u} \frac{(\Sigma_{p2}+\Sigma_s)\phi_o \Sigma_p e^{-(u-u')}}{(1-\alpha_2)\Sigma_t} du' \qquad 3.18$$

$$= \Sigma_p \phi_o \left\{1+\eta\left(\tan^{-1}\frac{x+\delta}{\beta_1} - \tan^{-1}\frac{x}{\beta_1}\right)\right\} \qquad 3.19$$

where $\delta = \dfrac{2E_r(1-\alpha_2)}{\Gamma}$,

and $\beta = \sigma_p/\sigma_o$,

$$\eta = \frac{\sigma_{p1}(\beta_1^2 - \beta^2)}{(\sigma_{p1}+\sigma_{p2})\beta_1\delta} .$$

The term $\tan^{-1}\dfrac{x+\delta}{\beta_1}$ on the right hand side of equation 3.19 is symmetric about

$$x = -\frac{\delta}{2} .$$

The asymptotic value of the flux for large u is ϕ_o, whereas it should be $p\phi_o$, where p is the resonance escape probability. The Goldstein result does not include the flux decrease due to neutron absorption.

To modify the result of equation 3.19, allowing for the reduction in neutron population, we first use the NR flux of equation 3.16 as a first iterant in equation 3.6. The second iterant becomes

$$\phi_2 = \frac{\Sigma_p \phi_o}{\Sigma_t} \left\{1 - \frac{\Gamma_a}{2\beta\bar{\xi}E_r} \int_x^\infty \frac{1}{\beta_1^2 + x^2}\, dx\right\}$$

where the usual approximation is made to the integral. Hence

$$\Sigma_t \phi_2 = \Sigma_p \phi_o \left\{1 - \frac{\Gamma_a}{2\beta\beta_1\bar{\xi}E_r} \left(\frac{\pi}{2} - \tan^{-1} x/\beta_1\right)\right\} \qquad 3.20$$

Further iteration gives additional terms which have as coefficients higher powers of $\frac{\Gamma_a}{2\bar{\xi}\beta\beta_1 E_r}$. The rate of convergence of the iteration procedure is determined by the value of $\frac{\Gamma_a}{2\bar{\xi}\beta\beta_1 E_r}$, which is smallest when the mixture contains only a small amount of resonant material.

If, now, we use the approximation of equation 3.20 as a first iterant for Goldstein's method, the second iterant becomes

$$\begin{aligned}\Sigma_t\phi = \Sigma_p\phi_o &\left\{1+\eta\left(\tan^{-1}\frac{x+\delta}{\beta_1} - \tan^{-1}\frac{x}{\beta_1}\right)\right\}\left(1 - \frac{\Gamma_a}{4\bar{\xi}\beta_1\beta E_r}\pi\right) \\ &+ \frac{\Gamma_a}{2\bar{\xi}\beta_1\beta E_r}\Sigma_p\phi_o \left\{\int_{u-\ell n\ 1/\alpha_1}^{u} \frac{\Sigma_{p1}\, e^{-(u-u')}}{\Sigma_t(1-\alpha_1)} \tan^{-1}\frac{x}{\beta_1}\, du'\right. \\ &\left. + \int_{u-\ell n\ 1/\alpha_2}^{u} \frac{(\Sigma_s+\Sigma_{p2})\, e^{-(u-u')}}{\Sigma_t(1-\alpha_2)} \tan^{-1}\frac{x}{\beta_1}\, du'\right\} \qquad 3.21\end{aligned}$$

The integrals of the last equation can be approximated and simplified by giving the term $\tan^{-1}\frac{x}{\beta_1}$ its value at the mid-point of the integration range. By this procedure the integrals of equation 3.21 reduce to the same form as that of equation 3.18. Hence

$$\begin{aligned}\Sigma_t\phi = \Sigma_p\phi_o &\left\{1+\eta\left(\tan^{-1}\frac{x+\delta}{\beta_1} - \tan^{-1}\frac{x}{\beta_1}\right)\left(1 - \frac{\Gamma_a}{4\bar{\xi}\beta_1\beta E_r}\pi\right)\right\} + \\ &\frac{\Gamma_a}{2\beta\ \beta\bar{\xi}E_r}\Sigma_p\phi_o\left\{\tan^{-1}\frac{x_1}{\beta_1} + \eta\tan^{-1}\frac{x_2}{\beta_1}\left(\tan^{-1}\frac{x+\delta}{\beta_1} - \tan^{-1}\frac{x}{\beta_1}\right)\right\} \qquad 3.22\end{aligned}$$

where $$x_i = \frac{x(1+\alpha_i)+4}{2\alpha_i} .$$

It is of interest to see whether the flux predicted by equation 3.22 is in agreement with the correct flux values in regions well removed from the resonance. When $x \to +\infty$

$$\Sigma_t\phi = \Sigma_p\phi = \Sigma_p\phi_o \left(1 - \frac{\Gamma_a \pi}{4\bar{\xi}\beta\beta_1 E_r}\right) + \Sigma_p\phi_o \frac{\Gamma_a \pi}{4\bar{\xi}\beta\beta_1 E_r}$$

$$= \Sigma_p\phi_o$$

and when $x \to -\infty$.

$$\Sigma_t\phi = \Sigma_p\phi = \Sigma_p\phi_o \left\{1 - \frac{\Gamma_a \pi}{2\beta_1\bar{\xi}F_r\beta}\right\}$$

$$\simeq p\ \Sigma_p\phi_o .$$

The expression for the flux will go to the correct asymptotic value on condition that the NR approximation can be used, i.e.

$$\frac{\Gamma_a \pi}{2\beta\beta_1\bar{\xi}E_r} = 1 - p.$$

The quantity $\frac{\Gamma_a \pi}{2\beta\beta_1\bar{\xi}E_r}$ could be replaced by 1-p in equation 3.22, so that it no longer depends on the NR approximation. The modified form of equation 3.22 would give the exact flux value below the resonance.

In section 7.2 (p.60) the predicted value of the flux obtained by use of equation 3.22 is checked against the flux obtained by numerical solution of the slowing down equation. The agreement is to within 4% and equation 3.22 is considered to be a better approximation than equation 3.19.

4. APPROXIMATION FOR ABSORPTION IN CENTRAL RESONANCE REGION

4.1 Introduction

The shape of the Placzek function would suggest that evaluation of equation 3.5 would give a flux depression near a lethargy greater by $\ell n\ 1/\alpha_1$, than u_r. In Chapter 3, this possibility was ignored by taking

$$\int_{u-\ell n\ 1/\alpha_1}^{u} \frac{\Sigma_{pl}\ \phi\ e^{-(u-u')}}{1-\alpha_1}\ du' \simeq \Sigma_{pl}\ \phi\ .$$

Evaluation of equation 3.5 is not possible because of the complexity of the functions forming the integrand. Polynomial approximation for the quantity $\Sigma_a\phi$ would allow evaluation of the integral, but for high order polynomials, the result is quite complicated. In the interests of comparative simplicity, and in order to use Simpson's integration rule, a pair of parabolas symmetrically placed about $E=E_r$ is used for approximation purposes. Since only the central region of a resonance gives a large flux perturbation effect, an approximation is obtained for the central region only.

4.2 Parabolic Approximation for $\Sigma_a\phi$, at zero temperature

It is to be noted that the points x=0,1,2,3; y=1,.5,.2,.1 lie on both the curves

$$y = \frac{1}{1+x^2}$$

and

$$10y = (x-3)^2+1\ .$$

The slope of the parabola is zero at x=3, and the areas under the curves for $0 \leq x \leq 3$, are 1.23 and 1.2 units respectively.

The absorption reaction rate, for a resonance, using the NR flux approximation, is

$$\Sigma_a \phi = \frac{N \Gamma_a}{\Gamma E_r} \frac{\sigma_p}{(1+\frac{1}{\beta})+x^2} \phi_o \qquad 4.1$$

where β is again σ_p/σ_o.

If we put $\sqrt{1+1/\beta}\ \zeta = x$, then

$$\Sigma_a \phi = \frac{N \Gamma_a}{\Gamma E_r} \frac{\sigma_p}{(1+1/\beta)} \frac{1}{1+\zeta^2} \phi_o \qquad 4.2$$

which we may approximate as

$$\Sigma_a \phi = \frac{N \Gamma_a}{\Gamma E_r} \frac{\sigma_o \sigma_p}{\sigma_o+\sigma_p} \frac{\phi_o}{10} \{(\zeta-3)^2+1\}, \quad 0 \leq \zeta \leq 3,$$

$$= \frac{N \Gamma_a}{\Gamma E_r} \frac{\sigma_o \sigma_p}{\sigma_o+\sigma_p} \frac{\phi_o}{10} \{(\zeta+3)^2+1\}, \quad 0 \geq \zeta \geq -3. \qquad 4.3$$

4.3 Parabolic Approximation for $\Sigma_a \phi$, allowing for Temperature

In order to obtain a parabolic approximation for $\Sigma_a \phi$ for any temperature, it is necessary to first reduce the function

$$\frac{\psi(x,\theta)}{\sigma_p+\sigma_o\ \psi(x,\theta)} \qquad \text{(i)}$$

by approximating to a standard form

$$\frac{c}{1+\zeta^2} \qquad \text{(ii)}$$

whence the results of the previous section can be applied. If we take ζ to be of the form

$$= \frac{E-E_r}{G/2} \qquad 4.4$$

estimates of the quantities c, and G are needed.

Applying the criterion that the two values of functions (i) and (ii) are to coincide at $E=E_r$, it follows that

$$c = \frac{\psi_o}{\sigma_p+\sigma_o\ \psi_o} \qquad 4.5$$

where $\psi_o = \psi(0,\theta)$.

If, in addition, the function of ζ corresponding to $\psi(x,\theta)$ is to have the same integral over the range $x = \pm\infty$, as has $\psi(x,\theta)$; then

$$\int_{-\infty}^{\infty} \frac{c}{1-\sigma_o c+\zeta^2}\, dx = \int_{-\infty}^{\infty} \frac{\psi(x,\theta)}{\sigma_p}\, dx \ ,$$

and as $\quad G\ d\ \zeta = \Gamma\ dx$

so, $$\int_{-\infty}^{+\infty} \frac{\sigma_p c}{1-\sigma_o c+\zeta^2}\ \frac{G}{\Gamma}\, d\zeta = \pi.$$

Hence

$$\frac{\sigma_p c\ G}{\sqrt{(1-\sigma_o c)}\,\Gamma} = \pi$$

and using result 4.5, gives

$$G = \frac{\Gamma\sqrt{(\sigma_p+\sigma_o\ \psi_o)}}{\sqrt{\sigma_p\ \psi_o}} \ . \qquad 4.6$$

When $T = 0$, $\psi_o = 1$.

$$G = \frac{\Gamma\sqrt{(\sigma_p+\sigma_o)}}{\sqrt{\sigma_p}} \ .$$

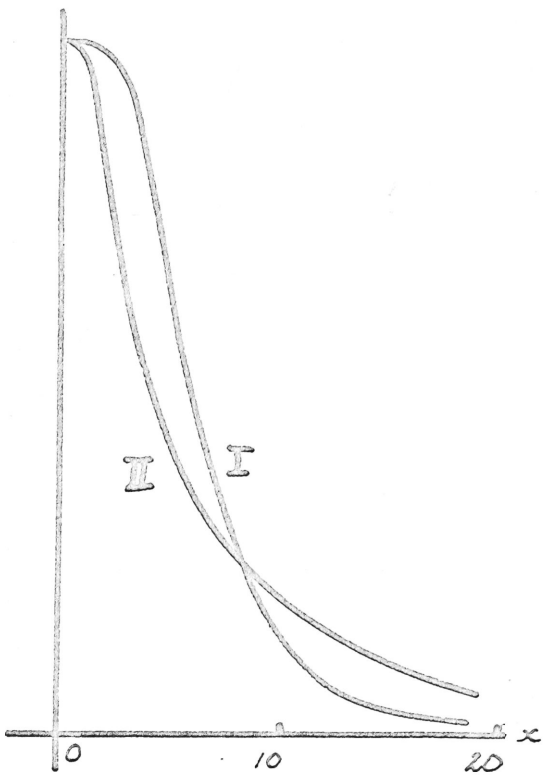
Using equations 4.3, an approximation to $\Sigma_a\phi$ is

$$\Sigma_a\phi = \frac{N\ \Gamma_a}{\Gamma\ E_r}\ \frac{\sigma_o\ \sigma_p}{\sigma_p+\sigma_o\ \psi_o}\ \frac{\phi_o}{10}\ \{(\zeta-3)^2+1\}, \quad 0\leq x\leq 3 \ ,$$

$$= \frac{N\ \Gamma_a}{\Gamma\ E_r}\ \frac{\sigma_o\ \sigma_p}{\sigma_p+\psi_o\ \sigma_o}\ \frac{\phi_o}{10}\ \{(\zeta+3)^2+1\}, \quad 0\geq x\geq -3 \ . \qquad 4.7$$

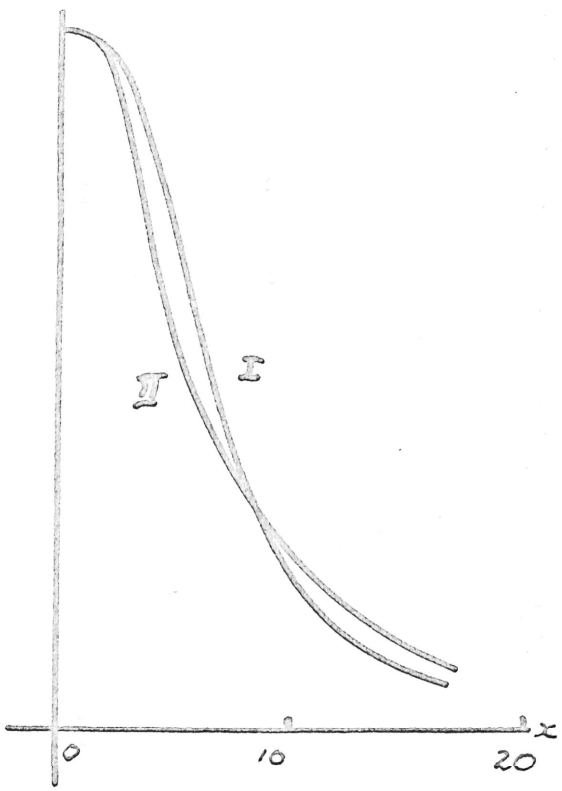
Fig II B Comparison of (I) $\psi / (\sigma_p + \sigma_0 \psi)$

(II) $\left\{ \psi_0 / (\sigma_p + \sigma_0 \psi_0) \right\} \times \frac{1}{1+\varphi^2}$



$T = 300^\circ K$

$G = 5.3\,\Gamma$



$T = 600^\circ K$

$G = 6.3\,\Gamma$

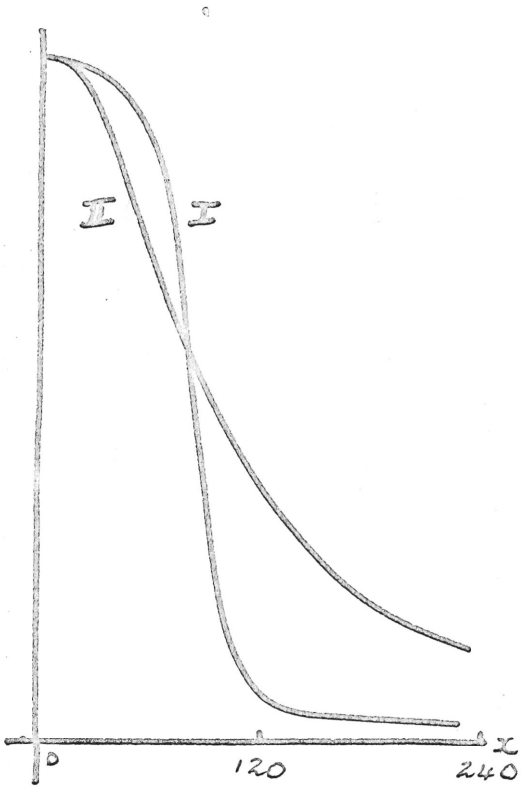
Common Data:- $E_r = 189.6$ e.v. , $\Gamma_n = 0.068$ e.v

$\Gamma_\gamma = 0.1$ e.v. , $\Gamma_f = 0.0$ e.v

$\sigma_p = 2000b$, $g = 1.0$

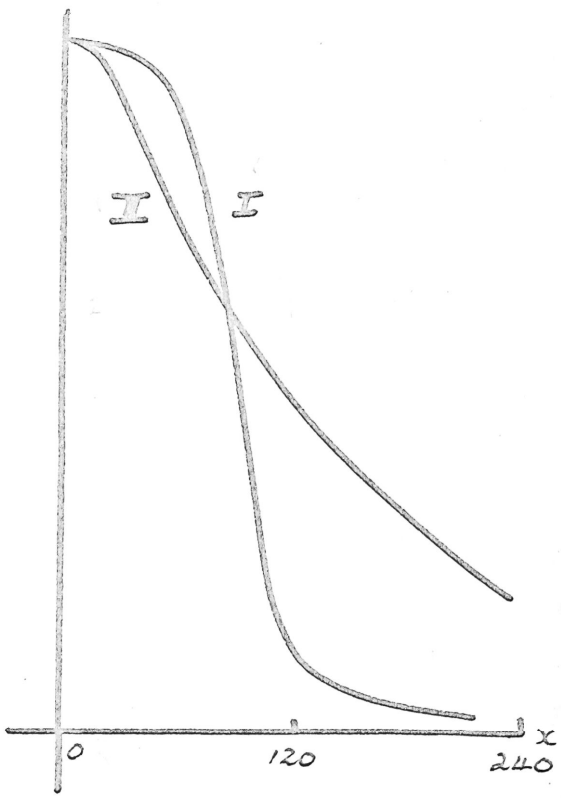
Fig II(A) Comparison of (I) $\psi / (\sigma_p + \sigma_0 \psi)$

(II) $\{ \psi_0 / (\sigma_p + \sigma_0 \psi_0) \} \times \frac{1}{1+\zeta^2}$



$\sigma_p = 2000 b$

$G = 87.9 \Gamma$



$\sigma_p = 500 b$

$G = 120.6 \Gamma$

Common Data:- $E_r = 6.67$ ev, $\Gamma_m = 0.0025$ ev

$\Gamma_\gamma = 0.025$ ev, $\Gamma_f = 0.$ ev

$g = 1.0$, $T = 300^\circ$ K.

It is of interest to compare

$$\int_0^\infty \frac{\sigma_o\, c}{1+\zeta^2}\, dx \text{ with } J(\theta,\beta)$$

for extreme values of the parameters.

We have

$$\int_0^\infty \frac{\sigma_o\, c}{1+\zeta^2}\, dx = \int_0^\infty \frac{\sigma_o\, c}{1+\zeta^2}\, \frac{G}{\Gamma}\, d\zeta$$

$$= \frac{\sigma_o\, \psi_o}{\sigma_o\, \psi_o+\sigma_p}\, \frac{\sqrt{(\sigma_p+\sigma_o\, \psi_o)}}{\sqrt{\sigma_p\, \psi_o}}\, \pi/2 \qquad 4.8$$

When $T\to\infty$ ($\psi_o\to 0$) or when β is large, $\left(\beta=\frac{\sigma_p}{\sigma_o}\right)$, the RHS of 4.8 reduces to $\frac{\pi}{2\beta}$, which agrees with the result for $J(\theta,\beta)$ and which was evaluated in section 2.7.1.

When $\sigma_p << \sigma_o$, the result 4.8 simplifies to

$$\frac{\pi}{2\sqrt{(\beta\, \psi_o)}}$$

which is not the correct value. The reason for the disagreement is that in the wings of the resonance, the asymptotic values of the two functions do not agree; they are

$$\frac{\beta\psi_o}{(\beta+\psi_o)(\beta+\psi_o x^2)} \text{ and } \frac{1}{\beta+1+x^2}\ .$$

In Fig.II, a comparison is made between the values for $\Sigma_a\phi/K$, for the Breit Wigner profile,

$$\Sigma_a\phi = K\psi/(\sigma_p+\sigma_o\psi)\ ,$$

and the approximation

$$\Sigma_a\phi \simeq K\psi_o/(\sigma_p+\sigma_o\, \psi_o)(1+\zeta^2)\ ,$$

where $K = \Sigma_p\, \phi_o\, \sigma_o \frac{\Gamma_a}{\Gamma}$,

for two different resonances.

It is to be noted that for small G/Γ the curves are in close agreement, but the agreement is not close for large G/Γ.

However, for a study of flux perturbations, the wings are not so important since the major contribution comes from the region where $\Sigma_a\phi$ is largest. An estimate of the absorption is obtained by integration over the central region of the curve for $\Sigma_a\phi$, and the errors observable in Fig.II tend to cancel.

5. EFFECT OF FLUX PERTURBATIONS FROM ONE RESONANCE, ON THE ABSORPTION BY A SECOND RESONANCE

5.1 Introduction

The problem of resonance overlap, when the central portions of the two resonances overlap to some extent has been considered by Corngold and Schermer (1959) and O'Halloran and Keane (1966). The present discussion is restricted to resonances which have greater separation than the separation which gives a negligible overlap effect when flux perturbations from the higher resonance are not considered. The major portion of any flux perturbation effect will be caused by the central region of a resonance. Only flux perturbations which fall on the central region of a resonance will produce any appreciable change in the absorption by that resonance.

5.2 Reduction in Resonance Absorption by a δ-Resonance because of Flux Perturbations from another δ-Resonance

For a δ-resonance, with resonance escape probability p_1, where the subscript 1 refers to the resonance of greater energy, the flux for $u>u_{r_1}$, is given by equation 3.1, namely

$$\Sigma_t\phi = \Sigma_p\phi_o\{1 - \bar{\xi}(1-p_1)\ P_n(u-u_{r_1})\}$$

and the absorption in the second resonance will apparently be

$$A = \Sigma_p\phi_o\{1 - \bar{\xi}(1-p_1)\ P_n(u_{r_2}-u_{r_1})\}\bar{\xi}(1-p_2)\ .$$

The reduction in absorption by the second resonance will apparently be

$$\delta A = (1-p_2)(1-p_1)\ \bar{\xi}^2\ P_n(u_s) \qquad 5.1$$

where $u_s = u_{r_2} - u_{r_1}$, and n is the number of nuclear species present in the mixture.

However, the absorption by a narrow resonance is approximately

$$N\Gamma_a \sigma_p \phi_o J(\theta,\beta)$$

and for zero temperature it is

$$\frac{N\pi\Gamma_a \sigma_p \phi_o}{2\sqrt{\{(1+\beta)\beta\}}} ,$$

where $\beta = \frac{\sigma_p}{\sigma_o}$ as before.

If the practical width of a resonance is defined to be $|x_1-x_2|$, where x_1,x_2 are the roots of the equation

$$\frac{\sigma_o}{1+x^2} = \sigma_p$$

then $$x_1,x_2 = \pm\sqrt{(\beta-1)}.$$

The absorption within a practical width of a resonance is

$$N\Gamma_a \sigma_p \phi_o \int_o^{\sqrt{(\beta-1)}} \frac{dx}{\beta x^2+\beta+1} = \frac{\Gamma_a \sigma_p}{\sqrt{\{(1+\beta)\beta\}}} \tan^{-1} \frac{\sqrt{(\beta-1)}}{\sqrt{(\beta+1)}} N\phi_o$$

and for a resonance in which $\sigma_o >> \sigma_p$, the total absorption reduces to

$$\frac{\pi \sigma_p \Gamma_a}{2\sqrt{\{(\beta+1)\beta\}}} N\phi_o$$

while the absorption within a practical width is

$$\frac{\pi \sigma_p \Gamma_a}{4\sqrt{\{(\beta+1)\beta\}}} N\phi_o$$

At best no more than half of the total absorption by a resonance occurs within a practical width.

In view of the above remarks, the estimate of equation 5.1 ought to be modified to

$$\delta A = \varepsilon(1-p_2)(1-p_1)\bar{\xi}^2 \, P_n(u_s) \qquad 5.2$$

where $0<\varepsilon<1$

since the central region of a resonance gives the major flux perturbation effect.

5.3 Reduction in the Resonance Absorption of a δ-Resonance because of flux perturbations from a Narrow Resonance

The flux from a narrow resonance was given by equation 3.5 (NR approximation), and the flux change due to flux perturbations is given by

$$\delta\phi = -\int_0^u P_3(u-u')\Sigma_a\phi \, du' \qquad 5.3$$

when the two resonances are of different species (two resonant species and one moderating species). Since we are concerned with large separations

$$u_s > 3 \, \ell n \, 1/\alpha_i$$

where the subscript i refers to species other than the moderator, and $P_3(u)$ is defined by equation A4, Appendix A. If we assume the concentration of the resonant species is low, then $P_3(u)$ can be replaced by $P_1(u)$ in equation 5.3 to give

$$\delta\phi = -\int_0^u P_1(u-u')\Sigma_a\phi \, du' \, . \qquad 5.4$$

The flux change due to the central region of the resonance may be expressed as

$$\delta\phi = -\int_{u_1}^{u_2} P_1(u-u')\Sigma_a\phi \, du' \, , \qquad 5.5$$

where u_1, u_2 are the chosen limits of the central region. If we consider that the resonance is narrow, then

$$u_2 - u_r \simeq u_r - u_1$$

where u_1 and u_2 are now taken to correspond to the extremes of the approximation given by equation 4.3. By using the relations

$$\delta u \simeq \frac{dE}{E_r} \; ; \quad \delta E = \delta\zeta \frac{G}{2} \; ; \quad \delta\zeta = \frac{3}{2}$$

to obtain the numerical integration interval δu, and using the points

$$\zeta = -3, \; -3/2, \; 0, \; 3/2, \; 3$$

$$\Sigma_a \phi = \left(\frac{1}{10} \; , \; \frac{13}{40} \; , \; 1 \; , \; \frac{13}{40} \; , \; \frac{1}{10}\right) \; \frac{N\Gamma_a \, \sigma_o \, \sigma_p \, \phi_o \, \psi_o}{E_r(\sigma_p + \sigma_o \, \psi_o)}$$

(corresponding to equation 4.3) for Simpson's integration rule, we get

$$\delta\phi(u) = \frac{\Gamma_a \, \sigma_o \, \sigma_p \, G \, N\phi_o \, \psi_o}{\Gamma(\sigma_p + \psi_o \, \sigma_o) E_r \; 40} \left\{ P_1\left(u_s - \frac{3G}{2E_r}\right) + 13P_1\left(u_s - \frac{3G}{4E_r}\right) + 20P_1(u_s) \right.$$

$$\left. + \, 13P_1\left(u_s + \frac{3G}{4E_r}\right) + P_1\left(u_s + \frac{3G}{2E_r}\right) \right\} \; , \qquad 5.6$$

where $u = u + u_s$.

The result 5.6 changes the single discontinuous jump of the Placzek function, $P_1(u)$, at $u = \ell n \, 1/\alpha_1$, to a set of smaller discontinuities. Only analytical integration can remove the discontinuity from the flux equation. It is unlikely that one of the values of $P_1(u)$ in equation 5.6 should require, in a practical problem, evaluation at the point of discontinuity, but if so the mean value would be used.

If we average the values inside the bracket of equation 5.6, the result is

$$\delta\phi(u) = -\frac{\Gamma_a}{\Gamma}\,\frac{6\,\sigma_o\,\sigma_p\,\psi_o\,N\,G\,\phi_o}{5(\sigma_p+\sigma_o\,\psi_o)\,E_r}\,P_1(u_s) \qquad 5.7$$

If there is a δ-resonance at $u=u_{r_2}$, whose resonance escape probability is p_2, then the change in absorption is

$$\delta A = \frac{1.2N\Gamma_{a1}}{\Gamma_1\,E_{r_1}}\,\frac{\sigma_{o1}\,\sigma_p}{\sigma_p+\sigma_{o1}\,\psi_{o1}}\,G_1\bar{\xi}\,P_1(u_s)\phi_o\,(1-p_2)\,, \qquad 5.8$$

where $u_s = u_{r_2} - u_{r_1}$. The subscript 1 has been added to indicate the resonance of higher energy. In view of the remarks of section 5.2, equation 5.8 should be modified to read

$$\delta A = \frac{1.2\varepsilon\,N\Gamma_{a1}}{\Gamma_1\,E_{r_1}}\,\frac{\sigma_{o1}\,\sigma_p}{\sigma_p+\sigma_{o1}\,\psi_{o1}}\,G\bar{\xi}\,P_1(u_s)\phi_o\,(1-p_2)\,. \qquad 5.9$$

5.4 Reduction in Absorption by a Narrow Resonance because of Flux Perturbations from another Narrow Resonance

Flux perturbations which fall on the wings of the second resonance will contribute little to the change in the absorption by the second resonance, and only the effect of flux perturbations on the absorption in the centre of the second resonance need be considered.

The change in absorption is given by

$$-\delta A = \int_{u_1}^{u_2} (\delta\phi)\Sigma_a\,du'\,, \qquad 5.10$$

where $\delta\phi$ is given by equation 5.7, and represents the flux change caused by the upper resonance. If once again we use the approximation of equation 4.3 to assist in evaluating equation 5.10, and use Simpson's Rule as

before:-

$$-\delta A = \frac{1.2N\Gamma_1}{\Gamma_1 E_{r_1}} \frac{\sigma_{o_1}\sigma_p}{\sigma_p+\sigma_{o_1}\psi_{o_1}} G_1 \frac{1}{40}\left\{P\left(u_s - \frac{3G_2}{2E_{r_2}}\right) + 13P\left(u_s - \frac{3G_2}{4E_{r_2}}\right)\right.$$

$$\left. + 10P(u_s) + 13P\left(u_s + \frac{3G_2}{4E_{r_2}}\right) + P\left(u_s + \frac{3G_2}{2E_{r_2}}\right)\right\} \frac{\Gamma_{\gamma_2}\sigma_{o_2} G_2 \phi_o}{\Gamma_2 E_{r_2}(\sigma_p+\sigma_{o_2}\psi_{o_2})}$$

If we average the values of P(u) we get

$$-\delta A = \frac{1.44\, N\, \Gamma_{a_1}\Gamma_{a_2} G_1 G_2 \sigma_{o_1}\sigma_{o_2}}{\Gamma_1\Gamma_2 E_{r_1} E_{r_2}(\sigma_p+\sigma_{o_1}\psi_{o_1})(\sigma_p+\sigma_{o_2}\psi_{o_2})} \Sigma_p \phi_o P(u_s) ,$$

where again $u_s = u_{r_2} - u_{r_1}$.

By substituting from equation 4.6 for the values G_1, G_2, then

$$-\delta A = 1.44\, \Sigma_p \phi_o \frac{\Gamma_{a_1}\Gamma_{a_2}}{E_{r_1} E_{r_2}} \frac{\sigma_{o_1}\sigma_{o_1} P(u_s)}{\sigma_p \psi_{o_1}\psi_{o_2}} \left(\frac{1}{(\sigma_p+\psi_{o_1}\sigma_{o_1})(\sigma_p+\psi_{o_2}\sigma_{o_2})}\right)^{\frac{1}{2}}. \qquad 5.12$$

5.5 Two Resonances with 'No Flux Perturbation' Profiles

In section 3.4 a resonance profile was derived so that a resonance with such a profile would not cause flux perturbations. The resonance was assumed to be isolated. The overlap effect for two resonances with 'no perturbation' profiles becomes zero when the resonances are separated by a lethargy greater than twice a moderator collision interval. For two resonances with Breit Wigner profiles, the separation at which the overlap effect can be neglected is a function of temperature, because of Doppler broadening.

Two resonances with 'no perturbation' profiles would cause perturbation effects when any overlap of the resonances occurs. Thus, though the resonance profile for no flux perturbations can be tailored to suit an isolated resonance, such a profile is not suitable for resonances which are close together.

6. NUMERICAL SOLUTION OF SLOWING DOWN EQUATION - THE PROGRAMME 'EXPEAS'

6.1 Introductory Remarks

EXPEAS was designed to calculate, for an infinite homogeneous mixture, the flux in the region of, and the absorption by, two resonances which are close together, by stepping through the resonance and solving the slowing down equation at each step. The calculation starts at a lethargy well below and ends at a lethargy well above, the lethargies of resonance. It is to be noted that for practical use, the programme is best used for low energies (<10eV), since it was written to obtain flux perturbation effects, and use at high energies would use considerable computer time.

To evaluate the effect of one resonance on the other, the resonance absorption for each resonance is first calculated as if the other resonance were not present, and the calculation is repeated with both resonances present.

The equation solved is a specific form of equation 2.1 and is

$$\sigma_t\phi = \sum_{i=1,2} \int_{u-\ell n\ 1/\alpha_i}^{u} \frac{(\sigma_{si}+\sigma_{pi})\phi\ e^{-(u-u')}du'}{(1-\alpha_i)} + \int_{u-\ell n\ 1/\alpha_3}^{u} \frac{\sigma_{p3}\phi\ e^{-(u-u')}du'}{(1-\alpha_3)} \qquad 6.1$$

where (1) the subscript 3 refers to the moderator.

(2) σ_{pi} (i=1,2) is the potential scattering cross section for the species having the i^{th} resonance, if the resonances are of different species, but, σ_{pi} is half the potential scattering cross section of the resonant species if both resonances belong to the same species.

(3) σ_{si} is the resonance scattering cross section of the i^{th} resonance.

(4) The microscopic cross sections are given per nucleus of the species which has the resonance of higher energy.

The resonances are taken as having the single level Breit Wigner Doppler broadened profile, and interference between potential and resonance scattering is ignored.

6.2 Numerical Procedure

The numerical procedure follows closely the method used by Pollard (1964) in his programme PEAS.

6.2.1 Choice of Grid

Part of the input information determines the number N_3, of steps into which each interval of lethargy for the moderator, $\Delta n\ 1/\alpha_3$, is divided to give an approximate step length of the grid for the calculation.

The step length, δu, is then adjusted so that,

$$M = \frac{u_{r_2} - u_{r_1}}{\delta u}$$

where M is an even integer. By adjusting u, the resonance cross sections can be calculated at intervals δu, by stepping out from the centre of each resonance, and the calculated values correspond to points of the grid, for both resonances.

Because of the adjustment to δu, each interval of integration, $\ell n\ 1/\alpha_i$, i=1,2,3, does not necessarily consist of an integral number of subdivisions. Even numbers N_i(i=1,2,3), (N_3 being redefined), are defined so that

$$\frac{\ell n\ 1/\alpha_i}{\delta u} - 2 \leq N_i \leq \frac{\ell n\ 1/\alpha_i}{\delta u} \quad .$$

Each range of integration may have a small section, less than $2\delta u$, which is not included in the numerical integration. Due allowance is made, and each numerical integration is adjusted by an appropriate amount.

The computation starts at a lethargy $u_{r_1} - 2N_3\delta u$ which is very nearly 2 lethargy intervals of the moderator, below the lethargy corresponding to E_{r_1}, and ends at a lethargy $u_{r_2} + 2N_3\delta u$. The region of any large Placzek perturbations is included in the calculation.

6.2.2 Generation of $\psi(x,\theta)$

Near the centre of a resonance, the differential equation for $\psi(x,\theta)$, equation 2.35, is solved numerically for values of x corresponding to the grid values of lethargy.

For each resonance, the energies corresponding to the grid values of lethargies

$$u_{r_i} \pm n\delta u \quad , \quad i=1,2$$

which, for suitable n, are all the points of the chosen grid, are given as

$$E^{\pm}_n = E_{r_i}\ e^{\mp(n\delta u)} \quad i=1,2$$

In general $$E_k = E_{k-1}\, e^{-\delta u}$$

and $$x_k = x_{k-1} - dE_{k-1}$$

where $$d = \frac{2}{\Gamma}(e^{-\delta u} - 1)$$

To minimise round-off errors, the code uses

$$d = -\frac{2\delta u}{\Gamma}\left\{1 - \frac{\delta u}{2} + \frac{\delta u^2}{6} - \frac{\delta u^3}{24}\right\} .$$

Using the above equations, an iterative procedure for the generation of $\psi(x,\theta)$ can be written as:-

$$\delta x_k = - dE_{k-1}$$

$$x_k = x_{k-1} + \delta x_k$$

$$E_k = E_{k-1} + \frac{\Gamma}{2}\delta x_k$$

$$\psi_k = \psi_{k-1} + \delta x_k\, \psi'_{k-1} + \frac{\delta x_k^2}{2}\psi''_{k-1} + \frac{\delta x_k^3}{6}\psi'''_{k-1}$$

$$\psi'_k = \psi'_{k-1} + \delta x_k\, \psi''_{k-1} + \frac{\delta x_k^2}{2}\psi'''_{k-1}$$

$$\psi''_k = \tfrac{1}{4}\theta^4 - \theta^2 x_k\, \psi'_k - \tfrac{1}{4}\theta^2(2+\theta^2+\theta^2 x_k^2)\psi_k$$

$$\psi'''_k = -\theta^2 x_k\, \psi''_k - \tfrac{1}{4}\psi'_k - \tfrac{1}{4}\theta^2(6+\theta^2+\theta^2 x_k^2)\psi'_k - \tfrac{1}{2}\theta^4 x_k\, \psi_k$$

where primes denote differentiation with respect to x.

The solution starts at x = 0, where $\psi(x,\theta)$ has the initial conditions

$$E_j = E_r$$

$$x_j = 0$$

$$\psi_j = \theta\ \mathrm{erc}\ \frac{\theta}{2}$$

$$\psi'_j = 0$$

To evaluate $\psi(0,\theta)$ we use the relations

$$\text{erc } y = \tfrac{1}{2}\sqrt{\pi}\, e^{y^2} \text{ erfc } y$$

$$= \sum_{1}^{5} a_i \eta^i$$

provided $y \lesssim 1.5$, where

$$\eta = \frac{1}{(1+py)}$$

The constants p, and a_i (i=1,5) are given by Hastings (1955).

When x_k has been increased so that

$$|x_k| \gtrsim 12/\theta^2$$

the function $\psi(x,\theta)$ is obtained from its asymptotic series, equation 2.39, and when x_k reaches a value so that

$$[(3x_k^2-1) + (15x_k^2(x_k^2-2)+2)V_k]V_k \lesssim 10^{-4},$$

the function $\psi(x,\theta)$ is obtained from a further truncation of its asymptotic series, namely

$$\psi_k = \frac{1}{1+x_k^2} \quad .$$

It is to be noted that the iteration procedure has to be worked both ways from the centre of the resonance as

$$-x_{-k} \neq x_k$$

and the symmetry of $\psi(x,\theta)$ cannot be used.

6.2.3 Method of Integration

Equation 6.1 can be written, using Simpson's Rule

$$\sigma_t\phi - \sum_{i=1,3} \frac{\sigma_{pi}}{1-\alpha_i}\frac{\delta u}{3} - \sum_{i=1,2} \frac{\sigma_{si}}{1-\alpha_i}\frac{\delta u}{3} = \sum_{i=1,3} (Y_i+R_i)\frac{\delta u}{3(1-\alpha_i)} \qquad 6.2$$

where $Y_i = \sum_{K=L+1}^{L+N_i} \{S_K(\sigma_{pi}+\sigma_{si})\phi_K \frac{e^{-(K-L)\delta u}}{1-\alpha_i} + (\sigma_{pi}+\sigma_{si})\phi_{N_i+L+1} \frac{e^{-N_i\delta u}}{1-\alpha_i}\}$

and S_K = 2 or 4, depending on whether K-L is odd or even, and L is a grid point

Two separate values of Y_i, for each i, are used in the calculation through the resonances, and are used alternately. If one value of Y_i is given as

$$Y_{i_1} = \{4(\sigma_{pi}+\sigma_{si})\phi_L\ e^{-\delta u} + 2(\sigma_{pi}+\sigma_{si})\phi_{L+1}\ e^{-2\delta u} + \ldots\}$$

the corresponding value for Y_i for the next calculation of ϕ at the next point of the grid will be

$$Y_{i_2} = \{4(\sigma_{pi}+\sigma_{si})\phi_{L-1}\ e^{-\delta u} + 2(\sigma_{pi}+\sigma_{si})\phi_L\ e^{-2\delta u} + \ldots\}$$

but for the one after, will be

$$Y_{i_3} = \{4(\sigma_{pi}+\sigma_{si})\phi_{L-2}\ e^{-\delta u} + 2(\sigma_{pi}+\sigma_{si})e^{-2\delta u}\phi_{L-1} + 4(\sigma_{pi}+\sigma_{si})\phi_L\ e^{-3\delta u}\ldots\}$$

The pattern of numerical integration repeats itself every alternate step on stepping through the resonances. Each of the values Y_{i_1} and Y_{i_2} are adjusted by a product of $e^{-\delta u}$ and suitable subtraction and addition of terms after each evaluation of equation 6.2.

The terms R_i are evaluated by extrapolation, using the last four terms of the summation Y_i. Cubic extrapolation is used (since Simpson's

Rule is cubic in accuracy) to obtain the values of the integrand at points $\frac{r}{2}$ and r above the last term of the Simpson summation, where

$$r = \ell n\ 1/\alpha_i - N_i\ \delta u.$$

Simpson's Rule is then applied to the section of the integral which has not been covered by the integral rule, to give

$$R_i = (4w_3\ y^3 + \tfrac{4}{3}\ w_2\ y^2 + 2w_1 y + 2w_o)r$$

where the w_j are the coefficients of the cubic extrapolation based on abscissae 0,1,2,3 and

$$y = \frac{r}{2\delta u}\ .$$

6.2.4 Initial Values of Flux-Upper End Correction

The first value of ϕ_L calculated from equation 6.2 corresponds to a lethargy of $u_{r_1} - 2N_3\delta u$, and the initial values of ϕ_K, K>L used to begin the stepping through procedure are obtained by evaluating the resonance integrals and using equations 2.16, 2.17, 2.18.

For each resonance with $E_a >> E_r$

$$p \doteq \exp\left\{\int_{\infty}^{x_a} \frac{\Gamma_\gamma}{\xi 2E_r}\ \frac{\sigma_p}{(1+\beta)+\beta x^2}\ \phi_o\ dx\right\}$$

$$\doteq \exp\left\{-\frac{\Gamma_\gamma\ \sigma_p}{\xi 2E_r\sqrt{\{\beta(\beta+1)\}}}\left(\frac{\pi}{2} - \tan^{-1} x_a\sqrt{\frac{\beta}{\beta+1}}\right)\right\}$$

The initial values of flux are given by

$$\phi = \frac{\sigma_p\ p_1\ p_2}{\sigma_t}\ \phi_o$$

the above resonance flux being normalised to unity for printed output of EXPEAS.

6.2.5 Calculation of Resonance Absorption

The resonance absorption probability is calculated using Simpson's Rule, and is progressively evaluated at every second evaluation of the flux during the stepping through procedure. The equation used for the evaluation is

$$A_c = \frac{1}{\xi} \int_{u_1}^{u_2} \sigma_a \, \phi \, du' \ .$$

This is then corrected for the truncation of the lower wings of the resonances assuming that

$$\psi(x,\theta) = \frac{1}{1+x^2}$$

and using

$$A_e = \frac{1}{\xi} \int_{u_1}^{+\infty} \frac{\Sigma_a(u')}{\Sigma_t(u')} F(u')du'$$

where $$F(u) = \Sigma_t(u_2)\phi(u_2)$$

and $$u_2 = u_{r_2} + 2N_3 \, \delta u$$

The total absorption probability is then

$$A = A_e + A_c$$

6.2.6 Calculation of p

The resonance escape probability is simply

$$p = 1 - A \ .$$

6.3 Output Information

At regular intervals during the stepping through procedure, the quantities, energy, flux, absorption for both resonances, the value of $\Sigma_t\phi/q$, and the combined resonance escape probability is typed out.

6.4 Accuracy of EXPEAS

EXPEAS was used to calculate the absorption for a single resonance of a single absorbing species, with moderator present. Results were compared with the results from PEAS (Pollard 1963) and were in agreement to within .1%.

TABLE I FLUX THROUGH A RESONANCE

x	EXPEAS CALCULATION	PREDICTED VALUE
30	.979	.977
25	.970	.967
20	.952	.945
10	.848	.840
5	.582	.580
0	.005	.005
-5	.581	.560
-10	.812	.823
-20	.873	.881
-25	.906	.875
-30	.911	.874

Resonance Data

E_r = 6.68 ev, Γ_γ = 0.25 ev, Γ_n = .00148 ev

Γ_f = 0. , g = 1 , σ_{pl} = 1200. b

σp_2 = 12.6 b , A_1 = 9. , A_2 = 238

TABLE II RESONANCE ABSORPTION COMPARISON

Γ_r	Γ_γ	Γ_n	σ_{pl}	T	A	B	C
7	.04	.01	1200	300	.361	.376	.348
6.5	.04	.01	1200	300	.400	.410	.381
6.0	.04	.01	1200	300	.447	.440	.419
5.5	.04	.01	1200	300	.503	.480	.463
5.0	.04	.01	1200	300	.574	.525	.515
4.5	.04	.01	1200	300	.660	.580	.575
4.0	.04	.01	1200	300	.776	.638	.644
7	.04	.01	1200	900	.430	.432	.368
6.5	.04	.01	1200	900	.477	.466	.400
6.0	.04	.01	1200	900	.527	.502	.437
5.5	.04	.01	1200	900	.590	.538	.477
5.0	.04	.01	1200	900	.680	.590	.534
4.5	.04	.01	1200	900	.782	.642	.592
4.0	.04	.01	1200	900	.917	.700	.659
7.0	.04	.01	1200	450	.384	.396	.359
4.5	.04	.01	1200	450	.698	.600	.579
7.0	.04	.01	120	600	.632	.832	.780
4.5	.04	.01	120	600	.880	.970	.956
7.0	.04	.01	600	600	.570	.533	.470
4.5	.04	.01	600	600	1.03	.746	.708
7.0	.01	.04	1200	600	.220	.234	.323
4.5	.01	.04	1200	600	.372	.390	.551

Constant Data:- $\sigma_{p_2} = 12.6$ b, $A_1 = 9.0$, $A_2 = 232.$

7. NUMERICAL RESULTS AND CONCLUSIONS

7.1 Introduction

The programme EXPEAS was used to calculate several resonance overlap problems, and the output was compared with several results obtained in previous sections.

7.2 Flux through a Resonance - Numerical Data

Table I shows a comparison of the flux through a resonance (obtained as part of the output from the programme) with the flux as predicted by equation 3.22. The predicted value compares well with the calculated value for positive x, but there is not a close comparison for negative x. This is not unexpected since the value of the resonance escape probability used in the evaluation is only approximate. The predicted flux could be used as a second approximation for the flux through a resonance in order to improve the N.R. estimate of the absorption in the resonance.

7.3 Approximation to Resonance Absorption

The absorption probability for various resonances has been evaluated and the results are tabulated in Table II. In the column headed 'A', the evaluation is obtained by use of the expression on the R.H.S. of equation 5.7 (where $P_1(u)$ is replaced by its asymptotic value), namely

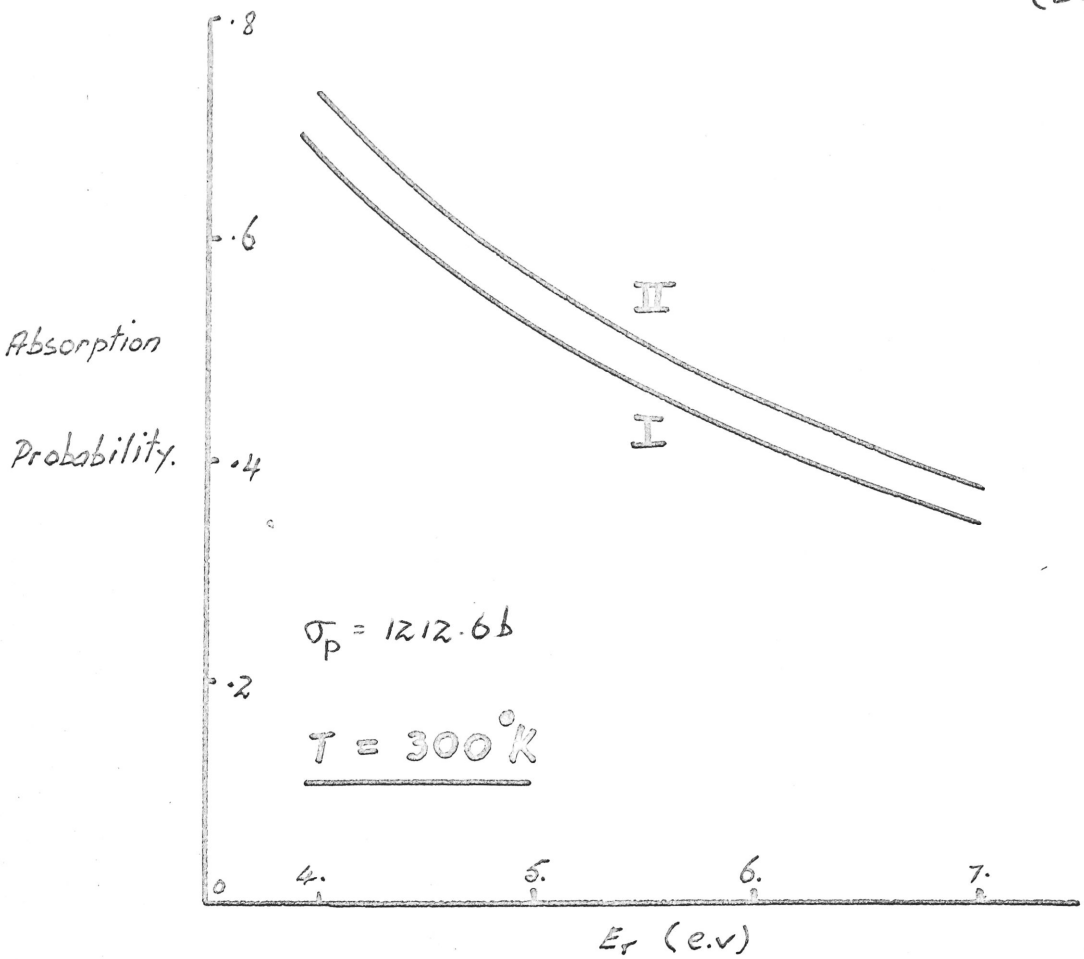
$$1-A = p \simeq \frac{1.2\ \Gamma_a\ \sigma_o\ \psi_o\ G}{\Gamma(\sigma_p+\sigma_o\ \psi_o)E_r\ \bar{\xi}}\ , \qquad 7.1$$

the above resonance flux being equated to unity. Under 'B', the

Fig III Variation of Absorption with E_r

I EXPEAS Value

II Formula (Equation 7.2)



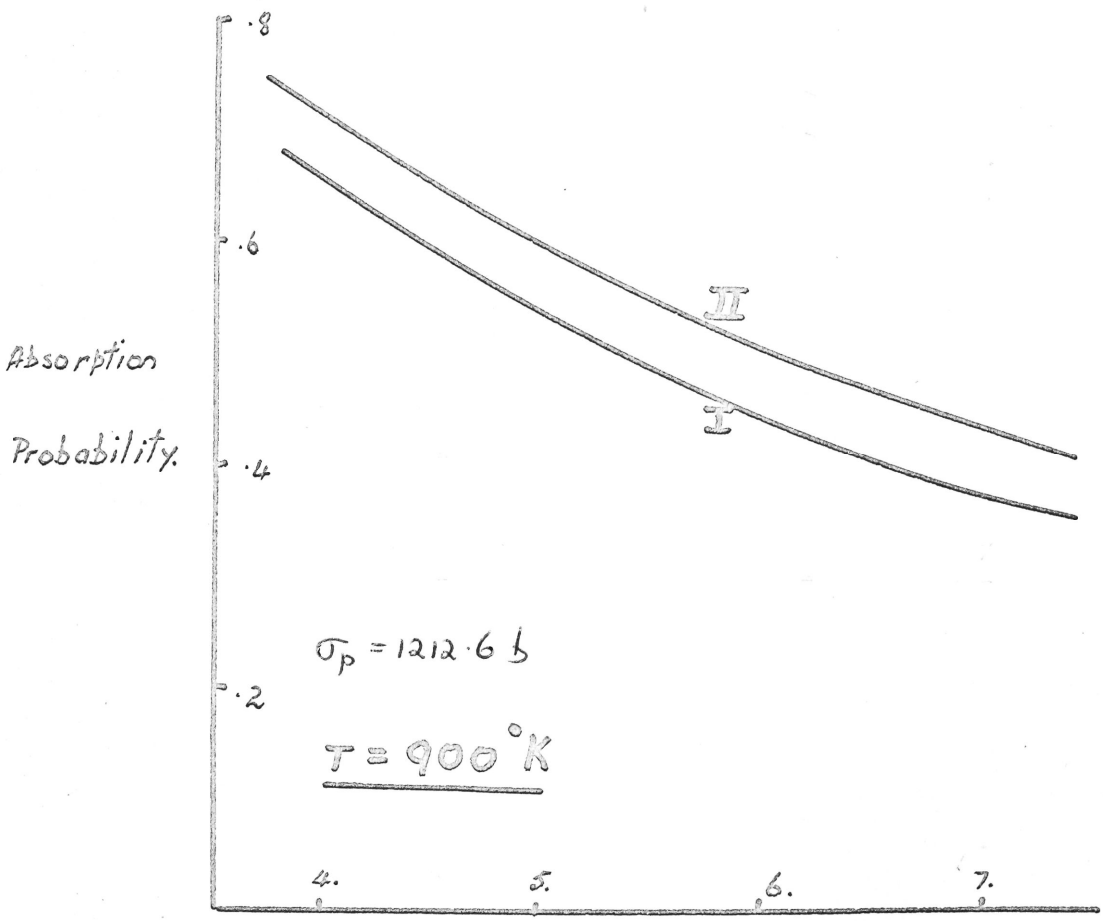
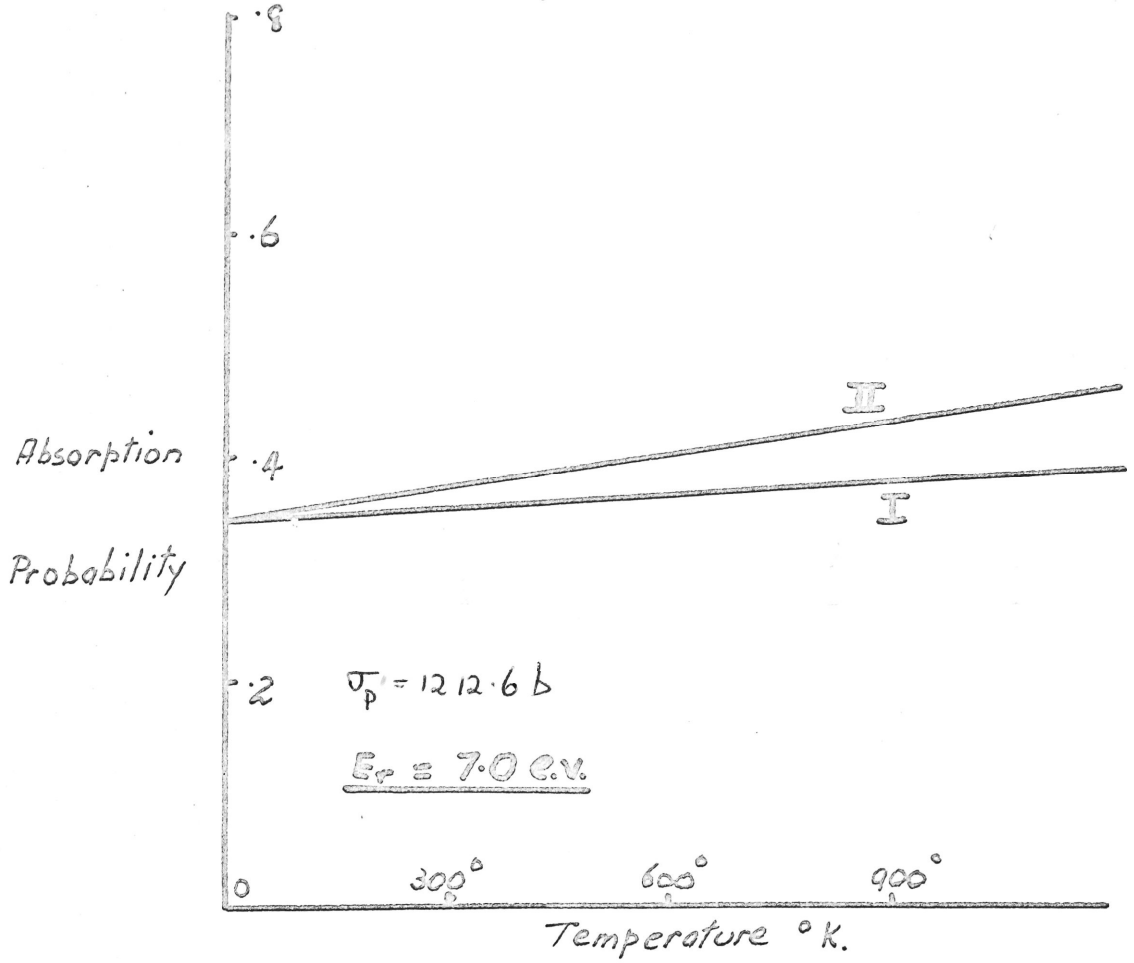


Fig IV Variation of Absorption with Temperature I Experimental Value

II Formula (Equation 7-2)



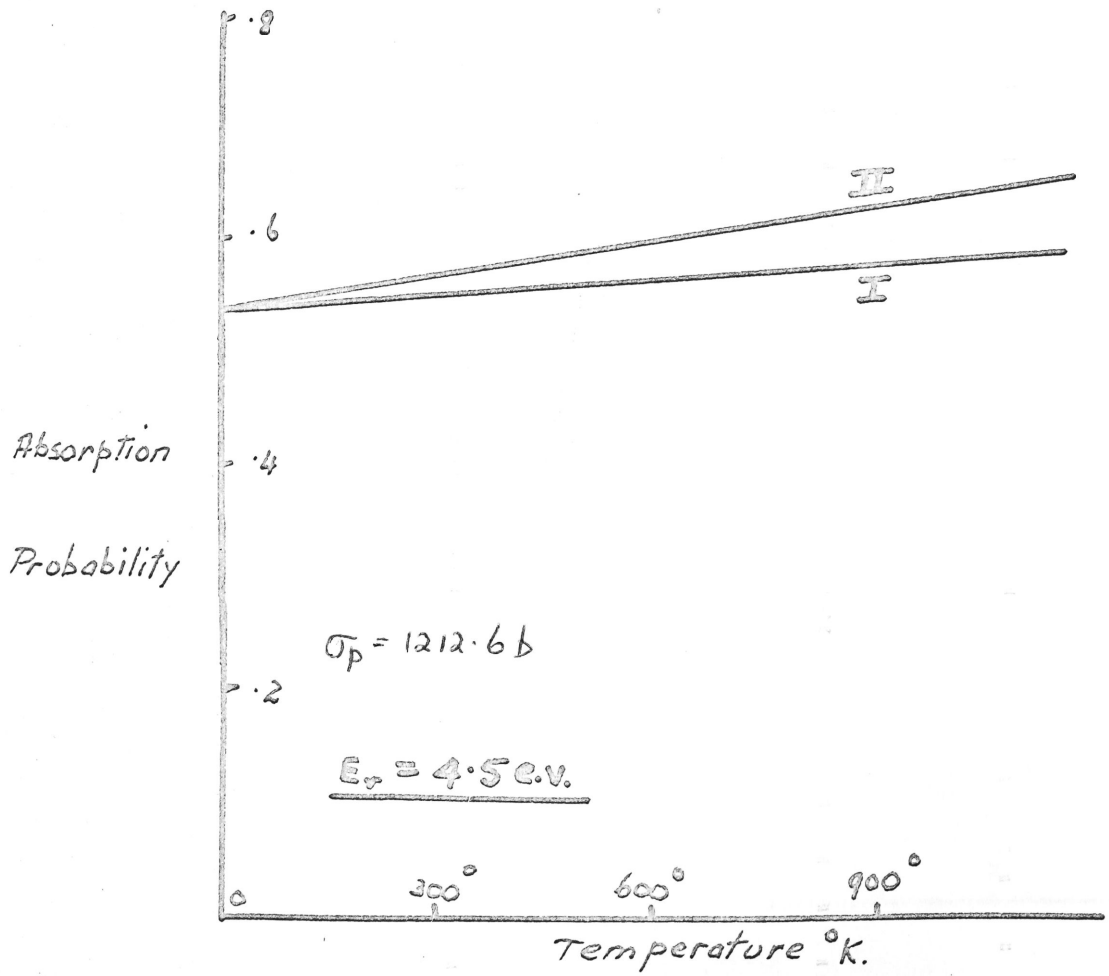
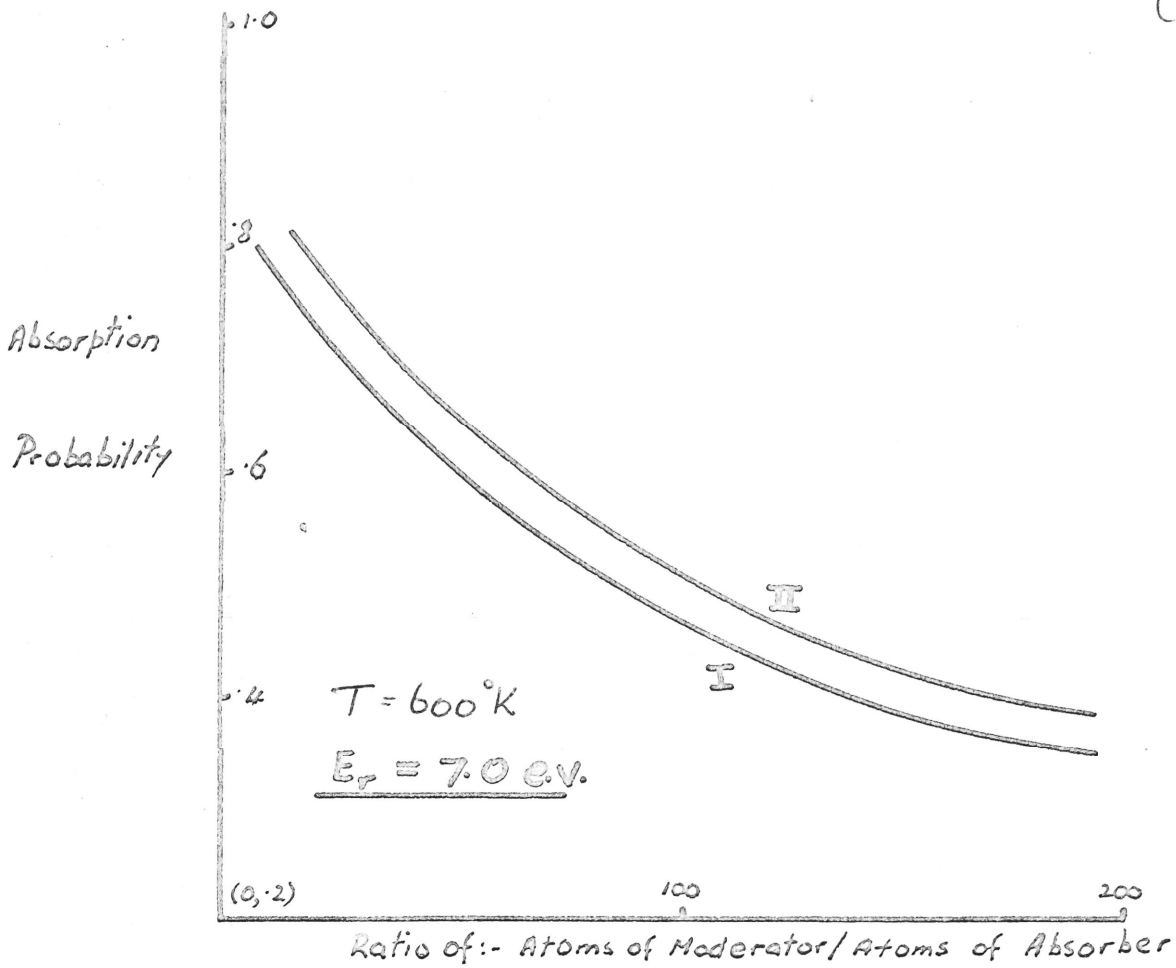
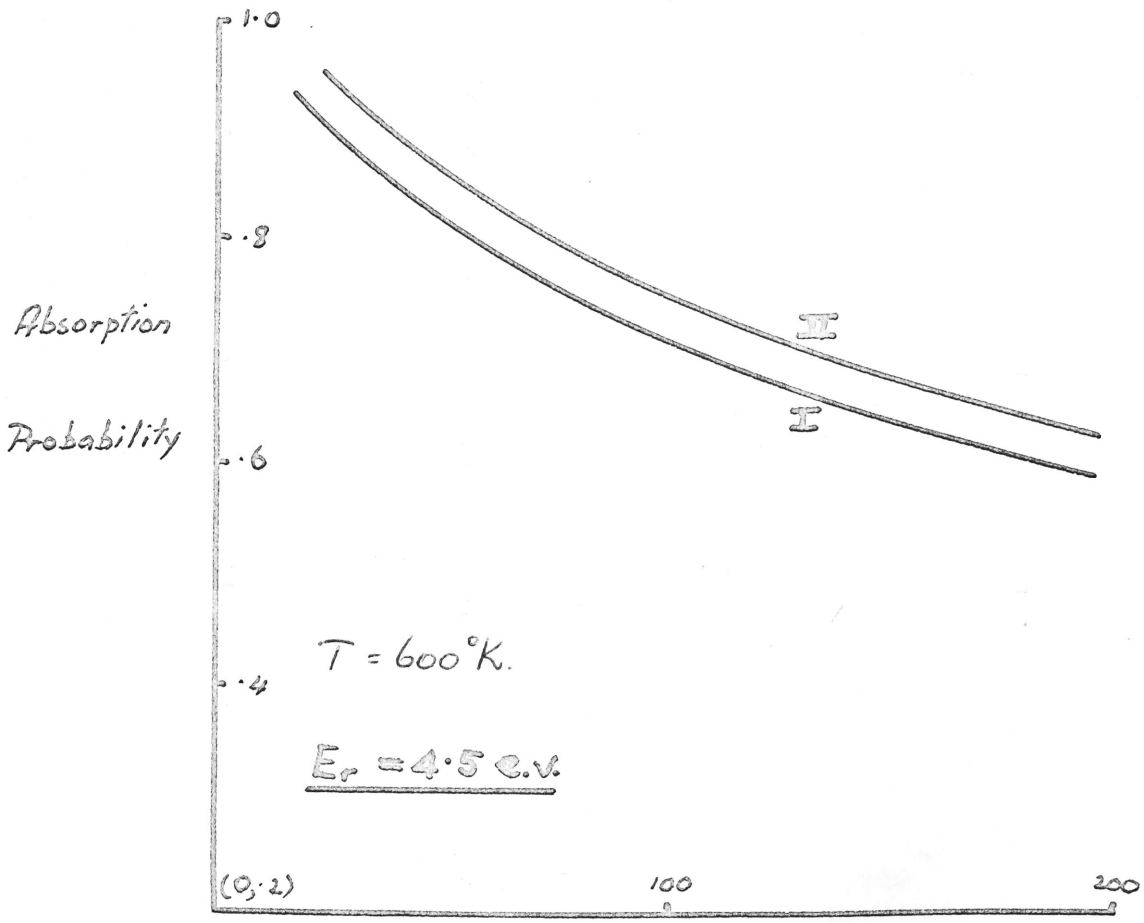


Fig V Variation of Absorption with Concentration

I Experimental Value
II Formula
(Equation 7·2)





evaluation was obtained by use of the expression,

$$1-A = p \simeq \exp - \left(\frac{\pi \Gamma_a \sigma_o \psi_o G}{2\Gamma(\sigma_p+\sigma_o \psi_o)E_r \bar{\xi}}\right) \qquad 7.2$$

where the R.H.S. of equation 5.7 has again been used, but in the exponential form of equation 2.17. The factor 1.2 appearing in equation 7.1 has been replaced in equation 7.2, by the factor $\pi/2$, to give agreement with the N.R. approximation for zero temperature. In the column headed 'C', are the evaluations obtained from the EXPEAS code. The figures indicate that the exponential form, (equation 7.2) is a more suitable approximation.

In figs. iii, iv, v, the absorption probability is plotted as a function of E_r, T, and σ_p, respectively. The curves indicate that the functional dependence of the absorption probability on E_r and σ_p is satisfactory for the approximation 7.2.

The temperature relationship is not good though the curves exhibit similar behaviour. It may be possible to improve the estimate of p(equation 7.2) by modifying the expression for G to give better temperature dependence.

7.4 Calculation of Flux Perturbation due to Absorption

The bracketed term

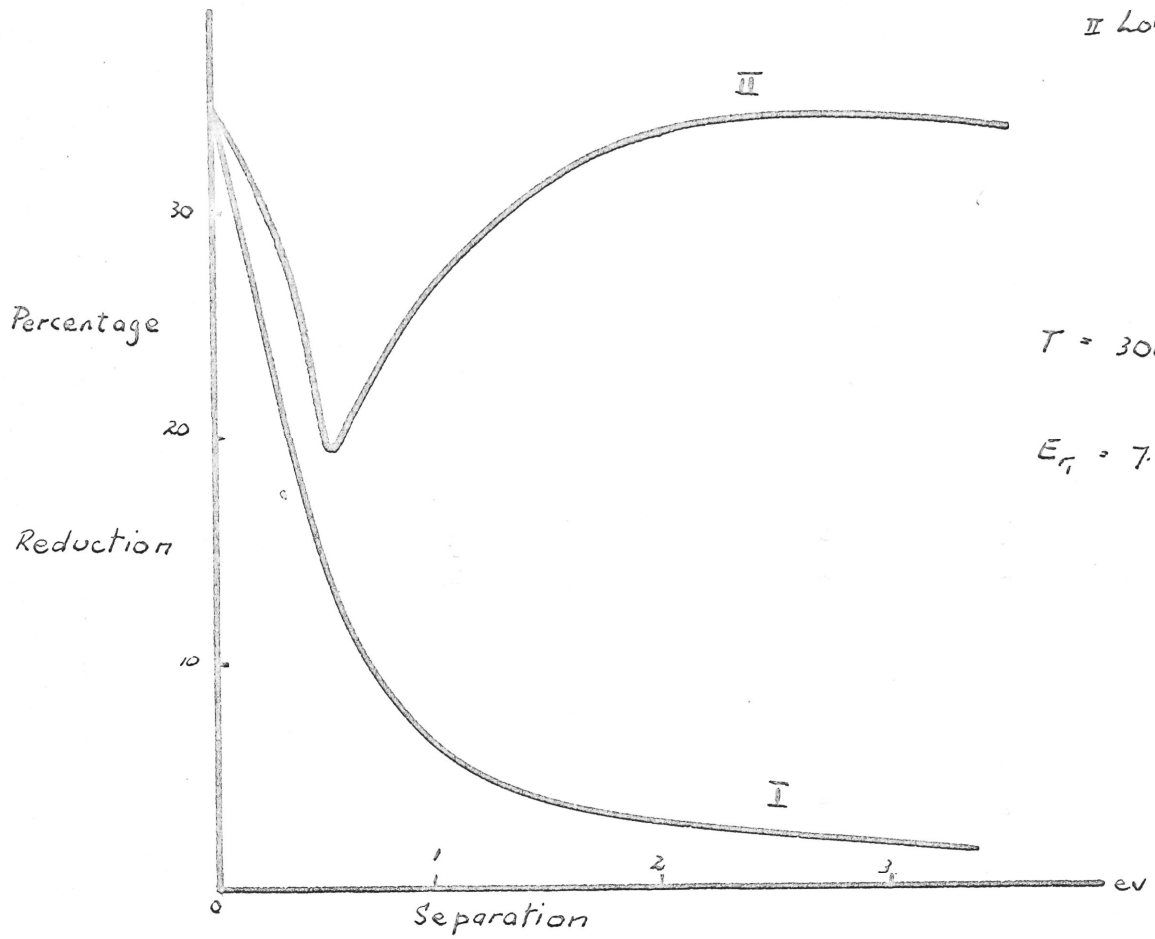
$$\frac{1}{40}\left\{P_1\left(u_s - \frac{3G}{2E_r}\right)+13P_1\left(u_s - \frac{3G}{4E_r}\right)+20P_1(u_s)+13P_1\left(u_s + \frac{3G}{4E_r}\right)+P_1\left(u_s+ \frac{3G}{2E_r}\right)\right\}$$

of equation 5.6 was used to estimate the flux perturbation effect, expressed as a percentage, for two different temperatures. The function $P_1(u)$ was first expressed as a percentage of its asymptotic value, and

Fig VI Variation of percentage Reduction in Absorption with Separation:-

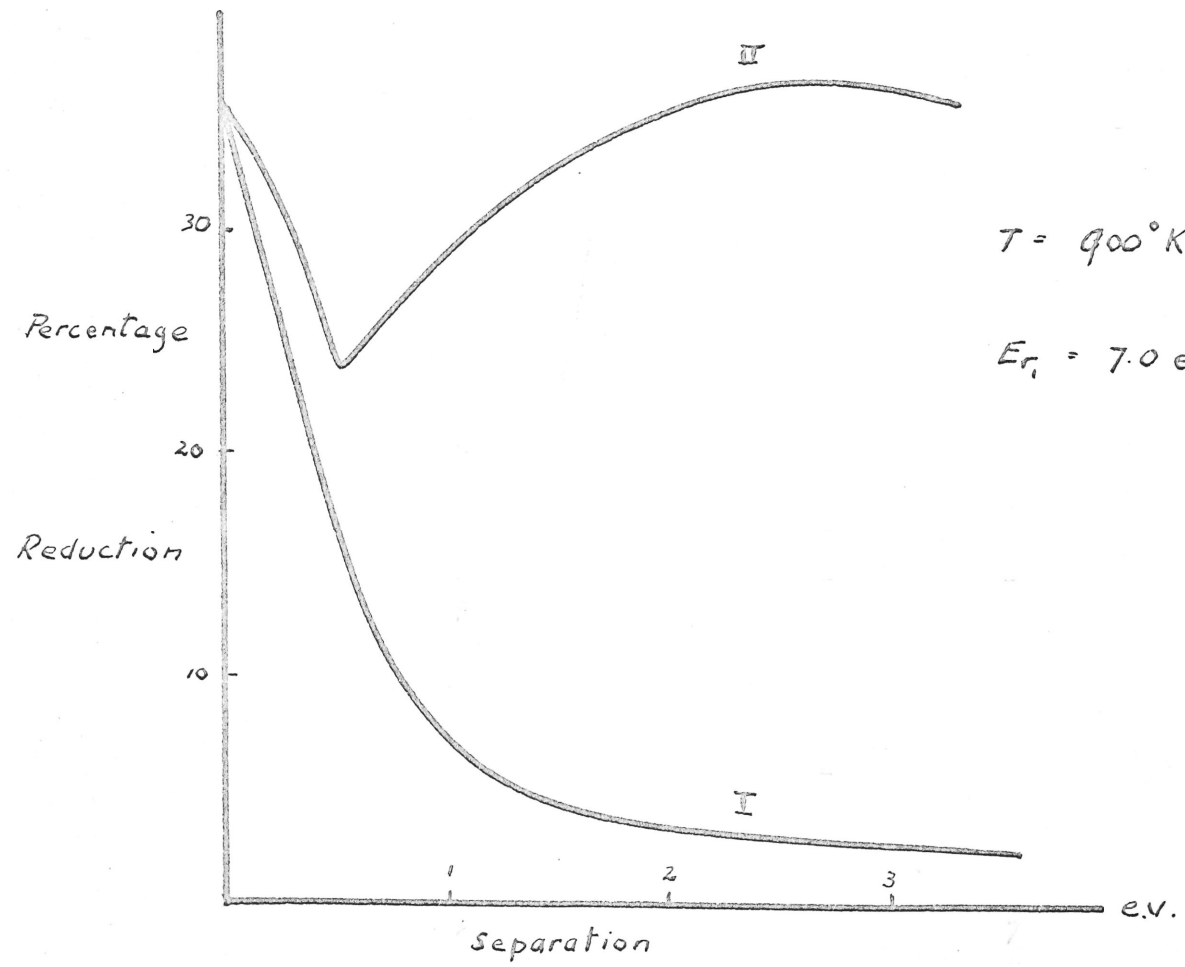
I Upper Resonance

II Lower Resonance.



$T = 300°K$

$E_{r_1} = 7.0$ e.v.



$T = 900°K$

$E_{r_1} = 7.0$ e.v.

TABLE III FLUX PERTURBATION

	Fraction of $\ell n\ 1/\alpha_m$ above U_{r_1}						
	.4	.7	.8	.9	1.0	1.1	
Placzek Function	.788	1.000	1.083	1.172	1.2688 .9025	.927	
Averaged Placzek	.788	1.000	1.083	1.172	1.077	.927	T=300°K
Estimate by Eq 5.6	.790	1.002	1.085	1.125	1.060	.967	T=300°K
Calculated value (EXPEAS)	.830	1.000	1.065	1.110	1.050	.972	T=300°K
Averaged Placzek	.788	1.000	1.083	1.172	1.075	.927	T=900°K
Estimate by Eq 5.6	.803	1.001	1.060	1.101	1.035	.985	T=900°K
Calculated value (EXPEAS)	.820	.994	1.045	1.105	1.055	.960	T=900°K

Resonance Data

$E_r = 7.0$, $\Gamma_\gamma = .04$ ev, $\Gamma_n = 0.01$ ev, $\Gamma_f = 0.$

$g = 1.$, $\sigma_{p_1} = 1200$ b, $\sigma_{p_2} = 12.6$, $A_1 = 9$

$A_2 = 232.$

in order to remove the discontinuity in the above evaluation, the discontinuity in the Placzek function was first removed by averaging the Placzek function in the region of its discontinuity. The average was taken over the lethargy interval δu, where

$$\delta u = \frac{3\sqrt{\{1+\psi_o/\beta\}}}{4F_r\,\psi_o} = \frac{3G}{4E_r} .$$

In Table III, the Placzek function, the averaged Placzek function, and the estimate (by eq 5.6) of the flux perturbation, together with the flux perturbation as obtained from an EXPEAS output are listed. All figures are expressed as a percentage, and for the EXPEAS output, the flux decrease, $1-\phi$, was expressed as a percentage of $1-\phi_o$, where ϕ_o was the value of the flux when

$$\frac{\Sigma_t \phi}{p} = 1.$$

It is to be noted that the perturbation is due to the removal of neutrons, which also gives the overall flux decrease. The perturbation is thus expressed as a percentage of the flux decrease, rather than of the flux. A value of the perturbation above 100% indicates a flux depression. The above estimate is based on the parabolic approximation and is reasonably satisfactory.

7.5 Interference between Two Resonances

The interference effects for a pair of resonances at various separations were calculated, and the results are graphically represented in fig. VI.

The data used was;

σ_p = 1212.6 b, and for both resonances

Γ_γ = ·04ev, Γ_n = ·01ev, Γ_f = 0.ev, g = 1, with the upper resonance located at E_r = 7e.v. The percentage reduction in absorption for both the upper and lower resonances, is plotted as a function of separation at two different temperatures.

The reduction in absorption for the upper resonance follows the pattern obtained by Corngold and Schermer (1959) and O'Halloran (1966), but does not reach zero as obtained by them. This is not unexpected since for large separations the mutual shielding is negligible, but the upper resonance has a reduced absorption due to neutron absorption by the upper wing of the lower resonance.

For the lower resonance the reduction in absorption is caused by the same factors which effect the upper resonance. The mutual shielding effect is dominant when the separation is small, but with larger separations the percentage reduction in absorption by the lower resonance is near the absorption probability (expressed as a percentage) of the upper resonance. There is a peak in the reduction of absorption by the lower resonance when

$$\frac{E_{r_1}}{E_{r_2}} \simeq \frac{1}{\alpha_m}, \quad E_{r_2} < E_{r_1}$$

where α_m refers to the moderator. The peak corresponds to the flux depression which was discussed in the previous section.

7.6 Estimation of Flux Perturbation effect from one Resonance on the Absorption by a Lower Resonance

Any estimate of the effect of the neutron population decrease (caused by absorption in the upper resonance), for large separations depends on the accuracy of the estimate of the resonance escape probability for the upper resonance. For large separations the flux change caused by the upper resonance can be considered satisfactorily as being discontinuous at the upper resonance, the magnitude of the discontinuity being equal to the resonance absorption probability of the upper resonance.

In order to estimate the percentage change in the decrease in absorption by the second resonance, the factor

$$\frac{1}{40}\left\{R(u_s-\frac{3G_2}{2E_{r_2}})+13R(u_s-\frac{3G_2}{4E_{r_2}})+20R(u_s)+13R(u_s+\frac{3G_2}{4E_{r_2}})+R(u_s+\frac{3G_2}{2E_{r_2}})\right\}$$

was again used to average the effect over the central region of the lower resonance, where the subscript, 2, refers to the lower resonance, and where R(u) is taken to be the flux perturbation effect previously calculated in section 7.3. The flux effect on the lower resonance was expressed as a percentage of the decrease in absorption for reasons given in the previous section.

For the output of EXPEAS, two separate results are obtained, namely the flux perturbation effect on the absorption in the central region of the lower resonance, and the effect on the absorption in the lower resonance. The absorption in the central region of the lower resonance was taken to be the absorption over the range

TABLE IV ESTIMATE OF REDUCTION IN ABSORPTION BECAUSE OF FLUX DEPRESSION

	Lower Resonance Energy			
	5.ev	4.5 ev	4.ev	
EXPEAS	101.5%	101.6%	98.7%	T=300°
EXPEAS (Central)	103.7%	104.3%	99.1%	T=300°
Estimate	102.5%	103.9%	100.5%	T=300°
EXPEAS	101.5%	101.9%	98%	T=900°
EXPEAS (Central)	103.8%	102.1%	99.5%	T=900°
Estimate	101.8%	102.2%	100.3%	T=900°

Resonance Data:

$E_{r_1} = 7.0ev$, $\Gamma_\gamma = .04$ ev , $\Gamma_n = .01$ ev , $\Gamma_f = 0.ev$

$g = 1.0$, $\sigma_{p_1} = 1200b$, $\sigma_{p_2} = 12.6b$, $A_1 = 9.0$

$A_2 = 232.$

$$U_{r_2} \pm \frac{3G_2}{2E_{r_2}}$$

where the subscript, 2, refers to the lower resonance. For both calculations the perturbation effect was expressed by

$$\frac{A_{L1} - A_{L2}}{A_{L1}(1-p_1(u_{r_2}))} \times 100\%$$

where (i) A_{L1} is the absorption in the lower resonance, over the appropriate range of u, when the upper resonance is not present, (ii) A_{L2} is the absorption in the lower resonance, over the appropriate range of u, when the upper resonance is present, and (iii) $p_1(u_{r_2})$ is the resonance escape probability for the upper resonance at the centre of the lower resonance.

In Table IV, the estimated, and the calculated (from EXPEAS output) perturbation effects are tabulated for various resonances. As to be expected, the estimated effect agrees fairly well with the result when the central region only, is considered in the EXPEAS output.

The figures relating to the central region of a resonance show greater variation than those relating to the whole resonance, because flux perturbations have little effect on the absorption in the wings of a resonance. Comparison between the values for the central region, and the estimated values suggests that a lower value of G, defined by equation 4.6, would give a better comparison. Correlation between the curves of Fig. IIA (p.40) would be improved by a lower value of G.

TABLE V PERCENTAGE CHANGE IN REDUCTION OF ABSORPTION

T	Γ_{γ_1}	Γ_{γ_2}	Γ_{n_1}	Γ_{n_2}	σ_{p_1}	Placzek % Depression	Reduction % Change
0	.04	.04	.01	.01	1200	110.1	101.8
300	.04	.04	.01	.01	1200	111.8	101.6
450	.04	.04	.01	.01	1200	110.2	101.4
900	.04	.04	.01	.01	1200	111.4	101.9
600	.01	.04	.04	.01	1200	105.3	101.1
600	.01	.01	.04	.04	1200	105.3	102.0
600	.04	.01	.01	.04	1200	110.5	102.0
600	.04	.04	.01	.01	600	108.7	100.8
600	.04	.04	.01	.01	200	103.2	99.5
*600	.04	.04	.01	.01	1200	111.8	101.4

Other Data:

$A_1 = 9$, $A_2 = 232$, $\sigma_{p_2} = 12.6b$

*$A_3 = 238$, $\sigma_{p_3} = 9.$, Ratio of Atoms $N_2 : N_3 = 1 : 1$

In Table V are listed the perturbation effects on the lower 4.5 e.v. resonance, caused by the upper 7.0 e.v. resonance under a variety of circumstances, and also the flux depression, expressed as a percentage, caused by the 7.0 e.v. resonance is listed. The chosen resonances give a separation of very nearly one moderator collision range.

The change in concentration of the mixture is shown to have a marked effect on the flux depression caused by the upper resonance. An increase in concentration broadens the curve for $\Sigma_a\phi$, and has the effect of decreasing the flux depression, but broadening the region of the depression. The reduction in the perturbation effect on the lower resonance reflects the change in the flux depression.

The value of the flux depression from a predominantly scattering upper resonance is considerably different from the flux depression from a predominantly absorbing resonance, and the change in the flux depression is reflected in the different values for the perturbation effect on the lower resonance. If the resonance is assumed to be a δ-resonance, then investigation of the slowing down equation yields

$$\Sigma_p\phi = S(u) - (1-p)\frac{\Gamma}{\Gamma_\gamma} - (1-p)\frac{\Gamma}{\Gamma_\gamma}H(u-u_r) + \bar{\xi}\,P_2(u) + (1-p)\frac{\Gamma_n}{\Gamma_\gamma}\frac{e^{-(u-u_r)}}{1-\alpha_2}H(u-u_r)$$

$$H(u_r+\ell n\ 1/\alpha_2-u) + \int_{u_r}^{u_r+\ell n\ 1/\alpha_2}\frac{\Gamma_n}{\Gamma_\gamma}\frac{(1-p)e^{-(u-u')}}{1-\alpha_2}P(u-u')du' - (1-p)\frac{\Gamma}{\Gamma_\gamma}P_2(u-u_r)\bar{\xi}\ ,$$

where the subscript, 2, refers to the absorbing species, and the above resonance flux is $\frac{1}{\Sigma_p}$ from a δ-source.

TABLE VI - Doppler Coefficients

Separation e.v.	ΔA Lower Resonance	ΔA Upper Resonance
0	.0093	.0093
0.5	.0107	.0159
1.0	.0080	.0226
1.5	.0047	.0218
2.0	.0004	.0209
2.5	-.0026	.0230
3.0	-.0046	.0246

RESONANCE DATA : As for fig. vi. (top page 68).

The last two terms give the resonance perturbation effects and tend to cancel out (being of opposite sign). For a predominantly scattering resonance the neutrons tend to 'bunch' near the resonant energy, and this 'bunching' causes a flux peak, one moderator collision range below the resonance energy, whereas a predominantly absorbing resonance causes a flux depression at this energy.

The last entry in Table V is the result of an EXPEAS calculation in which Th_{232} has a 4.5 ev resonance, and U_{238} has a resonance at 7.0 ev. The figures indicate that the percentage change in the reduction in absorption is not significantly different from when both resonances belong to Th_{232}.

7.7 The Doppler Coefficient

The change in absorption for the temperature of 300^{o} to 900^{o} is denoted by

$$\Delta A = A(900^{o}) - A(300^{o})$$

for any resonance, where A(T) is the absorption probability at T^{o}.

In Table VI, estimates of ΔA are listed for both the lower resonances and the upper 7 ev resonance at various values of separation. The values are obtained from the output of EXPEAS.

The negative values of ΔA obtained for the lower resonances are caused primarily by the increase in the absorption of the upper resonance with increase of temperature. The figures in the second column suggest that flux perturbations have little effect on the value of ΔA.

It is of interest to note that for the upper resonance at a separation of 2 ev, the value of ΔA is about 10% lower than the values for 1.5 ev and 2.5 ev. This is due to variation in the screening effect of the Doppler broadened lower resonance.

7.5 Results and Conclusions

In Chapter 3, the expression obtained by Goldstein (1964) for the flux in the region of a resonance was modified. Goldstein's expression gave an incorrect value for the below resonance flux. The modified expression corrects this defect. Comparison of the flux obtained by using the modified expression, and the flux obtained from an EXPEAS output shows close agreement.

A parabolic approximation was developed in Chapter 4 in order to estimate the absorption in the central region of a resonance at zero temperature. The parabolic approximation was then generalised so that it would be applicable to resonances at any temperature. It was shown that the approximations give simple formulae for the absorption in a resonance, but the formulae give excessive temperature variation. The formulae seem adequate in terms of the other parameters. The method of approximating was not entirely satisfactory. By further research it may be possible to improve the method so as to give a more satisfactory approximation.

The parabolic approximation was used to estimate the amount of flux perturbation caused by neutron absorption in a resonance. There

is a flux decrease below a resonance due to removal of neutrons. It was found that there is a further variation in the flux due to perturbation effects. A flux decrease occurs in the region of one moderator collision range below the resonance. For a predominantly absorbing resonance, the maximum total decrease was about 110% of the decrease due to neutron absorption. The maximum decrease occurs about .9 of a moderator collision range below the resonance. The calculated flux decrease, and the predicted flux decrease, were found to agree, as regards the maximum amount of decrease, and also as regards the value of the lethargy at which the maximum decrease occurs.

The parabolic approximation for a second resonance was used to assess the effect flux perturbations from a first resonance have on the absorption by the second resonance. The EXPEAS calculations showed that flux perturbations cause about 2-4% reduction in absorption in the central region of the second resonance, while the amount of absorption in the wings of the second resonance is not greatly affected by flux perturbations. The reduction in absorption by the lower resonance was found to be about 1-2%. The estimated value of the reduction was found to be about 2-4%. There was reasonable agreement between the predicted amount of reduction in absorption, and the calculated (EXPEAS) amount.

The change in absorption with temperature, for both resonances, was found to be not significantly affected by flux perturbations. In the calculation of Doppler coefficients, the effect of flux perturbations could be ignored.

8. ACKNOWLEDGMENTS

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9. REFERENCES

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APPENDIX A

THE PLACZEK FUNCTION

The method followed is similar to that used by Teichmann (1960). The general slowing down equation, when no absorption is present, is

$$\Sigma_p \phi = \sum_{i=1}^{n} \int_{u-\ell n\ 1/\alpha_i}^{u} \frac{\Sigma_{pi} \phi\ e^{-(u-u')} du'}{1-\alpha_i} + S(u) \qquad A.1$$

where $$\Sigma_p = \sum_{i=1}^{n} \Sigma_{pi} \quad .$$

If we assume that the neutron source, S(u) is a unit δ-source at u=0, the Laplace transform of equation A.1 is

$$\mathcal{L}\{\Sigma_p \phi\} = \sum_{i=1}^{n} K_i(p) \mathcal{L}\{\Sigma_{pi} \phi\} + 1 \qquad A.2$$

where $$K_i(p) = \frac{(1-\alpha_i)^{p+1}}{(1-\alpha_i)(p+1)}$$

By taking the Σ_{pi} as constant, equation A.2 may be rearranged thus:-

$$\mathcal{L}\{\Sigma_p \phi\} = \frac{1}{1 - \sum_{i=1}^{n} K_i(p) \frac{\Sigma_{pi}}{\Sigma_p}} \qquad A.3$$

$$= 1 + \sum_{r=1}^{\infty} \left\{ \sum_{i=1}^{n} \frac{\Sigma_{pi}}{\Sigma_p} K_i(p) \right\}$$

The term

$$\sum_{i=1}^{n} \frac{\Sigma_{pi}}{\Sigma_p} K_i(p) = \sum_{i=1}^{n} \frac{1}{p+1} \left\{\frac{1}{1-\alpha_i} - \frac{\alpha_i^{p+1}}{1-\alpha_i}\right\} \frac{\Sigma_{pi}}{\Sigma_p}$$

$$= \frac{1}{(1-\alpha)(p+1)} \left\{1 - \sum_{i=1}^{n} \frac{(1-\alpha)\Sigma_{pi}\alpha_i^{p+1}}{(1-\alpha_i)\Sigma_p}\right\} ,$$

where

$$\sum_{i=1}^{n} \frac{\Sigma_{pi}}{(1-\alpha_i)} = \frac{\Sigma_p}{1-\alpha}$$

Hence

$$\left\{1 - \sum_{i=1}^{n} \frac{\Sigma_{pi}}{\Sigma_p} K_i(p)\right\}^{-1} = 1 + \sum_{r=0}^{\infty} \left[\frac{1}{(1-\alpha)(p+1)} \left\{1 - \sum_{i=1}^{n} \frac{(1-\alpha)\Sigma_{pi}\alpha_i^{p+1}}{(1-\alpha_i)\Sigma_p}\right\}\right]^r$$

$$= 1 + \sum_{r=1}^{\infty} \left[\frac{1}{(1-\alpha)(p+1)}\right]^r \left\{\sum_{t=1}^{r} {}^rC_t \left(\sum_{i=1}^{n} \frac{(-1)(1-\alpha)\Sigma_{pi}\alpha_i^{p+1}}{\Sigma_p(1-\alpha_i)}\right)^t\right\}$$

where ${}^rC_t = \frac{r!}{t!(r-t)!}$.

If r_i is the power associated with the i^{th} species, the coefficient of

$$\prod_{i=1}^{n} \left\{\frac{\Sigma_{pi}\alpha_i^{p+1}(1-\alpha)}{\Sigma_p(1-\alpha_i)}\right\}^{r_i}$$ is given by

$$\left\{\sum_{s=0}^{\infty} \frac{\left(\left(\sum_{i=1}^{n} r_i\right)+s\right)!}{\left[\prod_{i=1}^{n} (r_i!)\right] s! \left[(1-\alpha)(p+1)\right]^{\left(\sum_{i=1}^{n} r_i\right)+s}} (-1)^{\left(\sum_{i=1}^{n} r_i\right)+s}\right.$$

and corresponds to the Binomial expansion of

$$(-1)^{\sum_{i=1}^{n} r_i} \frac{\left(\sum_{i=1}^{n} r_i\right)!}{\left(\prod_{i=1}^{n} (r_i!)\right)[(1-\alpha)(p+1)]^{\sum_{i=1}^{n} r_i}\left(1-\frac{1}{(1-\alpha)(p+1)}\right)^{\left(\sum_{i=1}^{n} r_i\right)+1}}$$

$$= \left(\frac{-1}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i} \frac{\left(\sum_{i=1}^{n} r_i\right)!\,(p+1)}{\left[\prod_{i=1}^{n} (r_i!)\right]\left(p+1-\frac{1}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i+1}}$$

$$= \left(\frac{-1}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i} \left\{\frac{\left(\sum_{i=1}^{n} r_i\right)!}{\left[\prod_{i=1}^{n} (r_i!)\right]}\left[\frac{1}{\left(p-\frac{\alpha}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i+1}} + \frac{1}{(1-\alpha)\left(p-\frac{\alpha}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i}}\right]\right\}.$$

By putting $\alpha^{p+1} = \alpha\, e^{-p \ell n\, 1/\alpha}$, the inversion of the general term

$$(-1)^{\sum_{i=1}^{n} r_i} \prod_{i=1}^{n}\left\{\left(\frac{\Sigma_{pi}\,\alpha_i}{\Sigma_p (1-\alpha_i)}\right)^{r_i} \frac{1}{(r_i!)}\right\}^{\sum_{i=1}^{n} r_i}\left[\frac{1}{\left(p-\frac{\alpha}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i+1}} + \frac{1}{1-\alpha}\cdot\frac{1}{\left(p-\frac{\alpha}{1-\alpha}\right)^{\sum_{i=1}^{n} r_i}}\right]$$

$$e^{-\left\{\sum_{i=1}^{n} r_i\, \ell u\, 1/\alpha_i\right\}}$$

which is denoted by S, is

$$S = \prod_{i=1}^{n}\left\{\left(\frac{\Sigma_{pi}\,\alpha_i}{\Sigma_p (1-\alpha_i)}\right)^{r_i} \frac{1}{r_i!}\right\} (-1)^{\sum_{i=1}^{n} r_i} \left(\sum_{i=1}^{n} r_i\right)!\; e^{\frac{\alpha}{1-\alpha}\left(u - \sum_{i=1}^{n} r_i\, \ell n\, 1/\alpha_i\right)}$$

multiplied by

$$H\left(u-\sum_{i=1}^{n} r_i \ell n\, 1/\alpha_i\right)\left[\frac{\left(u-\sum_{i=1}^{n} r_i \ell n\, 1/\alpha_i\right)^{\sum_{i=1}^{n} r_i - 1}}{\left(\left(\sum_{i=1}^{n} r_i\right)-1\right)!} + \left(u-\sum_{i=1}^{n} r_i \ell n\, 1/\alpha_i\right)^{\sum_{i=1}^{n} r_i}\right],$$

and $(-1)!$ is taken to be infinite.

We define

$$P_n(u) = \sum_{r_1=0}^{\infty} \cdots \sum_{r_n=0}^{\infty} S \,. \qquad \text{A.4}$$

When n=1, equation A.4 reduces to

$$P_1(u)=\frac{1}{1-\alpha}\, e^{\frac{\alpha}{1-\alpha} u} + \sum_{r=1}^{\infty} \frac{(-1)^r (u-r\ \ell n\ 1/\alpha)^{r-1}}{(1-\alpha)^r (n-1)!}\left[1 + \frac{u-r\ \ell n\ 1/\alpha}{r(1-\alpha)}\right]$$

$$e^{\frac{\alpha}{1-\alpha}} H(u-r\ \ell n\ 1/\alpha) \qquad \text{A.5}$$

which is the Placzek Function; the subscript 1, on the R.H.S. has been omitted.

Inversion of equation A.3 is, therefore,

$$\Sigma_s \phi = \delta(u) + P_n(u) \,.$$