GEOMETRICAL EFFECTS ON THE RESONANCE ABSORPTION OF NEUTRONS

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ABSTRACT

GEOMETRICAL EFFECTS ON THE RESONANCE

ABSORPTION OF NEUTRONS

by Hans Ludewig

An investigation was conducted to estimate the error when the flat-flux approximation is used to compute the resonance integral for a single absorber element embedded in a neutron source.

The investigation was initiated by assuming a parabolic flux distribution in computing the flux-averaged escape probability which occurs in the collision density equation. Furthermore, also assumed were both wide resonance and narrow resonance expressions for the resonance integral. The fact that this simple model demonstrated a decrease in the resonance integral motivated the more detailed investigation of the thesis.

An integral equation describing the collision density as a function of energy, position and angle is constructed and is subsequently specialized to the case of energy and spatial dependence. This equation is further simplified by expanding the spatial dependence in a series of Legendre polynomials (since a one-dimensional case is considered). In this form, the effects of slowing-down and flux depression may be accounted for to any degree of accuracy

desired. The resulting integral equation for the energy dependence is thus solved numerically, considering the slowing down model and the infinite mass model as separate cases.

From the solution obtained by the above method, the error ascribable to the flat-flux approximation is obtained. In addition to this, the error introduced in the resonance integral in assuming no slowing down in the absorber is deduced. Results by Chernick for bismuth rods, and by Corngold for uranium slabs, are compared to the latter case, and these agree to within the approximations made.

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CHAPTER I

INTRODUCTION

An important element in the balance relationship describing the fate of neutrons in a chain reactor cycle is resonance absorption. This refers to the radiative capture of neutrons having energies within a band in which the absorption probability, or cross-section, fluctuates strongly for many materials common to nuclear reactors (e.g. U^{238}). The accepted definition of the resonance escape probability, P, is (W1)*: "the ratio of the number of neutrons which reach the $1/v$ region during slowing down, to the number which reach the resonance region." The $1/v$ region is the energy band below the lowest resonance.

The probability P is not only important in the determination of reactivity (a measure of the amount of "imbalance" in the chain reaction), but in the conversion factor as well. The latter factor describes the amount of fissionable material transmuted from fertile material. The reactivity is proportional to P while 30% to 50% of the conversion factor is proportional to (1-P). For example if P were of the order of 0.85, a 10% uncertainty in (1-P) would cause a 1.5% uncertainty in reactivity and a 3% to 5% uncertainty in the conversion factor. Both these factors are of considerable importance in the economics of power reactors.

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*Refer to Bibliography

Following convention we will consider for the most part, the resonance integral I, which may be written (M1):

$$I = 1 - P = \int_V \int_{E'} \frac{F(\vec{r},E')\ \Sigma_a(E')}{q(\vec{r},E')\ \Sigma_t(E')}\, dE'\, \frac{dV}{V} \qquad (1)$$

where

$F(\vec{r},E)dE$ = neutron collision density at energy dE about E and at position $\vec{r}$

$= \Sigma_t(E)\ \phi(\vec{r},E)$.

$q(\vec{r},E)$ = neutron slowing down density past E, at $\vec{r}$, which would obtain in the pure, infinite moderator.

$\phi(\vec{r},E)dE$ = neutron flux at an energy dE about E and at position $\vec{r}$.

$\Sigma_t(E)$ = macroscopic total cross-section as a function of energy.

$\Sigma_a(E)$ = macroscopic absorption cross-section as a function energy.

V = volume of absorber material.

The first significant calculations of resonance integrals were semi-empirical formulas (W3, G1). Improvements over these methods made use of:

(i) more detailed cross-section vs. energy information,

(ii) increased knowledge of flux as a function of energy and position.

The functional dependence of the cross-section on energy was determined by Wigner and Breit (W2) and subsequently, using a different method, by Blatt et al. (B1), Vogt (V1), and Lane et al. (L1). The derivation of the latter method appears in Appendix A. The resonance cross-section as computed by the above methods appears to be satisfactory for the purpose of determining the resonance integral. Therefore increasing the accuracy of the calculation of I should result mainly from improving the determination of $\phi(\vec{r},E)$.

In early approaches the flux was assumed to be spatially constant. This simplifies the resonance integral and the equation used to determine the flux. This model is known as the flat flux approximation, and is physically valid only under certain conditions, to be discussed in Chapter II.

On intuitive grounds, Chernick (C1) proposed an equation for determining the flux of neutrons, independent of position, in a single lump of absorbing material surrounded by a source of neutrons. The equation has the following form:

$$\phi(E)\ \Sigma_t(E) = \left[1 - p(E)\right] \int_E^{E/\alpha} \frac{\phi(E')\ \Sigma_s(E')}{(1 - \alpha)\ E'}\, dE' + S(E) \qquad (2)$$

where

$p(E)$ = average neutron escape probability from the absorber lump, at energy E

$S(E)$ = independent source of neutrons in the lump at energy E

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

$A = M/m$

M = nuclear mass

m = neutron mass

An equation of the above form was also constructed for a lattice of absorber lumps in a source of neutrons (R1).

In spite of the fact that Eq. (2) is considerably simplified by neglecting the detailed spatial effects, it is still rather difficult to solve. Thus further approximations are necessary. As an initial simplification, only one resonance will be considered at a time. The cross-section is thus described by a constant scattering cross-section for all energies, to which is added the resonant scattering and absorption components at the appropriate energy. The cross-section of the absorber appears as in Fig. 1.

The width of the resonances usually considered varies over a large range (BNL-325). In view of this fact two assumptions which permit approximation of the integral term in Eq. (2) are (C1, D1, M1):

(i) The resonance width is narrow compared to the maximum energy-loss-per-collision of neutrons with absorber nuclei. In other words, the resonance is narrow compared to the range of integration in Eq. (2). This is known as the narrow resonance approximation, and will be subsequently referred to as the N.R. approximation.

(ii) The resonance width is wide compared to the maximum energy loss per collision of neutrons with absorber nuclei, i.e., the resonance is wide compared to the range of integration in Eq. (2). This is known as the wide resonance approximation, and will be subsequently referred to as the W.R. approximation.

In the case of the N.R. approximation the width of the resonance is considered to be so small that it has a negligible effect on the energy distribution of neutrons. To obtain the first order solution to Eq. (2) in this case, it is thus permissible to substitute the asymptotic flux solution into the integrand. The asymptotic flux may be obtained from the integral equation by setting $\Sigma_s(E')$ equal to the potential cross-section, shown in Fig. 2, and letting the flux in the integrand vary as 1/E (M1). The integral can now be evaluated, and the resulting solution for the flux may now be used to calculate the resonance integral.

In the W.R. approximation, the resonance is considered to be so large that it is impossible for a neutron to scatter out of its range when colliding with absorber nuclei. In this case, the assumption is made that the product $\phi(E)\ \Sigma_s(E)$ is constant over the range of integration, and as a first order approximation the integrand is evaluated for convenience, at the lower limit. Physically, the following meaning may be ascribed to the approximation: the absorber nucleus is assumed to have an infinite mass compared to the mass of the neutron, and thus allows no change in energy during a collision.

In view of this, the W.R. approximation is also known as the infinite mass approximation. In this case, the flux is represented by a linear equation which may be solved. The resulting flux may then be used to compute the resonance integral. The approximations outlined above have also been used by Dresner (D1) and Blässer (B2, B3) to compute the resonance integral. The validity of the N.R. and W.R. approximations is discussed at the end of Chapter II.

Chernick et al. (C2) subsequently refined the above procedure by iterating once the N.R. and W.R. solutions to the flux equation. This iterated result is a more realistic solution to the integral equation, since it is of the Fredholm type (C9). Using this improved flux, a more realistic estimate of the resonance integral may be obtained. Thus by comparing the more realistic N.R. and W. R. approximation to the unaltered N.R. and W.R. approximation for the resonance integral, it is possible to obtain an estimate of the error involved. Furthermore, it is of interest to note that the difference between the improved W.R. approximation and the unaltered W.R. approximation is a measure of the error introduced in neglecting energy changes of the neutron when colliding with absorber nuclei, i.e., in neglecting slowing down of the neutron. A further discussion of this slowing-down effect appears in Chapter III. Müller (M2), using an iteration method similar to Chernick's, has carried out an analogous computation of the resonance integral and an estimate of the corresponding errors.

The method outlined above, due to Chernick, was extended by Levine (L2), and the results of this extension were compared with the results of Monte Carlo calculations. A perturbation scheme was constructed by Chernick et al. (C3) to solve an equation similar to Eq. (2) for the case where the absorbing nucleus is Bi^{209}. In computing the flux by this method, the absorption of the nucleus was neglected. This flux was then used to compute an improved resonance integral. The values of the resonance integral for the N.R. and W.R. approximations were also computed. In addition to this, the resonance integral was computed by a Monte Carlo method. Assuming that the Monte Carlo estimate of the resonance integral is closer to the true value, the corresponding errors introduced by the approximation could be estimated, including the error introduced by neglecting slowing down, i.e., a comparison with the W.R. approximation. In an analysis by Corngold (C4), the error introduced by assuming infinite absorber mass has been estimated for a uranium-water lattice. The equation used for this analysis was similar to Eq. (2). This error is identical to the error introduced by assuming a W.R. approximation, or no slowing down.

Finally, a method which was first applied to a homogeneous case by Goldstein and Cohen (G2), and subsequently to a heterogeneous case by Forti (F1), has been used for cases where the resonance is neither wide nor narrow. In this method, a linear combination of the N.R. and W.R. approximations is iterated once in the integral equation. This results in an improved solution for the

flux which may then be used to compute a resonance integral for a resonance of intermediate width. The proportion of N.R. and W.R. solution used in the initial solution is determined by the width of the resonance under consideration.

In all the above heterogeneous cases considered, no detailed account was taken of the spatial flux variations within the absorber element. The spatial effects were integrated out, and it will be shown in Chapter II that Eq. (2) is a volume-averaged transport equation. Equation (2) may be derived from the general transport equation by neglecting angular effects, integrating out the volume effects, and by assuming that the flux is spatially flat. This is thus commonly known as the flat flux equation, as pointed out previously.

Corngold and Takahashi (C5, T1, T3) were among the first to consider the effect of including a spatial variation in the computation of the resonance integral. The geometrical configurations considered were slab and rod lattices, respectively. In both cases the starting point was the exact transport equation. This equation was simplified, by neglecting angular effects and evaluating the integral term which accounts for slowing down of the neutrons by collisions with absorber nuclei, by means of the W.R. approximation, i.e., no slowing down in the absorber lump was considered in this approach. By comparing the W.R. approximation using the solution to the flat flux equation, to the W.R. approximation using the solution of the equations developed in (C5) and (T1), it was possible to estimate the

error introduced by neglecting spatial variation of the neutron flux within the absorber lump.

Further estimates of the error introduced in the resonance integral by the flat flux approximation have been made by Dresner (D1), Goldstein (G3), and Berg (B6). Dresner's estimates of the error considered only the cases where $\Sigma_t(E)\vec{\ell} \gg 1$ and $\Sigma_t(E)\vec{\ell} \ll 1$, where $\vec{\ell}$ = mean chord length of the lump. However, there is a large range of practical interest between these two limits. In the computation by Goldstein and Berg, a variational method was utilized to estimate the error. Goldstein expressed the error in closed form as a function of mean chord length of the absorber lump. The computation carried out by Berg was based on a numerical technique. The methods of Goldstein and Berg, together with the general problem of the error associated with the flat flux approximation, will be considered in greater detail in Chapter III. In these error estimates no account was taken of the slowing down effects, i.e., in all cases the W.R. approximation was used.

In all the above calculations, except those appearing in (C5), (T1), (M2), (G2) and (B6), the Wigner rational approximation was used for the average escape probability p(E). This approximation is given by (M1):

$$p(E) = \frac{1}{1 + \vec{\ell}\,\Sigma_t(E)} \qquad (3)$$

The use of this expression introduces further errors. However it simplifies the analysis to the point where purely analytical methods are possible. Furthermore, certain convenient similarities between heterogeneous and homogeneous computations for the resonance integral exist when this approximation is used — these will be pointed out in Chapter II. Efforts to improve the accuracy of the Wigner rational approximation, while still retaining its basic structure, were made by Bell (B4), Nordheim (N1), Sauer (S1) and Otter (O1).

Finally, it should be noted that the resonance integral can be obtained directly by a variational technique. All approximations are then introduced in the functional. This approach has been used by Goldstein and Cohen (G2) for homogeneous systems, and by Gast (G4) for heterogeneous systems. In the computation carried out by Gast, a volume averaged functional was used, thus neglecting spatial effects.

It is evident from the foregoing discussion that all past theoretical estimates of the resonance integral have included at least one, and in some cases two, of the following approximations:

(i) Neutrons do not slow down when colliding with absorber nuclei, i.e., W.R. approximation.

(ii) The neutron distribution within the absorber elements has no spatial structure (flat flux approximation).

(iii) The average escape probability may be approximated by the Wigner rational approximation.

In this thesis the resonance integral is computed for a slab of absorbing material in a source of neutrons, without resorting to any of the above approximations. From this computation, the effect which these approximations have on the resonance integral is evaluated. In Chapter III a rough approximation is made of the error introduced in the resonance integral by neglecting the spatial variation of the flux. An exact collision density equation is formulated in Chapter IV. In Chapter V the resonance integral and fractional errors in the resonance integral are formulated. Chapter VI is devoted to a discussion of the numerical methods used to solve the integral equation and resonance integrals. A discussion of the results and conclusions follows in Chapter VII.

CHAPTER II

BASIC PHYSICAL CONCEPTS

It has been pointed out that the problem of accurately computing the resonance integral is two-fold:

(i) The cross-sections have to be known as a function of energy.

(ii) The flux has to be known as a function of energy and position.

In this chapter the energy dependence of the cross-sections involved is discussed and the basic transport equation, which will subsequently be used to determine the flux, is derived. In addition, the flat flux equation is derived, and the N.R. and W.R. approximations to the resonance integral are discussed. Finally the validity of the N.R. and W.R. approximations is considered.

A. Single Level Breit-Wigner Line Shape for Low Energy Resonances

The total, absorption, and scattering resonance cross-sections for the nuclei involved are given by (M1);

$$\sigma_t(E) = \frac{\pi}{k^2} g_J \frac{\Gamma_n \Gamma}{(E-E_r)^2 + (\Gamma/2)^2} + \frac{4\pi R}{k} g_J \frac{\Gamma_n (E-E_r)}{(E-E_r)^2 + (\Gamma/2)^2} + 4\pi R^2$$

$$\sigma_a(E) = \frac{\pi}{k^2} g_J \frac{\Gamma_n \Gamma_\gamma}{(E-E_r)^2 + (\Gamma/2)^2}$$

$$\sigma_s(E) = \frac{\pi}{k^2} g_J \frac{(\Gamma_n)^2}{(E-E_r)^2 + (\Gamma/2)^2} + \frac{4\pi R}{k} g_J \frac{\Gamma_n (E-E_r)}{(E-E_r)^2 + (\Gamma/2)^2} + 4\pi R^2 \qquad (4)$$

where

k = wave number of the neutron in the neutron-nucleus center of mass system

g = statistical spin factor $\frac{(2J + 1)}{2(2I + 1)}$

J = spin quantum number of compound nucleus

I = spin quantum number of target nucleus

R = potential scattering radius

E = neutron energy in center of mass system

E_r = resonance energy

Γ_n = neutron resonance width (in units of energy)

Γ_γ = radiative resonance width

Γ = total resonance width.

Equations (4) may be simplified somewhat by defining the following quantities:

$$\sigma_o = \frac{4\pi}{k^2} g_J \frac{\Gamma_n}{\Gamma}$$

$$\sigma_p = 4\pi R^2$$

$$x = \frac{2}{\Gamma} (E-E_r) \qquad (5)$$

where σ_p is the potential scattering cross-section — actually a measured constant from which R may be determined — and σ_o is the maximum value of the resonance cross-section at $E = E_r$.

Substituting definitions (5) into Eqs. (4) gives:

$$\sigma_t = \frac{\sigma_o + 2x\left[\sigma_o \sigma_p g_J \frac{\Gamma_n}{\Gamma}\right]^{1/2}}{1 + x^2} + \sigma_p$$

$$\sigma_a = \frac{\sigma_o \Gamma_\gamma}{\Gamma\,(1 + x^2)}$$

$$\sigma_s = \frac{\sigma_o \Gamma_n}{\Gamma\,(1 + x^2)} + \frac{2x\left[\sigma_o \sigma_p \frac{\Gamma_n}{\Gamma}\right]^{1/2}}{1 + x^2} + \sigma_p \qquad (6)$$

A derivation of these formulae appears in Appendix A.

B. The Transport Equation

To determine the energy and space dependence of the neutron flux we use a form of the general transport equation. This has been described often in the literature (D2, M1, W4). It will be useful to outline the assumptions involved and discuss the construction of the equation.

The following assumptions will be made regarding the motion of neutrons through matter:

(i) The motion of neutrons is described in terms of point collisions with nuclei. This results from disregarding all but the short-range nuclear forces. Neutron-neutron collisions are neglected since the neutron densities are many orders of magnitude lower than densities of the nuclei. This linearizes the transport equation.

(ii) Between collisions, the neutrons travel in straight lines at a constant speed.

(iii) Since atomic radii are large compared to nuclear radii (the ratio being approximately 10^{-4}), the neutron will, on the average, pass through a large number of atomic systems between collisions. Hence for neutrons traveling at a given speed through a given medium, the interaction probability per unit path length is independent of position and direction.

The above assumptions are all physically reasonable, and a mathematical model based on them describes the motion of neutrons in a nuclear reactor quite well.

With the above assumptions in mind, we construct an integral equation, which describes the collision density in a non-reentrant lump of absorbing material, surrounded by a neutron source. The following notation will be used:

$\vec{r}$ = the position vector of a neutron within the lump.

$\vec{\Omega}$ = the unit vector in the direction of motion of the neutron within the lump.

E = the energy of the neutron considered.

$F(\vec{r},\vec{\Omega},E)dVd\vec{\Omega}dE$ = the total collision rate in the volume element dV about point $\vec{r}$, for neutrons traveling in a direction $d\vec{\Omega}$ about $\vec{\Omega}$, and having an energy dE about E.

$$= \Sigma_t(E)\ \phi(\vec{r},\vec{\Omega},E)dVd\vec{\Omega}dE$$

$S(\vec{r},\vec{\Omega},E)dVd\vec{\Omega}dE$ = that part of the total collision rate in the volume element dV about point $\vec{r}$, for neutrons traveling in a direction $d\vec{\Omega}$ about $\vec{\Omega}$, and having an energy dE about E, which arises from an independent source, inside or outside the lump.

Two factors contribute to the collision rate of neutrons within the lump in the volume element dV about $\vec{r}$, traveling in direction $d\vec{\Omega}$ about $\vec{\Omega}$, and having energy dE about E:

(i) a contribution from the collision rate within the lump from dV' about position $\vec{r}'$, traveling in direction $d\vec{\Omega}'$ about $\vec{\Omega}'$ and having an energy dE' about E' (slowing down source), and

(ii) a contribution in the volume element dV about position $\vec{r}$, traveling in a direction $d\vec{\Omega}$ about $\vec{\Omega}$, and having energy dE about E, from the independent source. In our case the independent source is entirely external to the lump.

The general transport equation in the form that is useful here, is simply the combination of these two contributions. Thus:

$$F(\vec{r},\vec{\Omega},E)dVd\vec{\Omega}dE = S(\vec{r},\vec{\Omega},E)dVd\vec{\Omega}dE + \int_{E'}\int_{\vec{\Omega}'}\int_{V'} F(\vec{r}',\vec{\Omega}',E')\ \frac{\Sigma_s(E')}{\Sigma_t(E')}$$

$$K(E'\vec{\Omega}' \rightarrow E\vec{\Omega})\ \frac{\Sigma_t(E)\exp(-\Sigma_t(E)|\vec{r}-\vec{r}'|)}{4\pi|\vec{r}-\vec{r}'|^2}\ dV'd\vec{\Omega}'dE'dVd\vec{\Omega}dE \qquad (7)$$

where

$K(E', \vec{\Omega}' \rightarrow E\vec{\Omega})dE$ = probability that as a result of a scattering event, a neutron will change from a direction $d\vec{\Omega}'$ about $\vec{\Omega}'$, and an energy dE' about E', to a direction $d\vec{\Omega}$ about $\vec{\Omega}$ and an energy dE about E.

$\Sigma_t(E)$ = total macroscopic cross-section at energy E.

$= N\, \sigma_t(E)$

N = density of nuclei

$\sigma_t(E)$ = total microscopic cross-section at energy E.

$\Sigma_s(E)$ = macroscopic scattering cross-section at energy E.

We have used assumption (iii) to write the probability that a neutron having energy in dE about E will travel from dV' about $\vec{r}'$ to dV about $\vec{r}$ and undergo a collision in dV, as

$$\frac{\Sigma_t(E)\, \exp\left(-\Sigma_t(E)\,|\vec{r}-\vec{r}'|\right)}{4\pi\,|\vec{r}-\vec{r}'|^2}$$

Equation (7) is perfectly general, and with the assumptions stated gives an exact description of the total neutron collision density.

C. The Flat Flux Approximation

Developing the flat flux approximation from Eq. (7) enables us to show the restrictions implied by the assumption. The following procedure is followed:

(i) Equation (7) is integrated over the lump. A volume averaged collision density is defined. By this step the direct spatial dependence is removed from the flux.

(ii) The scattering is assumed to be isotropic in the center mass system. Then by integrating over $\vec{\Omega}$ all angular effects are removed from the equation.

(iii) Finally the flux is assumed to be spatially flat.

Assuming isotropic scattering the following averaged quantities are now introduced.

$$f(E) = \frac{1}{4\pi V}\int_{\vec{\Omega}}\int_{V} F(\vec{r},\vec{\Omega},E)\,dV\,d\vec{\Omega} = \text{collision rate averaged over volume and angle}$$

$$s(E) = \frac{1}{4\pi V}\int_{\vec{\Omega}}\int_{V} S(\vec{r},\vec{\Omega},E)\,dV\,d\vec{\Omega} = \text{source rate averaged over volume and angle.}$$

The probability that a neutron in dV will not have a collision in volume element dV', integrated over the lump is denoted by by $P(\vec{r},E)$ and is given by:

$$P(\vec{r},E) = 1 - \int_{V'} \frac{\Sigma_t(E)\,\exp\left(-\Sigma_t(E)\,|\vec{r}-\vec{r}'|\right)}{4\pi\,|\vec{r}-\vec{r}'|^2}\,dV'$$

$P(\vec{r},E)$ is thus the probability of a neutron escaping from the lump at an energy dE about E, from a volume element dV about $\vec{r}$. The collision density equation now becomes

$$f(E) = \frac{1}{V} \int_{V'} \int_{E'} \frac{\Sigma_s(E')}{\Sigma_t(E')} F(\vec{r}',E') \; k(E' \rightarrow E)\left[1 - P(\vec{r}',E)\right] d\vec{r}' dE' + s(E) \tag{8}$$

where

$$F(\vec{r},E) = \frac{1}{4\pi} \int_{\vec{\Omega}} F(\vec{r},\vec{\Omega},E) d\vec{\Omega} \; .$$

Now introducing the volume-averaged escape probability

$$p_V(E) = \frac{1}{V} \int_V P(\vec{r},E) dV \; ,$$

adding and subtracting this quantity from the term in brackets in Eq. (8), it is seen that it may be written as:

$$f(E) = \left[1 - p_V(E)\right] \int_{E'} \frac{\Sigma_s(E')}{\Sigma_t(E')} f(E') \; k(E' \rightarrow E) dE' + s(E)$$

$$- \frac{1}{V} \int_{\vec{r}'} \int_{E'} \frac{\Sigma_s(E')}{\Sigma_t(E')} F(\vec{r}',E') \; k(E' \rightarrow E) \left[P(\vec{r}',E) - p_V(E)\right] d\vec{r}' dE' \tag{9}$$

From the definition of $p_V(E)$ it is seen that the third term on the right hand side of Eq. (9) vanishes in the case of a spatially flat flux distribution.

Thus the remainder of this equation constitutes the flat flux equation. To proceed further we assume that outside the lump the neutron flux is spatially flat. We may then make use of the fact that the spatially-flat flux inside the lump, produced by a spatially-flat flux outside the lump, is equal to the product of

the average escape probability and the flux outside the lump (M1, C6). Since s(E) is a collision density, it may thus be written

$$s(E) = \Sigma_t(E)\ \phi_o(E)\ p_v(E)$$

where

$\phi_o(E)dE$ = the spatially-flat flux outside the lump in energy dE about E.

For the sake of convenience, the energy variable is changed to a lethargy variable, where lethargy is defined by:

$$u = \ell n \frac{E^*}{E}$$

where

E^* = reference energy

Furthermore, the assumption is made that the spatially-flat flux in the moderator is that which would result from slowing down in an infinite, non-absorbing moderator. Since this asymptotic distribution in terms of lethargy variables is a constant, the flux in the moderator is constant with respect to both lethargy and spatial variables. In lethargy variables $k(E' \rightarrow E)$ can be shown to be given by (M1):

$$k(E' \rightarrow E)dE' = \frac{e^{u'-u}}{1-\alpha}\, du'$$

Thus, Eq. (9) can be written

$$f(u) = \left[1 - p_v(u)\right] \int_{u-\Delta}^{u} \frac{\Sigma_s(u')}{\Sigma_t(u')}\, f(u')\, \frac{e^{u'-u}}{(1-\alpha)}\, du' + \phi_o\, \Sigma_t(u)\, p_v(u) \qquad (10)$$

where

$$\Delta = \ell n \frac{1}{\alpha}$$

Equation (10) is of the same form as Eq. (2), which was proposed on intuitive grounds by Chernick. The assumptions which were necessary to derive Eq. (10) restrict its applicability in the following manner (M1):

(i) The absorbing lumps must be widely spaced relative to the slowing down distance in the moderator.

(ii) The size of the absorbing lump must be larger than the mean free path in the moderator.

D. The W.R. and N.R. Approximations

To compute the resonance integral, Eq. (10) has to be solved to obtain the flux. This may be done either by a numerical method, or by an approximate analytic method. The approximations used are usually the N.R. or the W.R. approximations defined in Chapter I (M1, D1, C1). The cross-sections used are described by the single level Breit-Wigner relation, given by Eq. (6). The use of this cross-section implies that only one resonance will be considered at a time.

Finally, the volume-averaged escape probability $p_v(u)$ may be obtained by evaluating the integral defining it. However, even for the simplest geometrical shapes, this leads to a complicated function, and it is not possible to calculate the resonance integral in closed form.

An approximation, developed by Wigner (W3) is introduced. This is known as the Wigner rational approximation, as defined in Chapter I:

$$p_v(u) = \frac{1}{1 + \vec{\ell}\,\Sigma_t(u)} \qquad (11)$$

where

$\vec{\ell}$ = mean chord length = $4\,\frac{V}{S}$ (C6)

V = volume of lump

S = surface area of lump

It is possible to use this approximate relation for all geometrical shapes, since the dependence of $p_v(u)$ on geometry is not strong. It is particularly good for small values of $\vec{\ell}\,\Sigma_t(u)$ and for large values of $\vec{\ell}\,\Sigma_t(u)$. The maximum error is of the order of 10% (M1). It is thus possible to obtain analytic solutions for all geometrical shapes.

Using this technique the resulting resonance integrals are (M1):

$$I_{NR} = \frac{\phi_o\,\pi\,\sigma_o\,\Gamma_\gamma}{2E_r\left[1 + \frac{1}{\beta}\,(1 - \delta)\right]^{1/2}} \qquad \text{(narrow resonance approximation)}$$

$$I_{WR} = \frac{\phi_o\,\pi\,\sigma_o\,\Gamma_\gamma}{2E_r\left[1 + \left(\frac{\sigma_o\,\Gamma_\gamma}{\sigma\,\Gamma}\right)\right]^{1/2}} \qquad \text{(wide resonance approximation)} \qquad (12)$$

where

$$\beta = \frac{\sigma_p + \sigma_o}{\Gamma_o} \qquad \sigma = \frac{1}{\ell N}$$

$$\delta = \frac{\sigma_p \, g_J \, \Gamma_n}{(\sigma_p + \sigma)\Gamma}$$

It is of interest to note that by merely including the constant σ the heterogenous resonance integral may be deduced from the homogeneous resonance integral (M1). This equivalence is useful for predicting resonance integrals from measurements or calculations. However, it should be noted that the equivalence is only true within the assumptions stated regarding the flat flux equation and the Wigner rational approximation.

An attempt has been made (G2, F1) to include resonances which are neither narrow nor wide. The salient idea used in this approach is to make a linear combination of the N.R. and W.R. solutions to the collision density equation; i.e.

$$f(u) = \lambda \, f_{NR}(u) + (1 - \lambda) \, f_{WR}(u) \qquad (13)$$

The above solution is iterated once more in the integral equation (10), and since it is of the Fredholm type, the iterated solution is closer to the exact solution than the first approximation (C9). The resonance integrals are now computed using both solutions and equated to obtain a transcendental equation for the value of λ. This value for λ, which is a function of the resonance parameters, is then used to compute the resonance integral.

E. Validity of the W.R. and N.R. Approximations

Generally, as indicated in the definition in Chapter I, the total resonance width is compared with the maximum-energy-loss per neutron collision. It has been pointed out recently (C10) that this approach is not quite correct. For some isotopes the total width is large whereas the absorption width is small. Therefore a better comparison is the "absorption probability width" measured by $a(E) = \Sigma_a(E)/\Sigma_t(E)$. This is called the "practical width." This practical width is different from that suggested in the literature (M1, N2).

The value of a(E) varies with energy, as shown in Fig. 3. To find the half-width at half-maximum, first the value of $x = 2/\Gamma(E-E_r)$ is computed at which the maximum value of a(E) occurs. Using this value of x, it is possible to determine the value of the half-maximum value of a(E), $a_{max}/2$. Since the half width at the half-maximum value is desired, the value of $a_{max}/2$ is equated to a(E) and from this the value of x at half-maximum may be obtained. From this value of x the practical half-width may be defined.

Proceeding thus in the above manner, the absorption probability is given by:

$$a(E) = \frac{\sigma_a(E)}{\sigma_t(E)} = \frac{\sigma_o \Gamma_\gamma}{\Gamma\left\{\left[\sigma_p + \sigma_o\right] - \frac{b^2}{\sigma_p} + \left[x + \frac{b}{\sigma_p}\right]^2 \sigma_p\right\}} \qquad (14)$$

where

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

$$b = \left[\sigma_o \sigma_p \, g_J \, \frac{\Gamma_n}{\Gamma}\right]^{1/2}$$

The maximum value of a(E) occurs when $x = -b/\sigma_p$, thus the half-maximum value is given by

$$\frac{a_{max}}{2} = \frac{\sigma_o \, \Gamma_\gamma}{2\Gamma\left[\sigma_p + \sigma_o - \frac{b^2}{\sigma_p}\right]}$$

To find the width at half-maximum $a_{max}/2$ is equated to a(E), and the corresponding value for x is determined. From this the energy at half-maximum can be obtained, and with this relation the practical width at half-maximum may be defined, i.e.,

$$\frac{x_{max}}{2} = \pm\left[\frac{\sigma_p + \sigma_o}{\sigma_p} - \frac{b^2}{\sigma_p}\right]^{1/2} - \frac{b}{2} = \frac{2}{\Gamma}\left[\frac{E_{max}}{2} - E_r\right]$$

$$\frac{E_{max}}{2} = \pm\left[\frac{\sigma_p + \sigma_o}{\sigma_p} - \frac{b^2}{\sigma_p}\right]^{1/2} \frac{\Gamma}{2} - \frac{\Gamma b}{2\sigma_p} + E_r \quad .$$

Thus by definition

$$\Gamma_{prac} = \Gamma\left[1 + \frac{\sigma_o}{\sigma_p}\left(1 - g_J \, \frac{\Gamma_n}{\Gamma}\right)\right]^{1/2} \qquad (15)$$

It is thus seen that $\Gamma_{prac} > \Gamma$ since in most practical cases the term in brackets is greater than unity. Since the maximum energy loss

for neutrons when colliding with nuclei at energy dE about E is $(1 - \alpha)E$, the criterion for a resonance to be narrow or wide at a resonance energy E_r is

$$\Gamma_{prac} \ll (1 - \alpha)E_r \qquad \text{narrow resonance}$$

$$\Gamma_{prac} \gg (1 - \alpha)E_r \qquad \text{wide resonance} \tag{16}$$

Between these two limits a numerical solution of the collision density equation should be carried out, or an intermediate resonance formulation used.

CHAPTER III

THE SPATIALLY FLAT-FLUX AND INFINITE MASS APPROXIMATIONS

In the previous chapter, approximate solutions to the collision density equation are outlined, and these solutions may be used to determine the resonance integral. The approximations made are concerned with the spatial structure of the neutron flux and the mass of the absorbing nucleus. In the former approximation, the flux is considered spatially flat, and in the latter the mass of the absorbing nucleus is assumed to be infinite.

The first section of the present chapter will be devoted to a discussion of the error introduced in the resonance integral by the approximation concerning the nuclear mass of the absorber. This approximation is known as the infinite mass approximation. As previously noted it is identical to the W.R. approximation.

The second section of this chapter contains a discussion of the error introduced in the resonance integral by the spatial approximation to the flux distribution. This approximation is known as the flat flux approximation.

A. Infinite Mass Approximation

The infinite mass approximation affects the collision density, and thus the resonance integral, in two different ways. These depend upon whether the resonance is primarily absorbing, or primarily scattering.

To investigate these effects, let us consider a lump of absorbing material which is larger than the total mean free path of neutrons $\lambda_t = 1/\Sigma_t$, at resonance energy. Near the resonance energy two sources of neutrons exist in the lump:

(i) Neutrons in the resonance energy range may enter the lump from a spatially external source. These neutrons are absorbed, primarily, in a thin layer close to the surface of the lump. This layer is the depth of penetration, and is of the order of a mean free path in the predominantly absorbing case. It is therefore seen that the nuclei inside this layer have a low probability of reacting with the neutrons from a source external to the lump. The nuclei within the boundaries of this layer are thus shielded from the neutron flux. This effect is known as self-shielding.

(ii) Neutrons of higher energy may also enter into the resonance energy range by collisions with nuclei inside the lump. These neutrons appear, with equal probability, throughout the volume of the absorbing lump.

A closer consideration of the scattering and absorbing resonance types will now be undertaken.

(a) Absorbing Resonance

In the case of a predominantly absorbing resonance the absorption half-width is larger than the scattering half-width, i.e., $\Gamma_\gamma > \Gamma_n$.

With the above two source terms in mind, the infinite mass approximation will be considered. In this case only the first source contributes to the neutron flux. This follows from the fact that the nuclear mass is assumed infinite, and thus no neutrons lose energy when colliding with a nucleus. Neutrons which contribute to the flux in the resonance energy range originate from outside the lump. Thus, due to the self-shielding effect pointed out above, the volume of absorber in the central region, which is subjected to a low neutron flux, plays a relatively unimportant part in the absorption of neutrons.

In actual fact neutrons enter the resonance energy range from both sources mentioned above. Hence one should expect that the collision density, and thus the resonance integral, will be underestimated by the infinite mass approximation. This conclusion holds only for primarily absorbing resonances.

(b) Scattering Resonances

If the resonance is primarily scattering, the scattering half-width is larger than the absorbing half-width ($\Gamma_n > \Gamma_\gamma$).

Again only the first source term contributes to the neutron flux in the infinite mass approximation. Since neutrons are permitted to remain at the energy at which they enter the lump, they

undergo a large number of collisions in this case. In the real case a collision with an absorbing nucleus lowers the energy of the neutron. After a certain number of collisions the neutron may be completely removed from the resonance energy range.

The collision density is over-estimated in this case by the infinite mass approximation. Thus the resonance integral will be over-estimated. This result is only true for primarily scattering resonances.

Approximate computational investigations of the above effects have been carried out for several resonances in U^{238} (C4), and for one resonance in Bi^{209} (C3). These computations confirm the above conclusions.

It should be pointed out that the flat flux approximation was used in the above mentioned computations. Furthermore, in the case of the Bi^{209} computation, neutron absorption was neglected in the collision density equation.

B. The Geometrical Approximation

The geometrical approximation which is introduced in the collision density equation is known as the flat flux approximation, and follows from the fact that the flux is assumed spatially flat. This assumption has the effect of over-estimating the collision density, and thus over estimates the resonance integral. Three methods exist by which the fractional error introduced in the resonance integral may be estimated:

(i) The first approach is based on the last term of Eq. (9) of Chapter II. This term is zero when the flux is flat, and positive when the flux is depressed in the interior. Since this term is positive the collision density is reduced in the case where a spatial variation is taken into account. This consequently reduces the resonance integral.

Investigations by Goldstein (G3) and Berg (B6), using this approach, have indicated that the flat-flux approximation over-estimates the resonance integral. They consider a single absorber element surrounded by a neutron source. The absorbing nucleus is assumed to have a single resonance described by the Breit-Wigner single resonance line shape. Use is made of the infinite mass approximation to solve the energy integral in the collision density equation. A variational technique is used to determine the magnitude of the correction term. With this correction, the correction to the resonance integral is determined.

Goldstein (G3) makes use of the Wigner rational approximation to evaluate the correction to the resonance integral in closed form. The following relation is obtained for the fractional error introduced, by a flat flux approximation, in the resonance integral:

$$\epsilon = \frac{\frac{\Gamma_\gamma}{\Gamma}\left[\left(1 + \Sigma_p \vec{\ell}\right)^3 \left(1 + \bar{\ell}\left(\Sigma_p + \Sigma_o\right)\right)\right]^{1/2}}{\left[1 + \Sigma_o \vec{\ell}\,\frac{\Gamma_\gamma}{\Gamma}\right]\left\{1 - \frac{\frac{\Gamma_n}{\Gamma} - 2\Sigma_p \Gamma_\gamma \vec{\ell}\,\Gamma^{-1}}{\left[1 + \frac{\Sigma_o \Gamma_\gamma \vec{\ell}\,\Gamma^{-1}}{1 + \left(\Sigma_o + \Sigma_p\right)\vec{\ell}}\right]^{1/2}}\right\}} - 1 \qquad (17)$$

Berg(B6) uses an exact expression for the average escape probability, and consequently is unable to determine the desired fractional error in closed form. In this case a numerical estimate of the combined fractional error for a number of resonances in U^{238} was computed. The resonances included were at 6 ev, 6.8 ev, 21 ev, 36.8 ev, 66.3 ev, 102.8 ev and 190 ev. The geometrical configuration assumed, was a slab of thickness 0.5 cm. This computation indicated that the flat-flux approximation over-estimates the combined resonance integral, for these resonances, by 1.6%.

(ii) A second approach has been formulated by Corngold (C5) and Takahashi (T1). In this approach an infinite lattice of slabs, in Corngold's investigation, and of rods in Takahashi's investigation is considered. Equations defining the neutron flux, as a function of energy, position and angle, in these systems are set up. They are solved by an appropriate choice of polynomial expansion. In both cases the angular variable is

removed by expanding it in Legendre polynomials. The spatial dependence is expressed by an appropriate Legendre polynomial series in the case of the slab lattice, and a Bessel function series in the case of the rod lattice. Finally, the equation for the energy-dependent expansion coefficient is solved by using the infinite mass approximation. The neutron flux is then determined to any desired degree of accuracy, depending on how many spatial and angular terms are retained in the series. Thus the resonance integral may be computed for either a spatially flat or varying flux distribution. From these results it is possible to compute the fractional error introduced in the resonance integral when a spatially flat flux is assumed.

These investigations indicated that the resonance integral computed using a spatially varying flux is larger than the resonance integral computed using a flat flux approximation. This result is contrary to the results obtained by Goldstein (G3) and Berg (B6).

(iii) Finally the third approach may be explained physically by considering the spatial distribution of neutrons. In an actual absorber element a spatial variation of the neutron flux is present, and a large proportion of the neutron flux will be close to the surface. Due to this spatial distribution of the neutron flux, the average

escape probability per neutron is larger in the actual case than in the case where a flat flux approximation is assumed. This may be seen by noting that the average escape probability for a neutron from a lump is dependent on its distance from the surface of the lump.

In this method, a flux averaged escape probability $p_f(E)$ is determined, as opposed to the usual volume averaged escape $p_v(E)$. It is thus possible to determine the escape probability for a flat flux $p_f{}^f(E)$ and a spatially varying flux $p_f{}^v(E)$. Since $p_f{}^v(E) > p_f{}^f(E)$, more neutrons can escape from the lump and avoid resonance absorption. Thus the resonance integral computed using a spatially varying flux is less than the resonance integral computed using a spatially flat flux.

To determine the order of magnitude of this error the following fractional error will be determined.

$$\frac{\delta I}{I} = \frac{\partial I}{\partial p} \cdot \frac{1}{I} \cdot \delta p$$

$$= Q\, \delta p \qquad (18)$$

where

I = resonance integral

p = average escape probability

$$\delta p = p_f{}^v(E) - p_f{}^f(E)$$

A one-dimensional slab of thickness "a" will be considered, as shown in Fig. 2. The value of δp will be determined by using a flux with a quadratic spatial dependence for computing $p_f^{v}(E)$. This is the simplest physically reasonable shape that deviates from a flat flux for a symmetric problem. No energy dependence will be taken into account when computing δp; which will be determined at resonance energy. Q is determined by using approximate expressions for the resonance integral as a function of p (M1). Once δp and Q have been determined, $\delta I/I$ may be estimated.

The flux averaged escape probability is given by (C6):

$$p_f(E) = \frac{\frac{1}{2}\int_o^a \phi(x)\left\{E_2\left[x\Sigma_t(E)\right] + E_2\left[(a-x)\ \Sigma_t(E)\right]\right\}dx}{\int_o^a \phi(x)\ dx} \qquad (19)$$

where

$\phi(x)$ = neutron flux as a function of position

$E_n(\xi)$ = exponential integral function $= \int_1^\infty \frac{e^{-u\xi}}{u^n}\ du.$ (20)

For a spatially flat flux the average escape probability is given by (C6)

$$p_f^{f} = \frac{1}{a\Sigma_t}\left\{\frac{1}{2} - E_3\left[a\Sigma_t\right]\right\} \qquad (21)$$

Now assume that the flux is given by the following quadratic distribution

$$\phi(x) = A\left(x - \frac{a}{2}\right)^2 + B \tag{22}$$

where A and B are constants which determine the flux shape.

Substituting Eq. (22) into Eq. (19), and evaluating the integrals, the following expression is obtained for the average escape probability:

$$p_f{}^v = \frac{\left\{\frac{Aa^3}{2} + 2Ba\right\}\frac{1}{a\Sigma_t}\left\{\frac{1}{2} - E_3\left[a\Sigma_t\right]\right\}}{\left[\frac{Aa^3}{6} + 2Ba\right]} + \frac{4Aa^3\left\{\frac{1}{a^3\Sigma_t{}^3}\left[\frac{1}{4} - E_5\left(a\Sigma_t\right)\right] - \frac{1}{2a^2\Sigma_t{}^2}\left[\frac{1}{3} + E_4\left(a\Sigma_t\right)\right]\right\}}{\left[\frac{Aa^3}{6} + 2Ba\right]} \tag{23}$$

To compute δp, the difference between Eq. (23) and Eq. (21) is taken, i.e.

$$\delta p = \text{Equation (23)} - \text{Equation (21)} \tag{24}$$

The determination of Q (Eq. 18) will now be carried out. Q may be determined for both the W.R. and N.R. approximations, depending on which approximation is chosen for the evaluation of I.

Considering the N.R. case first, the resonance integral is given by (M1)

$$I = \phi_o \int p(u)\,\Sigma_t(u) + [1 - p(u)]\,\Sigma_p\,\frac{\sigma_a(u)}{\sigma_t(u)}\,du$$

Hence

$$Q_{NR} = \frac{\partial I}{\partial p} \cdot \frac{1}{I} = \frac{\int \left[\sigma_t(u) - p_p\right] \frac{\sigma_a(u)}{\sigma_t(u)}\, du}{\int \left\{p(u)\ \sigma_t(u) + \left[1 - p(u)\right]\ \sigma_p\right\} \frac{\sigma_a(u)}{\sigma_t(u)}\, du} \qquad (25)$$

In the case of the W.R. approximation, the resonance integral is given by (M1):

$$I = \phi_o \int \frac{p(u)\ \Sigma_a(u)\ \Sigma_t(u)}{\left[\Sigma_t(u) + p(u)\ \Sigma_s(u)\right]}\, du$$

Thus

$$Q_{WR} = \frac{\partial I}{\partial p}\ \frac{1}{I} = \frac{\int \frac{\sigma_t(u)\ \left[\sigma_a(u)\right]^2}{\left[\sigma_a(u) + p(u)\ \sigma_s(u)\right]^2}\, du}{\int \frac{p(u)\ \sigma_a(u)\ \sigma_s(u)}{\left[\sigma_a(u) + p(u)\ \sigma_s(u)\right]}\, du} \qquad (26)$$

The integrals in Eqs. (25) and (26) are taken over the effective range of the resonance.

It is desirable to evaluate Q_{NR} and Q_{WR} in closed form. To make this possible the Wigner rational approximation is used for the average escape probability p(u). (An exact value of p(u) would necessitate a numerical solution.) The integration variable is changed from lethargy to energy, and is further modified by the following substitution:

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

The Breit-Wigner single resonance line shapes are used for the cross-section. They are given by Eq. (6) in Chapter II. No interference scattering is included in this calculation. The scattering cross-section is therefore given only by the potential scattering term σ_p and the resonance scattering term $\sigma_s(x)$. Equations (25) and (26) now reduce to:

$$Q_{NR} = \frac{\sigma_o^2}{\sigma_p^* \sigma_p} \frac{\int_{-\infty}^{\infty} \frac{dx}{\left[1 + x^2\right]\left[(1 + \beta) + x^2\right]}}{\int_{-\infty}^{\infty} \frac{dx}{\left[x^2 + (1 + \frac{1}{\beta})\right]}} \tag{27}$$

and

$$Q_{WR} = \frac{\beta \Gamma_\gamma}{\Gamma} \frac{\int_{-\infty}^{\infty} \left[\frac{Bx^2 + D}{x^2 + A}\right]^2 \frac{dx}{\left[1 + x^2\right]\left[x^2 + C\right]}}{\int_{-\infty}^{\infty} \frac{dx}{(x^2 + A)}} \tag{28}$$

where

$$\beta = \frac{\sigma_o}{\sigma_p}$$

$$\sigma_p^* = \sigma_p + \frac{1}{\vec{\ell} N}$$

$$A = 1 + \sigma_o \vec{\ell} N \frac{\Gamma_\gamma}{\Gamma}$$

$$B = 1 + \sigma_o \vec{\ell} N$$

$$D = 1 + \vec{\ell} N(\sigma_p + \sigma_o)$$

$$C = 1 + \beta$$

With the range of integration extending from $-\infty$ to $+\infty$, the integrals may be evaluated by integrating around a suitable contour in the complex plane.

On evaluating the integrals, the following results are obtained for Q:

$$Q_{NR} = \left[1 + \frac{\sigma_o}{\sigma_p^*}\right]^{1/2} \left\{\frac{[1+\beta]^{1/2} - 1}{[1+\beta]^{1/2}}\right\} \tag{29}$$

and

$$Q_{WR} = \beta \frac{\Gamma_\gamma}{\Gamma} [B]^{1/2} \left\{\frac{(D-A)^2}{(B-1)^2 (C-1)} + \frac{(D-AC)^2}{(B-C)^2 (1-C) [C]^{1/2}} + \frac{2(D-AB)^2 [B]^{1/2}}{(B-1)(B-C)} \left[\frac{2A}{(D-AB)} + \frac{1}{4B} + \frac{1}{(B-1)} + \frac{1}{(B-C)}\right]\right\} \tag{30}$$

Thus with the value of δp given by Eq. (24) and the values of Q_{NR} and Q_{WR} given by the above two equations, the value of $\delta I/I$ may be estimated for both the W.R. and N.R. approximations. In view of all the approximations included in this particular computation of $\delta I/I$, it should not be expected to indicate more than a very rough estimate of the error.

The value of $\delta I/I$ for the 104 ev resonance in uranium is shown in Fig. 21 by the dotted line. Only the N.R. approximation is shown, as the W.R. approximation indicated errors which seem to be reasonable only for extremely thin slabs.

The estimate of the fractional error, given by Goldstein, is expressed by Eq. (17). However, since this formula is only good for extremely thin slab sizes, it is not shown on Fig. 21. In the range of practical interest, Goldstein's formula grossly over-estimates the error. This indicates a positive fractional error for the range investigated.

CHAPTER IV

THE COLLISION DENSITY EQUATION

The following two factors motivate a further study of the fractional errors introduced in the resonance integral by the infinite mass and the flat flux approximations:

(i) The results obtained by various investigators, when estimating the effect of the flat flux approximation on the resonance integral are contradictory. These estimates are discussed in Chapter III.

(ii) The infinite mass approximation has an important effect on the resonance integral; over-estimating it when the resonance is primarily scattering, and under-estimating it when the resonance is primarily absorbing. The physical background to this phenomenon is also discussed in Chapter III.

This chapter is devoted to the reduction of the general transport Eq. (7) into a form more suitable for our purpose. From this equation the collision density of neutrons in an absorbing lump of material may be determined to various degrees of accuracy, depending upon the approximation made in its solution. It is therefore possible to obtain an infinite mass or a flat flux approximation to the collision density as well as various more accurate approximations.

In order to simplify the analytical method while maintaining the heterogeneous configuration of the problem, a slab geometry is selected. As shown in Fig. 4, an infinite slab of thickness "a", containing an absorber, is assumed to be embedded in a neutron source.

The general collision density Eq. (7), will be modified for this geometry, in which

$$|\vec{r}-\vec{r}'|^2 = (x-x')^2 + y'^2 = T^2(x, x', y')$$

$$dV' = 2\pi\, y'dy'dx' \tag{31}$$

Equation (7) now becomes:

$$F(x,\vec{\Omega},E)dxd\vec{\Omega}dE = \int_{E'}\int_{\vec{\Omega}'}\int_{o}^{a}\int_{o}^{\infty} \frac{\Sigma_s(E')}{\Sigma_t(E')}\, F(x',\vec{\Omega}',E')\, K(E'\vec{\Omega}' \rightarrow E\vec{\Omega})$$

$$\times \frac{\Sigma_t(E)\; e^{-\Sigma_t(E)|T(x,x',y')|}}{4\pi\; T^2(x,x',y')}\, 2\pi y'dy'dx'd\vec{\Omega}'dE'dxd\vec{\Omega}dt$$

$$+ S(x,\vec{\Omega},E)dxd\vec{\Omega}dE \tag{32}$$

The expression for $T(x,x',y')$ may be re-written by defining an angle ϕ, i.e.

$$T(x,x',y') = \frac{|x' - x|}{\cos\,\phi}\ .$$

Setting

$$t \equiv \frac{1}{\cos\,\phi}$$

it is seen that

$$T(x,x',y') = t\ |x - x'|\ . \tag{33}$$

By substituting Eq. (33) in Eq. (31), an expression is obtained for y'. This expression will be a function of t, x' and x, i.e.

$$y' = \sqrt{t^2 - 1} \quad |x - x'| \quad . \tag{34}$$

The new expression for dy' is

$$dy' = \frac{|x - x'| t \, dt}{\sqrt{t^2 - 1}} \, . \tag{35}$$

Substituting Eqs. (33), (34) and (35) into Eq. (32), it is seen that the integral over y' is replaced by an integral over t. The limits of integration for t range from 1 to ∞, as can be seen from the definition of t. The following equation results:

$$F(x,\vec{\Omega},E)dxd\vec{\Omega}dE = \frac{1}{2} \int_{E'} \int_{\vec{\Omega}'} \int_{o}^{a} \int_{1}^{\infty} \frac{\Sigma_t(E) e^{-\Sigma_t(E) t |x-x'|}}{t} F(x',\vec{\Omega}',E')$$

$$\times \frac{\Sigma_s(E')}{\Sigma_t(E')} K(E'\vec{\Omega}' \rightarrow E\vec{\Omega}) dt dx' d\vec{\Omega}' dE' dx d\vec{\Omega} dE$$

$$+ S(x,\vec{\Omega},E)dxd\vec{\Omega}dE \tag{36}$$

Now by making use of expression (20), the integral over t is written as an exponential integral function. Equation (36) becomes:

$$F(x,\vec{\Omega},E)dxd\vec{\Omega}dE = \frac{\Sigma_t(E)}{2} \int_{E'} \int_{\Omega'} \int_{o}^{a} \frac{\Sigma_s(E')}{\Sigma_t(E')} F(x',\vec{\Omega}',E') \; K(E'\vec{\Omega}' \rightarrow E\vec{\Omega})$$

$$\times E_1\left[\Sigma_t(E) \; |x - x'|\right] dx' d\vec{\Omega}' dE' dx d\vec{\Omega} dE$$

$$+ S(x,\vec{\Omega},E)dxd\vec{\Omega}dE \tag{37}$$

We now consider the case of a slab which is a uniform mixture of several nuclear species. The appropriate equation for describing the collision density in a slab of several nuclear species is obtained from a generalization of Eq. (37). The only change required involves the integral term, which is the contribution of neutrons from a position dx' about x', traveling in a direction $d\vec{\Omega}'$ about $\vec{\Omega}'$, and having an energy dE' about E'. For the mixture, this term must include the contributions from collisions with all the various nuclear types present. It is necessary then, to add a scattering integral for each nuclear species i.

Defining i = 1, 2, ... N species,

$\Sigma_s^{(i)}(E)$ = macroscopic scattering cross-section of i^{th} species.

$K^{(i)}(E'\vec{\Omega}' \rightarrow E\vec{\Omega})$ = scattering kernel for the i^{th} species.

$$F(x,\vec{\Omega},E)dxd\vec{\Omega}dE = \sum_{i=1}^{N} \frac{\Sigma_t(E)}{2} \int_{E'} \int_{\vec{\Omega}'} \int_{o}^{a} \frac{\Sigma_s^{(i)}(E')}{\Sigma_t(E')} F(x',\vec{\Omega}',E') K^{(i)}(E'\vec{\Omega}' \rightarrow E\vec{\Omega})$$

$$\times E_1\left[\Sigma_t(E)\ |x - x'|\right] dx'd\vec{\Omega}'dE'dxd\vec{\Omega}dE$$

$$+ S(x,\vec{\Omega},E)dxd\vec{\Omega}dE \qquad (38)$$

For a given $S(x,\Omega,E)$, the collision density is completely specified by Eq. (38).

The collision density and source terms are now expanded. Legendre polynomials are postulated for the spatial variation, and spherical harmonics for the angular variation. The energy dependence

of the collision density is expressed by an expansion coefficient, i.e.,

$$F(x,\vec{\Omega},E) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{\ell=-n}^{+n} \left(\frac{2m+1}{a}\right) Y_n^{\ell}(\vec{\Omega})\, P_m\left(\frac{2x}{a}-1\right) f_n^{m}(E) \qquad (39)$$

$$S(x,\Omega,E) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{\ell=-n}^{n} \left(\frac{2m+1}{a}\right) Y_n^{\ell}(\vec{\Omega})\, P_m\left(\frac{2x}{a}-1\right) s_n^{m}(E) \qquad (40)$$

where

$$Y_n^{\ell}(\vec{\Omega}) = \left[\frac{(2n+1)(n-\ell)!}{4\pi(n+\ell)!}\right]^{1/2} P_n^{\ell}(\mu)\, e^{i\ell\psi} \qquad (41)$$

and $\mu = \cos \phi$. The direction $\vec{\Omega}$ in which the neutron is traveling is defined by the polar coordinates ϕ and ψ.

The following orthogonality relations hold (S2, M1)

$$\int_{\vec{\Omega}} Y_n^{\ell}(\vec{\Omega})\, Y_{\alpha}^{\beta *}(\vec{\Omega}) d\vec{\Omega} = \delta_{\ell\beta}\, \delta_{n\alpha} \qquad (42)$$

$$\int_0^a P_m\left(\frac{2x}{a}-1\right) P_s\left(\frac{2x}{a}-1\right) dx = \left(\frac{a}{2m+1}\right) \delta_{ms} \qquad (43)$$

In general, the values of n and m in Eqs. (39) and (40) cover all positive integers, n = 0, 1, 2, ... However, for cases involving a symmetric source distribution, the odd coefficients of m will vanish.

The following assumptions will now be made regarding the slab and the neutron slowing down process:

(i) The slab is made up of an isotropic homogeneous medium.

(ii) The neutron slowing down is due only to elastic scattering.

(iii) All nuclei of the medium are stationary.

With these assumptions in mind, it follows that the final direction of motion will depend only on the scattering angle between the initial and final directions. The following function will now be defined:

$\ell^{(i)}(E,\mu_o;E',\vec{\Omega}')d\mu_o dE$ = probability that a neutron with energy dE' about E', traveling in direction $d\vec{\Omega}'$ about $\vec{\Omega}'$, is scattered through an angle $d\mu_o$ about μ_o and has final energy dE about E,

where

$\mu_o = \cos \phi_o$, ϕ_o = angle between incoming and outgoing neutron direction.

In the case of an azimuthally symmetric collision, $K^{(i)}(E'\vec{\Omega}' \rightarrow E\vec{\Omega})$ and $\ell^{(i)}(E,\mu_o;E',\vec{\Omega}')$ are connected in the following manner:

$$K^{(i)}(E'\vec{\Omega}' \rightarrow E\vec{\Omega}) = \frac{1}{2\pi} \ell^{(i)}(E,\mu_o;E',\vec{\Omega}') .$$

The assumption is now made that $\ell(E,\mu_o;E',\vec{\Omega}')$ may be expressed by the following expansion:

$$\ell^{(i)}(E,\mu_o;E',\vec{\Omega}') = \sum_{\eta=0}^{\infty} \left(\frac{2\eta + 1}{2}\right) \ell_\eta^{(i)} (E;E',\vec{\Omega}') P_\eta(\mu_o) \qquad (44)$$

where

$$\ell_{\eta}^{(i)}(E;E',\vec{\Omega}') = \int_{-1}^{+1} \ell^{(i)}(E,\mu_o;E',\vec{\Omega}')\, P_{\eta}(\mu_o)\, d\mu_o \qquad (45)$$

Expansion (44) will now be written in terms of the directions $\vec{\Omega}'$ and $\vec{\Omega}$, which describe the respective directions before and after the collision. Using the addition formula for Legendre polynomials, expression (44) becomes

$$\ell^{(i)}(E,\mu_o;E',\vec{\Omega}') = 2\pi \sum_{\eta=o}^{\infty} \sum_{\beta=-\eta}^{+\eta} \ell_{\eta}^{(i)}(E;E',\vec{\Omega}')\, Y_{\eta}^{\beta}(\vec{\Omega})\, Y_{\eta}^{\beta^*}(\vec{\Omega}') \qquad (46)$$

Expressions (46), (40) and (39) are now substituted in Eq. (38), and by using the orthogonality relation (42) to evaluate the integral over $\vec{\Omega}'$, the integral term of Eq. (38) reduces to

$$\sum_{i=1}^{N} \sum_{m'=o}^{\infty} \sum_{n=o}^{\infty} \sum_{\ell=-n}^{n} \frac{\Sigma_t(E)}{2}\, Y_n^{\ell}(\vec{\Omega}) \int_{E'}\int_{o}^{a} P_{m'}\left(\frac{2x'}{a} - 1\right)\left(\frac{2m'+1}{a}\right) x$$

$$f_n^{m'}(E')\, E_1\left[\Sigma_t(E)\,|x - x'|\right] \frac{\Sigma_s^{(i)}(E')}{\Sigma_t(E')}\, \ell_n^{(i)}(E;E',\vec{\Omega}')\, dx'\, dE'\, dx\, d\vec{\Omega}\, dE$$

Equation (38) may now be written

$$\sum_{m=o}^{\infty} \sum_{n=o}^{\infty} \sum_{\ell=-n}^{n} Y_n^{\ell}(\Omega) \left(\frac{2m+1}{a}\right) P_m\left(\frac{2x}{a} - 1\right) f_n^m(E)\, dx\, d\vec{\Omega}\, dE$$

$$= \sum_{n=o}^{\infty} \sum_{\ell=-n}^{n} Y_n^{\ell}(\Omega) \left[\sum_{m=o}^{\infty} \left(\frac{2m+1}{a}\right) P_m\left(\frac{2x}{a} - 1\right) s_n^m(E)\, dx\, dE \right.$$

$$+ \sum_{i=1}^{N} \sum_{m'=o}^{\infty} \frac{(2m'+1)\Sigma_t(E)}{2a} \int_{E'}\int_{o}^{a} P_{m'}\left(\frac{2x'}{a} - 1\right) E_1\left[\Sigma_t(E)\,|x - x'|\right] f_n^{m'}(E')$$

$$\left. \frac{\Sigma_s^{(i)}(E')}{\Sigma_t(E')}\, \ell_n^{(i)}(E;E',\vec{\Omega}')\, dx'\, dE'\, dx\, dE \right] d\vec{\Omega}\ . \qquad (47)$$

Multiplying Eq. (47) by $Y_\alpha^{\beta *}(\vec{\Omega})\, P_s(2x/a-1)$ and integrating over $\vec{\Omega}$ and x, the following equation is obtained:

$$f_n^m(E)dE = \sum_{i=1}^{N} \sum_{m'=0}^{\infty} \left(\frac{2m'+1}{2a}\right) \Sigma_t(E) \int_o^a \int_o^a P_{m'}\left(\frac{2x'}{a} - 1\right) E_1\left[\Sigma_t(E)\,|x-x'|\right]$$

$$\times P_m\left(\frac{2x}{a} - 1\right) dx dx' \int_{E'} \frac{\Sigma_s^{(i)}(E')}{\Sigma_t(E')}\, f_n^{m'}(E')\, \ell_n^{(i)}(E;E',\vec{\Omega}')dE'dE$$

$$+ s_n^m(E)dE \qquad (48)$$

The integration over x is carried out by using the orthogonality relation (43). The integral over $\vec{\Omega}$ is performed by using Eq. (42).

Reconsidering the scattering kernel, expression (44) may be rewritten by defining two conditional probabilities, i.e.,

(i) $h^{(i)}(\mu_o;E,E;\vec{\Omega}')d\mu_o \equiv$ probability that, given a neutron with initial energy E' direction $\vec{\Omega}'$ and final energy E, it has been scattered through an angle of θ_o.

(ii) $g^{(i)}(E;E',\vec{\Omega}')dE \equiv$ probability that given a neutron with initial energy E' and direction $\vec{\Omega}'$, it has final energy dE about E.

The scattering kernel thus becomes

$$\ell^{(i)}(E,\mu_o;E',\vec{\Omega}')dEd\mu_o = h^{(i)}\,(\mu_o;E,E',\vec{\Omega}')\; g^{(i)}(E;E',\vec{\Omega}')dEd\mu_o \qquad (49)$$

Since there is a unique angle $\zeta^{(i)}[E,E']$ through which the neutron can be scattered elastically, it is seen that $h^{(i)}(\mu_o;E,E',\vec{\Omega}')$ is a delta function, i.e.,

$$h^{(i)}(\mu_o;E,E',\vec{\Omega}') = \delta(\mu_o - \zeta^{(i)}[E,E']) \tag{50}$$

Substituting (50) into (47) and the resulting expression into Eq. (45), it is seen that

$$\ell_n^{(i)}(E,E',\vec{\Omega}') = g^{(i)}(E,E',\vec{\Omega}')\ P_n\left[\zeta^{(i)}(E,E')\right] \tag{51}$$

Finally, making the assumption that the scattering is isotropic in the center of mass system, an expression may be formulated for $g^{(i)}(E;E',\vec{\Omega}')$ (M1). The following expression results for $\ell_n^{(i)}(E;E',\vec{\Omega}')$:

$$\ell_n^{(i)}(E;E',\vec{\Omega}') = \frac{P_n\left[\rho^{(i)}(E',E)\right]}{(1-\alpha_i)E'} \quad \text{for } E \le E' \le E/\alpha_i \tag{52}$$

$$= 0 \text{ otherwise}$$

Assuming now that there is no angular dependence present in the collision density, i.e., n = 0 (this implies isotropic scattering in the laboratory system)

$$\ell_o^{(i)}(E,E',\vec{\Omega}') = \frac{1}{(1-\alpha_i)E'} \text{ for } E \le E' \le E/\alpha_i \tag{53}$$

$$= 0 \text{ otherwise}$$

Using Eq. (53) as the kernel, Eq. (48) may be written as follows:

$$\begin{bmatrix} f_o^{\,o}(E) \\ \vdots \\ f_o^{\,m}(E) \end{bmatrix} = \begin{bmatrix} a_{oo}(E) & \cdots & a_{om}(E) \\ & & \vdots \\ a_{mo}(E) & & a_{mm}(E) \end{bmatrix} \begin{bmatrix} \sum_{i=1}^{N} \int_E^{E/\alpha_i} \frac{\Sigma_s^{(i)}(E') f_o^{\,o}(E') dE'}{(1-\alpha_i)\Sigma_t(E')E'} \\ \vdots \\ \sum_{i=1}^{N} \int_E^{E/\alpha_i} \frac{\Sigma_s^{(i)}(E') f_o^{\,m}(E') dE'}{(1-\alpha_i)\Sigma_t(E')E'} \end{bmatrix} + \begin{bmatrix} s_o^{\,o}(E) \\ \vdots \\ s_o^{\,m}(E) \end{bmatrix} \tag{54}$$

where

$$a_{rc}(E) = \left(\frac{2r+1}{2a}\right) \Sigma_t(E) \int_o^a \int_o^a P_r\left(\frac{2x'}{a} - 1\right) E_1\left[\Sigma_t(E)|x-x'|\right] \times P_c\left(\frac{2x}{a} - 1\right) dx dx' \tag{55a}$$

$$s_o^{\,c}(E) = \int_o^a P_c\left(\frac{2x}{a} - 1\right) S(x,E)\, dx \tag{55b}$$

The source of neutrons from outside the slab has not yet been specified. In this problem the assumption is made that the source of neutrons external to the slab has an energy dependence that varies as 1/E, no spatial dependence, and no angular dependence. Inside the slab, the collision density distribution, due to this external source,

will be determined from first-flight transport theory. S(x,E) is thus given by (M1, C6)

$$S(x,E) = \frac{\Sigma_t(E)}{2E}\left[E_2\left[\Sigma_t(E)x\right] + E_2\left[\Sigma_t(E)(a-x)\right]\right] \qquad (56)$$

The first m terms of the collision density expansion are determined in the following manner:

(i) Evaluate $a_{oo}(E)$ . . . $a_{mm}(E)$, and $s_o^{\,o}(E)$ . . . $s_o^{\,m}(E)$ from Eq. (47).

(ii) Substitute these in Eq. (46) and solve it for $f_o^{\,o}(E)$... $f_o^{\,m}(E)$.

(iii) These may then be substituted into expression Eq. (39), and F(x,E) may be determined, to the desired degree of accuracy.

From Eq. (39) it is seen that if m = 0, the resulting collision density is the flat flux approximation for this problem. If m = 2, quadratic terms are included in the collision density. As the value of m is increased, better approximations to the spatial distribution of the collision density are obtained.

The infinite mass approximation may also be obtained from Eq. (54). In this approximation, use is made of the fact that neutrons lose no energy when colliding with a nucleus. By evaluating the scattering collision density under the integrals of Eq. (54)

at the lower limit, i.e., E' = E, Eq. (54) reduces to

$$\begin{bmatrix} f_o^{\,o}(E) \\ \vdots \\ f_o^{\,m}(E) \end{bmatrix} = \begin{bmatrix} a_{oo}(E) & \cdots & a_{om}(E) \\ \vdots & & \\ a_{mo}(E) & \cdots & a_{mm}(E) \end{bmatrix} \begin{bmatrix} \sum_{i=1}^{N} \frac{f_o^{\,o}(E)\Sigma_s^{(i)}(E)}{\Sigma_t(E)} \\ \vdots \\ \sum_{i=1}^{N} \frac{f_o^{\,m}(E)\Sigma_s^{(i)}(E)}{\Sigma_t(E)} \end{bmatrix} + \begin{bmatrix} s_o^{\,o}(E) \\ \vdots \\ s_o^{\,m}(E) \end{bmatrix} \quad (57)$$

The three steps outlined above, for obtaining the collision density from Eq. (54), also apply to Eq. (57).

It is of interest to observe:

(i) The infinite mass approximation may be made without making any assumptions regarding the spatial distribution.

(ii) The flat flux approximation may be made without making any assumption regarding the mass of the nucleus.

(iii) Finally, both assumptions may be made, resulting in the usual W.R. approximation.

In the analysis of the actual problem, nine matrix elements and the corresponding three source terms are evaluated. This makes it possible to include quartic effects in the spatial distribution of the collision density. The method for evaluating the integrals

is illustrated in Appendix B. The nine matrix elements and three source terms are given below:

$$a_{oo}(E) = 1 - \frac{1}{r(E)}\left(\frac{1}{2} - E_3[r(E)]\right) \qquad s_o^{\,o}(E) = -\frac{r(E)}{E}\left[a_{oo}(E) - 1\right]$$

$$a_{2o}(E) = X(E); \qquad a_{o2}(E) = 5X(E); \qquad s_o^{\,2}(E) = -\frac{r(E)}{E}X(E)$$

$$a_{22}(E) = 1 - \frac{5}{r(E)}\left(\frac{1}{2} - E_3[r(E)]\right) + \frac{60E_4[r(E)]}{r^2(E)} + \frac{300}{r^3(E)}\left(\frac{1}{20} + E_5[r(E)]\right)$$
$$+ \frac{720E_6[r(E)]}{r^4(E)} - \frac{720}{r^5(E)}\left(\frac{1}{6} - E_7[r(E)]\right)$$

$$a_{4o}(E) = Y(E); \qquad a_{o4}(E) = 9Y(E); \qquad s_o^{\,4}(E) = -\frac{r(E)}{E}Y(E)$$

$$a_{24}(E) = 9Z(E); \qquad a_{42}(E) = 5Z(E)$$

$$a_{44}(E) = 1 - \frac{9}{r(E)}\left(\frac{1}{2} - E_3[r(E)]\right) + \frac{360}{r^2(E)}E_4[r(E)]$$
$$+ \frac{6840}{r^3(E)}\left(\frac{1}{76} + E_5[r(E)]\right) + \frac{79920}{r^4(E)}E_6[r(E)]$$
$$+ \frac{3326400}{r^6(E)}E_8[r(E)] - \frac{624240}{r^5}\left(\frac{3}{578} - E_7[r(E)]\right)$$
$$+ \frac{11793600}{r^7(E)}\left(\frac{1}{104} + E_o[r(E)]\right) + \frac{25401600}{r^9(E)}$$
$$\times \left[r(E)\,E_{10}[r(E)] - \frac{1}{10} + E_{11}[r(E)]\right]$$

$$X(E) = -\frac{1}{r(E)}\left(\frac{1}{2} - E_3[r(E)]\right) + \frac{6}{r^2(E)}\left(\frac{1}{3} + E_4[r(E)]\right) - \frac{12}{r^3(E)}\left(\frac{1}{4} - E_5[r(E)]\right)$$

$$Y(E) = \frac{1}{r(E)}\left(\frac{1}{2} - E_3[r(E)]\right) + \frac{20}{r^2(E)}\left(\frac{1}{3} + E_4[r(E)]\right) - \frac{180}{r^3(E)}\left(\frac{1}{4} - E_5[r(E)]\right)$$
$$+ \frac{840}{r^4(E)}\left(\frac{1}{5} + E_6[r(E)]\right) - \frac{1680}{r^5(E)}\left(\frac{1}{6} - E_7[r(E)]\right)$$

$$Z(E) = -\frac{1}{r(E)}\left(\frac{1}{2} - E_3[r(E)]\right) + \frac{26}{r^2(E)}\left(\frac{7}{39} + E_4[r(E)]\right) - \frac{312}{r^3(E)}\left(\frac{3}{52} - E_5[r(E)]\right)$$
$$+ \frac{2160}{r^4(E)} E_6[r(E)] + \frac{8880}{r^5(E)}\left(\frac{5}{222} + E_7[r(E)]\right)$$
$$+ \frac{20160}{r^7(E)}\left[r(E)\, E_8[r(E)] - \frac{1}{8} + E_9[r(E)]\right] \qquad (58)$$

where

$r(E) = a\,\Sigma_t(E)$

a = slab thickness

$\Sigma_t(E)$ = total macroscopic cross-section as a function of energy

$E_n[r(E)]$ = exponential integral function, as defined by Eq. (20).

CHAPTER V

FRACTIONAL ERRORS INTRODUCED IN THE RESONANCE INTEGRAL

In the previous chapter a method is derived for determining the collision density of neutrons in a slab of absorbing material. In this chapter, the collision density is used to determine:

(i) the resonance integral to various approximations, and

(ii) the fractional changes or errors introduced in the resonance integral by the flat flux and infinite mass approximation.

The resonance integral was defined by (1). Assuming a source of one neutron per unit volume per unit time, we can re-write this definition in the form

$$I = N \int_E^\infty \int_o^a \frac{F(x,E')\ \sigma_a(E')}{a\ \Sigma_t(E')}\, dE'dx \tag{59}$$

for the slab case in which we are presently interested. N is the number density of absorber nuclei. The double integral can be thought of as an effective microscopic resonance integral (e.g. barns per nucleus). This parameter (I/N) is the one that is calculated here.

Substituting Eq. (39) which defines $F(x,\vec{\Omega},E)$ for the case n = 0 into Eq. (59), using the orthogonality relation (43), the resonance integral becomes

$$\frac{I}{N} = \int_E^\infty \frac{f_o^{\circ}(E')}{a\Sigma_t(E')}\, \sigma_a(E')\, dE' \qquad (60)$$

from which we observe that the resonance integral depends only on the first coefficient of the collision density expansion.

Note that the spatial dependence seemingly eliminated in (60) is actually included in the determination of $f_o^{\circ}(E)$ via Eqs. (54) and (55). The accuracy with which the spatial effect is accounted for increases as m increases.

The infinite mass approximation to the resonance integral may also be computed from Eq. (60) by employing Eq. (57) to determine $f_o^{\circ}(E)$. Furthermore the W.R. approximation (infinite-mass plus flat-flux) is obtainable from Eq. (60) by simply using Eq. (57) with $m = 0$.

Thus we can estimate the errors involved. Specifically, to calculate the error due to the flat flux assumption, we first find $f_o^{\circ}(E)$ from (54) with $m = 0$, for a given set of resonance parameters. Then this value of $f_o^{\circ}(E)$, substituted into (60) gives what we shall call I_o/N. For the same parameters, recalculating $f_o^{\circ}(E)$ for higher values of m (even values for symmetric problems) gives the more accurate value I_m/N. Then the fractional error is given by

$$\frac{\delta I}{I} = \frac{I_o - I_m}{I_m} \qquad (61)$$

This may be computed for various slab thicknesses and for various values of m.

Similarly, the error due to the infinite mass assumption may be estimated for any desired value of m. Equation (57) is used in this case to determine $f_o^{\circ}(E)$ which, when substituted in turn into (60) gives what we shall call I_m^{im}/N. Then the error is given by

$$\frac{\delta I}{I} = \frac{I_m^{im} - I_m}{I_m} \tag{62}$$

where I_m is the same as calculated for (61). Again this may be performed for various slab sizes and values of m.

Finally, the error due to the W.R. approximation is found from

$$\frac{\delta I^{WR}}{I} = \frac{I_o^{im} - I_m}{I_m} \tag{63}$$

and as before, may be found to any degree m and for various slab sizes.

CHAPTER VI

NUMERICAL METHODS

In the previous two chapters, equations are set up to determine the collision density, resonance integral, and fractional errors introduced in the resonance integral. In solving these equations we can use either an approximate analytical technique, or a numerical technique, utilizing computing machines.

The approximate analytical technique of solution would substantially reduce the accuracy of the fractional errors in the resonance integral. This reduction in accuracy would defeat the purpose of the investigation. Therefore in view of the complexity of the equation, and the accuracy desired, a numerical technique of solution was adopted.

In the first part of this chapter the method of computing the matrix elements, given by Eq. (58), is considered. Part two is concerned with the method used for solving the set of connected linear integral equations, (54). The evaluation of the resonance integral, and the fractional errors introduced in the resonance integral, is also dealt with in the second part. Finally, part three is devoted to the errors and limitations of the method used for solving Eq. (54).

A. Computation of the Matrix Elements

Particular difficulties are encountered in computing the matrix elements $a_{04}(E) \cdots a_{44}(E)$, using the expressions given by Eq. (58). These difficulties are due to numerical instabilities,

introduced by taking the difference of two large numbers with insufficient accuracy. This can be seen from the expressions given by Eq. (58). In the limit of small r(E), round-off errors in the difference terms are highly magnified and lead to erroneous results.

These difficulties may be overcome by computing the elements in double precision. However this leads to further computational difficulties. In a certain range, it is difficult to determine the exponential integral function in double precision. This range is given by $4 < |x| < 50$, where x is the argument of the exponential integral function.

A Taylor series may be used to compute the exponential integral function in the range $1 < |x| < 4$. The Taylor series takes the form

$$E_1(x) = \gamma + \ln|x| + x + \frac{x^2}{2.2!} + \frac{x^3}{3.3!} + \cdots \qquad (64)$$

where

$$\gamma = 0.5772157 = \text{Eulers constant}$$

Exponential integral functions of higher order may be determined from the recursion relation (C6):

$$E_n(x) = \frac{1}{n-1}\left[e^{-x} - x\,E_{n-1}(x)\right] \qquad (65)$$

In the case where $|x| > 50$, the following asymptotic form may be used (P1, C6):

$$E_n(x) = \frac{e^{-x}}{x+n}\left[1 \quad \frac{n}{(x+n)^2} + \frac{n(n-2x)}{(x+n)^4} + \frac{n(6x^2 - 8nx + n^2)}{(x+n)^6}\right] + R(n,x) \qquad (66)$$

where R(n,x), the remainder, is given by an integral (C6, P1).

With Eqs. (64), (65) and (66), it is possible to compute the value of $E_n(x)$ to as many decimal places as is desirable, in the ranges indicated. Thus the matrix elements may be computed with as much accuracy as is necessary, to give reasonable results in these ranges. However, in the range $4 < |x| < 50$, a complicated, time consuming method (H1, M3), is required to determine $E_n(x)$ in double precision. The range $4 < |x| < 50$ cannot be ignored, since it constitutes an important part of the solution. Since the matrix elements are energy-dependent they have to be re-calculated at every point considered, thus aggravating the situation. It is thus desirable to re-write the matrix elements in a different form. This form must be such that a sufficiently accurate estimate of the matrix elements is obtainable within a relatively short period of time, for all values of the argument x.

The new form is obtained by using the recursion relation (65). With the help of Eq. (65) all the exponential integral functions in the matrix elements are expressed in terms of $E_3(x)$. The details of this substitution are shown in Appendix B. In all cases, except $a_{oo}(E)$, the $E_3(x)$ functions cancel out. Therefore the remaining matrix elements and source terms are expressed in terms of exponential functions only. Written in this way the matrix elements and source terms can be obtained with sufficient accuracy, since it is relatively easy to obtain the exponential functions in double precision. $a_{oo}(E)$ can be determined with sufficient accuracy without

the help of double precision, since it does not contain any large numbers. The transformed matrix elements, and corresponding source terms are:

$$a_{oo}(E) = 1 - \frac{1}{r(E)}\left(\frac{1}{2} - E_3\,[r(E)]\right) \qquad s_o^{\,o}(E) = -\frac{r(E)}{E}\left(a_{oo}(E) - 1\right)$$

$$a_{02}(E) = X(E) \qquad a_{20}(E) = 5X(E) \qquad s_o^{\,2}(E) = -\frac{r(E)}{E}X(E)$$

$$a_{22}(E) = 5\left[\frac{1}{5} - \frac{1}{2r(E)} + \frac{e^{-r(E)}}{r^2(E)} + \frac{3}{r^3(E)} + \frac{ae^{-r(E)}}{r^3(E)} + \frac{24}{r^5(E)}\left(e^{-r(E)}\,[r(E)+1] - 1\right)\right]$$

$$a_{04}(E) = Y(E) \qquad a_{40}(E) = 9Y(E) \qquad s_o^{\,4}(E) = -\frac{r(E)}{E}Y(E)$$

$$a_{24}(E) = 5Z(E) \qquad a_{42}(E) = 9Z(E)$$

$$a_{44}(E) = 9\left[\frac{1}{9} - \frac{1}{r(E)} + \frac{e^{-r(E)}}{r^2(E)} + \frac{10}{r^3(E)} + \frac{37e^{-r(E)}}{r^3(E)} + \frac{612e^{-r(E)}}{r^4(E)} - \frac{360}{r^5(E)} + \frac{5820e^{-r(E)}}{r^5(E)} + \frac{34440e^{-r(E)}}{r^6(E)} + \frac{12600}{r^7(E)} + \frac{128520e^{-r(E)}}{r^7(E)} + \frac{282240}{r^9(E)}\left(e^{-r(E)}\,[r(E)+1] - 1\right)\right]$$

$$X(E) = -\frac{1}{2r(E)} + \frac{20}{3r^2(E)} + \frac{e^{-r(E)}}{r^2(E)} - \frac{3}{r^3(E)} + \frac{3e^{-r(E)}}{r^3(E)}$$

$$Y(E) = -\frac{1}{2r(E)} + \frac{20}{3r^2(E)} + \frac{e^{-r(E)}}{r^2(E)} - \frac{45}{r^3(E)} + \frac{17e^{-r(E)}}{r^3(E)}$$
$$+ \frac{168}{r^4(E)} + \frac{112e^{-r(E)}}{r^4(E)} - \frac{280}{r^5(E)} + \frac{280e^{-r(E)}}{r^5(E)}$$

$$Z(E) = -\frac{1}{2r(E)} + \frac{14}{3r^2(E)} + \frac{e^{-r(E)}}{r^2(E)} - \frac{18}{r^3(E)} + \frac{23e^{-r(E)}}{r^3(E)}$$
$$+ \frac{220}{r^4(E)} + \frac{200}{r^5(E)} + \frac{1060e^{-r(E)}}{r^5(E)}$$
$$+ \frac{2520}{r^7(E)}\left(e^{-r(E)}\,[r(E) + 1] - 1\right) \qquad (67)$$

where

$r(E) = a\,\Sigma_t(E)$

a = slab thickness

$\Sigma_t(E)$ = total macroscopic cross-sections as a function of energy.

With the above expressions for the matrix elements and source terms, it is possible to obtain a stable numerical representation of the matrix in Eqs. (54) and (57).

B. Solution of the Integral Equation

This section deals with the solution of Eq. (54). In addition, the evaluation of the resonance integral and the fractional errors introduced in the resonance integral are discussed.

Since Eq. (54) is of the Fredholm type, it is expected that iterating the source term would eventually converge to the solution (C9). It is found, however, that the rate of convergence is much

too slow. All efforts to increase the rate of convergence proved to be ineffective. These efforts included;

(i) using the infinite mass approximation as a starting point, instead of the source term. This was attempted since it was felt that the infinite mass approximation is closer to the actual solution than the source term. And,

(ii) employing the Aitkens δ^2 process (T2) to accelerate the convergence.

In view of the failure to solve the equation by conventional means, a new approach was necessary. Two such approaches were developed. The details of the first approach appear in Appendix C. This method was not followed to completion but a result, which was derived from this first approach, was instrumental in the success of the second approach in solving Eq. (54). This result is the solution for the energy dependent expansion coefficients, defined by Eq. (38), for the case of energy independent cross-sections. This solution is exact in the case where the source, external to the absorbing element, has an energy dependence which varies as 1/E. This solution, derived in Appendix C, is given by

$$\overrightarrow{f^{im}}(E) = \frac{1}{E} \frac{\text{adj } [\tilde{B}]}{|\tilde{B}|} \vec{D} \qquad (68)$$

where

$$\tilde{B} = \begin{bmatrix} 1 - a_{oo}\frac{\Sigma_s}{\Sigma_t} & \cdots & -a_{om} \\ \vdots & & \\ a_{mo} & \cdots & 1 - a_{mm}\frac{\Sigma_s}{\Sigma_t} \end{bmatrix}$$

$$\vec{D} = \begin{bmatrix} s_o^{\,o} \\ \vdots \\ s_o^{\,m} \end{bmatrix}$$

$$\overrightarrow{f^{im}}(E) = \begin{bmatrix} f_o^{\,o}(E) \\ \vdots \\ f_o^{\,m}(E) \end{bmatrix}$$

The above results hold for any geometrical configuration. Equation (68) is used as a starting point in the numerical method to be described below.

The second method, which is the one actually used for solving Eq. (54) will now be described. In this method all spatial modes, i.e. m = 0, 2, 4, ..., have to be considered separately. However, the methods are similar in principle.

First the flat flux case m = 0 is considered. To avoid undue complication the case with a single nuclear type present is discussed in detail. The method is then generalized to the case where a mixture of nuclear species is present. The equation describing

the flat flux approximation to $f_o^{\circ}(E)$ may be obtained from Eq. (54), and is given by

$$f_o^{\circ}(E) = a_{oo}(E) \int_{E}^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{f_o^{\circ}(E)}{(1-\alpha)E'} dE' + s_o^{\circ}(E) \qquad (69)$$

The solution to $f_o^{\circ}(E)$ is determined at discrete points as shown on Fig. 5. It takes the form $f_o^{\circ}(E_i)$, where i = 1, 2,...β, 1 and β being the terminal points considered. The terminal points are determined in general by the total cross-section of the nucleus. All energy dependence of the cross-section is assumed to be negligible beyond the β^{th} point.

Equation (69) will now be considered for the β^{th} point. It is given by

$$f_o^{\circ}(E_\beta) = a_{oo}(E_\beta) \int_{E_\beta}^{E_\beta/\alpha} \frac{f(E')\,\Sigma_s(E')}{\Sigma_t(E')(1-\alpha)E'} dE' + s_o^{\circ}(E_\beta) \qquad (70)$$

The integration interval in Eq. (70), E_β to E_β/α is now divided into k sub-intervals. Using a quadrature formula (T2), the integral of Eq. (70) will be written as a sum, becoming

$$f_o^{\circ}(E_\beta) = a_{oo}(E_\beta) \left[\frac{C_\beta f_o^{\circ}(E_\beta)\Sigma_s(E_\beta)}{(1-\alpha)E_\beta\Sigma_t(E_\beta)} + \sum_{j=\beta+1}^{\beta+k} \frac{C_j f_o^{\circ}(E_j)\Sigma_s(E_j)}{(1-\alpha)E_j\Sigma_t(E_j)} \right]$$

$$+ s_o^{\circ}(E_\beta) \qquad (71)$$

This equation may be written in the more convenient form,

$$f_o^{\circ}(E_\beta) = B(E_\beta)\, C_\beta\, f_o^{\circ}(E_\beta) + U_\beta + s_o^{\circ}(E_\beta) \tag{72}$$

where:

$$B(E_\beta) = \frac{a_{oo}(E_\beta)\ \Sigma_s(E_\beta)}{(1-\alpha)\ E_\beta \Sigma_t(E_\beta)} \tag{73}$$

$$U_\beta = a_{oo}(E_\beta) \sum_{j=\beta+1}^{\beta+k} \frac{C_j\ f_o^{\circ}(E_j)\ \Sigma_s(E_j)}{(1-\alpha)\ E_j\ \Sigma_t(E_j)} \tag{74}$$

From Eq. (72) it is possible to solve for the desired quantity $f_o^{\circ}(E_\beta)$, i.e.

$$f_o^{\circ}(E_\beta) = \frac{U_\beta + s_o^{\circ}(E_\beta)}{1 - B(E_\beta)\ C_\beta} \tag{75}$$

In Eq. (75) the quantities $s_o^{\circ}(E_\beta)$ and $B(E_\beta)$ are known. The unknown quantities are U_β and C_β and, if these two quantities could be determined, $f_o^{\circ}(E_\beta)$ could be determined explicitly.

The values of $C_\beta \ldots C_{\beta+k}$ depend upon the quadrature formula used. Since the function being integrated does not have any rapid changes in slope, Simpson's method is used. The reason for the relatively smooth variation of $f_o^{\circ}(E)$ with energy is that it has the same energy dependence as the collision density which is the product of flux and cross-section. When there is a peak in the absorption cross-section, there is a depression in the flux. The product of the two however, remains relatively smooth. The values of $C_\beta \ldots C_{\beta+k}$

are thus clearly defined, and are given by (T2):

$$C_{\beta} = \frac{h}{3}$$

$$C_{\beta+1} = \frac{4h}{3}$$

$$\vdots$$

$$C_{\beta+(k-1)} = \frac{4h}{3}$$

$$C_{\beta+k} = \frac{h}{3} \tag{76}$$

where h is the size of sub-interval into which the integral is divided.

E_{β} is the terminal point beyond which the cross-sections are considered to be energy independent. It is therefore permissible to assume that the solution beyond E_{β} is given by Eq. (68) which is based on energy independent cross-sections. Therefore the $f_o^{\circ}(E_{\beta+1})$ ... $f_o^{\circ}(E_{\beta+k})$ can be determined explicitly and the sum U_{β} may be computed. Although this is an approximation, it is rather good, and it may therefore be used to determine $f_o^{\circ}(E_{\beta})$ explicitly.

The value of $f_o^{\circ}(E_{\beta-1})$ can be computed in an analogous fashion, and is given by

$$f_o^{\circ}(E_{\beta-1}) = \frac{U_{\beta-1} + s_o^{\circ}(E_{\beta-1})}{1 - B(E_{\beta-1})\, C_{\beta-1}} \tag{77}$$

In this case the value of $f_o^{\circ}(E_{\beta})$ determined previously is used to evaluate the sum $U_{\beta-1}$. Thus one less solution to Eq. (68) is necessary to determine the sum $U_{\beta-1}$, than was necessary to find U_{β}. The values of $f_o^{\circ}(E_{\beta-2})$, $f_o^{\circ}(E_{\beta-3})$...$f_o^{\circ}(E_2)$, $f_o^{\circ}(E_1)$ may be computed

in the same way. As more and more solution points are determined, fewer and fewer values of the assumed solution are necessary in the sum given by Eq. (74). Eventually a point is reached where Eq. (74) contains only the computed values of $f_o^{\circ}(E_j)$.

In the case where a mixture of N nuclear species is present, the same method of solution applies. N separate integrals exist in this case, one for each species and each one has to be written in terms of a quadrature formula. These N integrals all have different ranges of integration, i.e. E to E/α_1, ...E to E/α_N. In this method all these integration ranges are divided into the same number of subdivisions, k, in spite of the fact that they have different ranges. With this assumption in mind, Eqs. (73) and (74) may be rewritten to take all the nuclear species into account. This is done by summing over all the nuclear species present, since for each specie there exists a $B(E_\beta)$ and a U_β. $B(E_\beta)$ and U_β become

$$B(E_\beta) = \sum_{i=1}^{N} \frac{a_{oo}(E_\beta)\Sigma_s^{(i)}(E_\beta)}{(1-\alpha_i)\, E_\beta\, \Sigma_t(E_\beta)} \tag{78}$$

$$U_\beta = \sum_{i=1}^{N} a_{oo}(E_\beta) \sum_{j=\beta+1}^{\beta+k} \frac{C_j\, f_o^{\circ}(E_j)\, \Sigma_s^{(i)}(E_j)}{(1-\alpha_i)\, E_j\, \Sigma_t(E_j)} \tag{79}$$

$f_o^{\circ}(E_\beta)$ for the mixture may be determined by substituting Eq. (78) and (79) into Eq. (75). In a manner identical to that outlined above $f_o^{\circ}(E_{\beta-1})$, $f_o^{\circ}(E_{\beta-2})$, ... $f_o^{\circ}(E_2)$, $f_o^{\circ}(E_1)$ may be determined.

The accuracy of the solutions obtained for $f_o^{\,o}(E_i)$ by this method may be increased by iterating it in the original Eq. (69). This iteration process may be continued, until a satisfactory solution is obtained.

The above discussion is limited to the flat-flux case, i.e. $m = 0$. The case where a parabolic spatial distribution ($m = 2$) is taken into account will now be considered. In this case Eq. (54) for the case of a single nuclear specie, becomes:

$$\begin{bmatrix} f_o^{\,o}(E) \\ f_o^{\,2}(E) \end{bmatrix} = \begin{bmatrix} a_{oo}(E) & a_{02}(E) \\ a_{20}(E) & a_{22}(E) \end{bmatrix} \begin{bmatrix} \int_E^{E/\alpha} f_o^{\,o}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} \\ \int_E^{E/\alpha} f_o^{\,2}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} \end{bmatrix} + \begin{bmatrix} s_o^{\,o}(E) \\ s_o^{\,2}(E) \end{bmatrix} \tag{80}$$

Equation (80) gives rise to the two-coupled linear integral equations,

$$f_o^{\,o}(E) = a_{oo}(E) \int_E^{E/\alpha} f_o^{\,o}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + a_{02}(E) \int_E^{E/\alpha} f_o^{\,2}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + s_o^{\,o}(E) \tag{81}$$

$$f_o^{\,2}(E) = a_{22}(E) \int_E^{E/\alpha} f_o^{\,2}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + a_{20}(E) \int_E^{E/\alpha} f_o^{\,o}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + s_o^{\,2}(E) \tag{82}$$

Because of the relatively small cross-section at an energy outside of the resonance range, there is very little spatial structure to the collision density. Therefore $f_o^2(E)$ is negligibly small, except in the region close to the resonance peak. Thus the solution to $f_o^0(E)$ obtained from Eq. (81) will not be very different from $f_o^0(E)$ obtained by solving Eq. (69).

It will now be assumed that Eq. (69) has been solved and all the corresponding $f_o^0(E_i)$ are known accurately. The value of $f_o^0(E)$ in Eq. (82) is approximated by the value of $f_o^0(E)$ obtained by solving Eq. (69). It is seen that $f_o^2(E)$ may now be determined from Eq. (82). The second integral in Eq. (82) is known approximately, and may be added to the source term $s_o^2(E)$, to make up a modified source $C_o^2(E)$. Equation (82) may thus be written as follows:

$$f_o^2(E) = a_{22}(E) \int_E^{E/\alpha} f_o^2(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + C_o^2(E) \qquad (83)$$

where

$$C_o^2(E) = a_{20}(E) \int_E^{E/\alpha} f_o^0(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + s_o^2(E) \qquad (84)$$

By comparing Eqs. (83) and (69) it is seen that they have the same form. Hence a method of solution may be used to determine $f_o^2(E)$, identical to that used to determine $f_o^0(E)$. This value of $f_o^2(E)$ is not the true value, since an approximate form of $f_o^0(E)$ was used. To obtain a better solution, the approximate solution of $f_o^2(E)$, obtained from Eq. (83), and the flat flux solution obtained

from Eq. (69) are substituted in the right hand side of Eq. (80). New values of $f_o^{\,0}(E)$ and $f_o^{\,2}(E)$ are obtained. These new values may be iterated again in Eq. (80) until satisfactory solutions are obtained.

In the case where a mixture of nuclear species is present, the $B(E_\beta)$ and U_β used in solving Eq. (83) have to be modified. The modification is identical to that used in the flat flux case.

Finally in the case where quadratic and quartic spatial variations are taken into account (m = 4), Eq. (54), for a single nuclear species becomes:

$$\begin{bmatrix} f_o^{\,0}(E) \\ f_o^{\,2}(E) \\ f_o^{\,4}(E) \end{bmatrix} = \begin{bmatrix} a_{00}(E) & a_{02}(E) & a_{04}(E) \\ a_{20}(E) & a_{22}(E) & a_{24}(E) \\ a_{40}(E) & a_{42}(E) & a_{44}(E) \end{bmatrix} \begin{bmatrix} \int_E^{E/\alpha} f_o^{\,0}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} \\ \int_E^{E/\alpha} f_o^{\,2}(E) \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} \\ \int_E^{E/\alpha} f_o^{\,4}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} \end{bmatrix}$$

$$+ \begin{bmatrix} s_o^{\,0}(E) \\ s_o^{\,2}(E) \\ s_o^{\,4}(E) \end{bmatrix} \qquad (85)$$

The equation analogous to Eq. (83) for this case is given by

$$f_o^{\,4}(E) = a_{44}(E) \int_E^{E/\alpha} f_o^{\,4}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + C_o^{\,4}(E) \qquad (86)$$

where

$$C_o^{\,4}(E) = a_{40}(E) \int_E^{E/\alpha} f_o^{\,0}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'}$$

$$+ a_{42}(E) \int_E^{E/\alpha} f_o^{\,2}(E') \frac{\Sigma_s(E')}{\Sigma_t(E')} \frac{dE'}{(1-\alpha)E'} + s_o^{\,4}(E) \qquad (87)$$

It is now assumed that the case for m = 2 has been solved. Hence $f_o^{\,0}(E)$ and $f_o^{\,2}(E)$ are known functions. By applying the same reasoning as before, it is assumed that the values of $f_o^{\,0}(E)$ and $f_o^{\,2}(E)$ given by the solution to the case where m = 2 will not change much in the case where m = 4. The only range in which a change will take place is in the resonance range.

Therefore, using the two values of $f_o^{\,0}(E)$ and $f_o^{\,2}(E)$ obtained from the case where m = 2, $C_o^{\,4}(E)$ is completely specified. Equation (86) is thus analogous to Eq. (69), and the same method used to solve Eq. (69) may be used to solve Eq. (86). Hence a first approximation may be obtained to $f_o^{\,4}(E)$. This first approximation to $f_o^{\,4}(E)$, together with the solution to the case where m = 2, i.e. $f_o^{\,0}(E)$ and $f_o^{\,2}(E)$, are then iterated in Eq. (85) until a satisfactory solution is obtained.

In the case where a mixture of nuclear species is present the same procedure is followed as outlined above for the cases m = 0 and m = 2. The values of $B(E_\beta)$ and U_β have to be suitably modified as indicated by Eqs. (78) and (79).

From the previous discussion it should be clear how the value of $f_o^{\,o}(E)$ can be determined for the cases m = 0, 2, 4. Therefore, flat flux, spatially quadratic, or spatially quartic terms may be included in the solution of $f_o^{\,o}(E)$. These solutions are designated by $f_o^{oo}(E)$, $f_o^{o2}(E)$ and $f_o^{o4}(E)$, respectively. From these values of the expansion coefficients the resonance integral corresponding to them is determined. From Eq. (60) the respective resonance integrals are

$$\frac{I_o}{N} = \int_E \frac{f_o^{\,oo}(E)}{a\Sigma_t(E)}\,\sigma_a(E)\,dE \tag{88}$$

$$\frac{I_2}{N} = \int_E \frac{f_o^{\,o2}(E)}{a\Sigma_t(E)}\,\sigma_a(E)\,dE \tag{89}$$

$$\frac{I_4}{N} = \int_E \frac{f_o^{\,o4}(E)}{a\Sigma_t(E)}\,\sigma_a(E)\,dE \tag{90}$$

The limits on the integrals are determined primarily by the absorption cross-section. Evaluating these integrals poses no special difficulties.

The fractional errors introduced in the resonance integral given by Eq. (62) may now be computed. For the infinite mass approximation we must solve the set of linear equations (57). This is a relatively straight forward procedure and will not be detailed here. The solutions are $f_{oim}^{oo}(E)$, $f_{oim}^{o2}(E)$ and $f_{oim}^{o4}(E)$, depending on whether no spatial structure, a quadratic spatial structure, or a quartic spatial structure is considered, respectively. The respective resonance integrals, as defined by Eq. (60), are given by

$$\frac{I_o^{im}}{N} = \int_E \frac{f_{oim}^{oo}(E)}{a\Sigma_t(E)} \sigma_a(E)\, dE \tag{91}$$

$$\frac{I_2^{im}}{N} = \int_E \frac{f_{oim}^{o2}(E)}{a\Sigma_t(E)} \sigma_a(E)\, dE \tag{92}$$

$$\frac{I_4^{im}}{N} = \int_E \frac{f_{oim}^{o4}(E)}{a\Sigma_t(E)} \sigma_a(E)\, dE \tag{93}$$

The limits of integration are again determined by the absorption cross-section.

C. Errors and Limitations of the Solution to the Integral Equation

In addition to the errors introduced by round-off, which are characteristic of numerical procedures, the approximations are among the major contributors to inaccuracies. Five sources of errors are discussed.

(i) It is found that the solution is critically dependent on the approximation used in evaluating the sum U_β, given by Eq. (74). This necessitates the commencement of the process of solution sufficiently far from the resonance peak such that the cross-sections may be considered energy-independent. Since Eq. (68) gives an exact solution for constant cross-sections the closer the cross-sections are to a constant value, the better is the starting solution given by Eq. (68). Thus by assuming a value of E_β sufficiently far from the resonance energy, the error due to an incorrect starting solution is reduced.

(ii) The type of quadrature formula used for the integration introduces another source of error. The Simpson formula which is used, introduces the following error (T2):

$$\epsilon = \frac{h\,\delta^4}{90}$$

where

h = integration step size

δ^4 = averaged fourth difference (T2)

This error can be reduced by using a different quadrature formula.

(iii) The criterion used for determining when a solution for $f_o^o(E)$ is satisfactory, may also introduce an error. Since the resonance integral is of prime interest here,

it is used as the criterion. The resonance integral is evaluated after each iteration, and compared to that of the previous iteration. When the agreement between the two resonance integrals is close, the solution is considered acceptable and the iteration process is terminated. It is seen that the solutions are not necessarily exact, although in most cases it was found that a satisfactory resonance integral also results in a satisfactory solution for $f_o^o(E)$.

(iv) In the case where a mixture of nuclear species is considered the different integration ranges are all divided into the same number of intervals. This means that some sub-intervals are larger than others and thus the errors are larger, since they are proportional to the step size (T2). This error is unavoidable in the method used.

(v) Finally it is of interest to note that the atomic masses A of the nuclei affect the accuracy. This is due to the fact that for light nuclei the integration range is larger than for heavy nuclei. For hydrogen the range is from E to ∞. Thus for lighter nuclei the approximate solution used to evaluate U_β initially, affects more points than in the case of heavier nuclei. This makes the computed solution more dependent on the

initial assumption for light nuclei than for heavier nuclei. This may be overcome by iterating the solution more times.

CHAPTER VII

RESULTS AND CONCLUSIONS

In this chapter the formalism for obtaining the collision density, the resonance integral, and the fractional errors introduced in the resonances integral is applied to slabs of bismuth, uranium, thorium, and thorium oxide. In all the computations considered, the absorbing nucleus is assumed to have a single resonance, with cross-sections which are described by Eq. (6). Where a mixture of nuclei is assumed, it will be made up of absorbing and moderating nuclei. In this case the moderating nuclei are considered to have constant, purely scattering cross-sections.

A. Description of Problems Solved

Table I gives the pertinent nuclear properties of the resonances considered.

TABLE I

	E_r (ev)	σ_o (barns)	σ_p (barns)	Γ (ev)	Γ_n (ev)	Γ_γ (ev)	Γ_γ/Γ
Bismuth (L3)	784	1821	10.4	4.34	4.30	0.04	0.092
Thorium (D2)	70	17700	12.0	0.082	0.039	0.043	0.524
Thorium Oxide (D2)	70	17700	19.7	0.082	0.039	0.043	0.524
Uranium (C4)	104	18000	10.0	0.095	0.07	0.025	0.263

Various slab thicknesses are also considered. These thicknesses are shown in Table II

TABLE II

	Slab thickness "a" in cm.					
Bismuth		0.5		2.5	7.5	35
Thorium	0.1	0.5		2.5	7.5	
Thorium oxide		0.5		2.5	7.5	
Uranium	0.1	0.5	0.8	2.5	7.5	

For all the materials, Eqs. (54) and (57) were solved for m = 0 and m = 2 with thicknesses "a" of 0.5 cm, 2.5 cm, and 7.5 cm. For thorium an additional set of problems was solved for m = 4 for the same thicknesses. The solutions mentioned above were then applied to the calculation of the resonance integrals using both the flat flux and infinite mass approximations.

For the other thicknesses mentioned in Table II Eqs. (54) and (57) were solved only for m = 0. These results are used only to estimate the fractional error introduced in the resonances integral by the infinite mass approximation.

B. Results Obtained for $f_o^o(E)$

The expansion coefficient $f_o^o(E)$ of the collision density defined by Eq. (39) is illustrated in Figs. 9 to 20. In each figure the $f_o^o(E)$ solution for m = 0 and m = 2 in Eqs. (54) and (57) is shown, except in the case of thorium. In this case $f_o^o(E)$ is shown for m = 0, and m = 4. The slab thickness and resonance parameters are held constant for each figure.

C. Evaluation of Resonance Integrals

The values of the resonances integrals, defined by Eq. (60), are shown in Tables III, IV, V and VI in barns/nucleus.

TABLE III - Bismuth

	a=0.5	a=2.5	a=7.5	a=35
I_o^{im}/N	0.1246	0.0807	0.0510	0.0236
I_o/N	0.0547	0.0403	0.0363	0.0397
I_2^{im}/N	0.1039	0.0533	0.0339	-
I_2/N	0.0530	0.0378	0.0332	-

TABLE IV - Uranium

	a=0.1	a=0.5	a=0.8	a=2.5	a=7.5
I_o^{im}/N	1.2933	0.4724	0.3720	0.2092	0.1181
I_o/N	0.7718	0.4069	0.3429	0.2246	0.1526
I_2^{im}/N	-	0.4683	-	0.1995	0.4069
I_2/N	-	0.4000	-	0.2168	0.1450

TABLE V - Thorium

	a=0.1	a=0.5	a=2.5	a=7.5
I_o^{im}/N	3.1731	1.0993	0.4915	0.2809
I_o/N	2.7290	1.1628	0.5929	0.3664
I_2^{im}/N	-	1.0943	0.4822	0.2678
I_2/N	-	1.1555	0.5827	0.3540
I_4^{im}/N	-	1.0876	0.4817	0.2665
I_4/N	-	1.1527	0.5815	0.3522

TABLE VI - Thorium Oxide

	a=0.5	a=2.5	a=7.5
I_o^{im}/N	1.2669	0.5645	0.3228
I_o/N	1.3792	0.8037	0.6257
I_2^{im}/N	1.2594	0.5527	0.3048
I_2/N	1.3716	0.7957	0.6182

From these results the fractional errors in the resonance integrals were computed.

D. Fractional Error Introduced in Resonance Integral by Flat Flux Approximation

Figure (21) illustrates the fractional error introduced in the resonance integral by neglecting the spatial variation in the neutron flux ($\delta I/I$). This fractional error is defined by Eq. (61) for m = 2. As can be seen from Fig. (21) this fractional error increases monotonically with increasing slab size, in the range of slab thicknesses investigated. It is also clear that it is always positive in this range. This general result indicates that the flat flux approximation is better for thinner slabs.

It is interesting to note that the flat flux approximation seems to be best for a nucleus with a high absorption component in its resonance. This phenomenon may be explained by considering the neutron sources which contribute to the flux at resonance energy. Two

sources exist, one from the source external to the slab, and the other from neutrons slowing down within the slab.

First we consider the case where the nuclei have large absorption components, i.e. Γ_γ/Γ large. In this case, neutrons which enter the slab from an external source at resonance energy penetrate a relatively small distance into the slab. They are primarily absorbed close to the surface of the slab. The resonance flux inside the slab due to slowing down is expected to be relatively flat. This lack of spatial variation is due to the fact that the cross-sections above the resonance are constant and non-absorbing. The resonance flux thus tends to be spatially flat inside the slab, and peaked near the surface. These source terms are illustrated schematically in Fig. 6.

It is thus seen that the neutron flux in this case can be approximated, with good accuracy, by a flat flux. Therefore the fractional errors introduced by a spatially flat flux are small.

Where the slab is made up of nuclei having a small absorption component, the same two sources exist. However, in this case the external source neutrons penetrate much deeper into the slab. The source due to slowing down of neutrons within the slab is unchanged. Figure 7 illustrates schematically how the resonance flux is made up in this case. Here the overall spatial structure of the flux cannot be approximated accurately by a spatially flat flux. Therefore the fractional error is larger than in the previous case.

The results for thorium oxide indicate that this resonance integral is least affected by the flat flux approximation. This may be attributed to the reduced density of thorium which increases the transparency to external source neutrons, and to the increased slowing-down ability due to the presence of oxygen. Figure 8 shows schematically the structure of the two sources.

In addition, illustrated on Fig. 21 is the fractional error computed using the approximate technique of Eq. (23), assuming the N.R. approximation. Values of A = 2 and B = 1 are assumed, and the comparison is to be made with the U^{238} results. It can be seen that the comparison is not very good, merely indicating the existence of a fractional error which has a positive sign and increases monotonically.

As discussed in Chapter III previous attempts to calculate this $\delta I/I$ have been made. Berg's results (B6) are qualitatively similar but cannot be compared closely with these results because they include a number of resonances. Corngold and Takahashi (C5, T1), on the other hand, obtained one value which gave a negative $\delta I/I$. They used an infinite mass approximation, but this in itself cannot account for the negative $\delta I/I$. Reference to Table IV gives a $\delta I/I$ for this case as (0.4724 - 0.4683)/0.4683, which is still positive. Thus Corngold's results cannot be explained by any of the results presented here.

E. Fractional Error Introduced in the Resonance Integral by the Infinite Mass Approximation

Figure 22 shows the fractional error introduced in the resonance integral by the infinite mass approximation, which neglects neutron slowing down when colliding with nuclei. This fractional error is defined by Eq. (62) for m = 0. It is seen that the fractional error decreases monotomically with increasing slab size, and at a certain thickness changes sign. The thickness at which the change of sign occurs is a function of the absorption probability a(E), increasing as the value of a(E) decreases.

A positive fractional error indicates that the resonance integral computed using the infinite mass approximation (I_o^{im}) is larger than the resonance integral computed taking slowing down into account (I_o). A negative fractional error results from $I_o^{im} < I_o$. The variation of the fractional error with thickness may be explained by considering the resonance neutron flux and the mechanisms by which neutrons can escape resonance absorption. Two mechanisms exist by means of which neutrons can escape resonance absorption. First, they can escape from the slab by scattering across the boundaries. Second, they can collide with a nucleus thereby losing enough energy to scatter out of the resonance range. In the case of the infinite mass approximation, only the source of neutrons external to the slab contributes to the neutron flux. Furthermore, the only mechanism by which neutrons can escape resonance absorption is by scattering out of the slab, since neutrons cannot lose energy.

Consider now a slab of absorbing material made up of nuclei with given resonance parameters. We start by letting the slab be relatively thin. In this case the external source neutrons can penetrate deeply into the slab. In the infinite mass model, these neutrons undergo many collisions until they are either absorbed or scattered out of the slab. In the case where slowing down of neutrons is accounted for, the external source neutrons, together with those from slowing down in the slab, undergo fewer collisions to escape the resonances. They either leak out of the slab or slow down past the resonance. For the thinner slab then, the collision density computed using the infinite mass model is larger than that determined from the model which takes neutron slowing-down into account. Therefore for relatively thin slabs, $I_o < I_o^{im}$, and the fractional error is positive.

As the slab size increases, the slowing-down source remains constant while the external source (per unit volume) decreases. Hence the infinite mass model predicts a larger reduction in average collision density than does the slowing-down model. Thus I_o^{im} begins to approach I_o. Where $I_o^{im} = I_o$, it may be inferred that the effect of slowing-down of neutrons into the resonance is balanced exactly by the effect of slowing-down out of the resonance. For greater thicknesses, slowing-down into the resonance is more important than slowing-down out of the resonance, and the sign of the error reverses.

Chernick et al. (C3) and Corngold (C4) have also carried out estimates of the effect of the infinite mass approximation on the resonance integral. The details of these approaches are given in Chapter III. Agreement with these estimates is seen to be reasonably good, as shown on Fig. 22.

F. The Fractional Error Introduced in the Resonance Integral by the W.R. Approximation

Shown on Fig. 23 is the fractional error which is introduced in the resonance integral by the W.R. approximation. This fractional error is defined by Eq. (63) for m = 2. Since the W.R. approximation is a combination of the flat flux and infinite mass approximations, the explanation for the results presented on Fig. 23 is a combination of the effects explained in sections D and E.

Using Eq. (15) to compute Γ_{prac}, and the criterion expressed by Eq. (16) it is evident that the resonances responsible for a large proportion of the resonance absorption in U^{238} and Th^{232} are relatively wide, as opposed to relatively narrow. The W.R. approximation is thus useful in estimating the resonance escape probability in reactor calculations. To correct the overall resonance integral, the results shown on Fig. 23 would have to include all the absorbing resonances.

G. Possible Extensions

Real nuclei usually have a number of important resonances. The above computations are therefore not sufficient, since only a single resonance was considered. Furthermore each resonance of any

nucleus has different parameters. It is evident from the results that for a given slab size the fractional errors either add to each other or subtract from each other, depending on the resonance parameters. It is thus conceivable that the total fractional error introduced in the resonance integral for a given slab size is either positive, zero or negative.

An interesting extension to this work would be the inclusion of a number of resonances in the computation. Kelber (K1) has carried out an investigation of this aspect.

It is usual in computations of the resonance integral to assume that the neutron flux outside of the absorbing lump is asymptotic in nature. This assumption is not entirely valid for resonances at low energies, since the resonances at the higher energies disturb the asymptotic distribution. Including the effect of the higher resonances would modify the energy dependence of the source term. Instead of it merely being 1/E it would be some function of energy, which would account for the depletion of neutrons due to the resonances at higher energies. Work on this aspect has be done by a number of authors (K2, B8).

Finally a different method may be considered to determine the neutron flux as a function of position, angular direction, and energy. A method developed by Case (C6) for solving the monoenergetic transport equation in one dimension has been generalized to include energy as a variable by Fuchs et al. (F2). By using

the method developed by Fuchs et al. to solve the transport equation, the neutron flux for a one-dimensional slab may be determined as a function of position, angular direction and energy. The resonance integral may be computed with great accuracy using this solution.

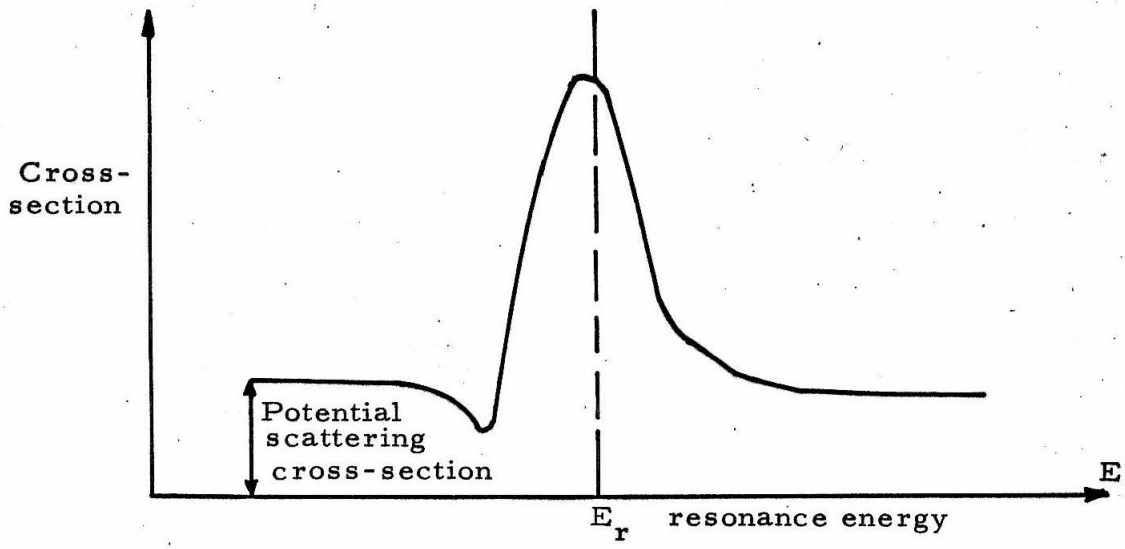

Fig. 1. Schematic illustration of a Breit-Wigner single level line

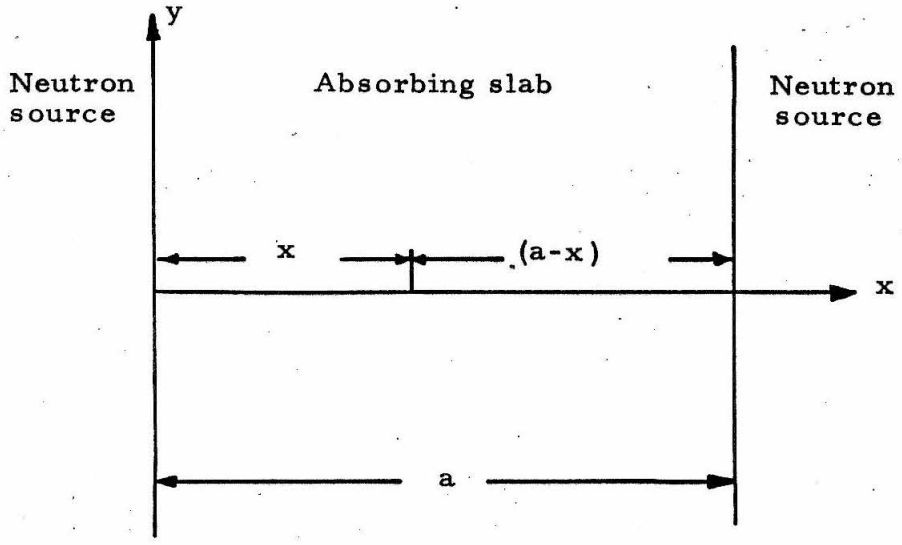

Fig. 2. Absorbing slab surrounded by a neutron source

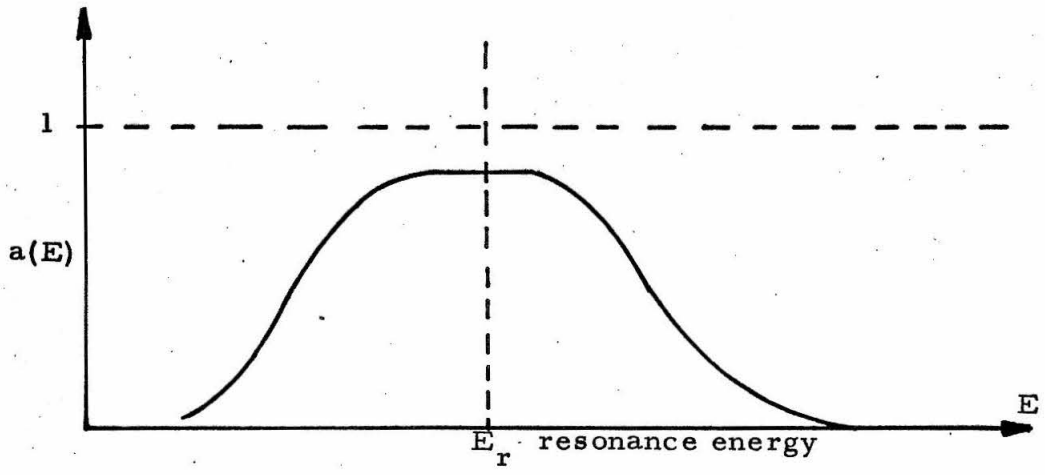

Fig. 3. Schematic illustration of the variation of the absorption probability a(E) with energy.

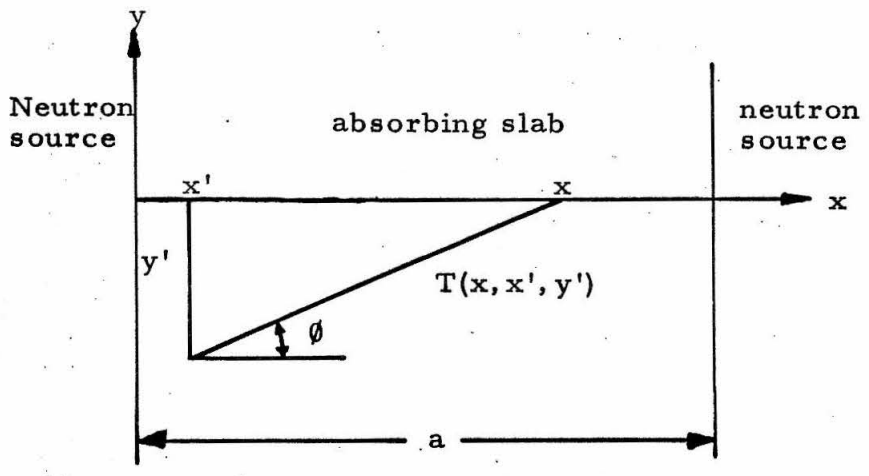

Fig. 4. Slab of absorbing material embedded in a neutron source.

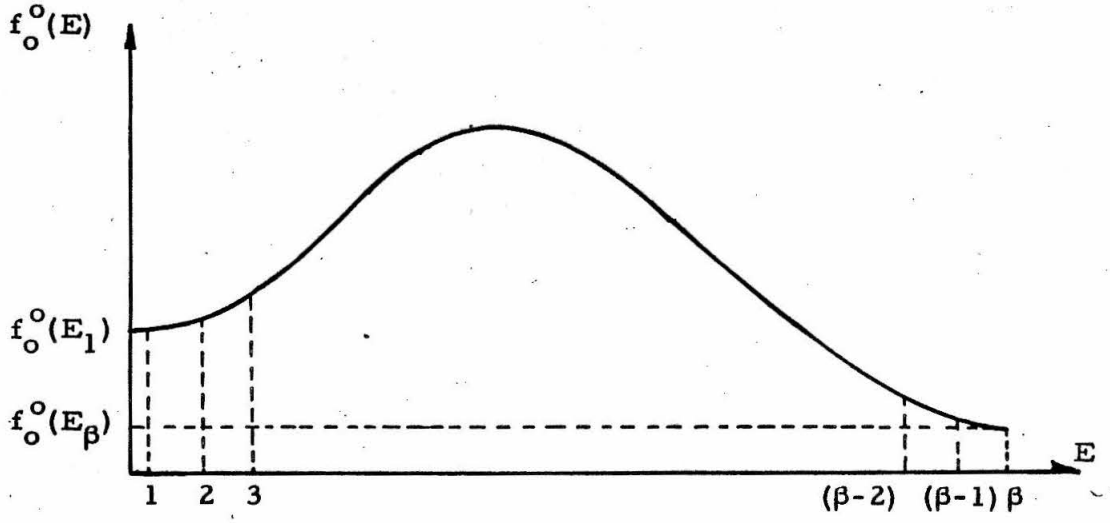

Fig. 5. Schematic illustration of the numerical solution to $f_o^o(E)$.

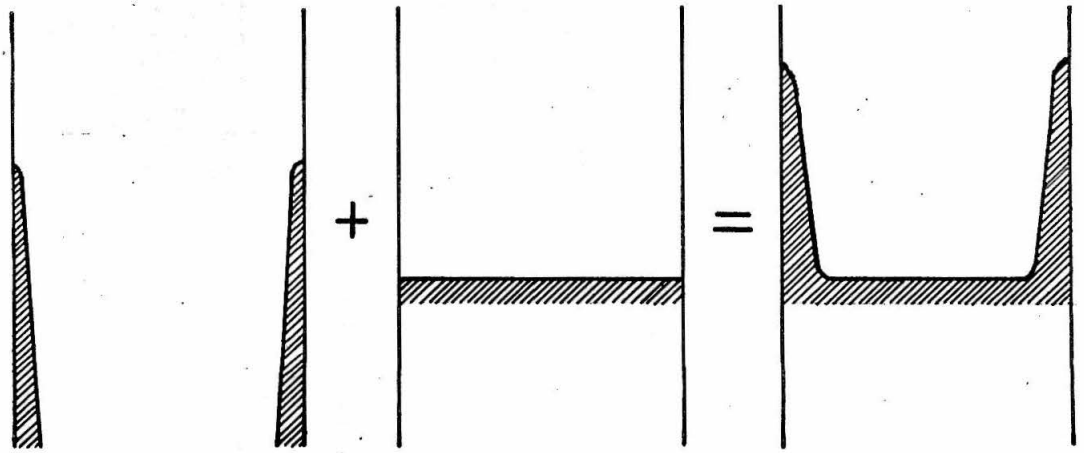

Fig. 6. Schematic illustration of the resonance flux for Γ_γ/Γ large.

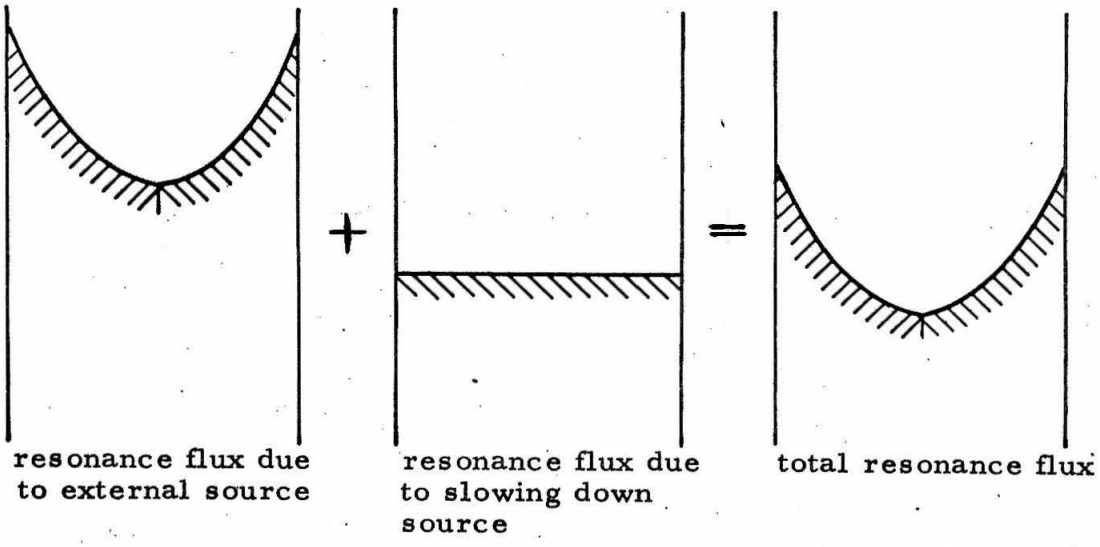

Fig. 7. Schematic illustration of the resonance flux for Γ_γ/Γ small.

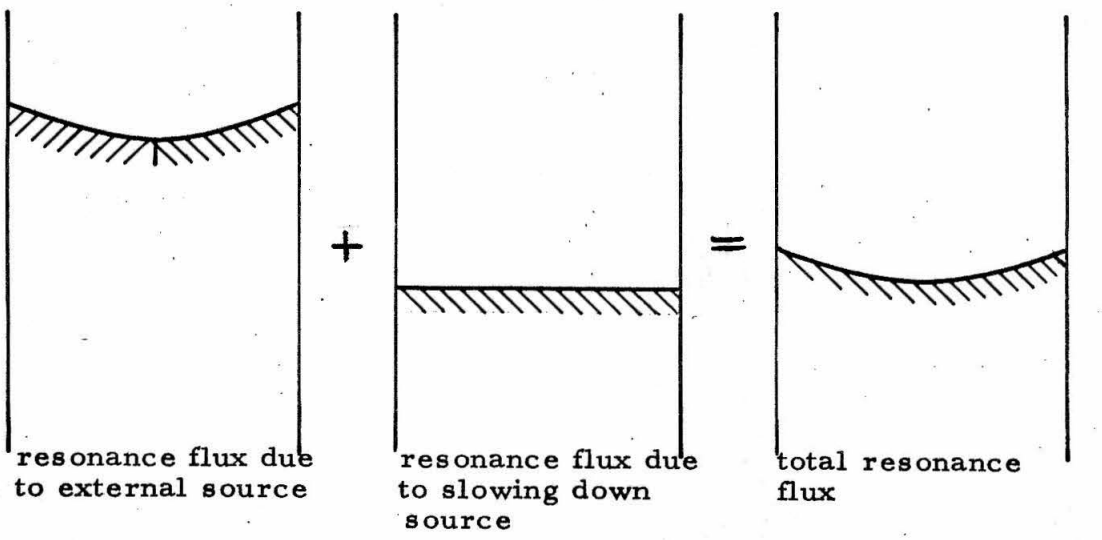

Fig. 8. Schematic illustration of the resonance flux for a mixture of nuclei.

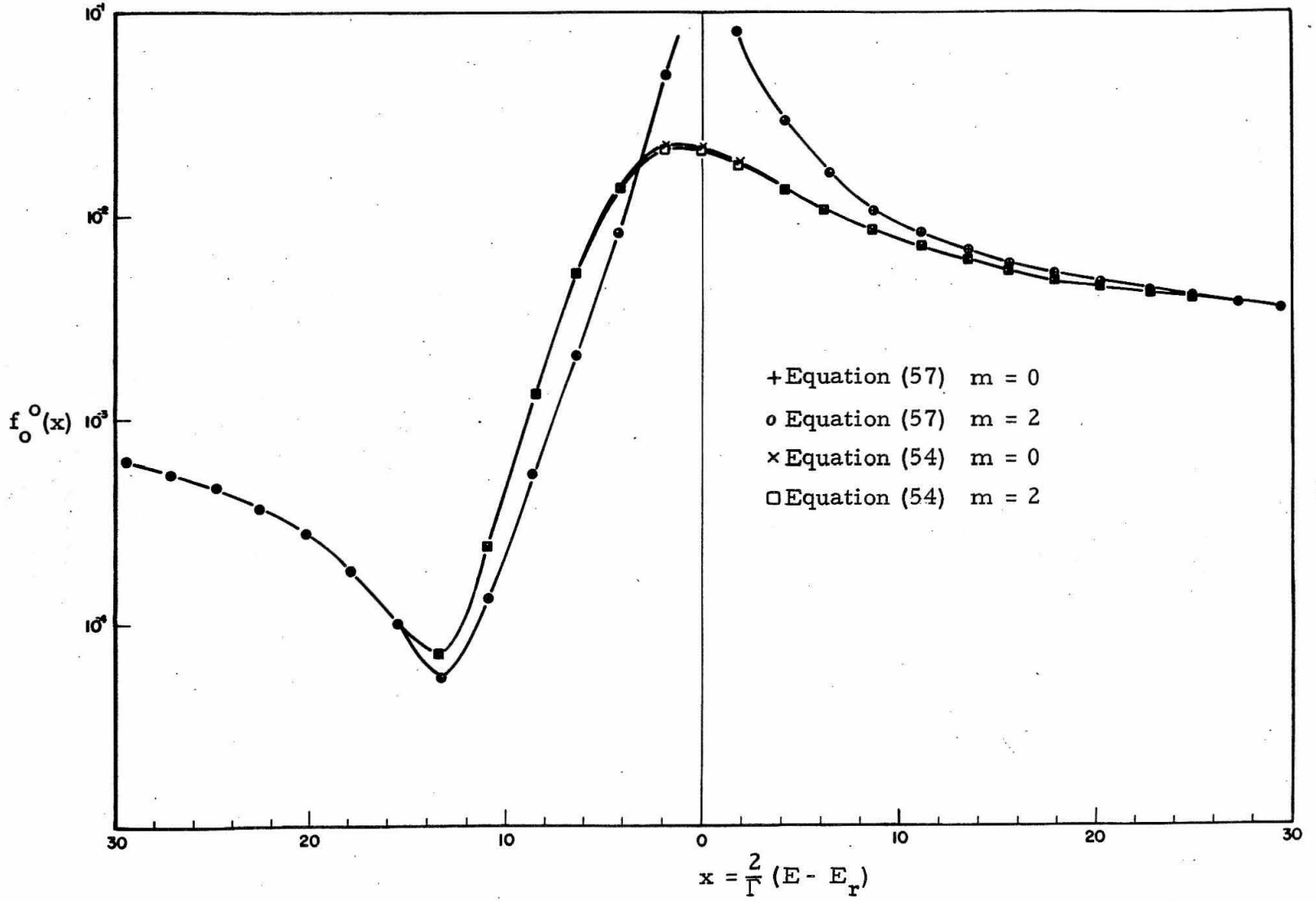

Fig. 9. Solutions for Bismuth. Slab thickness = 0.5 cm.

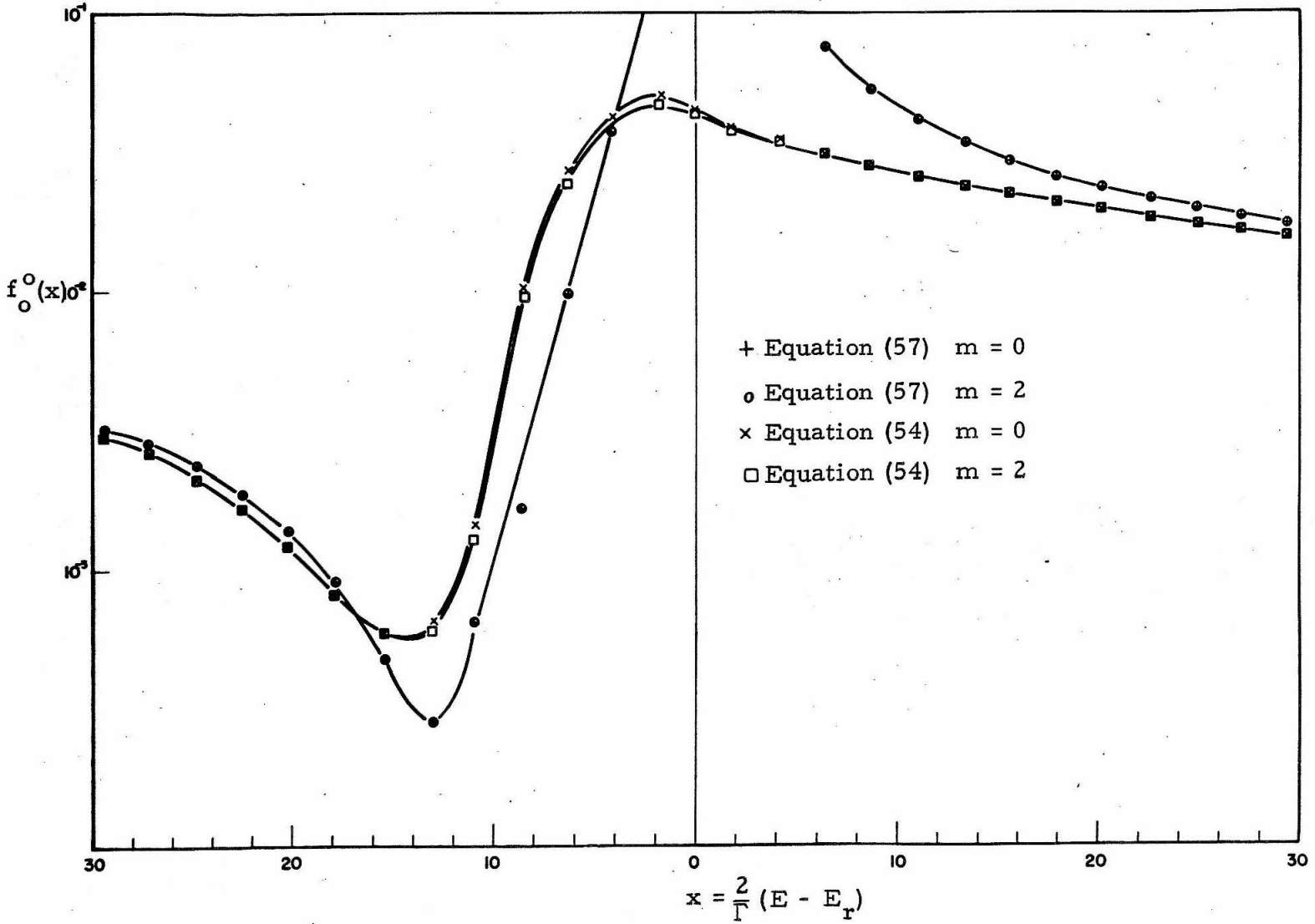

Fig. 10. Solutions for Bismuth, slab thickness = 2.5 cm

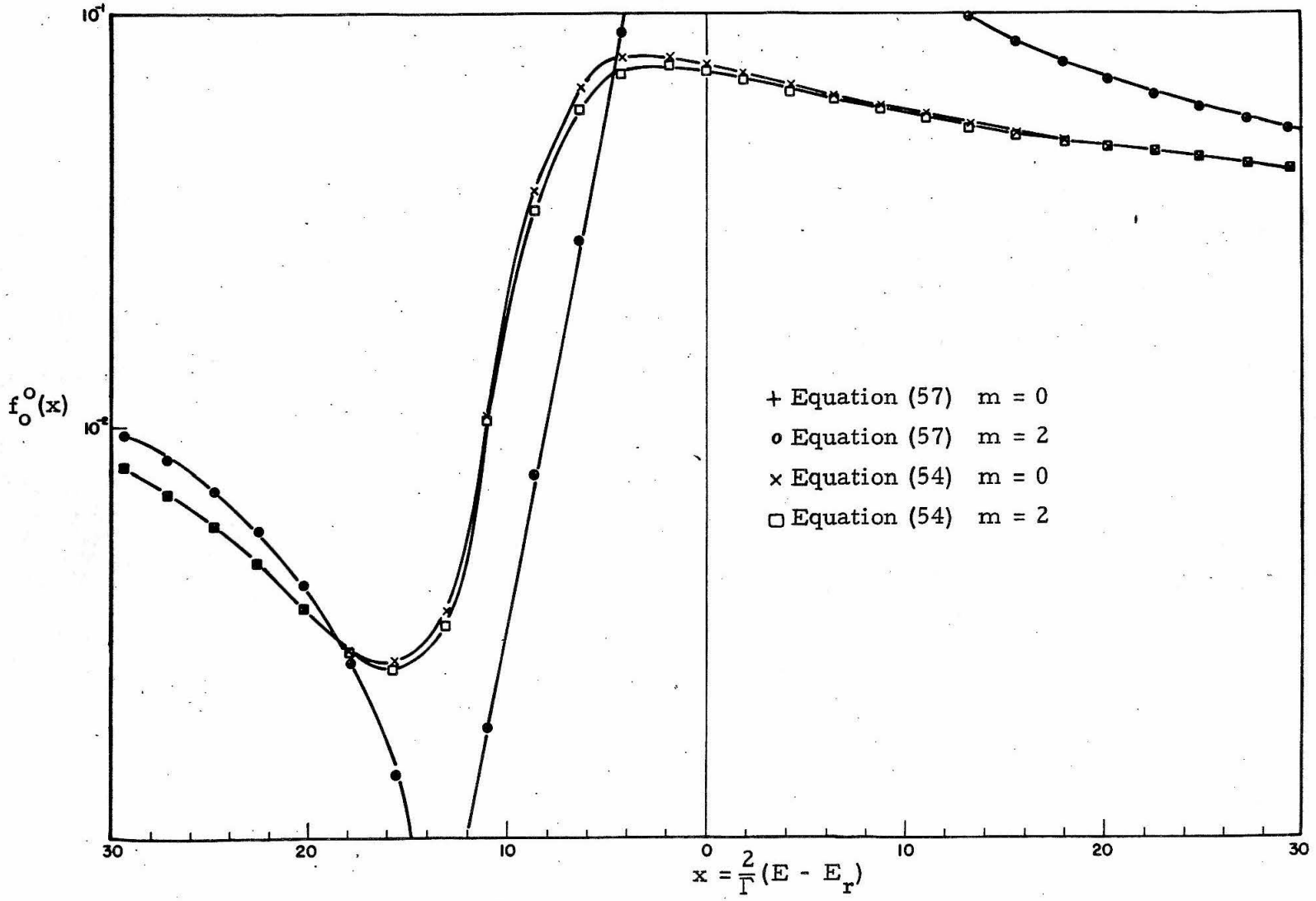

Fig. 11. Solutions for Bismuth, slab thickness = 7.5 cm.

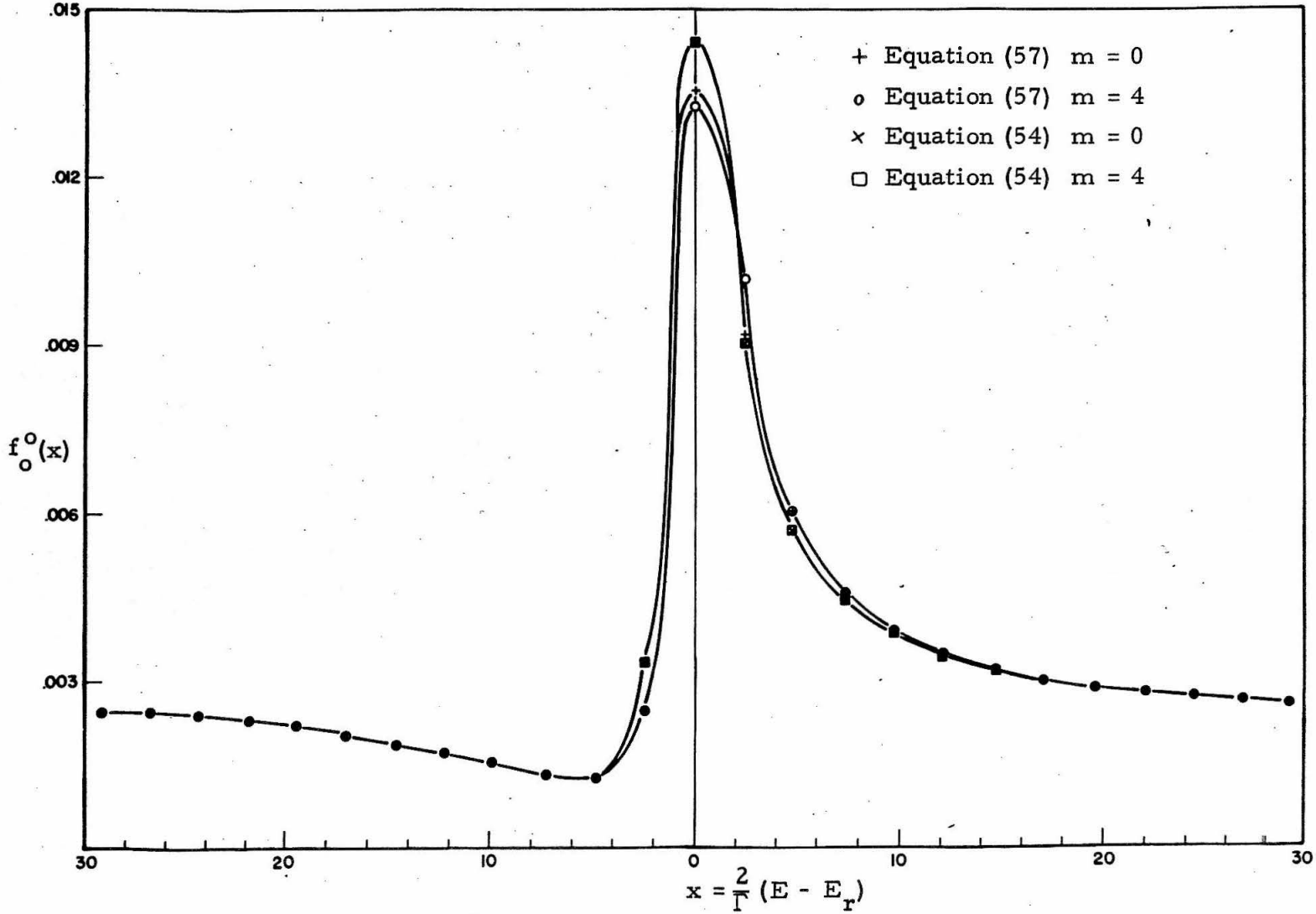

Fig. 12. Solutions for Thorium, slab thickness = 0.5 cm.

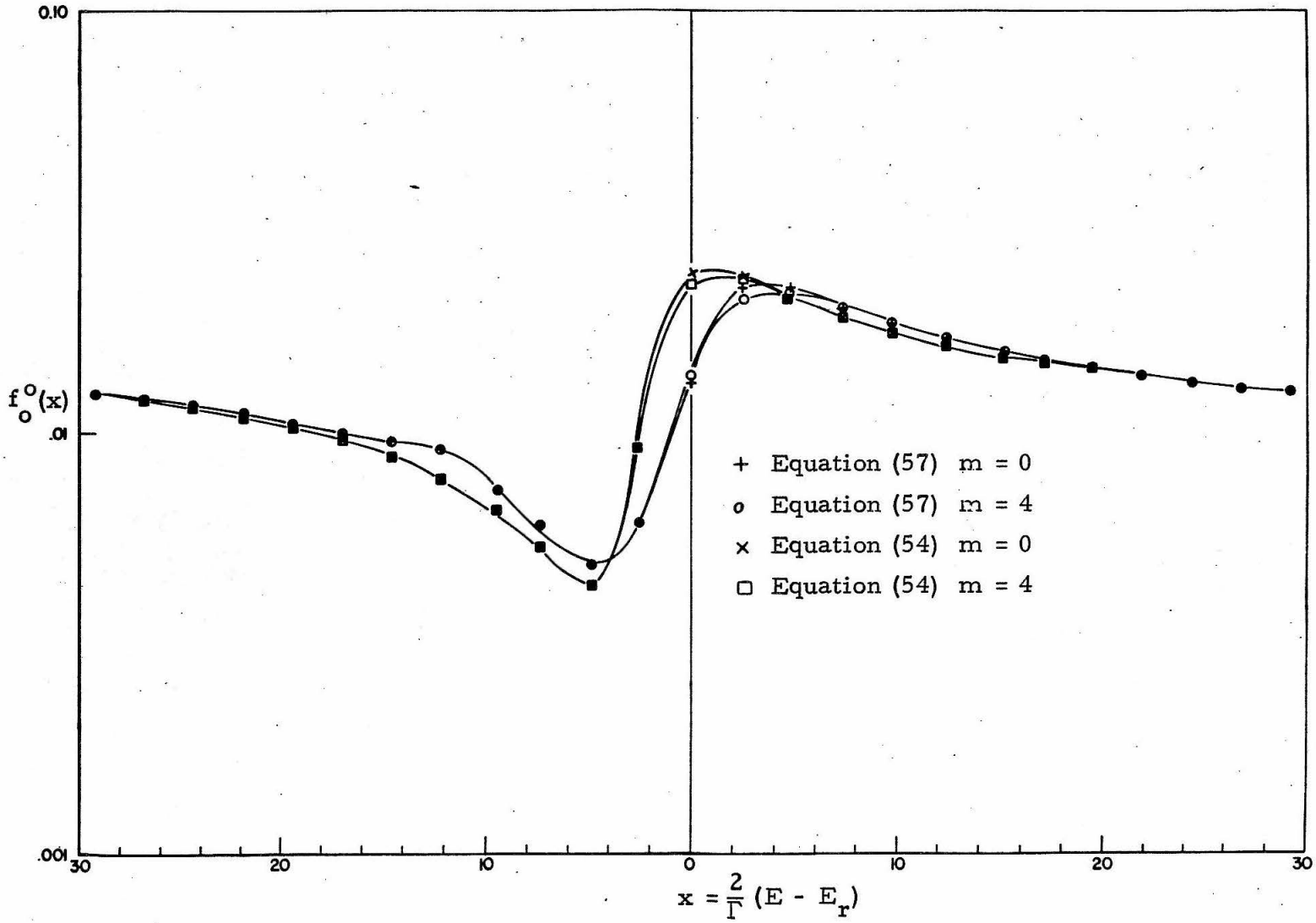

Fig. 13. Solutions for Thorium, slab thickness = 2.5 cm.

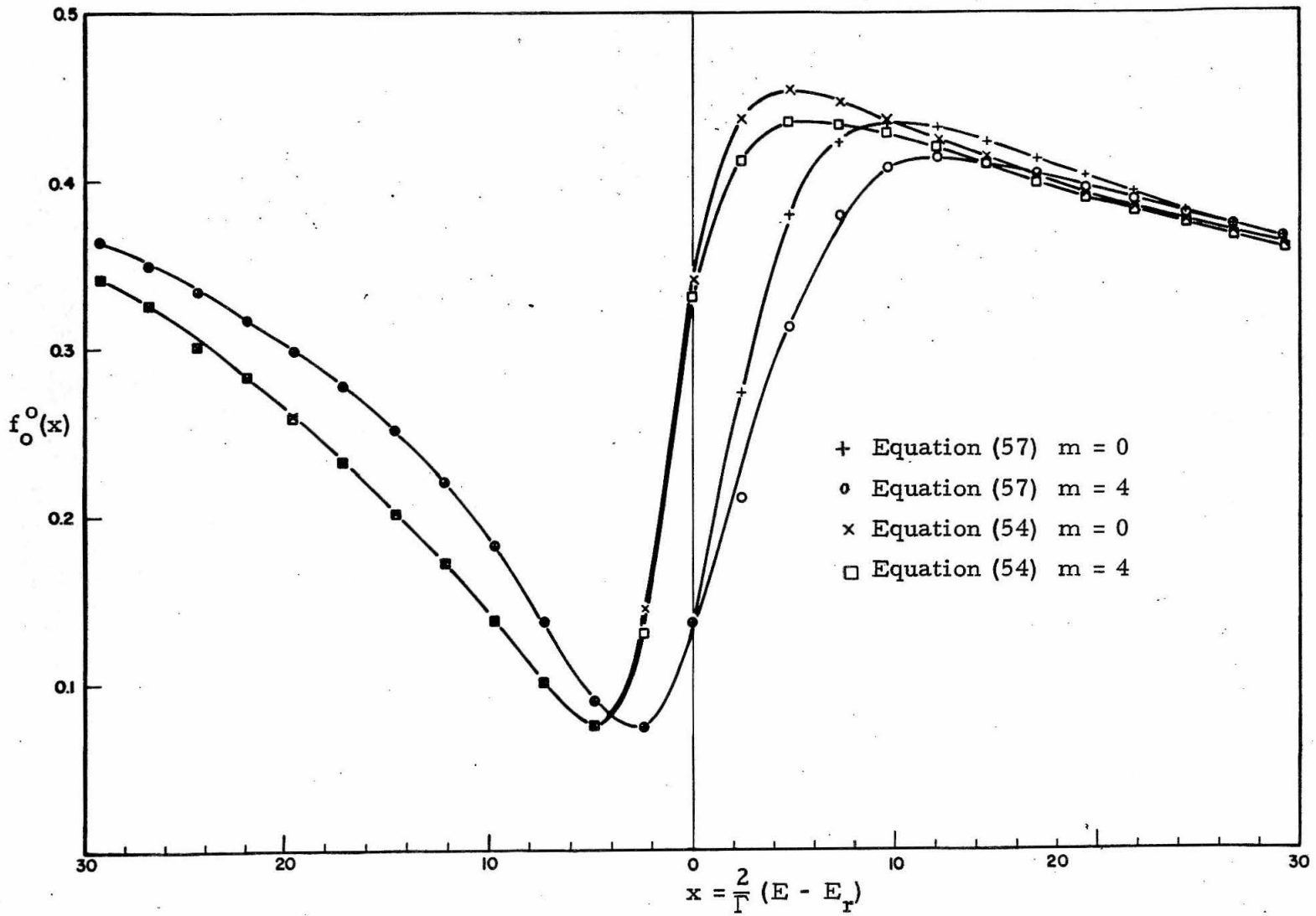

Fig. 14. Solutions for Thorium, slab thickness = 7.5 cm.

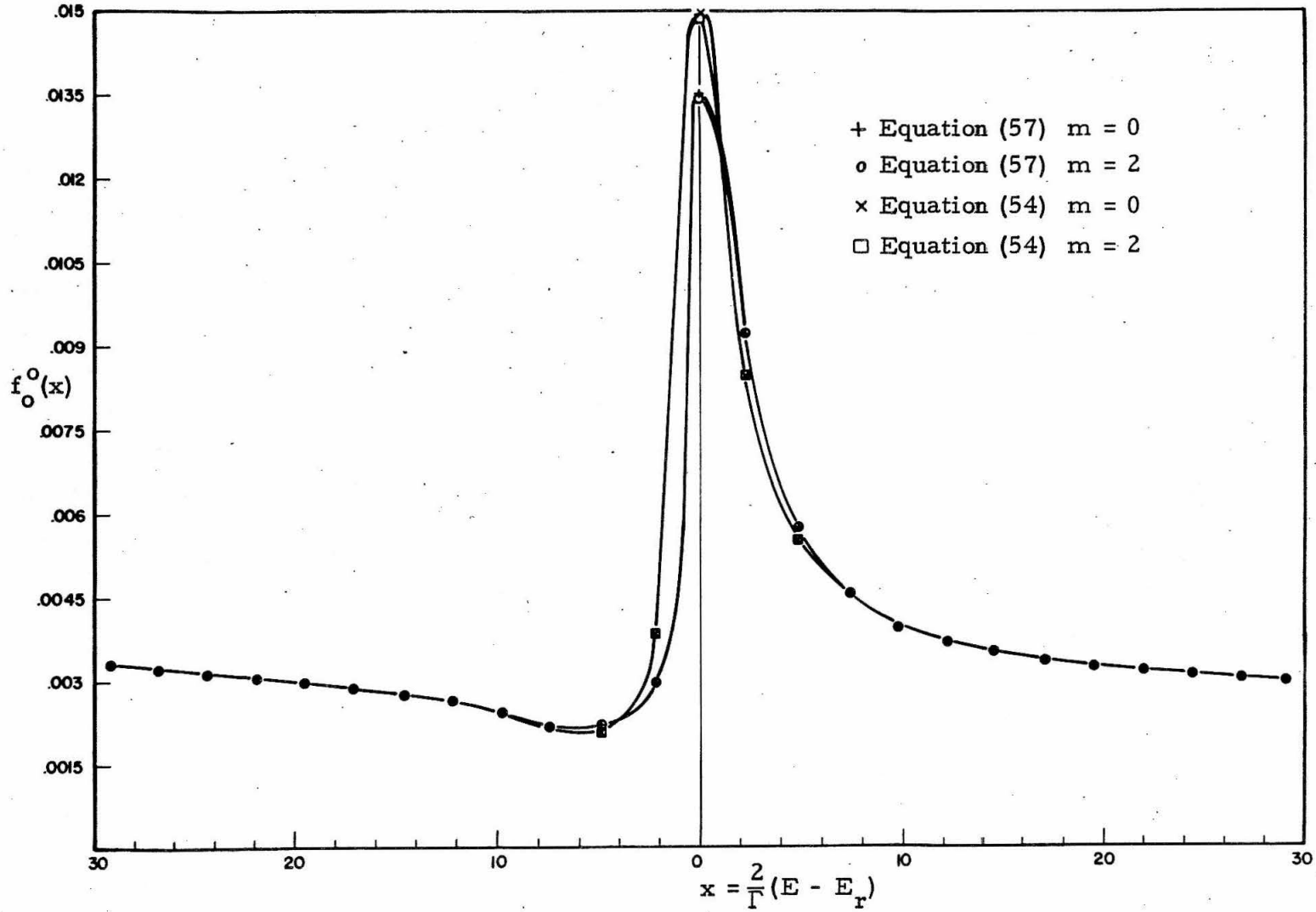

Fig. 15. Solutions for Thorium oxide, slab thickness = 0.5 cm.

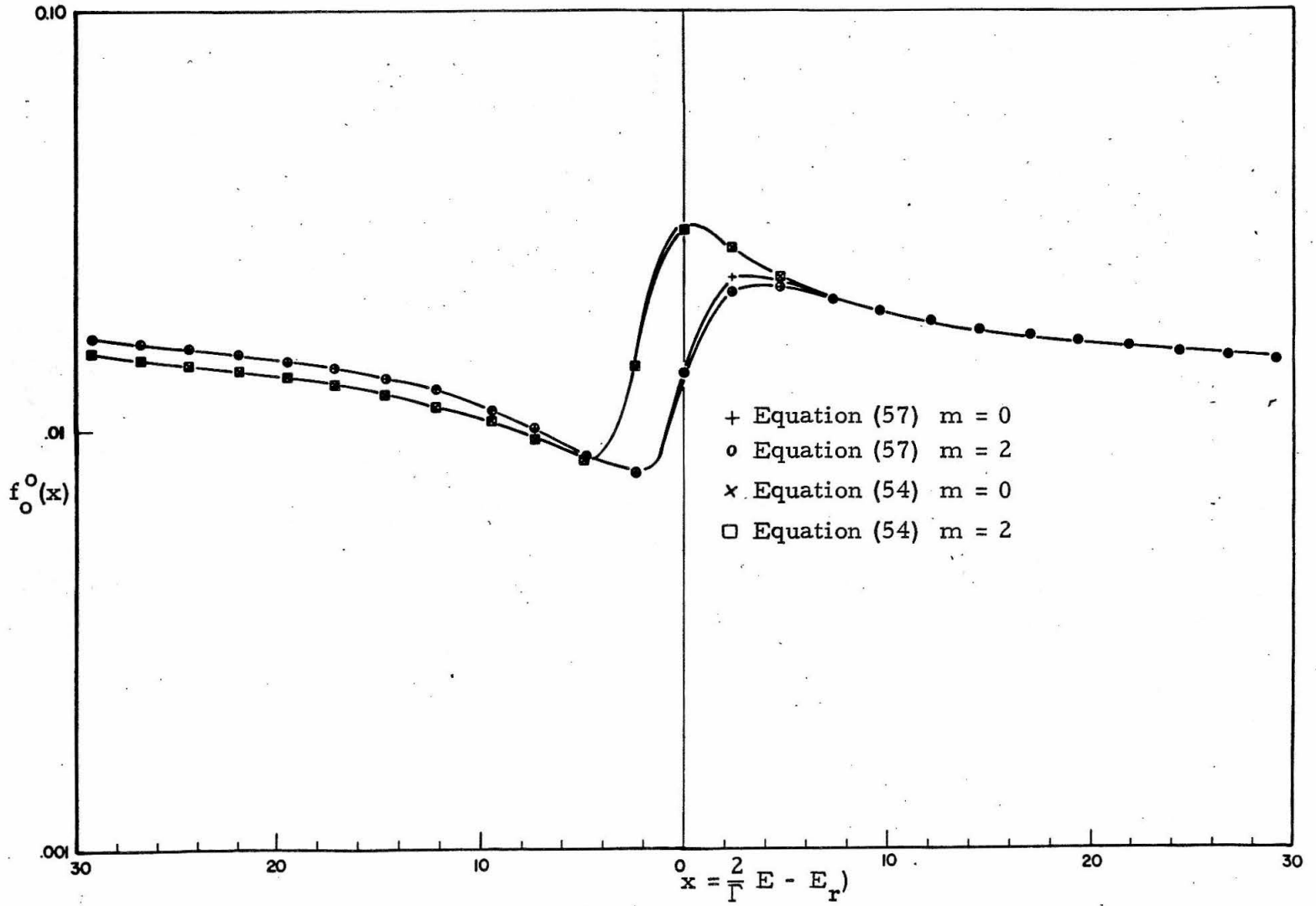

Fig. 16. Solutions for Thorium oxide, slab thickness = 2.5 cm.

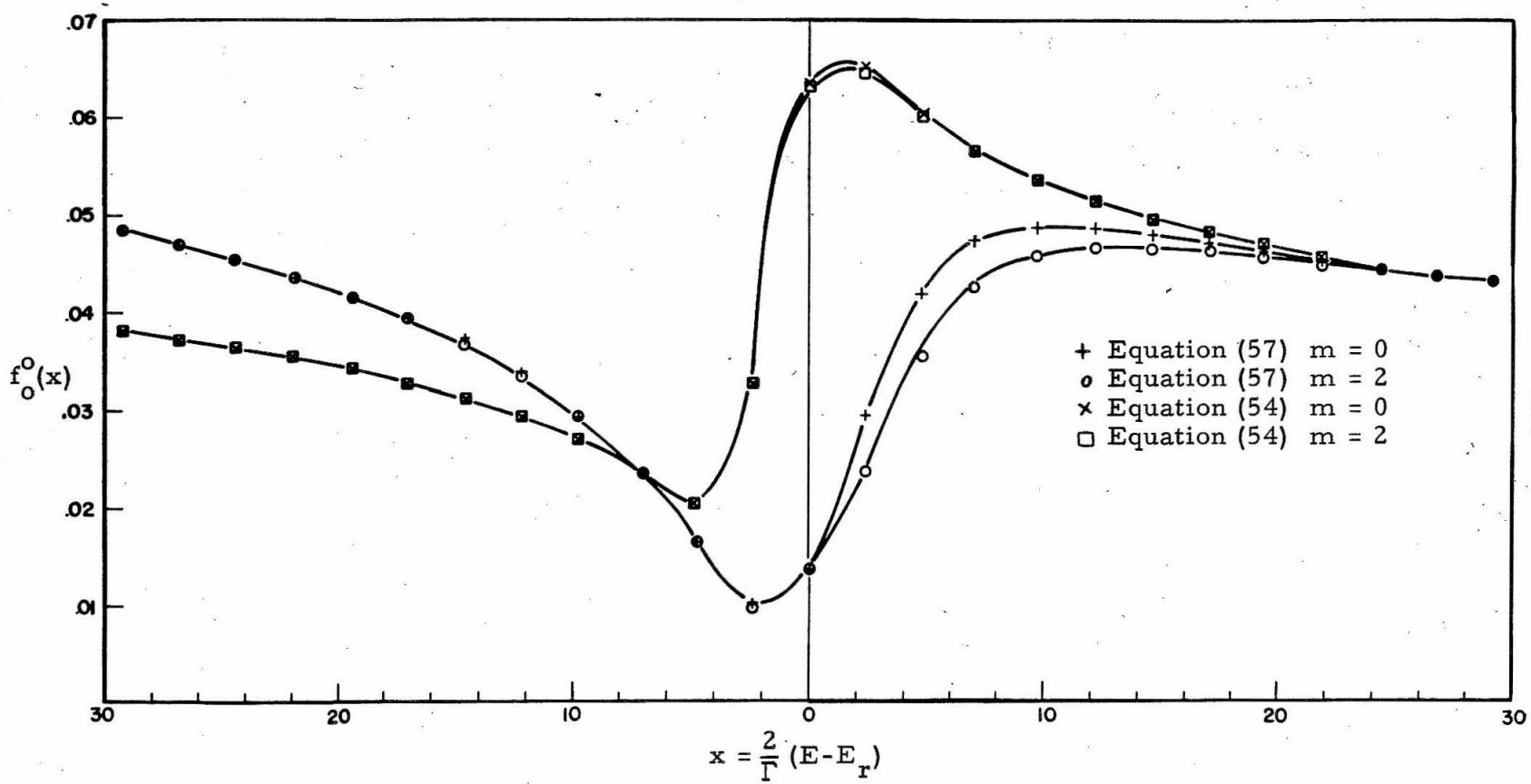

Fig. 17. Solutions for Thorium oxide, slab thickness = 7.5 cm.

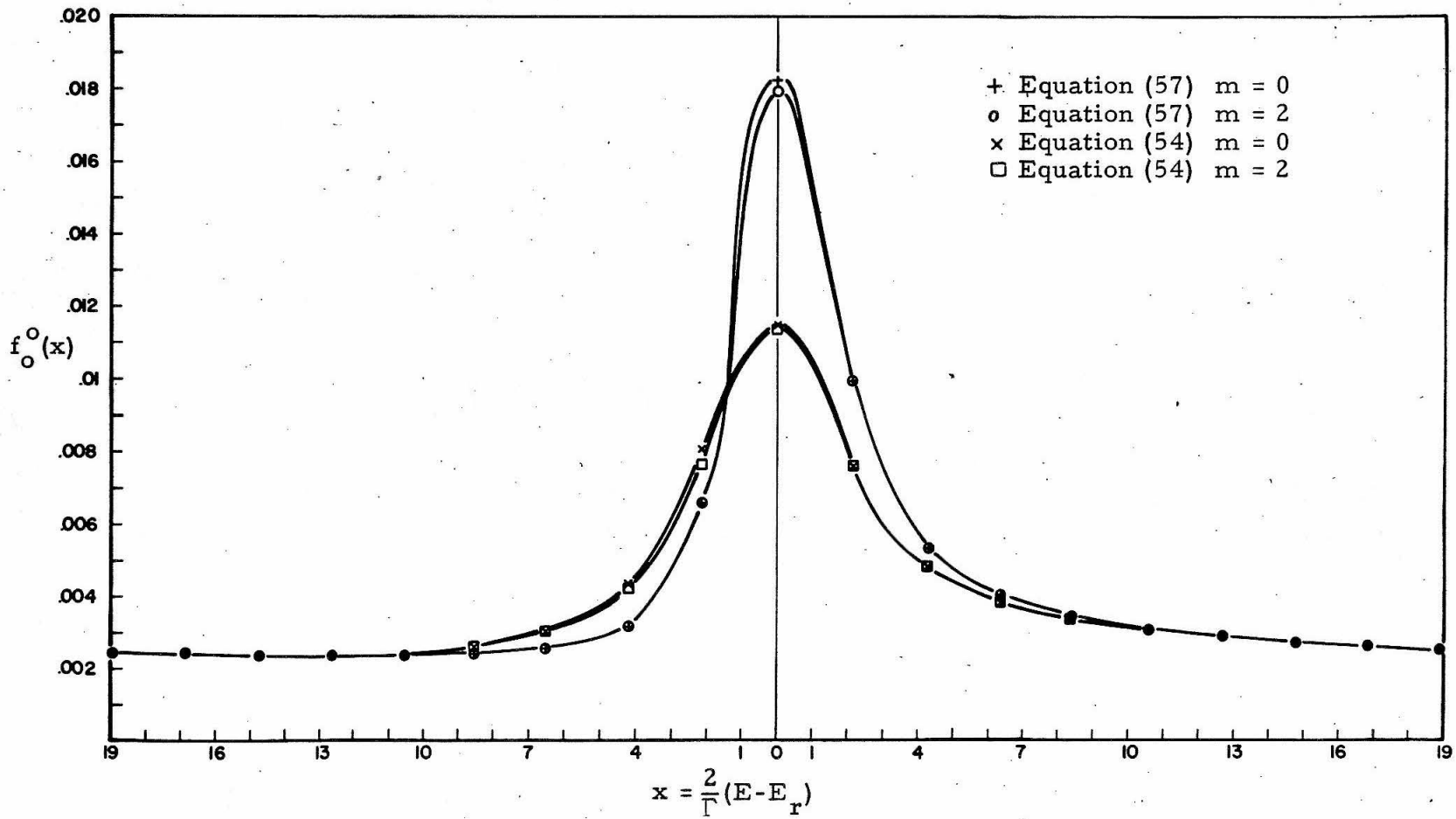

Fig. 18. Solution for Uranium, slab thickness = 0.5 cm.

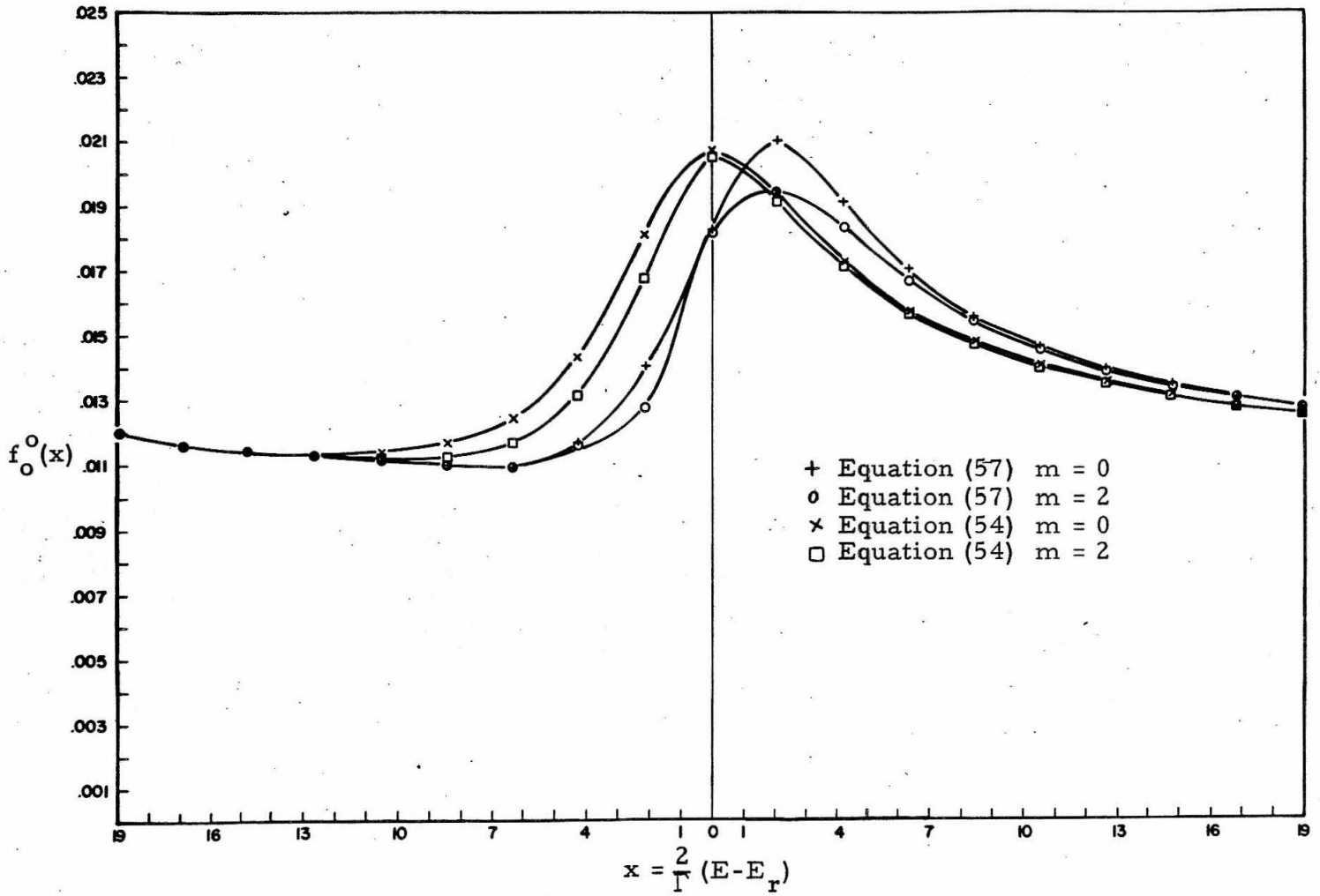

Fig. 19. Solutions for Uranium, slab thickness = 2.5 cm.

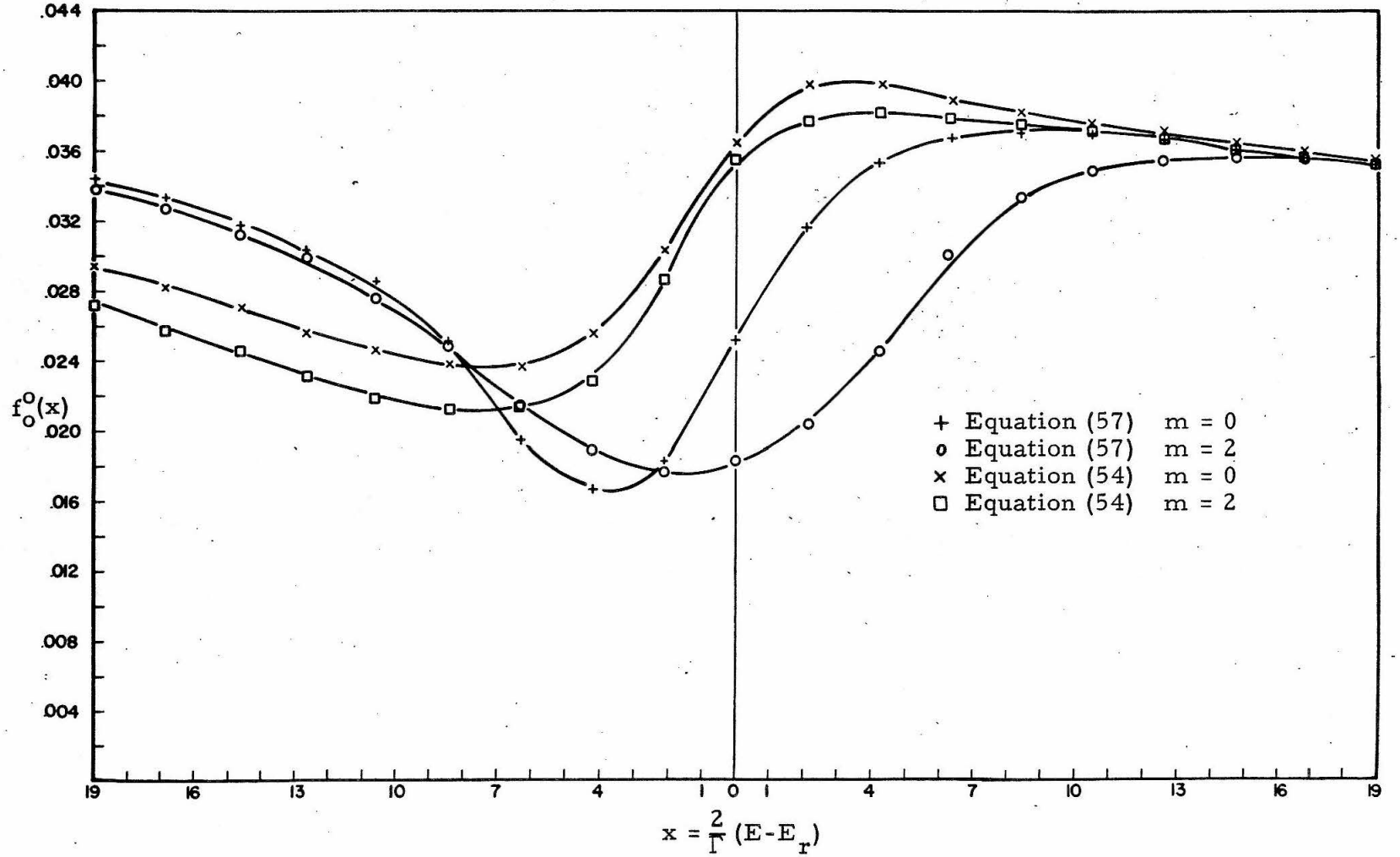

Fig. 20. Solutions for uranium, slab thickness = 7.5 cm.

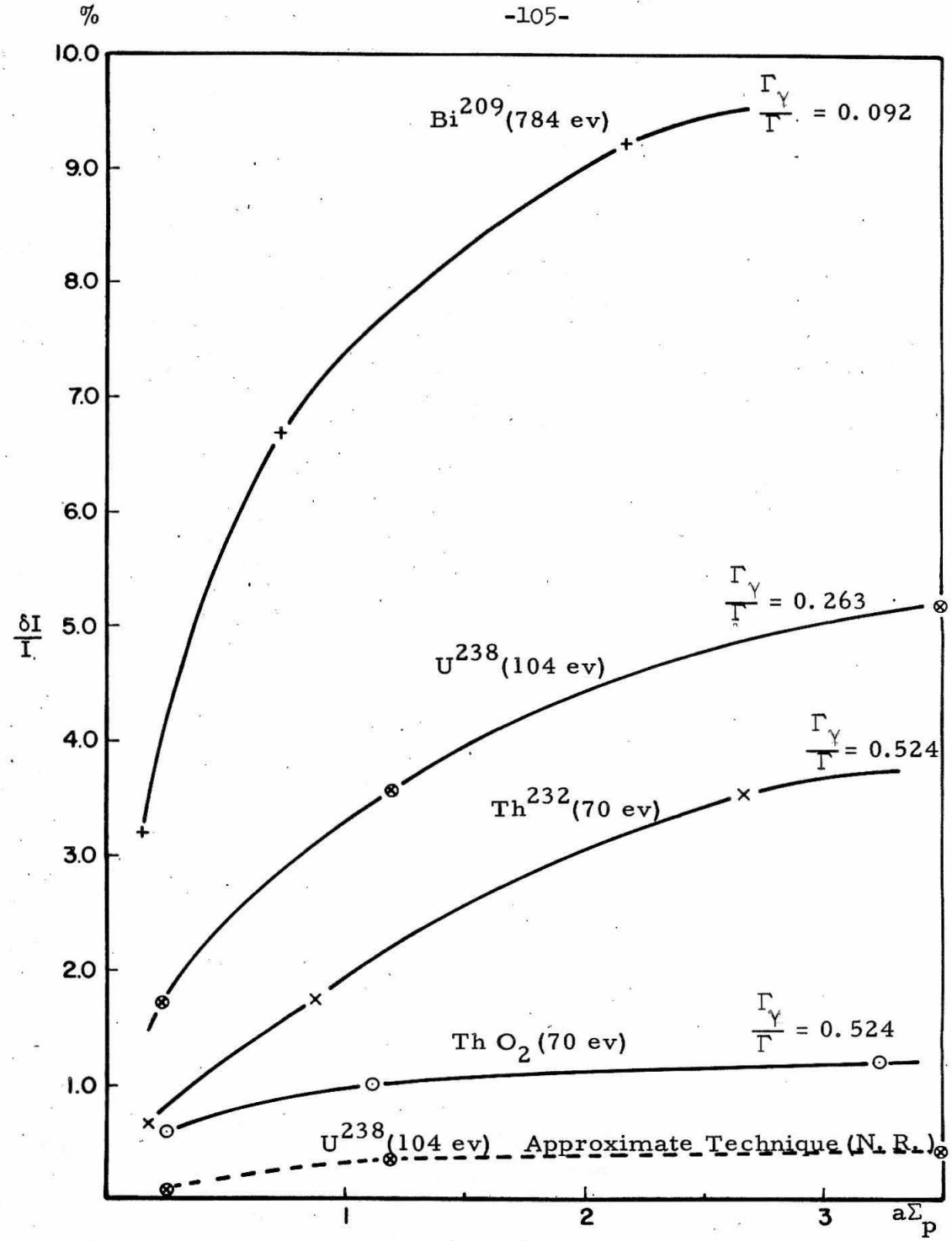

Fig. 21. Fractional error introduced in resonance integral by the flat flux approximation.

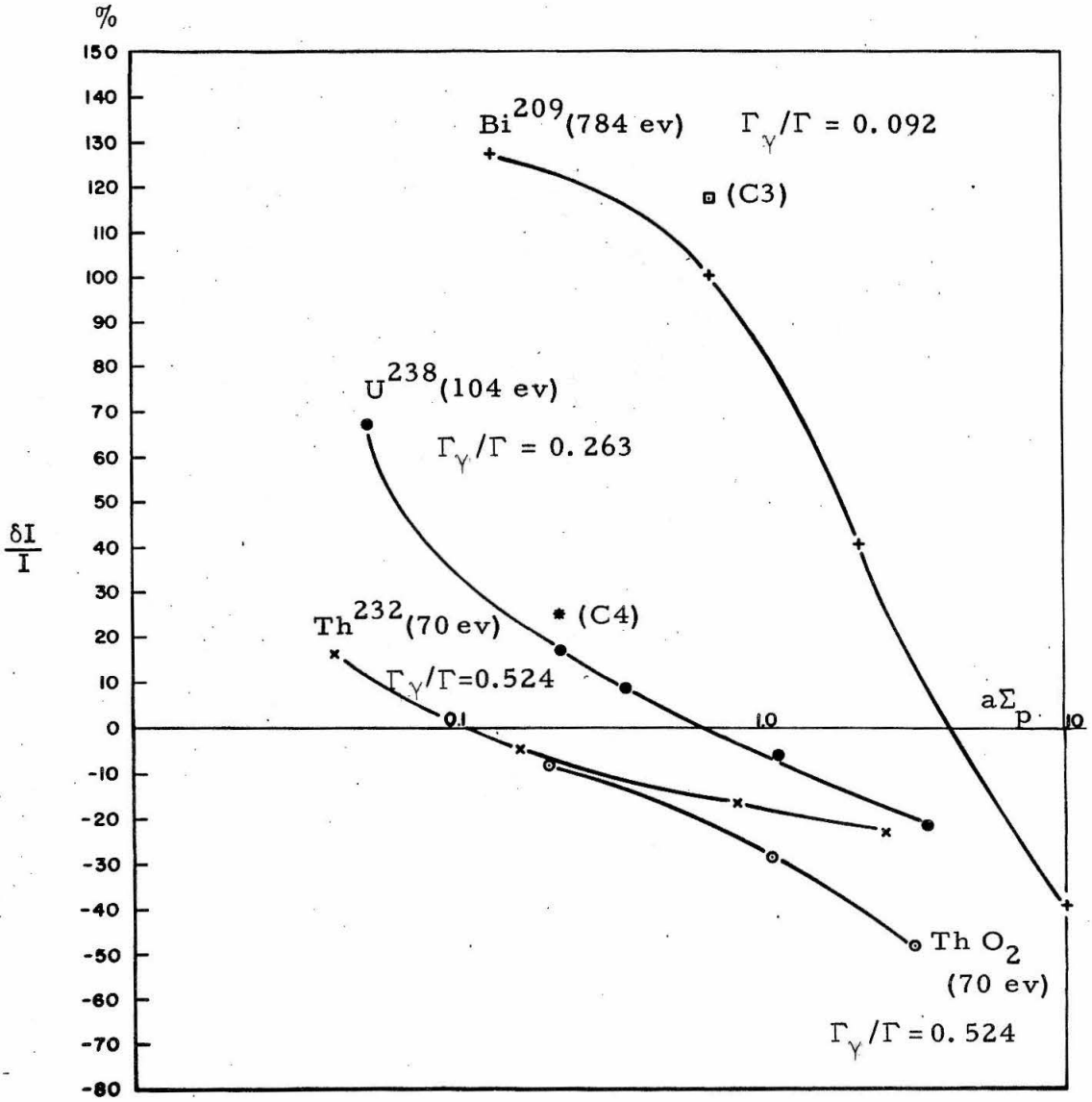

Fig. 22. Fractional error introduced in the resonance integral by the infinite mass approximation.

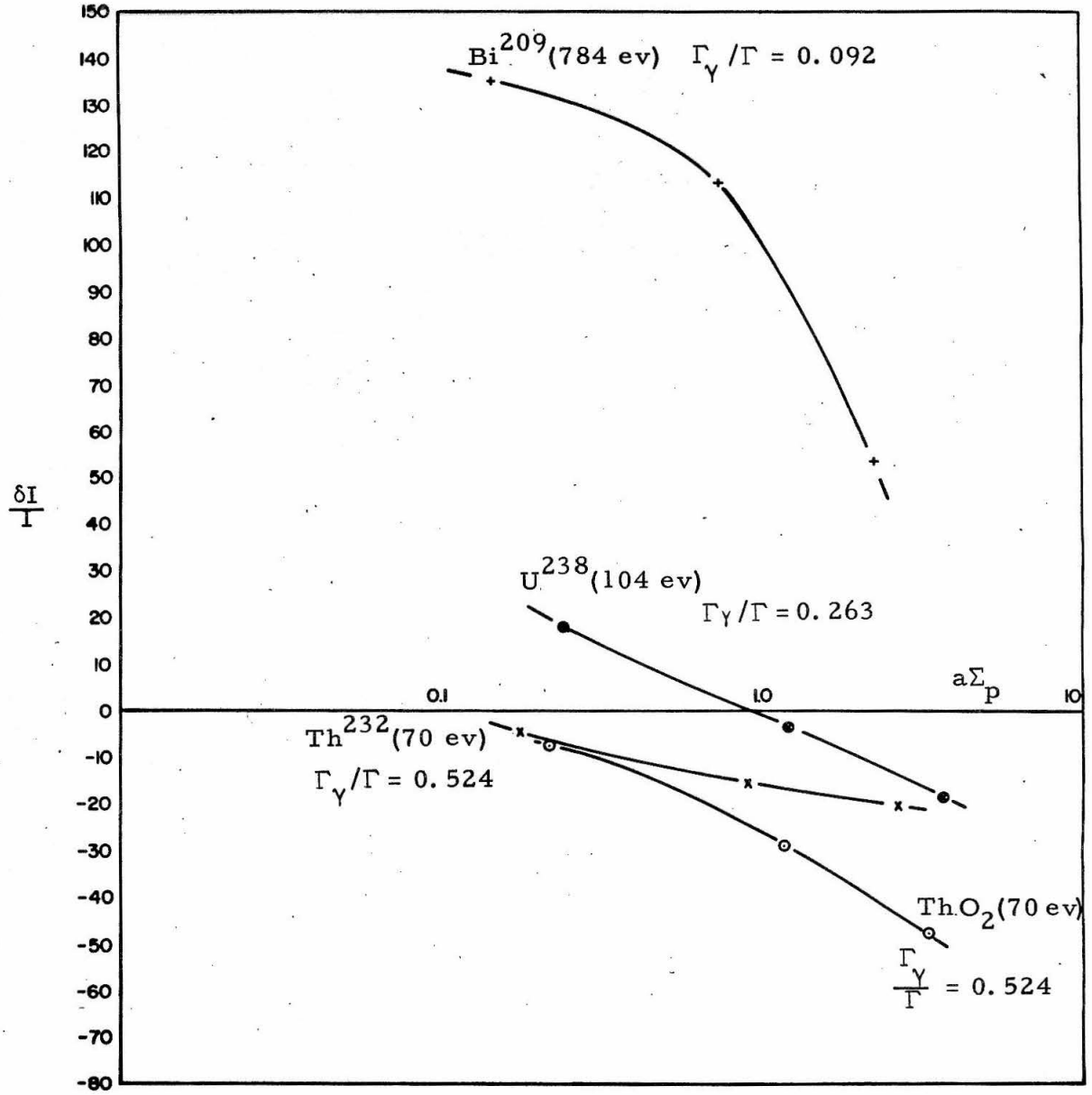

Fig. 23. Fractional error introduced in the resonance integral by the W. R. approximation.

APPENDIX A

THE SINGLE LEVEL BREIT-WIGNER LINE SHAPE FOR LOW ENERGY RESONANCES

A derivation of the Breit-Wigner resonance line shape is outlined in this appendix. The outline is based on published results (B1, V1 and L1). It is divided into two parts, as will be described below.

The derivation of nuclear cross-section may be divided into two distinct steps:

(i) The asymptotic part of the wave function is connected to the cross-section by means of the collision matrix. Asymptotic implies "far removed from the compound nucleus." The connection is a general one; that is, it has nothing to do with the nuclear problem in particular, and deals merely with the geometry of particle beams and the detection equipment.

(ii) The collision matrix is expressed in terms of the R-matrix, which contains the parameters of the nuclear resonant states. This step contains all the nuclear physics.

Reaction of the following type are considered:

$$a + X \rightarrow b + Y \qquad (1.a)$$

Particle a collides with nucleus X. After the collision particle b emerges at an angle θ, and the resulting nucleus recoils in the appropriate direction. Before the collision the system is described by the following three quantum numbers:

a = channel index, which defines the type of incoming particle

s = channel spin which is the total spin of the channel, and is the vector addition of the spin i of the incoming particle, and the spin I of the nucleus

$$\vec{s} = \vec{i} + \vec{I} \qquad (2.a)$$

$\vec{l}$ = the orbital angular momentum quantum number, of the two particles in the center of mass system

The states of the system after the collision are described by a', s', and l'.

Two invariant quantities of the reaction may be defined:

(i) The total angular momentum J, which is the vector sum of the orbital angular momentum l, and the channel spin s, i.e.

$$\vec{J} = \vec{l} + \vec{s} \qquad (3.a)$$

(ii) The second invariant quantity for reaction (1a) is the parity π.

The term channel is a convenient notation used to represent a collection of quantum numbers describing the motion of two particles, i.e.

$$C \equiv (\alpha,\ \ell,\ s,\ J,\ M) \tag{4.a}$$

where

$$M = \text{z-component of } J = J_z.$$

Thus the term channel refers collectively to the five quantum numbers in the right hand side of identity (4a).

I. The Relation Between the Scattering Matrix, and the Cross-Sections

The following approach has been outlined by Blatt et al. (B1):

Consider a nuclear state with total angular momentum J, which has a z-component $M = J_z$. The channel wave number is k_α, and the relative speed is V_α. Let $\Phi_{\alpha s}$ be a product of the wave function, of the nucleus and the particle a. Thus the most general wave function in channel a consists of a superposition of an ingoing and outgoing spherical wave. Each of these waves has spin and angular dependence. At distances large compared to the channel radius, i.e. radius of compound nucleus, the asymptotic wave function may be expressed by

$$\Psi_{\alpha s} = \frac{1}{r_\alpha \sqrt{V_\alpha}} \mathcal{Y}^M_{J\ell s}\ \Phi_{\alpha s} \left\{ A^{JM}_{\alpha s \ell} \exp\left[-i\left(k_\alpha r_\alpha - \frac{\ell\pi}{2}\right)\right] \right. \tag{5.a}$$

$$\left. - B^{JM}_{\alpha s \ell} \exp\left[i\left(k_\alpha r_\alpha - \frac{\ell\pi}{2}\right)\right] \right\}$$

where

$\mathcal{Y}^{M}_{J\ell s}$ = spin and angle dependent wave function with total angular momentum J, oribital angular momentum ℓ, and channel spin s.

$$\mathcal{Y}^{M}_{J\ell s} = \sum_{M_\ell=-\ell}^{\ell} \sum_{M_s=-s}^{s} (\ell s M_\ell M_s | \ell s J M)\, Y^{M_\ell}_{\ell}(\theta,\varphi)\, \chi_{s,M_s} \qquad (6.a)$$

M_s, M_ℓ = z-component of s and ℓ respectively

$(\ell s M_\ell M_s | \ell s J M)$ = Clebsch-Gordan coefficient (C8)

$Y^{M_\ell}_{\ell}(\theta,\varphi)$ = spherical harmonic

χ_{s,M_s} = spin wave function

Since $1/\sqrt{V_\alpha}$ is different in every channel, the coefficients correspond to an amplitude of probability flux. The coefficients $A^{JM}_{\alpha s \ell}$ and $B^{JM}_{\alpha s \ell}$ are not independent, and the relation between them is the scattering matrix

$$B^{JM}_{\alpha' s' \ell'} = \sum_{\alpha s \ell} U^{J}_{\alpha' s' \ell', \alpha s \ell}\, A^{JM}_{\alpha s \ell} \qquad (7.a)$$

It should be noted that the coefficients of the scattering matrix are independent of M, since different values of M may be obtained by merely rotating the co-ordinate system. The coefficients $A^{JM}_{\alpha s \ell}$ and $B^{JM}_{\alpha s \ell}$ will now be determined.

Consider now an incoming plane wave of the form $\exp(ik_\alpha Z_\alpha)\ \chi_{s,ms}\ \Phi_{\alpha s}$. Using the asymptotic form of the Bessel functions involved, this expression may be written as follows:

$$\exp(ik_\alpha Z_\alpha)\ \chi_{s,Ms}\Phi_{\alpha s} = \sum_{J=0}^{\infty}\sum_{M=-J}^{J}\sum_{\ell=|J-s|}^{(J+s)} \frac{i\sqrt{\pi}}{k_\alpha r_\alpha}\,\Phi_{\alpha s}(\ell s OM_s|\ell s MJ)$$

$$\times\, i^{\ell}\sqrt{2\ell+1}\,q^{m}_{J\ell s}\left\{\exp\left[-i(k_\alpha r_\alpha - \frac{\ell\pi}{2})\right]\right.$$

$$\left. + \exp\left[i(k_\alpha r_\alpha - \frac{\ell\pi}{2})\right]\right\} \qquad (8a)$$

Comparing this expression to Eq. (5a) and using Eq. (7a) the coefficients are seen to be given by

$$A^{JM}_{\alpha s\ell} = i^{(\ell+1)}\,\lambda_\alpha\sqrt{V_\alpha\pi(\alpha\ell+1)}\quad(\ell s OM_s|\ell s JM)$$

$$B^{JM}_{\alpha s\ell} = \sum_{\ell=|J-s|}^{(J+s)} i^{(\ell+1)}\,\lambda_\alpha\sqrt{V_\alpha\pi(\alpha\ell+1)}\quad(\ell s OM_s|\ell s JM)U^{J}_{a's'\ell';\alpha s\ell} \qquad (9a)$$

Equation (9a) holds in the αS channel.

$$A^{JM}_{\alpha s\ell} = 0$$

$$B^{JM}_{\alpha s\ell} = 0 \qquad (10a)$$

Equation (10a) holds in all other channels.

It will be of interest now to determine the wave function due to any reaction, and the corresponding differential cross-section. For $\alpha s = \alpha' s'$ the part of the wave function due to a reaction is of interest. Ψ the total wave function may thus be split up into an

incoming and reaction component, i.e.

$$\Psi = \Psi_{inc} + \Psi_{reac} \tag{11a}$$

Thus by substituting for the coefficients in Eq. (5a) from Eqs. (9a) and (10a), and comparing this to Eq. (8a) an expression may be extracted for Ψ_{reac}, i.e.

$$\Psi_{reac}(\alpha's') = i\,\lambda_\alpha \sqrt{\frac{\pi V_\alpha}{V_{\alpha'}}}\,\frac{\Phi_{\alpha's'}}{r_{\alpha'}} \sum_{J=0}^{\infty} \sum_{M=-J}^{J} \sum_{\ell=|J-s|}^{J+s} \sum_{\ell'=|J-s'|}^{J+s'} (\ell s 0 M_s \,|\, \ell s J M)\; i^{\ell} \sqrt{2\ell + 1}\, q^{M}_{J\ell's'} \exp\left[i\left(k_\alpha r_\alpha - \frac{\ell\pi}{2}\right)\right]$$

$$\times \left[\delta_{\alpha\alpha'}\,\delta_{ss'}\,\delta_{i\ell'} - U_{\alpha's'\ell';\alpha s\ell}\right] \tag{12a}$$

However, since detectors usually cannot select particles of total angular momentum J and orbital angular momentum ℓ, it is necessary to change Eq. (12a) to a system in which the measurements can be made. The assumption is made that the detectors can distinguish between particles of different spin M_s. $q^{M}_{J'\ell's'}$ is decomposed by means of Clebsch-Gordan coefficients, and Ψ_{reac} may be written as follows:

$$\psi_{reac}(\alpha's') = i\,\lambda_\alpha \sqrt{\frac{V_\alpha}{V_{\alpha'}}}\,\frac{e^{ik_{\alpha'}r_{\alpha'}}}{r_{\alpha'}}\,\Phi_{\alpha's'} \sum_{M_{s'}=-s'}^{s'} q_{\alpha's'M_{s'};\alpha s M_s}(\theta,\varphi)\,\chi_{s',M_{s'}} \tag{13a}$$

The angular dependent quantity $q(\theta,\varphi)$ is known as the reaction amplitude for the reaction $\alpha' s' M_{s'} \rightarrow \alpha s M_s$. The differential cross-section for this reaction corresponding to known spins M_s and $M_{s'}$, is measured in a detector at an angle $d\vec{\Omega}$ about $\vec{\Omega}$, and is given by

$$d\sigma_{\alpha' s' M_{s'}, \alpha s M_s} = \lambda_\alpha^2 \left| q_{\alpha' s' M_{s'}, \alpha s M_s}(\theta,\varphi) \right|^2 d\vec{\Omega} \qquad (14a)$$

The cross-section for an unpolarized beam of particles is obtained by averaging out the initial spin states and summing over the final state

$$d\sigma_{\alpha' s'; ds} = \frac{1}{2s+1} \sum_{M_s=-s}^{s} \sum_{M_{s'}=-s'}^{s'} d\sigma_{\alpha' s' M_{s'}; \alpha s M_s} \qquad (15a)$$

An explicit expression for $q(\theta,\varphi)$ is given in (B1). The total cross-section may be obtained by integrating over all angles in Eq. (14a), substituting this expression in Eq. (15a), and suitably modifying $q(\theta,\varphi)$, an expression for $\sigma_{\alpha' s'; \alpha s}$ is obtained. The details of the modification are given in (B1). The expression is

$$\sigma_{\alpha' s' \alpha s} = \frac{\pi \lambda_\alpha^2}{2s+1} \sum_{J=0}^{\infty} \sum_{\ell=|J-s|}^{J+s} \sum_{\ell'=|J-s'|}^{J+s'} (2J+1) \left| \delta_{\alpha\alpha'} \delta_{ss'} \delta_{\ell\ell'} - U^J_{\alpha' s' \ell'; \alpha s \ell} \right|^2 \qquad (16a)$$

In the case where $\alpha' = \alpha$ and $s' = s$, the total cross-section from α to α' is given by summing over s' and averaging over s. The total number of states of channel α is $(2J_X+1)(2J_Y+1)$. $(2s+1)$ of

these have channel spin s.

Hence

$$\sigma_{\alpha\alpha'} = \pi \lambda_\alpha^2 \sum_{J,\ell,\ell',ss'} g_\alpha^J \left| U^J_{\alpha' s' \ell';\alpha' s' \ell'} \right|^2 \qquad (17a)$$

In the case where $\alpha = \alpha'$ the same summing and averaging procedure is used. The elastic scattering cross-section is thus given by:

$$\sigma_{\alpha,\alpha} = \pi \lambda_\alpha^2 \sum_J g_\alpha^J \sum_{\ell s} \left[1 - 2\mathrm{Re}\, U^J_{\alpha' s' \ell', \alpha s \ell} + \sum_{\ell' s'} \left| U^J_{\alpha' s' \ell', \alpha s \ell} \right|^2 \right] \qquad (18a)$$

where

$$g_J^\alpha = \frac{2J + 1}{(2J_X + 1)(2J_Y + 1)} \qquad (19a)$$

J_X and J_Y = the total spins of nuclei X and Y. Re denotes the real part.

Equations (17a) and (19a) express the cross-section in terms of the collision matrix. These relations are purely geometrical, since no mention of the physics involved has been made.

II. Relation Between the Nuclear Properties and the Collision Matrix

The following approach has been considered by Vogt (V1) and Lane, et al. (L1). In this part the notation of a channel c will be used, since the geometrical section has been completed. As defined $c \equiv (\alpha, \ell, s, JM)$.

The assumption is now made that the total wave function inside the nucleus satisfies the same Schrödinger equation as that for the resonant states, i.e.

$$H\theta = E\theta$$

$$HZ_\lambda = E_\lambda Z_\lambda \tag{20a}$$

where

H = Hamiltonian

θ = total wave function inside nucleus

Z_λ = wave function for resonant states

In order to give resonant states, the functions Z_λ have to satisfy the following boundary condition:

$$Z_\lambda' = r_c \frac{dZ_\lambda}{dr_c} = b_c Z_\lambda \tag{21a}$$

where

r_c = channel radius, which is equivalent to the radius of the compound nucleus

Equation (21a) is evaluated at the surface of the compound nucleus S_c which is defined by the channel radius r_c.

The assumption is now made that the wave function θ can be written as a product. One element of the product describes the radial variation of the wave function, while the other element will be a function of all other variables. This product is summed over

all the channels, i.e.

$$\theta = \sum_c \eta_c(r)\, \mu_c \tag{22a}$$

This decomposition is only useful, if and only if, the following orthogonality relation holds:

$$\int_{S_c} \mu_c \mu_c^{*\prime}\, dS_c = \delta_{cc'} \tag{23a}$$

The functions Z_λ also form a complete orthonormal set, the orthogonality relation being:

$$\int_V Z_\lambda Z_\lambda^{*\prime}\, dV = \delta_{\lambda\lambda'} \tag{24a}$$

where V = volume of compound nucleus

It is possible to expand the actual wave function θ, in terms of the function Z_λ, i.e.

$$\theta = \sum_\lambda C_\lambda Z_\lambda \tag{25a}$$

using the orthogonality relation (24a)

$$C_\lambda = \int_V Z_\lambda^*\, \theta\, dV \tag{26a}$$

An expression for the radial part of θ is now derived. The first equation of Eq. (20a) is multiplied by Z_λ^*, and the complex conjugate of the second equation of Eq. (20a) is multiplied by θ. The resulting two equations are subtracted and integrated over the volume of the compound nucleus. The volume integrals are reduced

to surface integrals by Green's theorem. Using boundary conditions (21a), Eqs. (22a), (25a), and (26a), the following expression results for θ

$$\theta = \sum_c \eta_c(r)\mu_c = \sum_\lambda \sum_{c'} \frac{Z_\lambda \gamma_{\lambda c'}}{(E_\lambda - E)} \left[\frac{h^2}{2m_{c'} r_{c'}}\right]^{\frac{1}{2}} \left[\eta'_{c'} - b_{c'} \eta_{c'}\right] \tag{27a}$$

where

$$\gamma_{\lambda c} = \left[\frac{h^2}{2m_c r_c}\right]^{\frac{1}{2}} \int Z_\lambda^* \, \mu_c \, dS_c \tag{28a}$$

E_λ = level energy

Using Eq. (23a), Eq. (27a) becomes

$$\left[\frac{h^2}{2m_c r_c}\right]^{\frac{1}{2}} \eta_c(r) = \sum_{c'} \left[\frac{h^2}{2m_{c'} r_{c'}}\right]^{\frac{1}{2}} R_{cc'} \left[\eta'_{c'} - b_{c'} \eta_{c'}\right] \tag{29a}$$

where

$R_{cc'} \equiv$ Wigners R-matrix

$$= \sum_\lambda \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{(E_\lambda - E)} \tag{30a}$$

An expression for the radial part of the general wave function, $\eta_c(r)$ in terms of an incoming I wave function, an outgoing wave function O, and the collision matrix is now derived. Equating the result to Eq. (29a) will then yield the desired connection between the R-matrix and the collision matrix U. This expression of U may in turn be used in Eqs. (17a) and (18a) to determine the cross-sections.

The most general expression for the wave function θ is a combination of an incoming wave I, and an outgoing wave O. Using the definition of the collision matrix, Eq. (22a), and the orthogonality relation (23a), the radial part of the wave function may be written as

$$\eta_c(r) = \frac{1}{\sqrt{v_c}} \left[A_c I_c - \sum_{c'} U_{cc'} A_{c'} O_c \right] \qquad (31a)$$

Now equating Eqs. (31a) and (30a), writing the resulting expression in matrix form, the following relation between the R-matrix and the U-matrix is obtained.

$$U = (ka)^{\frac{1}{2}} O^{-1} [1-RL]^{-1} [1-RL^*] I (ka)^{-\frac{1}{2}} \qquad (32a)$$

The coefficients of A are arbitrarily set equal to unity

$$L_c = \frac{O_c'}{O_c} - b_c \equiv S_c + iP_c$$

$$L_c^* = \frac{I_c'}{I_c} - b_c \equiv S_c - iP_c$$

In principle Eq (32a) would be the desired result. It is more convenient though to introduce the concept of the level matrix $D_{\lambda\lambda'}$ which connects level λ to level λ'.

We define

$$\left[(1-RL)^{-1} (1-RL^*) \right]_{cc'} = \delta_{cc'} + \sum_{\lambda\lambda'} 2iP_{c'} \gamma_{\lambda c} \gamma_{\lambda' c'} D_{\lambda\lambda'} \qquad (33a)$$

Multiplying Eq. (33a) by (1-RL)

$$\sum_{\lambda\lambda'} 2iP_{c'} \frac{\gamma_{\lambda c}\gamma_{\lambda' c'}}{E_\lambda - E}\left[\delta_{\lambda\lambda'} - (E_\lambda - E) D_{\lambda'\lambda} + \sum_{\lambda''} \xi_{\lambda\lambda''} D_{\lambda\lambda''}\right] = 0 \qquad (34a)$$

where

$$\xi_{\lambda\lambda''} = \sum_{c''} \gamma_{\lambda c''}\gamma_{\lambda'' c''} L_{c''} = \frac{i}{2}\Gamma_{\lambda\lambda''} - \Lambda_{\lambda\lambda''}$$

The term in the brackets of Eq. (34a) must be zero independently, for it to be independent of $\gamma_{\lambda c}$ and $\gamma_{\lambda' c'}$. This defines the level matrix, i.e.

$$(D_{\lambda\lambda'})^{-1} = (E_\lambda - E)\,\delta_{\lambda\lambda'} + \Lambda_{\lambda\lambda'} - \frac{i\Gamma_{\lambda\lambda'}}{2}$$

Since the matrices I and O are diagonal, the combination $(k_c r_c)^{\frac{1}{2}} O_c^{-1} I_{c'}(k_{c'} r_{c'})^{-\frac{1}{2}}$ may be evaluated together. The incoming and outgoing waves may be written as a combination of a regular solution F_c and an irregular solution G_c of the Schrödinger equation, i.e.

$$I_c = O_c^* = G_c - iF_c \qquad (36a)$$

The functions f_c and G_c are normalized by the Wronskian

$$F_c' G_c - G_c' F_c = k_c r_c \qquad (37a)$$

It is now possible to compute $(k_c r_c)^{\frac{1}{2}} O_c^{-1} I_{c'}(k_{c'} r_{c'})^{-\frac{1}{2}}$

$$(k_c r_c)^{\frac{1}{2}} O_c^{-1} I_{c'}(k_{c'} r_{c'})^{-\frac{1}{2}} = e^{-i(\theta_c + \theta_{c'})} P_c^{\frac{1}{2}} P_{c'}^{-\frac{1}{2}} \qquad (38a)$$

where the θ_c's are the s-wave hard sphere phase shifts.

Hence by combining Eqs. (38a), (35a), (33a) and (32a) the relation for $U_{cc'}$ for a single level is given by

$$U_{cc'} = \delta_{cc'} e^{-2i\theta_c} + \frac{ie^{-i(\theta_c+\theta_{c'})}\left\{\Gamma_{\lambda c}\,\Gamma_{\lambda c'}\right\}^{\frac{1}{2}}}{(E_\lambda + \Lambda_\lambda - E) - \frac{i\Gamma_\lambda}{2}} \tag{39a}$$

To obtain the relation cross-section Eq. (39a) is substituted into Eq. (17a). For s-wave scattering, i.e. $\ell = 0$ the cross-section is given by

$$\sigma_{\alpha,\alpha'} = \frac{\sigma_o\,\Gamma_{c'}}{\Gamma\left\{1 + \left(\frac{2}{\Gamma}\left[E_r - E\right]\right)^2\right\}} \tag{40a}$$

where

$$\sigma_o = \pi\, g_J^{\alpha}\,\frac{\Gamma_c}{\Gamma}\,\lambda_2^{\,2}$$

$$E_r = E_\lambda + \Lambda_\lambda$$

Γ, $\Gamma_{c'}$,Γ_c = total reaction, and scattering half widths, at the half-maximum cross-section.

$\Gamma = \Gamma_{c'} + \Gamma_c$, if only one reaction is allowed. $\sigma_{\alpha\alpha'}$ has a maximum at $E = E_r$, the resonance energy.

The scattering cross-section is obtained by substituting Eq. (39a) into Eq.(18a). In addition, since the energies involved are low, only S-wave scattering will be considered. In this case $\theta_c \ll 1$, and this allows simplification regarding the exponential

functions in Eq. (39a). The scattering cross-section is given by

$$\sigma_{\alpha,\alpha} = \frac{\sigma_o \Gamma_c}{\Gamma\left\{1 + \left(\frac{2}{\Gamma}\left[E_r - E\right]\right)^2\right\}} + 2\left(\sigma_o \sigma_p g_J \frac{\Gamma_c}{\Gamma}\right)^{\frac{1}{2}} \frac{\frac{2}{\Gamma}(E_r - E)}{\left\{1 + \left[\frac{2}{\Gamma}(E_r - E)\right]^2\right\}} + \sigma_p \qquad (41a)$$

where

σ_p = potential scattering cross-section = $2\pi R^2$

R = radius of nucleus X

Equation (41a) consists of the following three terms:

(i) The first describes the resonance scattering, which has a maximum at $E = E_r$.

(ii) The second term is a measure of the intereference scattering.

(iii) The third term is the constant, energy independent background scattering.

The energies E and E_r are measured in the center of mass system. Γ, Γ_c, and Γ_c are physical parameters which have the units of energy. These parameters are called total width, Γ and partial width Γ_c, $\Gamma_{c'}$, $\Gamma_{c''}$, one width existing for each mode of decay.

APPENDIX B

COMPUTATION OF $a_{44}(E)$

The method used for computing the matrix elements will be outlined here, and as an example the $a_{44}(E)$ element will be considered.

From the definition, Eq. (55)(a) the element is given by

$$a_{44}(E) = \frac{9\Sigma_t(E)}{2a} \int_0^a \int_0^a P_4\left(\frac{2x'}{a} - 1\right) E_1\left[\Sigma_t(E)|x-x'|\right] P_4\left(\frac{2x}{a} - 1\right) dx dx' \quad (1.b)$$

Making use of the definition of the exponential integral function, interchanging the order of integration in such a manner that the integrals over x' and x are evaluated first, and introducing a new set of variables defined by:

$$\varphi = \left(\frac{2x'}{a} - 1\right)$$

$$\theta = \left(\frac{2x}{a} - 1\right) \quad (2.b)$$

the matrix element becomes

$$a_{44}(E) = \frac{9a\Sigma_t(E)}{8} \int_1^\infty \frac{du}{u} \int_{-1}^{+1} \int_{-1}^{+1} P_4(\theta) \exp\left[-\frac{ua\Sigma_t(E)}{2}|\theta-\varphi|\right]$$

$$\times P_4(\varphi)\, d\theta\, d\varphi \quad (3.b)$$

Substituting for $P_4(\theta)$ and $P_4(\varphi)$ and evaluating the integral over φ first, the following value for the matrix element is obtained:

$$a_{44}(E) = \frac{9a\Sigma_t(E)}{512}\int_1^\infty \frac{du}{u}\int_{-1}^{+1}\left[35\theta^4 - 30\theta^2 + 3\right]\left[\frac{140\,\theta^4}{au\,\Sigma_t(E)}\right.$$

$$\left. - \frac{120\,\theta^2}{au\,\Sigma_t(E)} + \frac{12}{au\,\Sigma_t(E)} + \frac{6{,}720\,\theta^2}{a^3u^3\,\Sigma_t{}^3(E)} - \frac{960}{a^3u^3\,\Sigma_t{}^3(E)} + \frac{53760}{a^5u^5\Sigma_t{}^5(E)}\right]$$

$$- A\left[u,\Sigma_t(E),a\right]\left(\exp\left[-au\theta\,\frac{\Sigma_t(E)}{2}\right] + \exp\left[+au\theta\,\frac{\Sigma_t(E)}{2}\right]\right)$$

where

$$A\left[u\,\Sigma_t(E)a\right] = \exp\left[-\frac{au}{2}\,\Sigma_t(E)\right]\left[\frac{16}{au\Sigma_t(E)} + \frac{320}{a^2u^2\Sigma_t{}^2(E)} + \frac{2880}{a^3u^3\Sigma_t{}^3(E)} + \frac{13440}{a^4u^4\Sigma_t{}^4(E)}\right.$$

$$\left. + \frac{26880}{a^5u^5\Sigma_t{}^5(E)}\right]$$

The integral over θ may now be evaluated, in a similar fashion as the one over φ, i.e.

$$a_{44}(E) = \frac{9a\Sigma_t(E)}{512}\int_1^\infty \frac{du}{u}\left[\frac{512}{9a\Sigma_t(E)} - \frac{512}{a^2u^2\Sigma_t{}^2(E)}\left(1 - e^{-a\Sigma_t(E)u}\right)\right.$$

$$+ \frac{20480\,e^{-au\Sigma t(E)}}{a^3u^3\Sigma_t{}^3(E)} + \frac{20480}{a^4u^4\Sigma_t{}^4(E)} + \frac{389120\,e^{-ua\Sigma_t(E)}}{a^4u^4\Sigma_t{}^4(E)}$$

$$+ \frac{4546560\,e^{-ua\Sigma t(E)}}{a^5u^5\Sigma_t{}^5(E)} - \frac{1105920}{a^6u^6\Sigma_t{}^6(E)} + \frac{35512320\,e^{-au\Sigma_t(E)}}{a^6u^6\Sigma_t{}^6(E)}$$

$$\left. + \frac{189235200}{a^7u^7\Sigma_t{}^7(E)} + \frac{670924800}{a^8u^8\Sigma_t{}^8(E)} + \frac{1445068800}{a^{10}u^{10}\Sigma_t{}^{10}(E)}\left[e^{-au\Sigma_t(E)}\left(1+au\Sigma_t(E)\right)-1\right]\right]$$

In evaluating the integral over u, use is made of the definition of the exponential integral function. Finally then, the matrix element is given by:

$$a_{44}(E) = 1 - \frac{9}{a\Sigma_t(E)}\left(\frac{1}{2} - E_3\left[a\Sigma_t(E)\right]\right) + \frac{360E_4\left[a\Sigma_t(E)\right]}{a^2\Sigma_t^{\,2}(E)}$$

$$+ \frac{6840}{a^3\Sigma_t^{\,3}(E)}\left(\frac{1}{76} + E_5\left[a\Sigma_t(E)\right]\right) + \frac{79920E_6\left[a\Sigma_t(E)\right]}{a^4\Sigma_t^{\,4}(E)}$$

$$+ \frac{3326400E_8\left[a\Sigma_t(E)\right]}{a^6\Sigma_t^{\,6}(E)} - \frac{624240}{a^5\Sigma_t^{\,5}(E)}\left(\frac{3}{578} - E_7\left[a\Sigma_t(E)\right]\right)$$

$$+ \frac{25401600E_{10}\left[a\Sigma_t(E)\right]}{a^8\Sigma_t^{\,8}(E)} + \frac{11793600}{a^7\Sigma_t^{\,7}(E)}\left(\frac{1}{104} + E_9\left[a\Sigma_t(E)\right]\right)$$

$$- \frac{25401600}{a^9\Sigma_t^{\,9}(E)}\left(\frac{1}{10} - E_{11}\left[\Sigma_t(E)a\right]\right) \qquad (4.b)$$

Now since it is desired to express the expression (4.b) in terms of exponentials and a single exponential integral function, the following recursion relation is used (C6):

$$E_n(x) = \frac{1}{n-1}\left[e^{-x} - x\,E_{n-1}(x)\right]$$

Thus

$$E_4(x) = \frac{1}{3}\left[e^{-x} - x\,E_3(x)\right]$$

$$E_5(x) = \frac{1}{4}\left[e^{-x} - \frac{xe^{-x}}{3} + \frac{x^2E_3(x)}{3}\right]$$

etc. (5.b)

In this way all the exponential integral functions occuring in the various matrix elements could be expressed in terms of $E_3\left[a\Sigma_t(E)\right]$ and $e^{-a\Sigma_t(E)}$. The following result was obtained for $a_{44}(E)$.

$$a_{44}(E) = 9\left[\frac{1}{9} - \frac{1}{2a\Sigma_t(E)} + \frac{e^{-a\Sigma_t(E)}}{a^2\Sigma_t{}^2(E)} + \frac{10}{a^3\Sigma_t{}^3(E)} + \frac{37e^{-a\Sigma_t(E)}}{a^3\Sigma_t{}^3(E)}\right.$$

$$+ \frac{612e^{-a\Sigma_t(E)}}{a^4\Sigma_t{}^4(E)} - \frac{360}{a^5\Sigma_t{}^5(E)} + \frac{5820e^{-a\Sigma_t(E)}}{a^5\Sigma_t{}^5(E)} + \frac{34440e^{-a\Sigma_t(E)}}{a^6\Sigma_t{}^6(E)}$$

$$+ \frac{12600}{a^7\Sigma_t{}^7(E)} + \frac{128520e^{-a\Sigma_t(E)}}{a^7\Sigma_t{}^7(E)}$$

$$\left. + \frac{282240}{a^9\Sigma_t{}^9(E)}\left\{e^{-a\Sigma_t(E)}\left(a\Sigma_t(E) + 1\right) - 1\right\}\right] \qquad (6.b)$$

The above mentioned substitution could have been carried out as part of the computer program. However, in an effort to minimize the round-off error which might be introduced and which would grow with increasing order of the exponential integral functions, it was decided to change the matrix elements by hand.

APPENDIX C

AN ALTERNATE METHOD FOR SOLVING THE INTEGRAL EQUATION

A method of solving Eq. (54), which yields an exact solution in the case of constant cross-sections, will now be outlined. This exact solution is important in the method used to solve Eq. (54) and is given by Eq. (68). Equation (54) may be re-written in the following manner for the case of one nuclear type:

$$\overrightarrow{f(E)} = \tilde{A}(E) \int_{E}^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \overrightarrow{f(E')} \frac{dE'}{(1-\alpha)E'} + \overrightarrow{s(E)} \qquad (1.c)$$

where

$$\overrightarrow{f(E)} = \begin{bmatrix} f_o^{\,o}(E) \\ \vdots \\ f_o^{\,m}(E) \end{bmatrix}$$

$$\tilde{A}(E) = \begin{bmatrix} a_{oo}(E) & \cdots & a_{om}(E) \\ \vdots & & \\ a_{mo}(E) & \cdots & a_{mm}(E) \end{bmatrix}$$

$$\overrightarrow{s(E)} = \begin{bmatrix} s_o^{\,o}(E) \\ \vdots \\ s_o^{\,m}(E) \end{bmatrix}$$

From Eq. (1.c), the infinite mass approximation may be derived by evaluating the scattering collision density at the lower limit of the integral i.e.

$$\overrightarrow{f^{im}}(E) = \tilde{A}(E) \frac{\Sigma_s(E)}{\Sigma_t(E)} \overrightarrow{f^{im}}(E) + \overrightarrow{s(E)} \tag{2.c}$$

Solving for $f^{im}(E)$ from this equation, we get

$$\overrightarrow{f^{im}}(E) = \left[\tilde{I} - \tilde{A}(E) \frac{\Sigma_s(E)}{\Sigma_t(E)}\right]^{-1} \overrightarrow{s(E)} \tag{3.c}$$

where I is the unit matrix.

Equation (1.c) may be re-written in the following manner

$$\overrightarrow{f(E)} = \tilde{A}(E)\left[\int_E^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \overrightarrow{f(E')} \frac{dE'}{(1-\alpha)E'} - \frac{\Sigma_s(E)}{\Sigma_t(E)} \overrightarrow{f(E)}\right] + \tilde{A}(E) \frac{\Sigma_s(E)}{\Sigma_t(E)} \overrightarrow{f(E)}$$

$$+ \overrightarrow{s(E)} \tag{4.c}$$

The following assumption is now made:

$$\overrightarrow{f(E)} = \overrightarrow{f^{im}}(E) + \sum_{n=1}^{\infty} \vec{\phi}_n(E)\, \epsilon^n \tag{5.c}$$

$\vec{\phi}_n(E)$ are correction terms to $\overrightarrow{f^{im}}(E)$, and ϵ^n are parameters. Giving the bracket in Eq. (4.c) a weight ϵ, since it is assumed to be small compared to the rest of the right hand side of Eq. (4.c), Eq. (5.c) is substituted into Eq. (4.c), and terms of equal order

in ϵ are equated i.e.

$$\vec{f}^{im}(E) + \sum_{n=1}^{\infty} \vec{\phi}_n(E)\epsilon^n = \epsilon\tilde{A}(E)\left[\int_E^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \vec{f}^{im}(E) \frac{dE'}{(1-\alpha)E'} - \frac{\Sigma_s(E)}{\Sigma_t(E)} \vec{f}^{im}(E)\right] + \sum_{n=1}^{\infty} \epsilon^{n+1}\tilde{A}(E)\left[\int_E^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \times \vec{\phi}_n(E') \frac{dE'}{(1-\alpha)E'} - \frac{\Sigma_s(E)}{\Sigma_t(E)} \vec{\phi}_n(E)\right] + \sum_{n=1}^{\infty} \epsilon^n\tilde{A}(E) \frac{\Sigma_s(E)}{\Sigma_t(E)} \phi_n(E) + \tilde{A}(E) \frac{\Sigma_s(E)}{\Sigma_t(E)} \vec{f}^{im}(E) + \vec{s}(E)$$

Using Eq. (2.c) and solving for $\vec{\phi}_n(E)$, the following equation results:

$$\sum_{n=1}^{\infty} \epsilon^n \left[\tilde{I} - \tilde{A}(E) \frac{\Sigma_s(E)}{\Sigma_t(E)}\right] \vec{\phi}_n(E) = \epsilon\tilde{A}(E)\left[\int_E^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \vec{f}^{im}(E') \frac{dE}{(1-\alpha)E'} - \frac{\Sigma_s(E)}{\Sigma_t(E)} \vec{f}^{im}(E)\right] + \sum_{n=1}^{\infty} \epsilon^{n+1} \tilde{A}(E)\left[\int_E^{E/\alpha} \frac{\Sigma_s(E')}{\Sigma_t(E')} \vec{\phi}_n(E') \frac{dE}{(1-\alpha)E'} - \frac{\Sigma_s(E)}{\Sigma_t(E)} \vec{\phi}_n(E)\right] \quad (7.e)$$

Now by equating equal orders in ϵ, it is seen that

$$\vec{\phi}_1(E) = \left[\tilde{I}-\tilde{A}(E)\frac{\Sigma_s(E)}{\Sigma_t(E)}\right]^{-1}\tilde{A}(E)\left[\int_E^{E/\alpha}\frac{\Sigma_s(E')}{\Sigma_t(E')}\frac{\vec{f}^{im}(E')}{(1-\alpha)E'}\,dE' - \frac{\Sigma_s(E)}{\Sigma_t(E)}\vec{f}^{im}(E)\right]$$

$$\vdots$$

$$\vec{\phi}_n(E) = \left[\tilde{I}-\tilde{A}(E)\frac{\Sigma_s(E)}{\Sigma_t(E)}\right]^{-1}\tilde{A}(E)\left[\int_E^{E/\alpha}\frac{\Sigma_s(E')}{\Sigma_t(E')}\frac{\vec{\phi}_{n-1}(E')}{(1-\alpha)E'}\,dE' - \frac{\Sigma_s(E)}{\Sigma_t(E)}\vec{\phi}_{n-1}(E)\right] \tag{8.c}$$

The value of ϵ in Eq. (5.c) is now equated to unity, since ϵ is arbitrary, and the solution is given by

$$\vec{f}(E) = \vec{f}^{im}(E) + \sum_{n=1}^{\infty}\vec{\phi}_n(E) \tag{9.c}$$

Thus to solve the equation the following method should be used:

(i) Using Eq. (3.c), the value of $\vec{f}^{im}(E)$ is determined.

(ii) Using Eq. (8.c), $\vec{\phi}_1(E)$ ... $\vec{\phi}_n(E)$ are determined.

(iii) These values are then substituted into Eq. (9.c), and the solution is obtained.

The case where the cross-sections are assumed to be constant yields a result of particular interest. In this case the only energy dependence of $\vec{f}^{im}(E)$ is due to the external source. In this particular case this varies as 1/E. This makes it possible to evaluate the integrals of Eq. (8.c). It is found that $\vec{\phi}_1(E) = 0$, and thus all

the other $\vec{\phi}(E)$'s are zero, since they all depend on $\vec{\phi}_1(E)$. The solution to the case of constant cross-section is thus given exactly by the infinite mass approximation

$$\vec{f}(E) = \vec{f}^{im}(E) = \left[\tilde{I} - \tilde{A}\frac{\Sigma_s}{\Sigma_t}\right]^{-1} \frac{\vec{D}}{E}$$

Set

$$\tilde{B} = \left[\tilde{I} - \tilde{A}\frac{\Sigma_s}{\Sigma_t}\right]$$

Then

$$\vec{f}(E) = \frac{1}{E} \frac{\text{adj}[\tilde{B}]}{|B|} \vec{D} \qquad (10.c)$$

Equation (10.c) is identical to Eq. (68).

This solution seems to be physically reasonable, since the infinite mass approximation and the wide resonance approximation are analogous. In the limit of an energy independent cross-section the wide resonance cross-section is exact, since this case may be thought of as an infinitely wide resonance.

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