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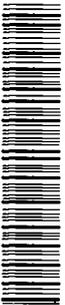
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THEORY OF EFFECTIVE CROSS SECTIONS

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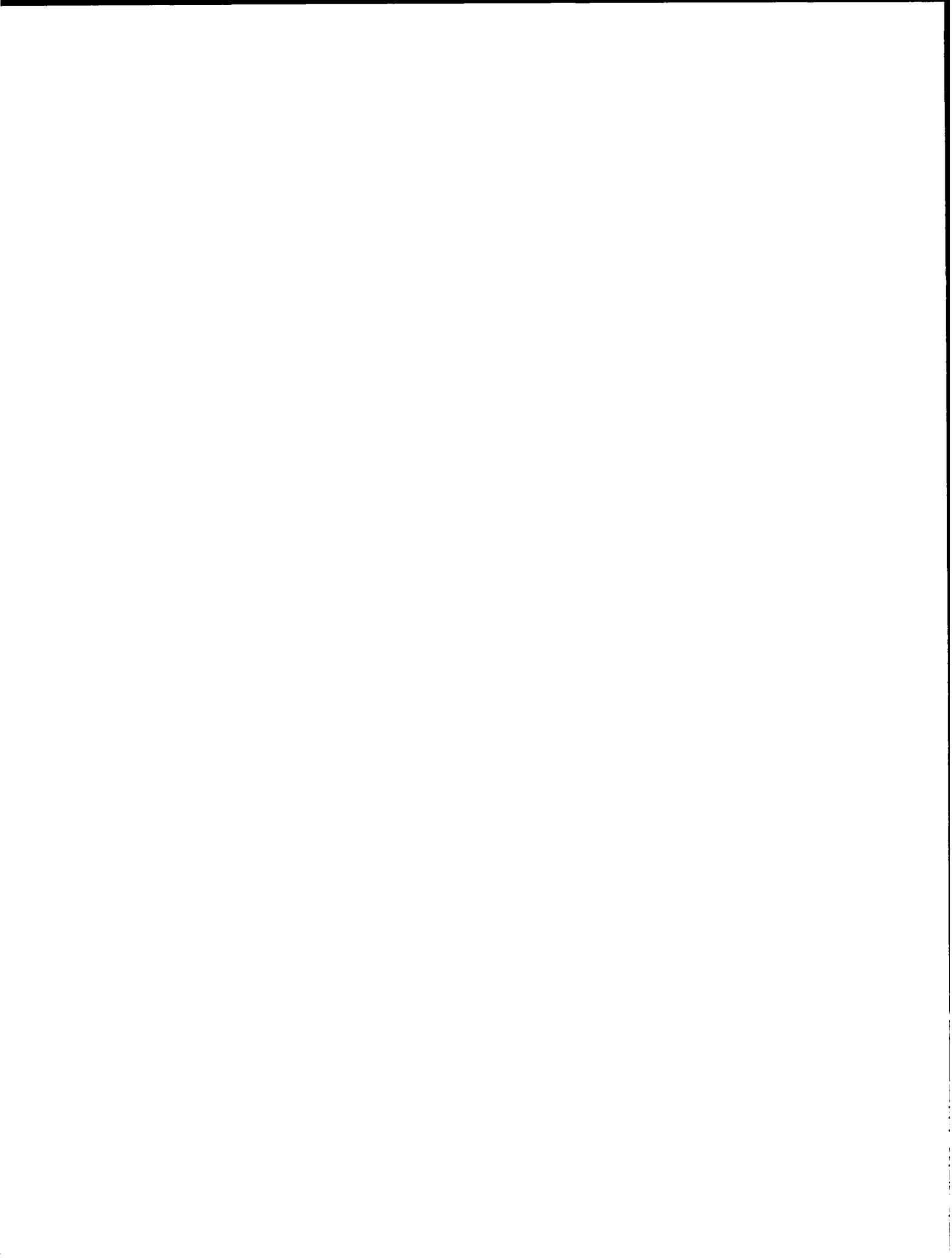
THEORY OF EFFECTIVE CROSS SECTIONS

by
George I. Bell

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ABSTRACT

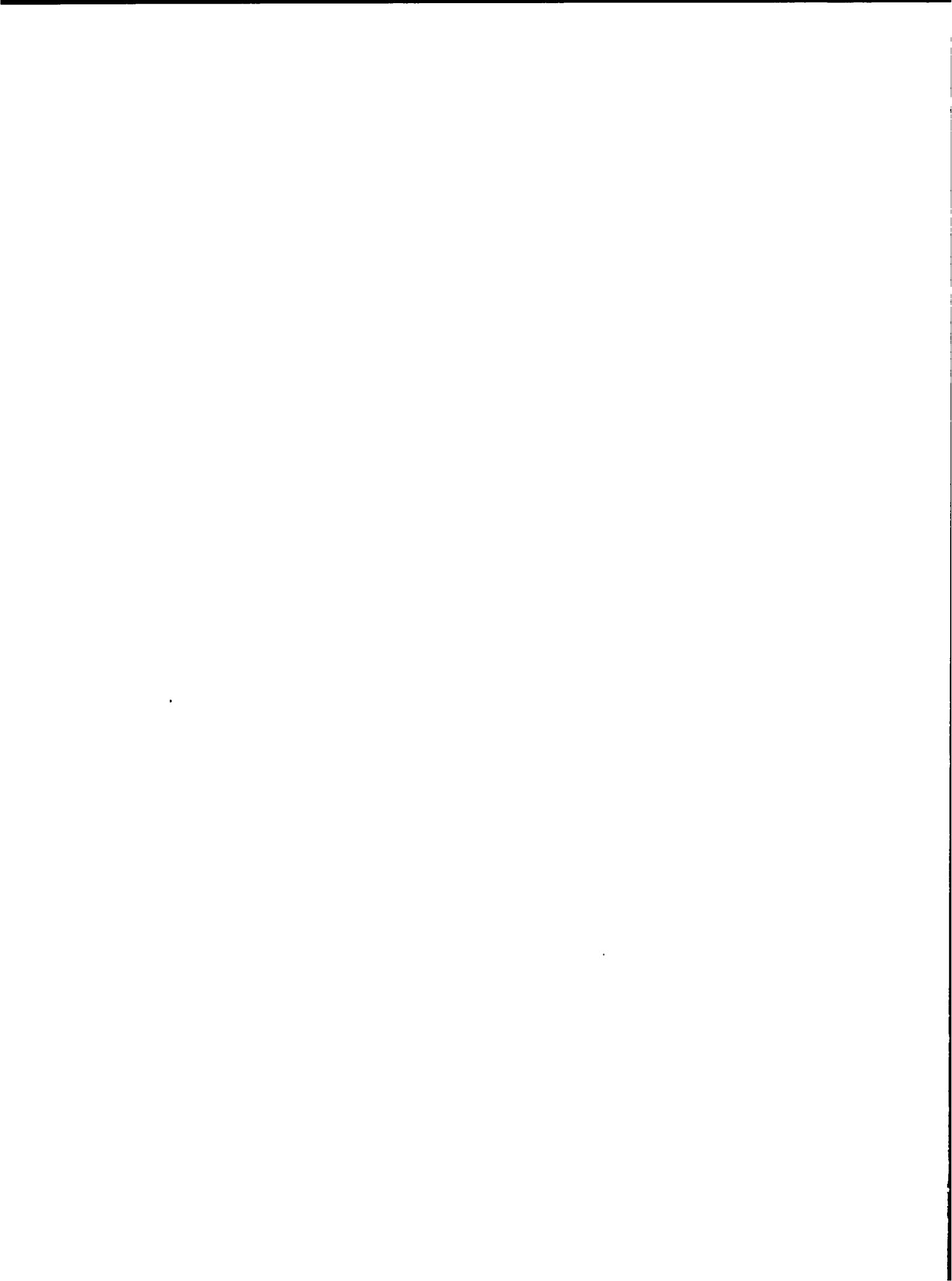
The theory of effective resonance cross sections for reactor calculations is reviewed in a general form. In section II, we discuss homogeneous mixtures and the NR and IM approximations. In section III, theory for capture in isolated lumps is discussed. IM, NR and canonical approximations are developed and it is noted how higher accuracy may be attainable by retention of the spatial heterogeneity in a multigroup calculation. In section IV theory is generalized to dense lattices and a simple transition between the homogeneous and isolated lump case. It is shown that quite complex lattices can be treated in canonical form. In section V we discuss further improvements for lumps with strong IM scattering.

Appendix A contains a discussion of the mathematical basis for improvements on the NR and IM theories and Appendix B notes various Breit-Wigner single level expressions and when they cannot be used.

An intent of this report is to provide a unified and general picture of effective resonance cross sections which will be used as the basis of a digital code for computing effective cross sections.

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I. Introduction

Neutron cross sections of most heavy elements exhibit prominent resonances in the energy region between roughly .1 ev and 10 kev. For reactors in which neutrons are present in the space-energy region of such resonances, the neutron flux* may be a rapidly varying function of both energy and position. The problem of taking these rapid variations of neutron flux into account has long been recognized as a central one in reactor physics, and its solution has usually been attempted by the introduction of effective cross sections, cross sections which are slowly varying functions of energy. An effective reaction cross section is generally defined by the requirement that when it is multiplied by a flux which is slowly varying in space-energy and the resulting product is integrated over an appropriate space-energy region, it must yield the correct reaction rate, which is given by the integral of the true rapidly varying cross section times rapidly varying flux.

The most important example of an effective cross section is the "effective resonance capture cross section" for the case of heterogeneous

*Flux is here taken to mean number of neutrons per unit volume times absolute value of neutron velocity.

natural uranium reactors. A theory for this difficult case was first developed by Wigner, et al., [1], [2]. Although the qualitative predictions of the theory were confirmed by experiment in the early 1940's, an accurate application of Wigner's theory was not possible at that time because of inadequate information on the U^{238} resonance parameters.

More recently, three developments have stimulated an advance in the theory of effective cross sections. First of all, resonance parameters have been measured fairly accurately for many of the low lying levels of U^{238} and other isotopes and are now available for use in calculations. Secondly, at the 1955 Geneva Conference, a Russian theory of effective resonance capture was reported [3] which appeared to be quite different from the Wigner theory. This apparent discrepancy prompted critical re-examination of both theories. Third, modern electronic computers have become available for performing Monte Carlo and other accurate calculations of a lengthy nature. These have afforded a number of checks on the various assumptions invoked in constructing simpler theories. As a result of these developments and considerable theoretical work, the theory of effective resonance cross sections is on quite firm ground in a number of practical cases, and difficulties and limitations are better understood. The status of the theory and comparison with experiment have been reviewed in a number of recent papers [4] - [10].

In this paper, we present a review and amplification of current theories in a general form applicable to a variety of multigroup calculations. We begin with the case of a homogeneous mixture of moderator and

absorber (section II), then discuss the case of isolated lumps of an absorber imbedded in a moderator (section III). The theory is then generalized to an array of lumps in a moderator (section IV) - a situation intermediate between the homogeneous and isolated lump case. A modification of the theory to account for broad resonances with much scattering is made (section V). In Appendix B some of the theoretical expressions are applied to single Breit-Wigner resonances, which are either unbroadened or simply Doppler broadened.

An intent of this report is to provide a unified and general picture of effective cross sections which will be used as the basis of a digital code for machine computation of effective cross sections. It is hoped that the theory is general enough to be applicable to such diverse situations as intermediate homogeneous reactors, heterogeneous reactors with either widely or closely spaced fuel lumps, resonance absorption in control elements, and critical assemblies in which fuel is inhomogeneously disposed.

Before proceeding to special cases we note a general principle which will be employed in constructing all subsequent expressions for effective resonance cross sections. Consider a resonance at energy E_0 and characterized by a practical width Γ_p over which "the resonance is important."

Let E be an energy within the range $E_0 - \frac{\Gamma_p}{2} < E < E_0 + \frac{\Gamma_p}{2}$, and let $S(E) dE$ be the source of neutrons being elastically scattered into the range of dE about E . We shall assume that this source of neutrons is

primarily due to collisions of neutrons which had energies before collision substantially greater than $E_0 + \Gamma_p/2$. This means that the source of neutrons at energies near E_0 will be very little perturbed by the resonance in question and that $S(E)$ will be a slowly varying function of E near the resonance. It is usually easy to make a good estimate of the source of neutrons $S(E)$ by neglecting the resonance. From this assumed source we then calculate the neutron flux in the space energy region of the resonance and from the calculated neutron flux we obtain the effective cross sections. The essential point is that in order to obtain a simple $S(E)$, the resonance in question should be narrow compared to the maximum energy loss in elastic scattering from the moderator. We then work from known source to flux to effective cross section.

II. Homogeneous Case

Theory for the homogeneous case has recently been reviewed by Chernick et al. [4, 5, 6, 10]. We shall employ essentially the NR and IM approximations.

Consider a homogeneous mixture of J isotopes and suppose that at energy E_0 , one isotope has a resonance which absorbs and scatters neutrons. The other isotopes are assumed to have constant scattering cross sections and no absorption near E_0 . Let the total macroscopic scattering cross section off resonance be $\sum_0 = \sum_{j=1}^J N_j (\sigma_j - \sigma_{res,j})$ where $\sigma_{res,j}$ is the contribution of the resonance to the total cross section, σ_j . Let us now

define the practical width (Γ_p) of the resonance, first introduced by Wigner [1], as that energy range about E_0 over which the total resonance cross section Σ_r exceeds Σ_0 . The practical width of a resonance is thus that energy interval over which the macroscopic cross section is predominantly due to the resonance. It depends on the ratio of moderator to absorber densities as well as on the microscopic cross sections.

For an isolated Breit-Wigner resonance and ignoring Doppler broadening and interference between potential and resonance elastic scattering, we would have

$$\Sigma_{\text{res}}(E) = \frac{\Sigma_{\text{max}}}{1 + \frac{4(E - E_0)^2}{\Gamma^2}} \quad \left\{ \begin{array}{l} \Sigma_{\text{res}}(E) = \Sigma_0 \\ E - E_0 = \frac{\Gamma_p}{2} \end{array} \right. \quad (1)$$

and hence

$$\Gamma_p = \Gamma \sqrt{\frac{\Sigma_{\text{max}} - \Sigma_0}{\Sigma_0}}$$

$$1 + \frac{4\Gamma_p^2}{\Gamma^2} = \frac{\Sigma_{\text{max}}}{\Sigma_0}$$

$$\Gamma_p^2 = \Gamma^2 \frac{\Sigma_{\text{max}} - \Sigma_0}{\Sigma_0}$$

For a low resonance, having $\Sigma_{\text{max}} \lesssim \Sigma_0$, instead of setting $\Gamma_p = 0$, it is more appropriate to replace it with the natural width, Γ , as a measure of the width of the energy region over which the resonance is important.

This suggests using a generalized practical width [5]:

$$\Gamma_p = \Gamma \sqrt{\frac{\Sigma_{\text{max}} + \Sigma_0}{\Sigma_0}} \quad (2)$$

For the homogeneous case, at energy E , the neutron flux, $\phi(E)$, will be given by the integral equation:

$$\sum_{j=1}^J N_j \sigma_j(E) \phi(E) = \sum_{j=1}^J \frac{1}{1 - \alpha_j} \int_E^{E/\alpha_j} N_j \sigma_{s,j}(E') \phi(E') \frac{dE'}{E'} \quad (3)$$

where $\sigma_{s,j}$ is the elastic scattering cross section of the j th isotope, and $\alpha_j = \left(\frac{A_j - 1}{A_j + 1}\right)^2$ is one minus the maximum fractional energy loss ($A_j =$ atomic weight). Equation (3) is exact for the energy range where neutron scattering is elastic and spherically symmetric in the neutron-nucleus center of mass system. This energy range ($.2 \text{ ev} \lesssim E \lesssim 10 \text{ kev}$) is precisely that of greatest interest for resonance reactions.

We now divide all isotopes into two classes depending on whether the maximum energy loss at E_0 , $(1 - \alpha_j) E_0$, is greater than or less than the practical width:

If $(1 - \alpha_j) E_0 \gg \Gamma_p$, clearly the resonance is narrow compared to energy losses in scattering from the j th material. For such narrow resonance (NR) scattering, the dominant contribution to the integral in equation (3) comes from $E' \gg E_0 + \Gamma_p/2$ where, for a single resonance, we know $\phi(E')$ is proportional to $1/E'$, say $\phi(E') = \bar{\phi}/E'$. Thus if the off resonance scattering cross section of isotope j is σ_{0j} , the j integral in equation (3) equals $\frac{N_j \sigma_{0j} \bar{\phi}}{E}$.

If, on the other hand, $(1 - \alpha_j) E_0 \ll \Gamma_p$, the resonance is wide compared to energy losses in elastic scattering from the j th material. For such an isotope, a first approximation is to neglect the energy loss

in elastic scattering. For such scatterings we treat the scatterer as if it had infinite mass (IM approximation) in which case the j th integral on the right hand side of equation (3) equals $N_j \sigma_{s,j}(E) \phi(E)$ and thus cancels the corresponding term on the left side. This is a particularly good approximation when applied to a material with a strong resonance since then $\sigma_{s,j}(E) \phi(E)$ tends to be constant over the resonance.

Let us now treat all terms in equation (3) which have $(1 - \alpha_j) E_0 \geq \Gamma_p$ by the NR approximation (right hand integral = $\sum_{o,j} \bar{\phi}/E$) and all terms which have $(1 - \alpha_j) E_0 < \Gamma_p$ by the IM approximation (right side cancels left). We obtain

$$\sum_{j=1}^J N_j (\sigma_{s,j}^{NR}(E) + \sigma_{a,j}(E)) \phi(E) = \sum_{j=1}^J N_j \sigma_{o,j}^{NR} \frac{\bar{\phi}}{E} \quad (4a)$$

where

$$\begin{aligned} \sigma_{s,j}^{NR}(E) &= \sigma_{s,j}(E); & \sigma_{o,j}^{NR} &= \sigma_{o,j} & \text{if } (1 - \alpha_j) E_0 &\geq \Gamma_p & (4b) \\ &= 0 & &= 0 & \text{if } (1 - \alpha_j) E_0 &< \Gamma_p \end{aligned}$$

If we now let:

$$\begin{aligned} \sum_o^{NR} &= \sum_{j=1}^J N_j \sigma_{o,j}^{NR} \\ \sum_t^{NR} &= \sum_{j=1}^J N_j (\sigma_{s,j}^{NR}(E) + \sigma_{a,j}(E)) \end{aligned} \quad (5a)$$

equation (4a) may be rewritten:

$$\phi(E) = \frac{\sum_o^{NR} \bar{\phi}}{\sum_t^{NR}(E) E} \quad (5b)$$

For any reaction cross section, $\sigma_r(E)$, which may be a part or all of the resonance absorption cross section, the reaction rate ^{per atom} is the product $\phi(E) \sigma_r(E)$. We now define the effective reaction cross section $\tilde{\sigma}_r$ corresponding to an energy interval $E_1 \leq E \leq E_2$ as the integral of the reaction rate divided by the integral of the flux, or with the flux from equation (5b):

$$\tilde{\sigma}_r = \frac{\int_{E_1}^{E_2} \frac{\sigma_r(E)}{\sum_t^{NR}(E)} \frac{dE}{E}}{\int_{E_1}^{E_2} \frac{1}{\sum_t^{NR}(E)} \frac{dE}{E}} = \frac{\int_{E_1}^{E_2} \frac{\sigma_r(E) dE}{\sum_t^{NR}(E) E}}{\int_{E_1}^{E_2} \frac{dE}{\sum_t^{NR}(E) E}} \quad (6)$$

This is the fundamental result for the homogeneous case. Note that if $\sigma_r(E)$ were a constant, we would obtain $\tilde{\sigma}_r = \sigma_r$.

It is easy to see that equation (6) is equivalent to the requirements (a) that

$$\frac{\tilde{\sigma}_r}{\sum_t^{NR}} = \int_{E_1}^{E_2} \frac{\sigma_r(E)}{\sum_t^{NR}(E)} \frac{dE}{E} / \ln \frac{E_2}{E_1}$$

and (b) that if $\sigma_r(E)$ is a constant, then $\tilde{\sigma}_r = \sigma_r$. Thus we are essentially replacing the rapidly varying $\sigma_r(E)/\sum_t^{NR}(E)$ by its slowly varying average over an interval large compared to the resonance practical width.

For very narrow resonances ($\Gamma_p \ll E_2 - E_1$) the denominator of equation (6) departs from Σ_0^{NR} only over a small interval and we have

$$\tilde{\sigma}_r \approx \tilde{\sigma}'_r = \frac{\Sigma_0^{NR}}{\ln E_2/E_1} \int_{E_1}^{E_2} \frac{\sigma_r(E) dE}{\Sigma_t^{NR}(E) E} \quad (7)$$

This is evidently a good approximation whenever the average departure of the flux from $\bar{\phi}$ is small compared to $\bar{\phi}$, i.e., whenever

$$\int \phi(E) dE \approx \bar{\phi} \ln E_2/E_1 \quad (8)$$

A number of comments are now in order.

(a) Wide Resonances: If the resonance is wide for all scatterings, then the above treatment cannot be used. This is because the source in equation (4a) was given by NR scattering. In fact, only if the scattering is predominantly of the NR type (so that neutrons will usually skip over the resonance) can the source in equation (4) be so simply obtained. Thus it is necessary to have $\Sigma_0^{NR} \approx \Sigma_0$. For the general case of broad resonances, equation (3) must be integrated numerically.

(b) NR and IM Accuracy: The accuracy of the separation of the scatterings into NR and IM types has been investigated by Spinney [10] and Chernick [5,6]. From the integral equation (3), they derived the next order corrections to the NR and IM approximations for the source integrals. The general basis of these corrections is given in Appendix A. In addition,

for the particular case of a mixture of U^{238} and H (equal atomic densities) results were compared with numerical solutions of the integral equation. Reaction rates were computed for the resolved resonances and using alternatively NR, IM, and exact recipes for the U^{238} elastic scattering, as well as improved NR and IM expressions. For this case, equation (7) gives results correct to within about ten percent for each resonance. For more dilute systems (higher H/U ratio) the accuracy should be better. Comparable investigations are in progress for other moderators.

(c) Effective Scattering and Transport Cross Sections: Equation (6) was taken to define an effective reaction or resonant scattering cross section if such scattering is of the NR type. For such a case we would obtain an effective total cross section:

$$(\tilde{\Sigma}_t^{NR})^{-1} = \int_{E_1}^{E_2} \frac{1}{\Sigma_t^{NR}(E)} \frac{dE}{E} \ln \frac{E_2}{E_1} \quad (9)$$

In the absence of IM scattering this is, coincidentally, an appropriate total cross section for neutron transport in the diffusion approximation. If there is also IM scattering, it is appropriate to add the off resonant part of Σ_t^{IM} to $\tilde{\Sigma}_t^{NR}$ in order to obtain a total cross section for neutron transport. Normally transport and leakage of neutrons in the resonance region is not very important.

(d) General Practical Width: For Doppler broadened or overlapping resonances, the definition of the practical width, equation (2), needs amplification. The important physical point is that over a practical

width the probabilities of various reactions per collision should not change much. Thus if a macroscopic cross section exhibits a rise, $R(E)$, above a more or less constant background, B , the practical width is either the interval over which $R(E) > B$ or the width of $R(E)$ at half maximum, whichever is greater. For more general situations the practical width is not a very useful concept.

(e) Many Resonances: When more than one resonance is present, equation (6) still usually represents a good approximation for any energy interval (E_1, E_2) over which the slowing down density does not change much. For widely separated resonances, the reason is that between resonances, the neutron flux will usually recover to its asymptotic form ($\sim dE/E$) for no absorption in that region. This may be seen by considering absorption at a resonance energy as a negative source at that energy and noting that the resulting departures of the flux from its asymptotic value [11, 21] are generally unimportant. For relatively closely spaced resonances, the NR scattering source will average over many resonances and be little influenced by any particular one. We are currently investigating some of these points more quantitatively.

(f) Multigroup Limitations: If a substantial fraction of the neutrons within an energy group is absorbed, then the competition between absorption and other processes will not be accurately given by our simple effective absorption cross section. This is because the spectrum within the group will be strongly dependent on the absorption and will not be accurately given by our simple assumptions. The difficulty is common to

any group which has strong absorption, irrespective of whether it occurs in resonances. The denominator of σ_r , equation (7), will not take this difficulty into account. In this case we may still frequently replace the rapidly varying σ_r/Σ_t by its slowly varying average over an energy interval ($\tilde{\sigma}_r/\tilde{\Sigma}_t$) and treat the slowly varying capture cross sections by any appropriate multigroup means, for example as indicated by Hurwitz in [14].

Various analytical and numerical results for single Breit-Wigner resonances are noted in Appendix B.

III. Isolated Heterogeneous Case

Let us first consider isolated lumps of absorbing material imbedded periodically in a moderator. By isolated we mean that the lumps are separated by many moderator mean free paths. Since the array is periodic we confine our attention to a cell consisting of a single lump and its surrounding moderator. Let $P_i(E)$ be the probability that a neutron of energy E which originated in region i will make its next collision in region i , and let $i = 0$ denote absorber lump and $i = 1$ denote moderator. Following Chernick [10] we will express effective cross sections in terms of $P_0(E)$ and $P_1(E)$.

Let us again suppose that we have a single resonance at energy E_0 . For energies well above E_0 , we will have the unperturbed flux $\bar{\phi} \frac{dE}{E}$ throughout the lattice. For energies near E_0 , the flux will depend on whether we are dealing with a narrow or broad resonance (NR or IM scattering

in lump) and to make the distinction we must define the practical width of a resonance in the heterogeneous case. Let Σ_{00} be the lump scattering cross section off resonance, $\Sigma_{ot}(E)$ be the lump total cross section and $\Sigma_{or}(E) = \Sigma_{ot}(E) - \Sigma_{00}$. Then the quantity $\frac{\Sigma_{or}(E)}{\Sigma_{ot}(E)} P_0(E)$ represents the probability that a neutron ^{originating} in the lump will make its next collision "with the resonance," and in the lump. We define the practical width, Γ_p , of a resonance to be that energy interval, about E_0 , over which $\frac{\Sigma_{or}(E)}{\Sigma_{ot}(E)} P_0(E) > \frac{1}{2}$. This represents a logical generalization of the practical width for the homogeneous case. For weak resonances or thin lumps, for which $\frac{\Sigma_{or}}{\Sigma_{ot}} P_0$ never exceeds 1/2, we may as before let the practical width equal the full width of the resonance at half maximum.

We will now write down integral equations for the neutron fluxes, classify scatterings into NR and IM types - according to whether $(1 - \alpha) E_0$ is greater or less than Γ_p , and approximately evaluate the integrals for each type of scattering.

Let $\phi_i(E)$ be the space average flux in region i. Let V_i be the volume of region i, N_{ij} be the density of the jth isotope in region i, and let $\sigma_{sj}(E)$ be the scattering cross section of isotope j. Then, by definition of $P_i(E)$, the following exact integral equations hold*:

*Note that these equations are exact for an arbitrary array of absorbing lumps provided that region 0 is interpreted to include all lumps and region 1 all moderator. We assume, of course, s wave scattering.

$$\begin{aligned} \Sigma_{ot}(E) \phi_o(E) &= P_o(E) \sum_{j=1}^J \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} N_{oj} \sigma_{sj}(E') \phi_o(E') \frac{dE'}{E'} \\ &+ (1-P_1(E)) \frac{V_1}{V_o} \sum_{j=1}^J \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} N_{1j} \sigma_{sj}(E') \phi_1(E') \frac{dE'}{E'} \end{aligned} \quad (10a)$$

$$\begin{aligned} \Sigma_{1t}(E) \phi_1(E) &= P_1(E) \sum_{j=1}^J \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} N_{1j} \sigma_{sj}(E') \phi_1(E') \frac{dE'}{E'} \\ &+ (1-P_o(E)) \frac{V_o}{V_1} \sum_{j=1}^J \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} N_{oj} \sigma_{sj}(E') \phi_o(E') \frac{dE'}{E'} \end{aligned} \quad (10b)$$

Equation (10a) says that the collisions per unit volume in the lump ($\Sigma_{ot} \phi_o$) are equal to the number of neutrons per unit volume arriving at energy E in the lump (first sum of integrals) times probability that a neutron ^{originating} in the lump makes its next collision there ($P_o(E)$) plus number of neutrons per unit lump volume arriving at energy E in the moderator (V_1/V_o times second sum of integrals) times probability that a neutron ^{originating} in the moderator makes its next collision in the lump ($1-P_1(E)$). Equation (10b) has a similar interpretation with moderator and lump roles interchanged.

We now simplify the integrals exactly as for the homogeneous case. Thus for NR scattering [$(1-\alpha_j) E_o > \Gamma_p$] we approximate $\phi(E')$ in the integrand by $\bar{\phi}/E$, to obtain:

$$\frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} N_j \sigma_{sj} \phi(E') \frac{dE'}{E'} = N_j \sigma_{sj} \frac{\bar{\phi}}{E} \quad : \text{NR} \quad (11)$$

Here we have assumed σ_{sj} to be constant; if isotope j has the resonance, then σ_{sj} is the potential scattering cross section. For IM scattering $[(1-\alpha_j) E_0 < \Gamma_p]$, we assume that there is scattering without energy loss to obtain:

$$\frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} N_j \sigma_{sj}(E') \phi(E') \frac{dE'}{E'} = N_j \sigma_{sj}(E) \phi(E) \quad \text{IM} \quad (12)$$

We require that the moderator scattering should be primarily NR. This insures that $\phi_1 \approx \bar{\phi}/E$ for all energies and leads us to assume that all integrals over ϕ_1 may be approximated by the NR expression (equation (11)). In the lump, some scattering may be NR and some IM. For the NR scattering we use Σ_{oo}^{NR} , the off resonance scattering cross section, and for IM scattering we use $\Sigma_{os}^{IM}(E)$, the full scattering cross section. With this notation, we substitute equations (11) and (12) in (10) to obtain:

$$\begin{aligned} \Sigma_1 = \sum_{\text{mod.}} N_j \sigma_{sj} &= \text{moderator macroscopic scattering } \times \text{ sec} \\ \Sigma_{ot} &= \text{total} \\ \Sigma_{ot}(E) \phi_0(E) &= P_0(E) \left[\Sigma_{oo}^{NR} \frac{\bar{\phi}}{E} + \Sigma_{os}^{IM}(E) \phi_0(E) \right] \\ &+ (1-P_1(E)) \frac{V_1}{V_0} \Sigma_1 \frac{\bar{\phi}}{E} \end{aligned} \quad (13a)$$

$$\Sigma_{1t}(E) \phi_1(E) = P_1(E) \Sigma_1 \frac{\bar{\phi}}{E} + (1-P_0(E)) \frac{V_0}{V_1} \left[\Sigma_{oo}^{NR} \frac{\bar{\phi}}{E} + \Sigma_{os}^{IM} \phi_0(E) \right] \quad (13b)$$

Solving (13a) for $\phi_0(E)$, we find

$$\phi_0(E) = \frac{P_0(E) \Sigma_{oo}^{NR} + (1-P_1(E)) \frac{V_1}{V_0} \Sigma_1}{(1-P_0(E)) \frac{\Sigma_{os}^{IM}(E)}{\Sigma_{ot}(E)}} \frac{\bar{\phi}}{\Sigma_{ot}(E) E} \quad (14a)$$

and substituting this result in (13b), we have

$$\phi_1(E) = \frac{P_1(E) \Sigma_1 \bar{\phi}}{\Sigma_{1t}(E) E} + (1-P_0(E)) \frac{V_0}{V_1} \left[\Sigma_{00}^{NR} + \frac{\Sigma_{0s}^{IM} (P_0 \Sigma_{00}^{NR} + (1-P_1) \frac{V_1}{V_0} \Sigma_1)}{(1 - P_0 \Sigma_{0s}^{IM} / \Sigma_{ot}) \Sigma_{ot}} \right] \frac{\bar{\phi}}{\Sigma_{1t}(E)} \quad (14b)$$

Ordinarily, for isolated lumps, the second term in the expression for $\phi_1(E)$ is small compared to the first, because $(1-P_0) V_0/V_1$ is small. Also $P_1 \approx 1.0$ so that for a moderator without absorption

$$\phi_1(E) \approx \frac{\bar{\phi}}{E} \quad (15)$$

The number of reactions per atom per sec in the lump corresponding to a reaction cross section, σ_{ro} , is

$$\int_E^{E_2} \sigma_{ro}(E) \phi_0(E) dE$$

while the number of scatterings in the moderator is

$$\int_E^{E_2} \sigma_1 \phi_1(E) dE.$$

If we wish to homogenize the cell and use the real moderator scattering cross section and effective absorber cross sections, $\tilde{\sigma}_{ro}$, we must set

$$\tilde{\sigma}_{ro} = \frac{\int \sigma_{ro}(E) \phi_0(E) dE}{\int \phi_1(E) dE} \quad (16)$$

in order to preserve the correct competition between lump reactions and moderator scatterings. If we now approximate $\phi_1(E)$ by equation (15), use equation (14a) for $\phi_0(E)$ and denote the resulting effective cross section by $\tilde{\sigma}'_{ro}$,

$$\tilde{\sigma}'_{ro} = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{P_0(E) \Sigma_{oo}^{NR} + (1 - P_1(E)) \frac{v_1}{v_0} \Sigma_1 \sigma_{ro}(E)}{1 - P_0(E) \Sigma_{os}^{IM} / \Sigma_{ot}(E)} \frac{\sigma_{ro}(E)}{\Sigma_{ot}(E)} \frac{dE}{E} \quad (17)$$

This is the basic result for the isolated heterogeneous case. It will evidently hold for an array of resonances as well as a single resonance.

If we use the full expression for $\phi_1(E)$ (equation 14b) in equation (16) we find (assuming no absorption in moderator):

$$\tilde{\sigma}'_{ro} = \frac{\tilde{\sigma}'_{ro}}{1 - \frac{\tilde{\Sigma}'_{ot} - \tilde{\Sigma}'_{os}^{IM} - \Sigma_{oo}^{NR}}{\Sigma_1 v_1 / v_0}} \quad (18)$$

When simple approximations for $P_1(E)$ are introduced it will be seen that equations (17) and (18) are exactly analagous to equations (7) and (6) for the homogeneous case. We shall also show (section IV) how to arrange a simple transition between the isolated heterogeneous and homogeneous cases, thus treating a large class of homogeneous and heterogeneous problems on a unified basis.

Before considering expressions for $P_1(E)$, let us note how the effective cross sections should be treated if one does not wish to homogenize the cell but wishes to retain the spatial heterogeneity.

Indeed, in many practical cases one may wish to retain the heterogeneity in a calculation. For example, in a cell calculation one can thus compute the fast effect, resonance absorption, and thermal absorption in a single multigroup calculation. In such a treatment, resonance disadvantage factors appear as a result of the calculation rather than as somewhat ambiguous assumptions. The geometry will then be treated realistically and the cross sections simplified to be constant in each energy group. We seek effective cross sections for the lump: $\tilde{\Sigma}_{ot}^{\alpha}$, $\tilde{\Sigma}_{os}^{\alpha}$, $\tilde{\Sigma}_{oa}^{\alpha}$. For this case, equations (13) will still give the space averaged fluxes, with all cross sections replaced by effective cross sections independent of energy, and with the distinction between NR and IM now based on the group width - not resonance practical width. Thus, for example $\sum_{oo}^{NR} \frac{\bar{\phi}}{E}$ will be replaced by the source of neutrons scattered down from higher groups. This is usually a small contribution which may be ignored, so that we have $\tilde{\Sigma}_{ot}^{\alpha} \approx \tilde{\Sigma}_{oa}^{\alpha} + \tilde{\Sigma}_{os}^{\alpha}$.

Computing the reaction rate from (13a) with effective cross sections and equating it to the reaction rate in (17) we have:

$$\frac{(1 - \tilde{P}_1) \frac{v_1}{v_o} \sum_1}{1 - \tilde{P}_o \frac{\tilde{\Sigma}_{os}^{IM}}{\tilde{\Sigma}_{ot}^{\alpha}}} \frac{\sum_j}{\tilde{\Sigma}_{ot}^{\alpha}} = \frac{\int \frac{P_o(E) \sum_{oo}^{NR} + (1 - P_1(E)) \frac{v_1}{v_o} \sum_1}{\sum_{os}^{IM}(E)} \frac{\sum_j(E)}{\sum_{ot}(E)} \frac{dE}{E}}{1 - P_o \frac{\sum_{os}^{IM}(E)}{\sum_{ot}(E)}}{\int \frac{dE}{E}} \quad (19)$$

Note that \tilde{P}_1 and \tilde{P}_0 are determined by geometry, $\tilde{\Sigma}_1$, $\tilde{\Sigma}_{ot}$, and $\tilde{\Sigma}_{os}^{IM}$. Thus if we use equation (19) with $\tilde{\Sigma}_j(E)$ equal in turn to each reaction cross section and finally to $\tilde{\Sigma}_{ot}(E)$ we may use the results to obtain the corresponding effective cross sections. Later we will see that introduction of simple forms for $P_1(E)$ will make equation (19) very simple to use. Note that if the absorber contains considerable good moderator one can retain $\tilde{\Sigma}_{oo}^{NR}$ on the left side of (19). More simply one can use just equation (19) and set $\tilde{\Sigma}_{os}^{IM} = \tilde{\Sigma}_{ot} - \tilde{\Sigma}_{oa} - \tilde{\Sigma}_{oo}^{NR}$ with $\tilde{\Sigma}_{oo}^{NR}$ being a transfer cross section computed without resonances.

We must now consider appropriate expressions for $P_1(E)$ for isolated lumps. It has been found that it is generally a good approximation to compute $P_1(E)$ as if the source of neutrons at energy E were uniform in space and isotropic in angle in region i [4, 5, 6]. It is clear that this is a consistent assumption in the moderator, for we have assumed that the source of neutrons arriving at energy E in the moderator is unperturbed by the absorbing resonance, i.e., we have assumed NR moderator scattering. (However if the lump is strongly absorbing over a large range of energy, the NR scattering source in the moderator and moderator flux will be depleted near the lump and this must be taken into account. See discussion at the end of this section.) Likewise, if NR scattering is the primary source of neutrons in the lump, that source is uniform and isotropic.

However, if streaming from the moderator and IM scattering are the primary neutron sources in the lump, then for a sufficiently thick

lump and an energy near the resonance maximum the neutrons will be concentrated near the lump surface. In this situation, it would appear that $P_0(E)$ should not be computed for a uniform source. However, it has been shown [5] that when one considers the integration over an entire resonance, the lump absorptions are surprisingly uniform. The reason is that most absorptions will occur at energies of the order of the practical width of the resonance away from the maximum. For these energies the lump is not very thick and the neutron distribution is quite uniform. Thus for integration over an entire resonance $P_0(E)$ may still be reasonably approximated by its value for a uniform source. An additional practical justification for this approximation is that frequently $\sum_{os}^{IM} \ll \sum_{ot}$ so that a good approximation for $P_0(E)$ (in equation (17)) is unimportant. In section V we will consider other and better approximations to $P_0(E)$ for the case of large IM scattering contributions ($\sum_{os}^{IM} \approx \sum_{ot}$).

For the remainder of this section we shall assume that $P_0(E)$ and $P_1(E)$ are to be computed for uniform and isotropic sources. $P_1(E)$ then satisfies the general and exact reciprocity relation:

$$(1 - P_0(E)) \sum_{ot}(E) V_0 = (1 - P_1(E)) \sum_1(E) V_1 \quad (20)$$

as may be understood by the following argument. Suppose that everywhere in the lattice, there exists a flux $\phi(E)$ which is constant in space and isotropic. Thus there is zero net neutron current everywhere in the lattice. The total number of neutron collisions in region i is

$\phi(E) \Sigma_1(E) V_1$, and each collision removes a neutron from energy E . Such a distribution would be maintained by a source equal to $\phi(E) \Sigma_0(E)$ per unit volume in the lumps and $\phi(E) \Sigma_1(E)$ per unit volume in the moderator. Then the total flow of neutrons from lumps to moderator is

$$(1 - P_0(E)) \Sigma_0(E) V_0 \phi(E)$$

and the flow from moderator to lumps is $(1 - P_1(E)) \Sigma_1(E) V_1 \phi(E)$. The condition of zero net flow is just our reciprocity relation. Equation (20) is thus valid for any lump configuration - provided that P_0 and P_1 are to be computed for uniform and isotropic sources.

The reciprocity relation may be used to eliminate $P_1(E)$ from equation (17), obtaining:

$$\tilde{\sigma}'_{ro} = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{1 - P_0(E) \left(1 - \frac{\Sigma_{oo}^{NR}}{\Sigma_{ot}(E)}\right)}{1 - P_0(E) \frac{\Sigma_{os}^{IM}(E)}{\Sigma_{ot}(E)}} \sigma_{ro}(E) \frac{dE}{E} \quad (21)$$

$P_0(E)$ has been discussed and tabulated by Placzek et al. [12] for isolated slabs, spheres, and cylinders. For a slab of thickness t mean free paths,

$$P_0 = 1 - \frac{1}{t} \left(\frac{1}{2} - E_3(t) \right) \quad (22)$$

For a sphere of radius R mean free paths

$$\begin{aligned}
 \text{"Collision Prob."} \equiv P_0 &= 1 - \frac{3}{8R^3} \left[2R^2 - 1 + (1 + 2R) e^{-2R} \right] \\
 &= \frac{3}{8}D - \frac{1}{10}D^2 + \frac{1}{48}D^3 - \frac{1}{280}D^4 + \dots
 \end{aligned}
 \tag{23}$$

For cylinders P_0 is expressed in terms of Bessel functions and tabulated. [Note that our $P_0 = P_c$ of reference [12]]. Evidently these expressions can be inserted in equation (21) and effective cross sections can be thus computed.

A simple and useful approximation to P_0 for isolated lumps was originally suggested by Wigner [1], namely

$$P_0(E) \approx \frac{\sum_{ot}(E)}{s + \sum_{ot}(E)} \quad s = \frac{\text{Lump Surface}}{4 \text{ Lump Volume}}
 \tag{24}$$

Here s^{-1} is the mean chord length of the lump [12]. This approximation, variously termed the Wigner or canonical approximation has recently been much used by Chernick et al. [5, 6, 4], not only because of its simplicity but also because its introduction causes the equations for the isolated heterogeneous case to strongly resemble those for the homogeneous case as we show below. Furthermore, the canonical expression for $P_0(E)$ will be shown to be readily generalizable to lumps which are not isolated (Section IV) and for which more exact expressions for P_0 can be extremely complex.

If we introduce the canonical approximation to $P_0(E)$ in equation (21) we obtain:

$$\tilde{\sigma}'_{ro} = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{s + \sum_{oo}^{NR}}{s + \sum_{ot}^{NR}(E)} \sigma_{ro}(E) \frac{dE}{E} \quad (25)$$

where $\sum_{ot}^{NR} = \sum_{ot}(E) - \sum_{os}^{IM}(E)$. This is identical to equation (7) for the homogeneous case provided that s is interpreted as an added NR scattering cross section representing leakage from the lump. It has been shown [5] that this interpretation of s is more general than would be inferred from the above. In particular, if one merely makes the NR approximation for moderator scattering and then inserts the canonical forms for $P_1(E)$ in the integral equation (10a) one obtains an integral equation identical to equation (3) for the homogeneous case, with s appearing as an NR scattering cross section. From there on, any treatment one may wish to apply to the fuel scattering (NR, IM or improved versions) can be carried out identically for both homogeneous and heterogeneous cases. Also, from our discussion at the beginning of this section, we see that in computing the practical width of a resonance s may be used as a bona fide scattering cross section. We thus see that the canonical approximation leads to simple expressions for effective cross sections for isolated fuel lumps which are analagous to those for the homogeneous case.

Note that the canonical approximation does not make the denominator of equation (18) into a form similar to that for the homogeneous case, equation (6). This is clearly correct, for in the homogeneous case if σ_r is independent of energy $\tilde{\sigma}_r = \sigma_r$. However, in the isolated lump case $\tilde{\sigma}_r \neq \sigma_r$ even for constant σ_r .

We note also the appropriate canonical expression if one wishes to retain heterogeneity in the final calculation. Equation (19) becomes

$$\frac{s \tilde{\Sigma}_j}{s + \tilde{\Sigma}_{ot} - \tilde{\Sigma}_{os}} = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{s + \Sigma_{oo}^{NR}}{s + \Sigma_{ot}^{NR}(E)} \Sigma_j(E) \frac{dE}{E} \quad (26)$$

where all scattering on the left has been assumed of type IM. $\tilde{\Sigma}_j$ denotes a reaction or total cross section in the lump. Evidently if all scattering on the right is IM and all cross sections are constant, $\tilde{\Sigma}_j = \Sigma_j$. Equation (26) is probably more accurate than equation (25) since similar approximations were made to obtain both sides of equation (26) and errors in the approximations should cancel to some extent.

It remains to discuss the accuracy of the canonical approximation for $P_o(E)$. For large values of $\Sigma_{ot}(E)/s$, the canonical $P_o \rightarrow 1 - s/\Sigma_{ot}$ which is the correct limiting value [12]. For intermediate values of Σ_{ot}/s , the accuracy of the canonical approximation may be found by comparison with the exact values of P_o in Placzek's work [12]. Such a comparison is given in table I, where it is seen that the Wigner approximation systematically overestimates P_o (except for very thin slabs). An obvious possibility for improving the approximation is to use increased values of s in the Wigner expression. Numerical calculations for U^{235} and U^{238} in some heterogeneous lattices with exact P_o suggested increases of s by about 15% for slabs and 30% for spheres and cylinders. Values of P_o with increased s are also indicated in table I, where it is seen that they are in substantially better agreement with the exact values over a large range of s .

Table I

Collision Probabilities, P_0 , for Uniform Source

$\frac{s}{\Sigma_0} = \frac{\text{Surface}}{4 \text{ Volume}} = \frac{1}{2t}$ for slab with t = thickness in mean free paths

$= \frac{3}{4R}$ for sphere with R = radius in mean free paths

$= \frac{1}{2R}$ for cylinder with R = radius in mean free paths

$\frac{s}{V} = \frac{4\pi R^2}{\frac{4}{3}\pi R^3} = \frac{3}{R} = \frac{3}{2} \cdot \frac{1}{2R} = \frac{3}{2} \cdot \frac{s}{\Sigma_0}$

for sphere	$\frac{s/\Sigma_0}{D}$	Wigner Approximation $P_0(s) = \frac{1}{1 + s/\Sigma_0}$	Exact [12] *		Wigner Modified		$P_0(s) = \frac{1}{1 + 1.15 s/\Sigma_0}$	$P_0(s) = \frac{1}{1 + 1.3 s/\Sigma_0}$	$\left(\frac{1}{1 + 1.7 \frac{s}{\Sigma_0}} \right)$
			Slab	Sphere	Cylinder	$P_0(s) = \frac{1}{1 + 1.15 s/\Sigma_0}$			
.10	15	.909	.900	.901	.901	.897	.885	.855	
.20		.833	.806	.807	.807	.813	.794	.746	
.50	3.0	.667	.610	.589	.593	.635	.606	.540	
1.0	1.5	.500	.443	.393	.404	.465	.435	.370	
2.0	.75	.333	.299	.233	.247	.303	.277	.227	
5.0	.30	.169	.163	.104	.115	.148	.133	.105	
10.0	.15	.091	.099	.054	.061	.080	.071	.0555	
100.0	.015					.00562		.00585	

* Let $D = \text{optical diam.} = 2r\Sigma_0 = 2R = \frac{3}{2} \frac{1}{(s/\Sigma_0)}$

Then for $D \ll 1$ $\left\{ \begin{aligned} (1 - P_0) &= \left[1 - \frac{3}{8}D + \frac{1}{10}D^2 - \frac{1}{48}D^3 + \frac{1}{280}D^4 - \dots \right] = f_0 = \text{self-shielding factor} \\ P_0 &= \frac{3}{8}D - \frac{1}{10}D^2 + \frac{1}{48}D^3 - \frac{1}{280}D^4 + \frac{1}{1920}D^5 \pm \dots \end{aligned} \right.$

For $D \ll 1$ $\left\{ P_0 \sim \frac{3}{8}D \sim \frac{3}{8} \frac{3/2}{(s/\Sigma_0)} \sim \frac{9}{16} \frac{s}{\Sigma_0} \right.$ -29-

For an important resonance in a typical lattice of not very thick lumps ($s > \Sigma_{00}$), it can be shown that the dominant contribution to the effective cross section comes from the region $s \approx \Sigma_0$ which is shown in table I. If we consider a resonance for which $s \gg \Sigma_0$ throughout (thin lump), then there is little flux depression anywhere and the effective cross sections are nearly equal to average cross sections and insensitive to exact values of s . For a very thick lump, $s \ll \Sigma_{00}$ throughout, it is found that the simple Wigner expression (24) is preferable to any modified form. It is thus suggested that an expression of the form

$$s' = \frac{s(\Sigma_{00} + \alpha s)}{\Sigma_{00} + s} \quad \begin{array}{l} \alpha = 1.15 \text{ slab} \\ \alpha = 1.30 \text{ sphere, cylinder} \end{array} \quad (27)$$

is an even better approximation. It is believed that when such a value of s' is used to estimate $P_0(s)$ with equation (25), the resulting effective cross sections will deviate from those using exact values of P_0 by less than 5% for nearly all practical cases.

Alternative simple improvements on the canonical approximation to P_0 have been considered by Rothenstein [13]. His forms are slightly more complicated than our simple modification of s and appear to give results of roughly comparable accuracy.

The accuracy of the preceding theory has been checked by a number of authors. Adler, Hinman, and Nordheim [7] have applied equation

(21) to the computation of effective resonance integrals* for uranium, uranium oxide, and thorium rods. They used values of $P_0(E)$ which are exact for uniform sources in slabs, spheres, and cylinders [12], and obtained results in good agreement with experiment. Chernick et al. [6, 5] have applied equation (25) to lattices of uranium and water with the additional assumptions that all uranium scattering is IM and the resonances are not Doppler broadened. The results have been compared with Monte Carlo calculations on lattices for which the lumps are not completely isolated. The agreement is fairly good for those resonances and geometries for which the above additional approximations are good. At the end of section IV we will make a comparison with the same Monte Carlo results with allowance for NR scattering, lump interaction, and Doppler broadening.

For some lattices the neutron flux in the moderator may vary considerably with position in a cell. This might be the case if the fuel lumps were so widely separated that the flux between lumps was appreciably lower than the average or if the lumps were strongly absorbing and thus depleted the flux nearby. Either effect could be taken into account by retention of the heterogeneity in the calculation. Alternatively one could attempt to relate, by other calculations, the flux near the lump surface (which is essentially the assumed average flux $\bar{\phi}$ of our development) to the actual average flux in the moderator. Weinberg and

*Actually, their treatment of IM scattering was not identical with but closely equivalent to that in equation (17). See section V for further discussion of the comparison.

Wigner [21] have given a rather complete discussion of how this can be done with diffusion theory and the problems which arise. In many cases the above effect is unimportant. Where it is important, we advocate retention of heterogeneity.

Note that none of our effective cross sections can give the detailed spatial distribution of absorptions in a lump. For this a Monte Carlo calculation or detailed multigroup mock-up of the true resonance cross sections would seem necessary.

IV. Extension to Dense Lattices and Transition Between Homogeneous and Isolated Heterogeneous Case

In the preceding section we assume that $1 - P_0$ represented the neutron escape probability from a single fuel lump. We consider here the form of P_0 when the fuel lumps are so spaced that a neutron leaving a lump has a significant probability of colliding with some other lump. In such a case the flux depression near a resonance will be even greater than for isolated fuel lumps and the effective cross sections will be correspondingly smaller.

For simple slab lattices it is possible to compute P_0 in detail [13, 15] inasmuch as a neutron's angular coordinate will not change during flight. For cylindrical fuel lumps, the problem has been analysed by Dancoff and Ginsburg [2, 16] but the corrections are sometimes tedious and difficult to generalize. In the following, we shall show how a simple and logical generalization of the canonical approximation can be used for

dense lattices and to give a simple transition between isolated heterogeneous and homogeneous systems [17]. The approximation is, in addition, sufficiently accurate for many practical purposes.

Let:

$(1-P_0)_0$ = Escape probability for neutron born in an isolated fuel lump.

$(1-P_0)$ = Probability that neutron born in identical fuel lump of a lattice makes next collision in moderator.

G_1^i = Probability that neutron originating in fuel and incident on moderator from fuel, after i previous traversals of moderator, will collide in moderator before re-entering fuel.

G_0^i = Probability that neutron originating in fuel and incident on fuel lump, after i previous traversals of fuel lumps, will collide in lump.

With this notation:

(Prob. neut born in fuel dies in mod) *(Prob. neut born in fuel escapes its own lump)*

$$(1-P_0) = (1-P_0)_0 \left[G_1^0 + (1-G_1^0)(1-G_0^0) G_1^1 + (1-G_1^0)(1-G_0^0)(1-G_1^1)(1-G_0^1) G_1^2 + \dots \right] \quad (28)$$

(Prob. dies in mod 1st pass) *(Prob. survive 1st pass)* *(Prob. die in mod on 2nd pass)* *Prob survive 2nd pass* *Prob. die in mod on 2nd pass*

Let us next assume that G_0^i and G_1^i are independent of i . This

would appear to be reasonable if the G 's are small so that the changes of incident angular distribution with i are slight. Also for $(1-G^0)$ small, only the first two terms are important and other values of G^i may be set equal to G^0 . With this assumption:

not assumed in passing to Eq. (29). Latter retains all terms: $1 + X + X^2 + X^3 + \dots = \frac{1}{1-X}$

$$(1-P_o)_o = (1-P_o)_o \frac{G_1}{1 - (1-G_1)(1-G_o)} \quad (29)$$

Following the arguments of section III, we now assume that $(1-P_o)_o$ is the escape probability for a uniform and isotropic source in the lump. In order to estimate G_o and G_1 we assume that the angular distribution of neutrons crossing the fuel moderator surface is proportional to $|\hat{n} \cdot \Omega|$ per unit surface area, where \hat{n} is a unit normal and Ω a unit vector in the direction of neutron motion. For thick fuel lumps, this is a good approximation for G_1^o which is the only important G . For thin fuel and moderator it is presumably a good approximation for G^i on the average. For this assumed angular distribution:

$$G_i = \frac{4\sum_i V_i}{S} (1-P_i)_o = \frac{\sum_i}{s_i} (1-P_i)_o \quad \left. \begin{array}{l} \text{Proof: Case, de Hoffman} \\ \text{Placzek Eq 29} \\ \text{p 20.} \end{array} \right\} (30)$$

where S is the area of the fuel moderator interface and $s_i = S/4V_i$. This expression is justified by noting that for a region i with unit isotropic flux ϕ both inside and outside, $\frac{G_i S \phi}{4}$ represents a flow of neutrons into i which is just balanced by the flow of $\phi \sum_i V_i (1-P_i)_o$ out of i . A constant flux gives the required source distribution (uniform in i), for $(P_i)_o$ and the required angular distribution $(\hat{n} \cdot \Omega)$ for G_i .

If we now make the Wigner approximation for $(1-P_o)_o$,

$$(1-P_o)_o = \frac{s_o}{\sum_o + s_o}$$

equation (30) gives us

$$G_0 = \frac{\Sigma_0}{s_0} \frac{s_0}{\Sigma_0 + s_0} = \frac{\Sigma_0}{\Sigma_0 + s_0}$$

$$(1-G_0) = \frac{s_0}{\Sigma_0 + s_0} \rightarrow G_0 = \frac{\Sigma_0}{\Sigma_0 + s_0} \quad (31)$$

Substituting in equation (29) we have

$$(1-P_0) = \frac{s_0 G_1}{\Sigma_0 + s_0 G_1} \quad (32)$$

This approximation has been independently suggested by Rothenstein [13], who then used exact values of G_1 . Note that in (32), $s_0 G_1$ takes the same place as s_0 in the expression for $(1-P_0)_0$. The canonical approximation to G_1 is:

$$G_1 = \frac{\Sigma_1}{\Sigma_1 + s_1} \quad (33)$$

We obtain:

$$(1-P_0) = \frac{s_0 \Sigma_1}{\Sigma_0 \Sigma_1 + s_1 \Sigma_0 + s_0 \Sigma_1} \quad (34a)$$

Similarly

$$(1-P_1) = \frac{s_1 \Sigma_0}{\Sigma_0 \Sigma_1 + s_1 \Sigma_0 + s_0 \Sigma_1} \quad (34b)$$

If we introduce the notation,

$$\tau_0 = \frac{s_0 \Sigma_1}{\Sigma_1 + s_1} \quad \tau_1 = \frac{s_1 \Sigma_0}{\Sigma_0 + s_0} \quad (35)$$

we may write

$$1 - P_0 = \frac{\tau_0}{\Sigma_0 + \tau_0} \quad 1 - P_1 = \frac{\tau_1}{\Sigma_1 + \tau_1} \quad (36)$$

Equation (36) for P_i is our basic result for general lattices. It can be seen, by comparing equations (24) and (36), that for dense lattices, τ_0 plays exactly the same role as s ($\equiv s_0$) of the isolated lump case. This applicability of a canonical approximation to general lattices is very convenient.

The above expressions for P_i have a number of desirable properties:

(a) P_0 and P_1 are consistent with the reciprocity relation, equation (20). This is easily seen by substitution of (34) in (20).

(b) We approach the correct isolated heterogeneous limit of section III. The quantity Σ_1/s_1 is the average chord length in the moderator measured in mean free paths, so that the fuel lumps are isolated for $\Sigma_1/s_1 \gg 1$. In this limit $\tau_0 \approx s_0$ and $1 - P_0$ reduces to the canonical expression (equation (24)) for isolated lumps. Note that in this limit the fuel lumps may be thick or thin.

(c) We approach the correct homogeneous limit for thin fuel and moderator regions. This will obtain if $\Sigma_1/s_1 \ll 1$ and $\Sigma_0/s_0 \ll 1$.

Since $s_o/s_1 = V_1/V_o$, we have in this limit,

$$\tau_o \approx \sum_1 \frac{V_1}{V_o} \quad \tau_1 \approx \sum_o \frac{V_o}{V_1}$$

so that, for example

$$P_o \rightarrow \frac{\sum_o}{\sum_o + \sum_1 \frac{V_1}{V_o}} \quad (37)$$

as one would expect for a homogeneous limit. Simple substitution of (37) in the heterogeneous equation (21) leads to the homogeneous equation (7). Moreover, the heterogeneous flux depression factors (denominator in equation (18)) become identical to the homogeneous flux depression factor (denominator of equation (6)).

(d) The equations for all effective cross sections in the dense lattice are merely those for the canonical isolated heterogeneous lattice, with τ_o replacing s_1 . This follows from the form (36) of $1-P_o$ plus (a). Thus instead of equation (25) we have

$$\tilde{\sigma}'_{ro} = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{\tau_o + \sum_{oo}^{NR}}{\tau_o + \sum_{ot}^{NR}(E)} \sigma_{ro}(E) \frac{dE}{E}, \quad \text{with } \tau_o = \frac{s_o \sum_1}{\sum_1 + s_1} \quad (38)$$

By comparison with equations (25) and (7), we see that τ_o may be interpreted as a generalized NR pseudo-scattering cross section representing leakage from the lump. This interpretation may be maintained consistently throughout. Note that even if one wishes to do a multigroup

calculation for a dense lattice retaining spatial heterogeneity, effective cross sections should be computed using τ_0 instead of s_0 . Thus equation (26) should be used with τ_0 replacing s .

(e) For all lattices, $\tau_0 < s_0$ and $\tau_0 < \sum_1 V_1/V_0$. This means that for all lattices, there is stronger self shielding (lower $\tilde{\sigma}$) than for either the isolated heterogeneous or homogeneous approximations. This effect is physically correct.

Exact values of P_0 have been computed for a slab lattice [13] and by Monte Carlo for a cylindrical lattice [10, Chernick]. By comparing values of P_0 as given by equation (36) with the exact values, we find that our estimates of P_0 are somewhat higher than the exact values. The comparison is given in table II. It is seen that increasing s_0 , by 15% for slabs and 30% for cylinders (as suggested for isolated lumps) gives better agreement (to within $\sim 5\%$ typically) with exact values. This increase may be consistently effected by increasing the surface area of the fuel moderator interface (by 15% for slabs and 30% for cylinders and spheres).

In addition, Monte Carlo calculations have been made of capture probabilities in two uranium-water lattices [6]. The IM approximation was used for uranium scattering. In table III we give a comparison of results based on equation (38) with the Monte Carlo calculations for those resonances for which the IM approximation is sound. The capture probability (1-p) was taken to be

Table II

Collision Probabilities, P_o , for Two Lattices. P_o = probability that neutron born uniformly in fuel makes next collision in fuel. With notation of text:

$$P_o(s) = \frac{\Sigma_o/s_o}{\Sigma_o/s_o + \Sigma_1/(\Sigma_1+s_1)}$$

A. Cylindrical Uranium Rods ($r = .76$ cm) in H_2O ; Volume (U) = Volume (H_2O); [10, Chernick]

Σ_o/s_o (.073 σ_t)	P_o (Monte Carlo)	$P_o(s)$	$P_o(1.3 s_o)$
.73	.416 ± .005	.515	.471
1.46	.625	.680	.641
2.92	.763	.809	.781
5.84	.874	.895	.877
14.6	.948 ± .002	.955	.947

B. Slab Lattice [13], with $\Sigma_1/s_1 = 1.40$.

Σ_o/s_o	P_o (exact)	$P_o(s)$	$P_o(1.15 s_o)$
.25	.28	.300	.284
.50	.41	.462	.442
1.00	.56	.632	.613
2.00	.72	.774	.760
4.00	.84	.874	.864

Table III

Resonance Capture Probabilities (1-p) for Single U²³⁸ Resonances; Monte Carlo Results from [6] and Canonical Results from Equation (38) for .25 inch Uranium Rods

Resonance Energy	$v_{H_2O}/v_u = 4$		$v_{H_2O}/v_u = 1.0$	
	Monte Carlo	Canonical	Monte Carlo	Canonical
6.7	.0393	.0438	.1100	.1310
21.0	.0186	.0197	.0551	.0588
36.8	.0192	.0161	.0475	.0484
66.3	.00618	.00599	.0171	.0174
103	.00496	.00531	.0132	.0156
191	.00295	.00301	.0087	.0088

$$1-p = \frac{\tilde{\sigma}_{n,\gamma}}{21 \frac{N_H V_1}{N_u V_0}}$$

and τ_0/N_u was computed to be 32b and 18.25b (based on $s' = 1.3 s_0$) for the cases $V_1/V_0 = 4$ and $V_1/V_0 = 1$ respectively. The calculations included Doppler broadening, as noted in Appendix B. The Monte Carlo results are not very accurate so that, with the probable exception of the 6.7 ev resonance, canonical and Monte Carlo results are in agreement to within about the Monte Carlo accuracy. For these calculations, s/N_u was 42.5b, so that the dense lattice correction (replacement of s by τ_0) is of considerable importance for $V_1/V_0 = 1.0$ and much less significant for $V_1/V_0 = 4.0$.

The ideas of this section can be readily generalized to quite complicated lattices. Suppose, for example, that the fuel was in clusters of UO_2 rods cooled by D_2O and each cluster imbedded in graphite. First of all, for one rod we compute a τ_0 from equation (35) where s_0 is $1/4$ the surface to volume ratio of the rod, \sum_1 is the mean free path in D_2O , and $s_1=s_0$ times ratio of rod to D_2O volumes. Secondly, this τ_0 is added to \sum_{00}^{NR} (the constant NR scattering cross section in rod) and the sum is then interpreted as the macroscopic NR scattering cross section for the cluster which appears in equation (38). Another τ_0 is now computed for the cluster with s_0 equal to $1/4$ the surface to volume ratio of the cluster, \sum_1 the graphite mean free path, and $s_1=s_0$ times ratio of cluster to

graphite volumes. This value of τ_0 also is used in equation (38) to give the final effective cross section.

V. Refinement for Elastic Scattering in Broad Resonances

For broad resonances which have considerable elastic IM scattering, it is desirable to reconsider our treatment of thick lumps. In the absence of NR scattering in the lump, all neutrons which are absorbed at an energy E were assumed to have entered the lump at the same energy E and, within the practical width, the first collisions of such neutrons are concentrated near the lump surface. However it will be recalled that in section III we assumed that all scattered neutrons (including those first scattered) were uniformly distributed throughout the lump. We thus overestimated capture probabilities for neutrons incident on thick lumps. In this section we will examine the magnitude of this overestimate by considering one velocity capture probabilities.

In this one velocity problem, we consider that IM scattering leads to no energy change and that NR scattering is equivalent to absorption. Neutrons are, as usual, assumed incident with an angular distribution proportional to $\mu d\mu$. Let P_c be the probability that an incident neutron is captured in the lump before leaking out. The value of P_c which is implied by our development of section III, in particular equation (14a) for $\phi_0(E)$, is

$$P_c = \frac{4V_1}{A} \frac{(1-P_1(E)) \sum_1 \sum_{ot}^{NR}(E)}{\sum_{ot}(E) \cdot P_o(E) \sum_{os}^{IM}(E)}$$

with $A =$ lump area. This is exact for the one velocity problem and for exact $P_1(E)$. If we assume that $P_1(E)$ are to be computed for uniform isotropic sources, then the reciprocity relation (20) can be used to eliminate P_1 . To make the results easier to understand we simplify notation for the remainder of this section, calling

$$\sum_{os}^{IM}(E) = \sum_s$$

$$\sum_{ot}(E) = \sum_t$$

$$\sum_{ot}^{NR}(E) = \sum_a$$

Denoting the resulting capture probability by $P_{c,u}$ (uniform), we have

$$P_{c,u} = \frac{\sum_a}{s_o} \frac{(1-P_o(E))}{1 \cdot P_o(E) \frac{\sum_s}{\sum_t}} \quad (39)$$

where, as before, $s_o = A/4V_o$. If, in addition, we use the Wigner form for $P_o(E)$, $P_o = \sum_t / (s_o + \sum_t)$, we obtain $P_{c,w}$ (Wigner) and find:

$$P_{c,w} = \frac{\sum_a}{\sum_a + s_o} \quad (40)$$

In tables IV, pp. 47 and 48, $P_{c,u}$ and $P_{c,w}$ are given for various

spheres and slabs. Values of P_0 are taken from [12]. It is observed that in general $P_{c,w} < P_{c,u}$, which should be expected from the demonstration in table I that the Wigner approximation is an overestimate of P_0 . We note also that both expressions approach unity as $\Sigma_a/s_0 \rightarrow \infty$, irrespective of the ratio Σ_s/Σ_t . This is clearly incorrect and the error increases with increasing Σ_s/Σ_t . Both $P_{c,u}$ and $P_{c,w}$ are too large for thick lumps and in fact $P_{c,u}$ (being larger) is even a slightly worse approximation for such cases.

Before proceeding further, it is interesting to note an alternative but similar approach suggested by Wigner [1] and recently employed by Adler et al. [7]. In this approximation it is assumed that IM scattering of a neutron entering the lump will not change the neutron's escape probability. In other words, neutrons are attenuated as $\exp(-\Sigma_a r)$ where r is the path length, and thus $P_{c,a}$ (Adler) is

$$P_{c,a} = G_0(\Sigma_a)$$

For a μ_0 incident angular distribution, G_0 is given by equation (30) and

$$P_{c,a} = \frac{\Sigma_a}{s_0} (1 - P_0(\Sigma_a)) \quad (41)$$

If $\Sigma_s = 0$, $P_{c,u} = P_{c,a}$. We see from tables IV that unless the lumps are thick and also IM scattering is dominant, $P_{c,a}$ and $P_{c,u}$ are in close agreement (with $P_{c,a} \geq P_{c,u}$). Thus it is no surprise that Adler et al.

[7] found little difference between IM resonance integrals for U^{238} based on $P_{c,a}$ and $P_{c,u}$.

If the Wigner form for P_0 is inserted in equation (41) we obtain $P_{c,w}$ as given in equation (40). From tables IV, we see that $P_{c,a} \geq P_{c,w}$. Thus neither $P_{c,a}$ nor $P_{c,u}$ are improvements upon the simple Wigner approximation, $P_{c,w}$, for the case of thick lumps with much IM scattering.

Accurate values of the capture probability are readily computed by numerical solutions of the transport equation. This has been done for most of the cases of tables IV by use of the SNG code [18] with the S_{16} approximation. The accuracy of the solution may be checked by comparison with exact solutions for purely absorbing lumps or infinitely thick lumps. For purely absorbing lumps, $P_{c,u}$ and $P_{c,a}$ are exact, with P_0 taken from [12]. For infinitely thick lumps P_c may be computed from the work of Chandrasekhar [19]. If we let $P_{c,\infty}(\mu_0, w_0)$ be the capture probability for a neutron incident at an angle θ with the normal ($\cos\theta = \mu_0$) upon a semi-infinite plane medium (having w_0 neutrons emerging per collision or $w_0 = \Sigma_s/\Sigma_t$), then from [19],

$$P_{c,\infty}(\mu_0, w_0) = \sqrt{1 - w_0} H(\mu_0, w_0) \quad (42)$$

$H(\mu_0, w_0)$ is tabulated [19, table XI]. For an incident source proportional to μ_0 , we have

$$P_{c,\infty} = 2 \sqrt{1 - w_0} \int_0^1 H(\mu_0, w_0) d\mu_0 \quad (43)$$

This function has been computed by numerical integration and is given in tables IV. It has also been compared with the S_{16} results. From these comparisons, we conclude that for spheres the S_{16} results are accurate to better than .1% and for slabs to about .2%. S_{16} results are included in tables IV.

Further approximate expressions for the capture probability are available from diffusion theory; see, for example, Glasstone and Edlund [20]. For a slab of thickness t , the diffusion theory capture probability, $P_{c,d}$, is

$$P_{c,d} = \frac{\frac{4}{\sqrt{3}} \sqrt{\frac{\Sigma_a}{\Sigma_t}} \tanh\left(\frac{t}{2} \sqrt{3 \Sigma_a \Sigma_t}\right)}{1 + \frac{2}{\sqrt{3}} \sqrt{\frac{\Sigma_a}{\Sigma_t}} \tanh\left(\frac{t}{2} \sqrt{3 \Sigma_a \Sigma_t}\right)} \quad (44)$$

For very large t this approaches the diffusion theory capture probability for a semi-infinite medium, P_{c,d_∞} :

$$P_{c,d_\infty} = \frac{\frac{4}{\sqrt{3}} \sqrt{\Sigma_a / \Sigma_t}}{1 + \frac{2}{\sqrt{3}} \sqrt{\frac{\Sigma_a}{\Sigma_t}}} \quad (45)$$

Diffusion theory results are also given in tables IV. It is observed that, as expected, $P_{c,d}$ is most accurate for lumps where scattering

Table IV-a

Capture Probabilities - Slabs of thickness t . For the various approximations see equations in the text as follows:

- U: uniform, $P_{c,u}$ - equation (39)
- D: diffusion, $P_{c,d}$ - equation (44)
- A: Adler, $P_{c,a}$ - equation (41)
- W: Wigner, $P_{c,w}$ - equation (40)
- Exact = S_{16} or see page 45.

Approximation	$\frac{\Sigma_a}{\Sigma_t}$	$t \Sigma_a = .1$	$t \Sigma_a = .3$	$t \Sigma_a = 1.0$	$t \Sigma_a = 3.0$	$t \Sigma_a = 10.0$	$t \Sigma_a = \infty$
Exact	1.0	.167	.400	.781	.982	1.00	1.00
U	1.0	.167	.400	.781	.982	1.00	1.00
D	1.0	.182	.454	.894	1.07	1.07	1.07
Exact	.50	.170	.408	.747	.852	.853	.853
U	.50	.170	.408	.761	.923	.976	1.00
D	.50	.181	.446	.814	.898	.899	.899
Exact	.20	.173	.402	.635	.658	.658	.658
U	.20	.173	.406	.714	.882	.962	1.00
D	.20	.180	.426	.663	.681	.681	.681
Exact	.10	.173	.382	.518	.522	.522	.522
U	.10	.173	.397	.690	.871	.957	1.00
D	.10	.178	.396	.532	.535	.535	.535
W	*	.167	.375	.667	.857	.952	1.00
A	*	.167	.400	.781	.982	1.00	1.00

* Independent of Σ_a/Σ_t

Table IV-b

Capture Probabilities - spheres of radius r. For the various approximations see text as follows:

U: uniform, $P_{c,u}$ - equation (39)

D: diffusion theory

A: Adler $P_{c,a}$ - equation (41)

W: Wigner $P_{c,w}$ - equation (40)

Exact = S_{16} or see page 45.

Approximation	$\frac{\Sigma_a}{\Sigma_t}$	$r\Sigma_a = .1$	$r\Sigma_a = .3$	$r\Sigma_a = 1.0$	$r\Sigma_a = 3.0$	$r\Sigma_a = 10.0$	$r\Sigma_a = \infty$
Exact	1.0	.124	.323	.703	.946	.995	1.00
U	1.0	.124	.323	.703	.946	.995	1.00
D	1.0	.129	.329	.720	.965	>1.0	1.07
Exact	.50	.124	.319	.651	.808	.82	.853
U	.50	.124	.319	.665	.878	.963	1.00
D	.50	.126	.324	.663	.827	.819	.899
Exact	.20	.123	.307	.547	.626	.65	.658
U	.20	.123	.311	.617	.832	.943	1.00
D	.20	.124	.311	.554	.641	.669	.681
Exact	.10	.122	.290	.454	.50	.52	.522
U	.10	.122	.302	.595	.816	.937	1.00
D	.10	.124	.292	.460	.511	.528	.535
W	*	.118	.286	.571	.800	.930	1.00
A	*	.124	.323	.703	.946	.995	1.00

* Independent of Σ_a/Σ_t

predominates (and also for thin lumps in general).

From the numbers in tables IV, the following conclusions are drawn:

(a) Both $P_{c,u}$ and $P_{c,a}$ are quite accurate for thin lumps ($\Sigma_a/s_0 \lesssim 1.0$) or highly absorbing lumps ($\Sigma_a/\Sigma_s \gtrsim 1.0$). $P_{c,u}$ is more accurate than $P_{c,a}$. Both $P_{c,u}$ and $P_{c,a}$ are too large for finite Σ_s .

(b) For numerical work, accurate results would be obtained by always using the smaller of $P_{c,u}$ and $P_{c,d}$.

When considering resonance absorption in pure U^{238} , only three resonances (at 36.8, 103, and 191 ev) have both IM scattering and $\Sigma_a/\Sigma_s < 1.0$. These contribute about 20% to the U^{238} resonance integral [7].

Errors due to use of $P_{c,a}$ appear to be of the order of 10% for these resonances, leading to a net error of only about 2% in the resonance integral. There are numerous other uncertainties of comparable magnitude so that this effect does not appear to be of much importance for U^{238} (or Th^{232}).

For resonance absorption in a lattice containing normal tungsten, the considerations of this section are somewhat more significant because the most important resonance (W^{186} at 18.8 ev) has $\Gamma_n/\Gamma_\gamma \simeq 6.1$ and IM scattering. There are also several overlapping W resonances in this energy region so that a numerical integration of $\sigma_{n,\gamma}$ is appropriate and recipe (b) above could be used. For numerical work on some tungsten lattices, we have used, however, a somewhat different recipe. This follows the spirit of the canonical approximation for P_0 in that details of the

geometry enter only through the surface to mass ratio. We observe from tables IV that the smaller of $P_{c,w}$ or P_{c,d_∞} (diffusion theory result for semi-infinite medium) is always a fair approximation to the capture probability. A slight improvement upon P_{c,d_∞} is given by

$$\frac{\Sigma_t}{s_0 + \Sigma_t} \frac{4/\sqrt{3} \sqrt{\Sigma_a/\Sigma_t}}{1 + \frac{2}{\sqrt{3}} \sqrt{\Sigma_a/\Sigma_t}}$$

where the first factor represents the probability that an incident neutron makes a collision at all (in canonical approximation) and the second is the probability of reflection from a semi-infinite medium (from diffusion theory). Thus for our numerical work we used $P_{c,n}$ (numerical) where

$$P_{c,n} = \text{Min} \left(\frac{\Sigma_a}{s_0 + \Sigma_a}, \frac{\Sigma_t}{s_0 + \Sigma_t} \frac{4/\sqrt{3} \sqrt{\Sigma_a/\Sigma_t}}{1 + \frac{2}{\sqrt{3}} \sqrt{\Sigma_a/\Sigma_t}} \right) \quad (46)$$

$P_{c,n}$ is compared with exact values of the capture probability in table V. We see that it is least accurate for strongly absorbing lumps ($\frac{\Sigma_a}{\Sigma_t} \approx 1.0$) of moderate thickness ($\Sigma_t/s_0 \approx 1.0$). For these cases we have seen, table I, that increasing s_0 increases the accuracy of our approximation to P_0 . Equation (27) for s_0 would presumably lead to improved accuracy in effective cross sections obtained from $P_{c,n}$.

For several tungsten plane lattices, we have computed effective cross sections using $P_{c,n}$ and the relation

Table V

Capture Probabilities: values of $P_{c,n}$, from equation (46) which was used for some numerical work, are compared with exact values

<u>Plane:</u>	Σ_a/Σ_t	$t\Sigma_a=.1$	$t\Sigma_a=.3$	$t\Sigma_a=1.0$	$t\Sigma_a=3.0$	$t\Sigma_a=10.0$	$t\Sigma_a=\infty$
Exact	1.0	.167	.400	.781	.982	1.00	1.00
$P_{c,n}$	1.0	.167	.375	.667	.857	.952	1.00
Exact	.50	.170	.408	.747	.852	.853	.853
$P_{c,n}$.50	.167	.375	.667	.830	.877	.899
Exact	.20	.173	.402	.635	.658	.658	.658
$P_{c,n}$.20	.167	.375	.619	.659	.674	.681
Exact	.10	.173	.382	.518	.522	.522	.522
$P_{c,n}$.10	.167	.375	.509	.526	.532	.535
<u>Sphere:</u>	Σ_a/Σ_t	$r\Sigma_a=.1$	$r\Sigma_a=.3$	$r\Sigma_a=1.0$	$r\Sigma_a=3.0$	$r\Sigma_a=10.0$	$r\Sigma_a=\infty$
Exact	1.0	.124	.323	.703	.946	.995	1.00
$P_{c,n}$	1.0	.118	.286	.571	.800	.930	1.00
Exact	.50	.124	.319	.651	.808	.82	.853
$P_{c,n}$.50	.118	.286	.571	.799	.867	.899
Exact	.20	.123	.307	.547	.626	.65	.658
$P_{c,n}$.20	.118	.286	.571	.648	.671	.681
Exact	.10	.122	.290	.454	.50	.52	.522
$P_{c,n}$.10	.118	.307	.498	.522	.530	.535

$$\tilde{\sigma}' = \frac{1}{\ln \frac{E_2}{E_1}} \int_{E_1}^{E_2} \frac{s_0 \sigma(E)}{\Sigma_a(E)} P_{c,n}(E) \frac{dE}{E} \quad (47)$$

These were compared with detailed multigroup S_n slab calculations which used 12 energy groups between 8 and 23 ev. Effective cross sections from (47) agreed with the S_n values to within better than 10% in all cases tested. On the other hand values obtained with $P_{c,w}$ or $P_{c,u}$ instead of $P_{c,n}$ were in error by as much as 30%.

We conclude that for thick lumps with much IM scattering $P_{c,n}$ is a useful approximation, and that some such approximation is necessary to obtain accurate results.

APPENDIX A

Systematic Improvement of NR and IM Approximations

Consider the integral equation for the neutron collision density, $\psi(E)$, in an infinite homogeneous medium. Assuming that absorption and s scattering are the only significant processes, we have:

$$\psi(E) = \sum_{j=1}^J \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} \frac{\sum_{s,j} \sigma_{s,j}(E')}{\sum_t \sigma_t(E')} \psi(E') \frac{dE'}{E'} \quad (A1)$$

We abbreviate this as

$$\psi(E) = \int_E^{E_{\max}} K(E, E') \psi(E') dE' = K\psi \quad (A2)$$

where (A2) defines K , and E_{\max} is some finite energy sufficiently large that there is no contribution to the integrals from higher energies.

We are interested in the solution, $\psi(E)$, to this equation in the vicinity of a single resonance at $E = E_0$. Suppose that for E/E_0 sufficiently large, absorption is negligible, scattering cross sections have a constant ratio, and the solution is known to be $\psi_0(E)$. At all

energies let $\psi_0(E)$ be a solution of

$$\psi_0(E) = \int_E^{E_{\max}} K_0(E, E') \psi_0(E') dE' = K_0 \psi_0 \quad (A3)$$

where $K_0(E, E')$ is some kernel which is equal to K at high energies.

Then define

$$K(E, E') = K_0(E, E') + K_1(E, E') \quad (A4a)$$

$$\psi(E) = \psi_0(E) + \psi_1(E) \quad (A4b)$$

Substituting in equation (A2) and using (A3) we find that:

$$\psi_1 = K_1 \psi_0 + K \psi_1 \quad (A5)$$

However, $K_1 \psi_0$ is a known function, equal in fact to $K \psi_0 - \psi_0$. Thus equation (A5) says that ψ_1 is that collision density which is given by a source $K_1 \psi_0$. Equation (A5) is also an inhomogeneous Volterra integral equation which may be solved by a Neumann series, i.e., the sequence

$$\psi_1^{(0)} = K_1 \psi_0$$

$$\psi_1^{(1)} = K_1 \psi_0 + K K_1 \psi_0$$

$$\psi_1^{(n)} = K_1 \psi_0 + K K_1 \psi_0 + \dots + K^n K_1 \psi_0$$

converges to the solution of (A5). Thus the solution of (A1) is:

$$\psi = K_0\psi_0 + K_1\psi_0 + KK_1\psi_0 + K^2K_1\psi_0 + \dots$$

or

$$\psi = K\psi_0 + KK_1\psi_0 + K^2K_1\psi_0 + \dots \quad (A6)$$

Equation (A6) gives us a systematic procedure for finding the exact solution, ψ , from any approximate solution, ψ_0 . Of course, the procedure is efficient only if ψ_0 is a good approximation to ψ (usually in the sense that $K_1\psi_0 \ll K_0\psi_0$).

Before applying (A6) to the NR and IM approximations, it is interesting to note that equation (A5) may be written

$$\psi_1 = K_1\psi + K_0\psi_1 \quad (A7)$$

Weinberg and Wigner [21] have essentially used this equation for the case of a single scattering material plus absorption. Equation (A7) says that ψ_1 is that flux, due to a source $K_1\psi$, and in a medium characterized by kernel, K_0 . The solution may be written in terms of the source $K_1\psi$ and the Placzek function of the kernel, K_0 . To make further progress an approximation was then made for ψ . In equation (A7) the kernel, K_0 , is simple but the source, $K_1\psi$, is unknown. In equation (A5) the source, $K_1\psi_0$, is known but the kernel K is not simple.

Let us now see how equation (A6) may be used to systematically improve upon the NR approximation.

Suppose that one has a mixture of isotopes with constant scattering

cross sections and zero absorption, plus one (call it uranium) with a resonance, and that for all isotopes $(1-\alpha_j)E_0$ is larger than the resonance practical width. For this situation the NR approximation is appropriate. The integral equation is

$$\psi(E) = \sum_j \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} \frac{\sum_{s,j}(E')}{\sum_t(E')} \psi(E') \frac{dE'}{E'} + \frac{1}{1-\alpha_u} \int_E^{E/\alpha_u} \frac{\sum_{s,u}(E')}{\sum_t(E')} \psi(E') \frac{dE'}{E'} \quad (A8)$$

We know $\psi(E) = \psi_0 = 1/E$ for E sufficiently large, and for the NR approximation, we assume that in the integrals $\psi = \psi_0$. But ψ_0 satisfies the integral equation

$$\psi_0(E) = \sum_j \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} \frac{\sum_{s,j}}{\sum_{so}} \psi_0(E') \frac{dE'}{E'} + \frac{1}{1-\alpha_u} \int_E^{E/\alpha_u} \frac{\sum_{so,u}}{\sum_{so}} \psi_0(E') \frac{dE'}{E'} \quad (A9)$$

where \sum_{so} is the off resonance scattering cross section. The kernel K appears in equation (A8) and K_0 in equation (A9). Thus

$$K_1 \psi = \sum_j \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} \sum_{s,j} \left(\frac{1}{\sum_t(E')} - \frac{1}{\sum_{so}(E')} \right) \psi(E') \frac{dE'}{E'} \\ + \frac{1}{1-\alpha_u} \int_E^{E/\alpha_u} \left(\frac{\sum_{s,u}(E')}{\sum_t(E')} - \frac{\sum_{so,u}}{\sum_{so}} \right) \psi(E') \frac{dE'}{E'}$$

Note that this equation, for $\psi_0(E)$, could have been obtained without explicit use of K_0 , i.e., for $\psi = \psi_0$, the above equation is simply $K_1 \psi_0 = (K-1) \psi_0$. Introducing $\psi_0 = 1/E$, we find

$$\begin{aligned}
K_1 \psi_0 = & - \sum_j \frac{1}{1-\alpha_j} \int_E^{E/\alpha_j} \frac{\sum_{s,j} (\Sigma_t - \Sigma_{so})}{\Sigma_t \Sigma_{so}} \frac{dE'}{(E')^2} \\
& + \frac{1}{1-\alpha_u} \int_E^{E/\alpha_u} \frac{\sum_{s,u} \Sigma_{so} - \sum_{so,u} \Sigma_t}{\Sigma_t \Sigma_{so}} \frac{dE'}{(E')^2}
\end{aligned} \tag{A10}$$

If we now ignore interference between resonance and potential scattering, so that $\sum_{s,u} - \sum_{so,u} = \Gamma_n / \Gamma_\gamma \sum_a$, equation (A10) may be rearranged to read

$$\begin{aligned}
K_1 \psi_0 = & - \sum_j \frac{1}{1-\alpha_j} \frac{\sum_{sj} \Gamma}{\sum_{so} \Gamma_\gamma} \int_E^{E/\alpha_j} \frac{\sum_a(E')}{\Sigma_t(E')} \frac{dE'}{(E')^2} \\
& + \frac{1}{1-\alpha_u} \left[\frac{\Gamma_n}{\Gamma_\gamma} - \frac{\sum_{so,u}}{\sum_{so}} \left(1 + \frac{\Gamma_n}{\Gamma_\gamma} \right) \right] \int_E^{E/\alpha_u} \frac{\sum_a}{\Sigma_t} \frac{dE'}{(E')^2}
\end{aligned}$$

If we further assume that $\sum_a / \Sigma_t \approx 0$ for $E \geq E_1 < E/\alpha_u$, the upper limits of all integrals may be set equal to E_1 and we have

$$K_1 \psi_0 = - \frac{1}{1-\alpha_u} \left[1 - \sum_j \frac{\alpha_u - \alpha_j}{1 - \alpha_j} \frac{\sum_{sj} \Gamma}{\sum_{so} \Gamma_\gamma} \right] \int_E^{E_1} \frac{\sum_a}{\Sigma_t} \frac{dE'}{(E')^2} \tag{A11}$$

in agreement with the results of Spinney [10]. $\psi_0 + K_1 \psi_0$ furnishes an improved estimate of ψ . Note that the integral in (A11) is less than or of the order of $\frac{\Gamma_p}{(E_0)^2} \frac{\Gamma}{\Gamma}$ with Γ_p the practical width so that the correction, $K_1 \psi_0$, is small compared to ψ_0 if $(1-\alpha_u) E_0 \gg \Gamma_p$. This is just the condition for validity of the NR approximation.

In principle one could continue improving the approximation by computing $K K_{\perp} \psi_0$, etc. Each successive term would carry the source, $K_{\perp} \psi_0$, through one additional collision. This would be an inefficient way of obtaining the asymptotic neutron density. It is interesting to observe that the common approximation,

$$\psi_0 \approx e^{-\int_E^{E_{\max}} \frac{\Sigma_a(E')}{\Sigma_t(E')} \frac{dE'}{E'}}$$

does give the correct asymptotic flux in the sense that then

$$\int_{E_{\min}}^{E_{\max}} K_{\perp} \psi_0 dE = 0$$

(Here E_{\min} is some energy well below the resonance.) This means that the integral of the source for ψ_{\perp} is zero so that to a first approximation we have the correct flux at low energies also, i.e., the correct absorption.

The same technique can be applied to the case where IM scattering is also allowed. Then as a first approximation we would have

$$\psi_0(E) = \frac{\Sigma_t(E)}{\Sigma_t^{NR}(E)} \frac{1}{E} \quad (A12)$$

The correction term $K\psi_0 - \psi_0$ could be evaluated directly.

Actually, Chernick et al. [6,5] improved the IM approximation in a slightly different sense. They assumed that the NR approximation was exact for moderator scattering and thus had an equation for $\psi(E)$

of the form:

$$\psi(E) = \frac{1}{E} + \frac{1}{1-\alpha_u} \int_E^{E/\alpha_u} \frac{\sum_{s,u} s_u(E')}{\sum_t t(E')} \psi(E') \frac{dE'}{E'} \quad (A13)$$

For such an inhomogeneous equation, the solution corresponding to (A6)

is:

$$\psi = \frac{1}{E} + K \psi_0 + K K_1 \psi_0 + K^2 K_1 \psi_0 \quad (A14)$$

where the kernel, K, is given in (A13). Chernick computed the term $K\psi_0$, thus including the correction $K_1\psi_0$.

It has been shown [5,6] that the above first order corrections to the IM and NR approximations give results which are quite accurate for $(1-\alpha) E_0 \approx \Gamma_p$. Either improved approximation is quite accurate - but the IM usually more accurate.

It would appear that the above technique may have more general applicability.

APPENDIX B

Expressions for Single Resonances

1. Unbroadened Resonances

Consider a resonance which is described by the Breit Wigner single level expressions. Suppose that the target nucleus has zero spin and zero velocity in the laboratory system and the neutrons have $l = 0$. Then the elastic scattering cross section, σ_{el} , and absorption cross section, σ_a , are (in conventional notation [22])

$$\sigma_a = \pi \kappa^2 \frac{\Gamma_n \Gamma_a}{(E-E_0)^2 + \Gamma^2/4} \quad (B1)$$

$$\sigma_{el} = \pi \kappa^2 \left| \frac{i \Gamma_n}{(E-E_0) + \frac{1}{2} i \Gamma} + 2i\kappa R \right|^2 \quad (B2)$$

That part of the elastic scattering due to resonance scattering, $\sigma_{el,res}$, is

$$\sigma_{el,res} = \sigma_{el} - 4\pi R^2 = \pi \kappa^2 \left[\frac{\Gamma_n^2}{(E-E_0)^2 + \Gamma^2/4} + \frac{4\kappa R \Gamma_n (E-E_0)}{(E-E_0)^2 + \Gamma^2/4} \right] \quad (B3)$$

where the second term is the result of interference between potential and resonance scattering.

If we assume that the scattering cross sections of all other isotopes which are present are independent of energy over the range of the resonance, then effective cross sections may be computed analytically. If we choose an energy interval ($E_1 \leq E \leq E_2$) which includes all significant contributions of the resonance, and assume $\Gamma/E \ll 1$ so that $1/E$ may be taken out of the integral and Γ_n assumed energy independent, then from equation (7) for the homogeneous case (or equation (38) for the canonical heterogeneous case):

$$\begin{aligned} \tilde{\sigma}'_a \ln \frac{E_2}{E_1} &= \int_{E_1}^{E_2} \frac{\sum_0^{NR} \sigma_a(E')}{\sum_0^{NR} + \sum_a(E') + f \sum_{el, res}(E')} \frac{dE'}{E'} & (B4a) \\ &\approx \frac{1}{E_0} \int_{-\infty}^{\infty} \frac{\sigma_a(E')}{1 + \frac{\sum_a(E') + f \sum_{el, res}(E')}{\sum_0^{NR}}} dE' \end{aligned}$$

whence,

$$\tilde{\sigma}'_a \ln \frac{E_2}{E_1} = \frac{\pi \sigma_{\max} \Gamma_a}{2E_0} \left[1 + \frac{\sum_0^{NR}}{\sum_{\max}^{NR}} \left(1 - \frac{f \Gamma_n}{\Gamma} \frac{4\pi R^2 N_r}{\sum_0^{NR}} \right) \right]^{-\frac{1}{2}} \quad (B4b)$$

Here, $f = 1.0$ if the resonance scattering is NR, $f = 0$ if the resonance scattering is IM, and

$$\sigma_{\max} = 4\pi\lambda^2 \frac{\Gamma_n}{\Gamma}; \quad \sum_{\max}^{NR} = N_r \frac{f \Gamma_n + \Gamma_a}{\Gamma} \sigma_{\max}$$

with N_r the density of resonance nuclei. For the canonical heterogeneous case, replace \sum_o^{NR} by $\tau_o + \sum_{oo}^{NR}$. Similarly from equation (6) we have

$$\tilde{\sigma}_a = \frac{\frac{\pi}{2} \frac{\sigma_{\max} \Gamma_a}{E_o}}{\ln\left(\frac{E_2}{E_1}\right) \left[1 + \frac{\sum_o^{NR}}{\sum_o^{NR}} \left(1 - \frac{f\Gamma_n}{\Gamma} \frac{4\pi R^2}{\sum_o^{NR}} \right) \right]^{\frac{1}{2}} - \frac{\pi}{2} \frac{\sum_{\max}(\Gamma_a + f\Gamma_n)}{\sum_o^{NR} E_o} \left[1 - \frac{2f\Gamma_n}{\Gamma} \frac{4\pi R^2 N_r}{\sum_o^{NR}} \right]} \quad (B5)$$

In both equations (B4) and (B5) the factors

$$1 - \frac{f\Gamma_n}{\Gamma} \frac{4\pi R^2 N_r}{\sum_o^{NR}}$$

arise from interference between potential and resonance scattering.

Evidently they are frequently negligible. However, for very concentrated mixtures and $\Gamma_n/\Gamma \sim 1.0$ this interference can be appreciable.

2. Doppler Broadening with Maxwell Distribution

When considering nuclei at finite temperatures, the resonance will be Doppler broadened by motion of the nuclei. For a solid at temperatures above its Debye temperature, it is a resonance approximation to assume that the nuclei have a Maxwell distribution of velocities [23].

Consider a neutron moving in the $-z$ direction, $\hat{p} \perp \hat{z}$, having energy E_n in the laboratory system and E in the center of mass system, and let m_r be the reduced mass of the neutron-nucleus system. ($m_r = \frac{mM}{m+M}$). Let v_z, v_o be the components of nuclear velocity parallel and perpendicular to the neutron velocity. Then

$$E = \frac{1}{2} m_r \left[v_\rho^2 + \left(\sqrt{\frac{2E_n}{m}} + v_z \right)^2 \right] \quad (B6)$$

The cross section in the laboratory system will be for a Maxwell distribution of nuclear velocities:

$$\sqrt{\frac{E_n}{m}} \sigma(E_n) = \frac{\int_{-\infty}^{\infty} dv_z \int_0^{\infty} v_\rho dv_\rho \sqrt{\frac{E}{m_r}} \sigma(E) e^{-\frac{M}{2kT}(v_z^2 + v_\rho^2)}}{\int_{-\infty}^{\infty} dv_z \int_0^{\infty} v_\rho dv_\rho e^{-\frac{M}{2kT}(v_z^2 + v_\rho^2)}} \quad (B7)$$

Changing from variables v_ρ, v_z to E, v_z , integrating first over v_z , and setting $E' = \frac{m}{m_r} E$, $\frac{M}{m} = A$ we obtain:

$$\sqrt{E_n} \sigma(E_n) = \frac{\int_0^{\infty} \sqrt{E'} \sigma(E') e^{-\frac{A}{kT}(\sqrt{E_n} - \sqrt{E'})^2} - e^{-\frac{A}{kT}(\sqrt{E_n} + \sqrt{E'})^2} dE'}{\int_0^{\infty} \left[e^{-\frac{A}{kT}(\sqrt{E_n} - \sqrt{E'})^2} - e^{-\frac{A}{kT}(\sqrt{E_n} + \sqrt{E'})^2} \right] dE'} \quad (B8)$$

This expression was obtained, for example, by Feshbach and Goertzel [24].

Equation (B8) has been used by J. Devaney [25] together with single level expressions for $\sigma(E')$ for computing Doppler broadened cross sections for Pu^{239} , U^{238} , and W over a large range of temperatures (up to 100 ev). For moderate temperatures it is valid to expand E' and the exponents about E_n to obtain the usual expression:

$$\sigma(E_n) \approx \frac{\int_0^\infty \sigma(E') e^{-(E_n - E')^2 / \Delta^2} dE'}{\int_0^\infty e^{-(E_n - E')^2 / \Delta^2} dE'} \quad (B9)$$

with $\Delta^2 = 4kT E_n / A$.

It can be seen that in general, in going from (B8) to (B9) we neglect terms of relative order $(4kT/AE_n)^{1/2}$ which is usually a small quantity. It is interesting to note that the integral of $\sigma(E_n)$ is given more accurately, i.e., the error terms are here of order $4kT/AE_n$. Equation (B9) is, for common temperatures and resonance energies, a sufficiently accurate expression. It is commonly derived, following Bethe and Placzek [26], by simply neglecting the quadratic dependences of E on nuclear velocities.

For single level Breit Wigner expressions for $\sigma(E')$, equations (B1) and (B3);

$$\sigma_a(E_n) = \sigma_{\max} \Gamma_a / \Gamma \psi[2(E_n - E_0) / \Gamma, \Delta^2 / \Gamma^2]$$

where

$$\psi(x, \theta) = \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{e^{-(x-y)^2 / 4\theta}}{1 + y^2} dy \quad (B10)$$

$\psi(x, \theta)$ is a tabulated function [27]. Furthermore

$$\sigma_{e1, res}(E_n) = \sigma_{\max} \frac{\Gamma_n}{\Gamma} \psi\left(\frac{2(E_n - E_0)}{\Gamma}, \frac{\Delta^2}{\Gamma^2}\right) + \sqrt{4\pi R^2} \sigma_{\max} \frac{\Gamma_n}{\Gamma} \chi\left(\frac{2(E_n - E_0)}{\Gamma}, \frac{\Delta^2}{\Gamma^2}\right)$$

where

$$\chi(x, \theta) = \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{2y}{1+y^2} e^{-(x-y)^2/4\theta} dy \quad (\text{B11})$$

These expressions have been frequently used in computing resonance integrals. In particular if we ignore the interference term ($\chi(x, \theta)$), and consider the homogeneous case (or canonical heterogeneous case) we have (from equation (6)):

$$\tilde{\sigma}'_a \ln \frac{E_2}{E_1} = \frac{\Gamma}{\Gamma_a + f\Gamma_n} \frac{\sum_o^{NR} \Gamma_a}{N_r E_o} J\left(\frac{\Gamma}{\Delta}, \frac{\sum_o^{NR}}{\Gamma_a + f\Gamma_n}\right) \quad (\text{B12})$$

$N_r \sigma_{\max} \frac{\Gamma}{\Gamma}$

where

$$J(\xi, \beta) = \int_0^{\infty} \frac{\psi(x, 1/\xi)}{\beta + \psi(x, 1/\xi)} dx \quad (\text{B13})$$

The function $J(\xi, \beta)$ has been tabulated by Dresner [8] and Nordheim [7].

For the isolated heterogeneous case, non-canonical results are available from the work of Nordheim [7] for cylinders, spheres, and slabs. Interference between potential and resonance scattering was ignored. When only NR scattering is present the tabulations [7] correspond to use of our equation (21) with $P_o(E)$ from [12]. Nordheim's treatment of IM scattering is slightly different from ours, but as noted in the comparison of equations (39) and (41) the results should not be much different. For purely IM scattering in the heterogeneous case, some of Nordheim's tabulations are in error.

Rothenstein [13] has investigated the effect of interference between resonance and potential scattering at finite temperatures. He has expanded the denominator of equation (B4a) for small $\sum_{el, res}(E')$ and has computed the resulting interference term using equation (B11). The interference decreases with increasing temperature, thus partially cancelling the normal temperature broadening effects. As can be seen from equation (B4b) the effect is important if and only if (a) $f = 1.0$, i.e., the resonance scattering is NR, (b) $\Gamma_n/\Gamma \sim 1.0$, and (c) $4\pi R^2 N_r / (\tau_o + \sum_{oo}^{NR}) \sim 1.0$. If all these conditions are satisfied the temperature coefficient due to interference may be a moderate fraction ($\approx 20\%$) of that due to broadening.

3. Conditions Under Which the Single Level Results Are Inapplicable

Expressions which have been so far derived in this Appendix have been based on the assumption that the relevant absorption cross section could be represented by single level expressions, which do not noticeably overlap. This assumption is invalid under a number of conditions:

(a) The fission cross sections of the fissile isotopes show interference between various levels [28].

(b) For a single isotope the absorption cross sections due to various levels may seriously overlap if the levels are closely spaced. At sufficiently high temperatures [25] or neutron energies [24], Doppler broadening will make the overlap very serious.

(c) In a mixture of isotopes, overlap of resonances in the various isotopes may be serious.

In all the above cases, if the cross sections are known in detail, the desired integrations may evidently be performed numerically. An IBM 704 code (SET) was written at Los Alamos by B. Fagan to perform integrations corresponding to the homogeneous (and thus canonical heterogeneous) cases and, less conveniently, to equation (21) for the isolated heterogeneous case for spheres and slabs. Provision was made for use of equation (47) for broad scattering resonances. Cross sections were usually obtained from the work of Devaney [25]. The code does not decide whether scattering should be treated as IM or NR. The accuracy of the numerical integration is of the order of 1%.

In case the cross sections are strongly overlapping and known only statistically. Goertzel et al. [24] have used statistical considerations to compute effective cross sections.

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