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REPORT TITLE **IMPROVED CALCULATION OF EFFECTIVE RESONANCE CROSS
SECTIONS FOR FAST SPECTRUM ASSEMBLIES.**

AUTHOR
J. M. Otter

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ATOMICS INTERNATIONAL A Division of North American Aviation, Inc.		AI-AEC- TDR NO 12756	APPROVALS
TECHNICAL DATA RECORD		PAGE 1 OF 12	<i>H Otter</i>
AUTHOR DEPT & GROUP NO. J. M. Otter 731 - 141		DATE 11-5-68	<i>W. J. Davis</i>
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TITLE Improved Calculation of Effective Resonance Cross Sections for Fast Spectrum Assemblies		S/A NO 14610	TWR
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Alter, H. DA03 Bernath, L. BB16 Dunford, C. DA03 Fillmore, F. DA03 Hillig, O. SO09 Hubner, R. DA03 Levitt, L. DA03 Mahlmeister, J. BB32 Morewitz, H. BB18 Otter, J.(6) DA03 Ottewitte, E. BB22 Paschall, R. S100 Rhoades, W. BB22 Rood, H. BB22 Rose, P. DA03 Royden, H. S100 Sevy, R. BB10 Silberberg, M. DB01 Specht, E. BB32 Springer, T. DA03 Tuttle, R. S100 Vaughan, E. DA03 Vitti, J. BB32 Williams, R. BB13		STATEMENT OF PROBLEM Improve the accuracy of the treatment of unresolved resonances in the TRIX code to provide improved predictions of fast spectra, effective resonance cross sections, and Doppler coefficients.	
		ABSTRACT Modifications to the unresolved resonance subroutine in the TRIX code are described in both theoretical and practical detail. The effects dealt with include depletion of group fluxes by resonance absorption, and the energy dependencies of the absorber potential scattering cross section and level spacing. Also included are the value of the radius of the centrifugal potential well, elastic scatter with change of neutron angular momentum, and Doppler-broadened self-shielded scattering cross sections.	
		Calculations of infinitely dilute cross sections of U-238 are compared with optical model calculations and good agreement found.

I. INTRODUCTION

In fast spectrum assemblies several matters which can be neglected in thermal spectrum assemblies may be important to precise calculations of reactivities, spectra, and Doppler coefficients.

The following are judged worthy of consideration:

1. The value of the centrifugal potential well used in calculating penetrabilities of neutrons with non-zero angular momenta, l .
2. Elastic scatter to states with non-incident values of l .
3. Energy dependent potential scattering cross section for the resonance absorber including its effect on interference between resonance and potential scattering.
4. Doppler-broadened self-shielded resonance scattering integrals.
5. Depletion of group flux by unresolved resonances.
6. Energy dependent level spacing.
7. Competition from inelastic scattering.
8. Energy dependent radiative capture strength function.
9. Gross flux shape in an energy group.

The theory and approximation used for the first 6 items are discussed in turn and results of calculations which illustrate its importance are presented.

All these items were found to be of some importance below 100 kev, which was taken as the upper limit of the unresolved resonance range.

Finally, a detailed comparison of infinitely dilute cross sections of U-238 calculated by TRI-X with those from optical model calculations is made.

II. PENETRABILITY OF NEUTRONS WITH NON ZERO ANGULAR MOMENTA

The penetrabilities of neutrons with non zero angular momenta, $l > 0$, are functions of kR , where k is the wave number and R is the radius of the centrifugal potential well. The 'hard sphere' model in which $R = R_0 A^{1/3}$ is used. The value of the unit radius, R_0 , now recommended¹ is 1.25 fermi compared to the previous value of 1.44 fermi. The effect of this change is to reduce penetrabilities for p-wave neutrons in the unresolved resonance range by a maximum of about 25% at low energies down to about 20% at 100 kev. The corresponding reductions for d-wave neutrons are 43% and 41%, respectively. The routine was coded to permit values other than 1.25 fermi to be input.

Since it has not always been the case, it is worth noting that R is not determined with reference to the scattering length (or radius), a , in the formula for the s-wave potential scattering cross section, $\sigma_{\text{pot}} = \frac{4\pi}{k^2} \sin^2 ka$. Where the nuclear interaction is represented by a square well, the scattering length can vary from $-\infty$ to $+\infty$ depending on the well depth. Clearly, the potential well radius and not the scattering length should be used to calculate penetrabilities.¹

III. ELASTIC SCATTER WITH CHANGE OF NEUTRON ANGULAR MOMENTUM

The total level width is the sum of the partial widths of all available states with the same parity. For elastic scattering by neutrons with incoming angular momentum quantum numbers, ι_i , of 2 or 3 (d or f wave), an outgoing state with $\iota = \iota_i - 2$ is sometimes available. The width of this state is ordinarily much greater than that for the higher ι state because of the larger penetrability. Its inclusion reduces cross sections for competing processes, especially when their combined width is a minor fraction of the total width. In addition, its statistical distribution normally dominates fluctuation corrections and should be accounted for. Contributions to the

1. Letter 68AT-4735, C. L. Dunford to T. Stephenson, 10-2-68.

total width from neutrons with $\ell = \ell_i + 2$ are very small due to their reduced penetrabilities and are safely neglected.

The width is the same as for the formation of the compound nucleus by an $\ell_i - 2$ neutron. Therefore, the input data for that reaction, termed the (ℓ_i, J) state, can be used. The code is directed to the location of the input data for the desired state by an input number in the (ℓ_i, J) data set. The width at each energy is added to the elastic scattering and total level widths. Sampling from the distribution of widths with the number of degrees of freedom of the (ℓ_i, J) state is done independently from sampling for other processes.

This phenomenon occurs for isotopes with $I > 0$. For example, if $I = 1/2$ as in Pu-239, the $(\ell_i = 2, J = 1)$ state has an available $(0, 1)$ state, and the $(\ell_i = 3, J = 2)$ state has an available $(1, 2)$ state. If $I = 7/2$ as in U-235, $(\ell_i = 2, J = 3, 4)$ have available $\ell = 0$ states; $(\ell_i = 3, J = 2, 3, 4, 5)$ have available $\ell = 1$ states. For the $(2, 1)$ state of Pu-239 the dilute capture cross section is reduced by $1/3$ at 100 kev by including this additional scattering. The effect on the total capture cross section is a 2% reduction.

IV. ENERGY DEPENDENT POTENTIAL SCATTERING CROSS SECTION FOR THE RESONANCE ABSORBER

The scattering cross section for neutrons with angular momentum ℓ in the vicinity of an isolated resonance is²

$$\sigma_s^\ell = \frac{\pi}{k^2} \sum_J g_J |A_{\ell J}^{res} + A_{\ell J}^{pot}|^2$$

where J is the compound nucleus spin quantum number

g_J is the statistical weight factor

k is the neutron wave number

$A_{\ell J}^{res}$ is the resonance scattering amplitude

$A_{\ell J}^{pot}$ is the potential scattering amplitude

The single-level Breit-Wigner formula for the resonance scattering amplitude is used.

$$A_{\ell J}^{res} = \frac{i \Gamma_{\ell J}^{sc}}{(E - E_{\ell J}^{res}) + i \Gamma_{\ell J}^{sc}/2}$$

2. J. Blatt and V. Weisskopf, Theoretical Nuclear Physics, John Wiley & Sons, New York (1952) Chapt. 8.

where the symbols have their usual meanings. The potential scattering amplitude is given by

$$A_{lJ}^{\text{pot}} = \exp(2i\delta_{lJ}) - 1$$

where δ_{lJ} is the phase constant.

In the 'hard sphere' model approximation

$$\delta_{lJ} = kR_{lJ}$$

$$\delta_{1J} = kR_{1J} - \tan^{-1}(kR_{1J})$$

$$\delta_{2J} = kR_{2J} - \tan^{-1}\left[\frac{kR_{2J}}{1 - (kR_{2J})^2/3}\right]$$

In the TRIX code the usual assumption that the scattering potential radius R_{lJ} is independent of J is made, in which case the total potential scattering cross section would be

$$\sigma^{\text{pot}} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |A_{lJ}^{\text{pot}}|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_{lJ}$$

The potential scattering cross section is a function of energy through the neutron wave number, $k = \sqrt{2mE}/\hbar$ where m is the neutron mass and $\hbar$ is Planck's constant divided by 2π . $k = 2.197 \times 10^9 \sqrt{E}/\eta$ cm^{-1} where E is in electron volts, and R_l is the order of 10^{-12} cm, so that kR_l is roughly $0.002 \sqrt{E}$. $\eta = (M+m)/M$ is present because the energy is assumed to be measured in the laboratory frame of reference. Below 10 kev, kR is $\lesssim 0.2$, and $\sin kR \approx \tan kR \approx kR$. Then, $\sigma_0^{\text{pot}} \approx 4\pi R_0^2$, $\sigma_1^{\text{pot}} \approx 0$, $\sigma_2^{\text{pot}} \approx 0$, which were the approximations previously used. We now wish to consider energies to 100 kev, at which point $kR_l \approx 0.6$, which gives $\sin kR_l = 0.565$, $\tan^{-1} kR_l = 0.540$, $\delta_1 = 0.060$, $\delta_2 \approx .0015$, $\sigma_0^{\text{pot}} = 8.3\text{b}$, $\sigma_1^{\text{pot}} = .135\text{b}$, $\sigma_2^{\text{pot}} = .0001\text{b}$. σ_0^{pot} is reduced on the order of 10% from the energy independent approximation. The p and d-wave potential scattering cross sections are still very small at this energy and are neglected. The code derives R_0 from an input potential scattering cross section for slow neutrons, $\sigma_0^{\text{pot}}(0)$.

$$R_0 = [\sigma_0^{\text{pot}}(0)/4\pi]^{1/2} = a$$

$$\sigma^{\text{pot}} = \frac{4\pi}{k^2} \sin^2 kR_0$$

The potential scattering cross section of the resonance absorber enters the calculation of effective resonance integrals through the dilution parameter $\bar{\sigma}_p$, which is the potential scattering of all materials present per atom of resonance absorber, through the resonance scattering cross section by coherent interference, and through the total resonance absorber cross section both directly and by the scattering interference effect. In the narrow resonance approximation customarily employed for unresolved resonances

$$I_{\text{eff}}^x = \int_{\text{res}} \frac{(\sigma_m + \sigma_p) \sigma_x}{\sigma_m + \sigma_p + \sigma_t} \frac{c/E}{E}$$

$$\bar{\sigma}_m = \frac{1}{N} \bar{\sigma}_{\text{eff}} + \frac{\sum_i \sigma_i}{N}$$

where $\bar{\sigma}_{\text{eff}} = \frac{4V}{\bar{A} S_{\text{eff}}}$

V is the volume of lump

S_{eff} is the surface of lump corrected for Dancoff effects

$\bar{A}$ is the correction to the Wigner rational approximation to the escape probability.

N is the number density of resonance absorber.

$\sum_i \sigma_i$ is the scattering cross section of light scatterers homogeneous with the absorber

$$\bar{\sigma}_p = \bar{\sigma}^{\text{pot}} + \frac{\sum_p \sigma_p^h}{N}$$

where $\sum_p \sigma_p^h$ is the scattering cross section of heavy scatterers homogeneous with the absorber

$\bar{\sigma}_t$ is the total resonance cross section. For an isolated resonance,

$$\bar{\sigma}_t = \bar{\sigma}_n + \sum_x \sigma_x$$

$\bar{\sigma}_n$ is the cross section for elastic scattering without change in neutron angular momentum

$$\bar{\sigma}_h = \sigma_0 \left\{ \left(\frac{\Gamma_n}{\Gamma} - 2 \sin^2 \delta \right) \psi + \left(\frac{1}{2} \sin 2\delta \right) \chi \right\}$$

$$\sigma_x = \sigma_0 \frac{\Gamma_x}{\Gamma} \psi$$

where x is any process except n.

$$\sigma_0 = \frac{4\pi}{k^2} g \frac{\Gamma_n}{\Gamma}$$

ψ and χ are the symmetric and asymmetric line shape functions, respectively. Evaluating Γ_n , Γ , E , and σ^{pot} , at E_r and extending the limits of integration to $\pm \infty$, as is customary³

$$I_{\text{eff}}^x = \frac{\Gamma_\infty^x}{\pi} \int_{-\infty}^{\infty} \frac{\psi}{\psi + \beta + \frac{\tan 2\delta}{2} \chi} dx$$

$$\text{where } x = 2(E - E_r)/\Gamma$$

$$\beta = \frac{\sigma_m + \sigma_p}{\sigma_0 \cos 2\delta} ; \quad \Gamma_\infty^x = \frac{\pi \sigma_0^x \Gamma_x}{2E_r}$$

Following Rothenstein,⁴ the integrand is expanded in terms of $(\psi + \beta)^{-1}$

$$I_{\text{eff}}^x = \frac{\Gamma_\infty^x}{\pi} \int_{-\infty}^{\infty} \frac{\psi}{\psi + \beta + \frac{\tan 2\delta}{2} \chi} dx = \frac{\Gamma_\infty^x}{\pi} \int_{-\infty}^{\infty} \frac{\psi}{\psi + \beta} dx + \left(\frac{\tan 2\delta}{2} \right) \frac{\Gamma_\infty^x}{\pi} \int_{-\infty}^{\infty} \frac{\psi \chi}{(\psi + \beta)^2} dx + \dots$$

Since ψ is an even function and χ an odd function, a good approximation for the usual situation of small scattering interference is

$$I_{\text{eff}}^x = \frac{2\beta \Gamma_\infty^x}{\pi} \left[J(\theta, \beta) - \left(\frac{\tan 2\delta}{2\beta} \right) K(\theta, \beta) \right]$$

where

$$J(\theta, \beta) = \int_0^\infty \frac{\psi(\theta, \beta)}{\psi(\theta, \beta) + \beta} dx ; \quad K(\theta, \beta) = \int_0^\infty \frac{\psi(\theta, \beta) [\chi(\theta, \beta)]^2}{[\psi(\theta, \beta) + \beta]^3} dx$$

$$\theta = \Gamma(E) / (4k_B T E_r / A)^{1/2} *$$

Defining $f_1(\theta, \beta) = J(\theta, \beta) / J(\infty, \beta)$; $f_2(\theta, \beta) = K(\theta, \beta) / K(\infty, \beta)$

$$I_{\text{eff}}^x = \frac{\Gamma_\infty^x f_1(\theta, \beta)}{\sqrt{1 + \frac{1}{\beta}}} + \frac{\Gamma_\infty^x \left(\frac{\tan 2\delta}{2\beta} \right)^2 f_2(\theta, \beta)}{2(1 + \frac{1}{\beta})^{3/2}}$$

$$= \frac{\Gamma_\infty^x}{\sqrt{1 + \frac{1}{\beta}}} \left[f_1(\theta, \beta) + \left(\frac{\tan 2\delta}{2\beta} \right)^2 \frac{f_2(\theta, \beta)}{2(1 + \frac{1}{\beta})} \right]$$

3. L. Dresner, Resonance Absorption in Nuclear Reactors, Pergamon Press, New York (1960) p. 32.

4. W. Rothenstein, "Collision Probabilities & Resonance Integrals for Lattices," Nucl. Sci. Engrg. 7, 162 (1960).

* See Section VII for energy dependence of Γ .

f_1 and f_2 are interpolated from tables of values in the TRIX code.

Compared to the previous treatment the effective resonance integral is slightly reduced because of lower σ^{pot} values in β . Scattering interference gives rise to two terms in τ_s , namely, $(-2 \sigma_0 \sin^2 \delta) \psi$ and $(\frac{\sigma_0}{2} \sin 2\delta) \chi$. The first term was previously neglected in TRIX, as has been customary, in deference to $\sigma_0 \Gamma_n \psi / \Gamma$ because δ^2 is small below 10 kev. However, this term gives rise to the $\cos 2\delta$ term in β which increases β by $\sim 8\%$ at 10 kev and by about a factor of 3 at 100 kev. The change in the second scattering interference term is of relatively minor import. It is to be noted that, since both scattering interference terms are retained, β is different with and without scattering interference, and the procedure for generalizing to intermediate resonance formulas used for resolved resonances, namely

$$I(T) = I(0) f_1 + [I(T) - I(0)] f_2$$

is not valid here.

V. DOPPLER-BROADENED SELF-SHIELDED SCATTERING RESONANCE INTEGRALS

Self-shielding of the resonance scattering cross sections can have a significant influence upon the spectrum of compact fast reactors and give rise to a non-negligible 'scattering Doppler coefficient' according to S. C. Cohen et al.⁵ For scattering processes other than elastic scattering without change in neutron angular momentum, the resonance integral is that derived in the previous section. Otherwise, interference between resonance and potential scattering occurs, and we have, following the development of the previous section,

$$\begin{aligned} I_{eff}^n &= \int \frac{(\sigma_m + \sigma_p) \sigma_n}{\sigma_m + \sigma_p + \sigma_t} \frac{dE}{E} \\ &= \frac{I_{\alpha}^n \beta}{\pi} \int_{-\infty}^{\infty} \frac{(1 - \frac{2\Gamma}{\Gamma_n} \sin^2 \delta) \psi + (\frac{\Gamma}{2\Gamma_n} \sin 2\delta) \chi}{\psi + \beta + \frac{\tan^2 2\delta}{2} \chi} dx \end{aligned}$$

For small scattering interference, i.e., the neglect of terms containing χ to greater than the first power,

$$I_{eff}^n = \frac{2 I_{\alpha}^n \beta}{\pi} \left(1 - \frac{2\Gamma}{\Gamma_n} \sin^2 \delta \right) \left[J(T, \beta) + \left(\frac{\tan 2\delta}{2} \right)^2 K(T, \beta) \right]$$

5. S. C. Cohen et al, ANS Trans. 10, 579 (1967)

The total resonance scattering integral including inelastic scattering, index mark ie, and elastic scattering with change in k , index mark, k , becomes in general

$$I_{\text{eff}}^x = \frac{2\beta}{\pi} \left[I_{\infty}^{ie} + I_{\infty}^k + I_{\infty}^n \left(1 - \frac{2\Gamma}{\Gamma_n} \sin^2 \delta \right) \right] \left[J(0, \beta) + \left(\frac{\tan 2\delta}{2} \right)^2 K(0, \beta) \right]$$

$$= \frac{\sigma_0 \beta}{E_r} \left[\Gamma_{ie} + \Gamma_k + \Gamma_n - 2\Gamma \sin^2 \delta \right] \left[J(0, \beta) + \left(\frac{\tan 2\delta}{2} \right)^2 K(0, \beta) \right]$$

In TRIX scattering interference is neglected ($\delta = 0$) for $k > 0$, so that Γ_k and δ are never both non-zero for any (k, J) state. Self shielding reduces the scattering cross section for a 0.44 " d U-238 metal cylinder by 1% @ 50 kev, 9% @ 10 kev, and 40% @ 1 kev.

VI. DEPLETION OF GROUP FLUX BY UNRESOLVED RESONANCES

The effective group resonance cross section can be expressed as the effective group resonance integral divided by the group flux normalized to unity per unit lethargy in the absence of resonances.

$$\sigma_{\text{eff}}^x = \frac{I_{\text{eff}}^x}{\Phi}$$

In the narrow resonance approximation,

$$\phi(u) = \frac{\sigma_m + \sigma_p}{\sigma_m + \sigma_p + \sigma_t}$$

Then,

$$\Phi = \int_g \frac{\sigma_m + \sigma_p}{\sigma_m + \sigma_p + \sigma_t} du = \Delta u - \int_g \frac{\sigma_t}{\sigma_m + \sigma_p + \sigma_t} du$$

Using the treatment of section IV, we have

$$\Phi = \Delta u - \sum_g \frac{\Gamma}{E_r} \left[J(T, \beta) + \left(\frac{\tan 2\delta}{2} \right)^2 K(T, \beta) \right] = \Delta u - \frac{\pi}{2} \sum_g \frac{\Gamma}{E_r \beta} \frac{I_{\text{eff}}^x}{I_{\infty}^x}$$

TRIX computes unresolved cross sections by averaging samples from the distributions of level widths at each of a number of energy points across a group, so that the formula becomes

$$\Phi = \Delta u - \frac{\pi}{2} \sum_{(l, J)} \sum_E \left\langle \frac{\Gamma}{E \beta} \frac{I_{\text{eff}}^x}{I_{\infty}^x} \right\rangle_{l, J} \frac{\Delta E}{\bar{D}_{l, J}}$$

where the brackets denote averaging of the distributions of width and D is the average level spacing.

The neutrons scattered from within a resonance reappear, however, distributed in some fashion at lower energies. Assuming that the scatterings into a group are equal to those out of it, the real depletion of the group flux is just due to absorptions. Thus the formula used is

$$\phi = \Lambda_0 - \frac{\pi}{2} \sum_{(i,j)} \sum_E \left\langle \frac{\Gamma_a}{E} \frac{I_{a,i,j}}{I_{a,i,j}} \right\rangle \frac{\Delta E}{D_{i,j}}$$

The depletion of the flux by resonances in a 0.44" diameter U-238 metal cylinder is about 2% at 5 kev and 1/4% at 100 kev.

VII. ENERGY DEPENDENT LEVEL SPACING

The energy dependence of the density of levels is given in the free gas formulation of Gilbert and Cameron⁶ as

$$\rho(E, J) \propto \frac{\exp \left[2\sqrt{a}U - (J + \frac{1}{2})^2 / (0.1776 A^{2/3} \sqrt{a}U) \right]}{U^2}$$

where $U = E_B + E + \delta E$

E_B is the binding energy of the last neutron in the compound nucleus.

δE is the nucleon pairing correction of the compound nucleus

$a = (0.00917 S + 0.142) A$, undeformed nuclei

$a = (0.00917 S + 0.120) A$, deformed nuclei

A is the mass number of the compound nucleus

S is the shell correction of the compound nucleus

Values of E_B , δE , and S including empirical adjustments are given by J. L. Cook et al.⁷

6. A. Gilbert and A.G.W. Cameron. Can. J. Phys. 43, 1446 (1965).

7. J. L. Cook et al, 'Nuclear Level Densities in Intermediate and Heavy Nuclei,' AAEC/TM 392 (1966).

The values of level widths Γ_n^o , Γ^x are assumed to be proportional to $\bar{D}$ in TRIX* so that the energy dependence of $\bar{D}$ does not affect cross sections at 0°K. However, since Doppler broadening depends on the width independent of the spacing, it is changed because of the change in the total width necessary to maintain constant strength functions.

$$\Gamma(E) = \Gamma(0)/\gamma(E)$$

For Ta182 at 100 kev Γ and thus $\bar{D}$ are reduced about 14%.

VIII. COMPARISON OF U-238 TRIX CALCULATIONS WITH OPTICAL MODEL RESULTS

Calculations of the infinitely dilute capture cross sections of U-238 were made with TRIX and compared with recent optical model calculations.⁸ The parameters for the two calculations were matched at $E = 0$. The results for each ℓ, J series for $\ell = 0, 1, 2$ are compared between 1 kev and 45 kev, the first inelastic scattering threshold, in Figure 1.

The comparison is excellent. The slight falling of the TRIX results relative to the optical model results at higher energies may be due to the energy dependence of $\bar{D}$ in the optical model calculation. The small discrepancies at lower energies may be due to the fact that TRIX accounts for the distributions of level widths by averaging over a sample of a few points whereas the optical model calculation evaluates the integral by numerical integration using many more points.

* Except for consideration of item 8 in the Introduction, Section I.

8. C. L. Dunford, AI-68-TDR-44 (3-26-68) and private communication.

IX. CONCLUSION

The theory of resonance cross sections has been reviewed in several areas. Prescriptions sufficient for precise calculation of unresolved resonance cross sections in fast assemblies were formulated. The TRIX code was modified to incorporate these improvements. The new code provides an improved inexpensive analysis of effective resonance cross sections. The improved cross sections permit more precise determinations of resonance reaction rates and Doppler coefficients in fast spectra as well as the spectra themselves.