GENERAL ATOMIC
DIVISION OF
GENERAL DYNAMICS

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GA-2527
Physics
TID-4500 (16th ed.)

A PROGRAM OF RESEARCH AND CALCULATIONS
OF RESONANCE ABSORPTION

FINAL REPORT

Contract AT(04-3)-167
Project Agreement No. 8
U. S. Atomic Energy Commission

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Project 96

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Date: *03/10/2006*

August 28, 1961

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ABSTRACT

An improved method for the calculation of resonance integrals has been developed and programmed for the IBM-7090. It consists in a direct numerical solution of the integral equation for the average flux in the absorber, and thus obviates the formerly used distinction between narrow and wide resonances. Cross sections are calculated, inclusive of Doppler broadening, interference scattering, and the $E^{-1/2}$ factor in the absorption cross section. The unresolved resonances are calculated in the narrow-resonance approximation under consideration of the Porter-Thomas distribution of neutron widths. Available options include (1) choice of geometry--spherical, cylindrical, slab, and homogeneous; (2) Dancoff correction for absorbers of arbitrary transparency; and (3) integral treatment of admixed heavy scatterers.

The only input data required are the resonance parameters and specification of temperature, composition, and geometry. Everything else is handled automatically. The average computing time for the cross sections in one resonance is 2 millihours (mh), for one resonance integral is 0.5 mh, and for one set of unresolved resonances is 15 mh.

Resonance integrals have been computed for uranium and thorium metal and UO_2 and ThO_2 rods of various diameters and different temperatures and for homogeneous mixtures of uranium with moderators. Quantitative agreement with the best available measurements is reached for U^{238} , with respect to the absolute values of the resonance integrals as well as with respect to their temperature dependence. For Th^{232} , the agreement is not quite as perfect. The differences can, however, be traced to inconsistencies in the available cross-section data.

Examples are also given for the treatment of the Dancoff correction and a full integral treatment of admixed moderators.

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I. GENERAL METHOD

1. PROGRAM DISCUSSION

The theory of resonance absorption was developed during the days of the Manhattan Project by Wigner.⁽¹⁾ His work anticipated most of the later developments. An independent Russian treatment by Gourevich and Pomeranchouk⁽²⁾ looked superficially quite different, but was shown by Wigner⁽³⁾ to be different only in bookkeeping and emphasis. In the absence of sufficient resonance data, both theories were used only to produce semi-empirical formulas for the representation of experimental data.

One of the important points of Wigner's approach⁽¹⁾ was the recognition of the difference between the behavior of wide low-lying resonances and that of narrow resonances. The distinction is generally made according to whether or not

$$\Gamma_p \cong \Gamma \sqrt{\frac{\sigma_o}{\sigma_p}} \gtrless E_o \alpha_o, \quad (1.1)$$

that is, whether the practical width is Γ_p larger or smaller than the maximum energy loss in a collision. The practical width is the interval over which the resonance cross section is larger than the potential cross section. In Eq. (1.1), Γ is the natural width, σ_o is the cross section at resonance, σ_p is the potential scattering cross section, E_o is the resonance energy, and

$$\alpha = \frac{4A}{(A+1)^2}. \quad (1.2)$$

The first reasonably successful attempt to calculate resonance absorption from resonance data was made in 1956 by Dresner,⁽⁴⁾ who evaluated the resonance integrals for homogeneous assemblies. This was followed in 1958 by three independent calculations of resonance integrals

for heterogeneous assemblies by Adler, Hinman, and Nordheim,⁽⁵⁾ by Dresner,⁽⁶⁾ and by Chernick and Vernon,⁽⁷⁾ which were based on the same physics concepts and which yielded very similar results. In these calculations, the wide resonances are treated in the infinite-mass, or IM, approximation and the narrow resonances in the NR approximation, and provision has been made for the unresolved resonances. The main distinction is in the mathematical approximations. Chernick and Vernon, and to a lesser extent Dresner, try to use analytical procedures as much as possible, whereas Adler, Hinman, and Nordheim give an extensive set of tables, calculated with the actual escape probabilities and Doppler-broadened line forms, from which the resonance integrals can be interpolated for a wide variety of geometries and all temperatures. The latter method has been quite successful and has been widely applied with generally very good results. However, some important effects have been left out. The most serious of these is the necessity of using either the NR or the IM approximation. While the errors produced by this alternative tend to cancel out statistically, Spinney⁽⁸⁾ has pointed out that the errors for individual resonances may be quite large. Chernick and Vernon⁽⁷⁾ have introduced, therefore, an iteration procedure which closes the gap considerably. The ultimate in this type of effort is represented by the work of Rothenstein,⁽⁹⁾ who starts from analytical expressions to which he then adds a large number of corrections, partly analytical and partly to be read from tables. Aside from the fact that it is not evident that all these corrections can be simply added, the procedure is nearly self-defeating in its complexity when over fifty resonances have to be treated, as in U^{238} or Th^{232} .

An alternative method, which makes it possible to treat cases of arbitrary complication, is the Monte Carlo method. It has been successfully applied to resonance absorption by Richtmyer.⁽¹⁰⁾⁽¹¹⁾ However, the nature of the Monte Carlo method, and the very long times required to achieve reasonable accuracy with it, makes it very expensive to apply to production problems.

Nordheim,⁽¹²⁾ in his general discussion of resonance absorption, suggested, therefore, a direct numerical integration of the integral equation for the average collision density in the absorber. The present report deals with the implementation of this program. Part I describes the method of calculation, Part II presents a comparison with experimental data, and the details of the FORTRAN IBM-7090 code are given in GA-2525. Since the method employed is a numerical one, it has been possible to include effects which are otherwise difficult to treat. These include details of the cross sections, in particular, interference between potential and resonance scattering and the $E^{-1/2}$ factor in the absorption cross section; and the incorporation of the Dancoff correction for tight lattices in a form that is applicable to absorbers of arbitrary transparency.

As is shown in Part II, quantitative agreement has been reached with the newest experimental data on U^{238} , the resonance structure of which is the best known. This agreement covers the absolute values of the resonance integrals for a wide range of geometries, as well as their temperature coefficients. This shows, firstly, that resonance absorption can be calculated from resonance data, if the latter are sufficiently well known, and, secondly, that no physically important effects are left out in our treatment.

In the development of the program, great care has been taken to ensure a numerical accuracy so high that there are no limitations imposed by this factor, the greatest possible flexibility, and ease of practical application. In order to provide flexibility, a great number of options are made available. They include the following:

1. Choice of geometry--spherical, cylindrical, plane, and homogeneous. The latter makes it possible to test the rational approximation for the escape probabilities.
2. Incorporation of the Dancoff correction for tightly packed lattices. This makes the method available for a great variety of geometries.
3. Use of the full integral treatment for admixed heavy scatterers.

4. Use of the NR or the IM approximation when desired.
5. Retention or omission of interference scattering.
6. Adjustment of mesh size and integration intervals when desired.

The program is fully automatic, that is, it selects normally suitable mesh sizes and integration intervals by itself. The only input data required are the resonance parameters and specifications for temperature, composition, and geometry for the exact cases desired. The time for the computation of a set of cross sections for one resonance is about 2 mh. The cross sections are stored on tape and can be reused. Evaluation of one resonance integral takes about 0.5 mh and calculation of one set of unresolved resonances requires 15 mh. A complete calculation at 300°K of a resonance integral for U^{238} , for instance, which has 54 resolved resonances up to 1000 ev, for six geometries takes about 500 mh. The time may be somewhat longer at higher temperatures and with the integral treatment of admixed scatterers. The output is normally only the resonance integrals for each resonance and their algebraic sum. If desired, however, the cross sections and the collision densities can also be printed out.

Although the present program represents a fast and accurate method for computing resonance absorption, its availability does not mean that all problems in this field have been solved. A highly desirable next step would be the simultaneous treatment of two not widely separated resonances, which could be achieved with minor modification of the present code. Such a method would give an answer to the problems of interference between resonances and of mixtures of different resonance absorbers.

It is also to be remembered that the theory is adapted to the case of generally well-separated resonances, so that flux recovery can take place between them.

In the present method, the spatial distribution of absorption is not explicitly brought out. In fact, it is in this area that errors remain in the method. Though apparently these do not influence the results to any

appreciable extent, a closer study would seem to be very desirable. This could be done in part by analytical studies and in part by a Monte Carlo treatment of selected cases.

2. EQUATIONS TO BE SOLVED

The physical basis of the theory of resonance absorption has recently been discussed by the author,⁽¹²⁾ and we need here only a short recapitulation of the equations to be solved.

In the case of a homogeneous mixture of an absorber species, index 0, and a nonabsorbing moderator species, index 1, the flux distribution in energy $\phi(E)$ is determined by the integral equation

$$\phi(E)\Sigma_{t_0} = \frac{1}{\alpha_0} \int_E^{E/(1-\alpha_0)} \phi(E')\Sigma_{s_0} \frac{dE'}{E'} + \frac{1}{\alpha_1} \int_E^{E/(1-\alpha_1)} \phi(E')\Sigma_{s_1} \frac{dE'}{E'} , \quad (2.1)$$

where Σ_t and Σ_s are the macroscopic total and scattering cross sections. The two integrals on the right side represent the source terms due to scattering by the absorber and moderator, and the term on the left side the total removal rate. Dividing by the absorber density, N_0 , gives

$$\phi(E)\sigma_t = \frac{1}{\alpha_0} \int_E^{E/(1-\alpha_0)} \phi(E')\sigma_{s_0} \frac{dE'}{E'} + \frac{1}{\alpha_1} \int_E^{E/(1-\alpha_1)} \phi(E')\sigma_{s_1} \frac{dE'}{E'} , \quad (2.2)$$

where all cross sections are referred to one absorber nucleus. Above the resonance, the only cross sections are the potential scattering cross section of the absorber, σ_{p_0} , and of the scatterer, σ_{s_1} , and Eq. (2.2) admits the solution

$$\phi_{as} = \frac{1}{E} . \quad (2.3)$$

The resonance integral, I , is defined as

$$I = \int \phi \sigma_{a_0} dE \quad (2.4)$$

for the solution with the asymptotic behavior (Eq. (2.3)). It represents the microscopic effective cross section of the absorber. The escape probability through the resonance is

$$p_i = 1 - \frac{I_i}{\xi \sigma_s} \cong e^{-(I_i / \overline{\xi \sigma_s})}, \quad (2.5)$$

where

$$\overline{\xi \sigma_s} = \xi_0 \sigma_{p_0} + \xi_1 \sigma_{s_1}$$

and the escape probability through many resonances is

$$P = \prod p_i = \prod \left(1 - \frac{I_i}{\xi \sigma_s} \right) \cong e^{-(\sum I_i / \overline{\xi \sigma_s})} \quad (2.6)$$

For numerical work, it is useful to introduce the more slowly varying collision density

$$F = \phi \sigma_t \quad (2.7)$$

and the lethargy

$$u = \log \frac{E_1}{E}, \quad (2.8)$$

where E_1 is an energy above which the asymptotic form of the collision density,

$$F_{as} = (\sigma_{p_0} + \sigma_{s_1}) \frac{e^u}{E_1}, \quad (2.9)$$

holds. The integral equation for F then becomes

$$F(u) = \frac{1}{\alpha_0} \int_{u-\Delta_0}^u F(u') \frac{\sigma_{s0}}{\sigma_t} du' + \frac{1}{\alpha_1} \int_{u-\Delta_1}^u F(u') \frac{\sigma_{s1}}{\sigma_t} du' , \quad (2.10)$$

where

$$\Delta = \log \frac{1}{1 - \alpha} , \quad (2.11)$$

σ_t is the total cross section per absorber nucleus, and the resonance integral is

$$I = E_1 \int F(u) \frac{\sigma_{a0}}{\sigma_t} e^{-u} du . \quad (2.12)$$

Equation (2.10) can be solved numerically with the boundary condition (2.9). Since the energy loss in moderator collisions is generally large, it is sufficient in most cases to use the narrow-resonance (NR) approximation for the moderator term, that is, to insert for $F(u')$ its asymptotic value (2.9). One then obtains

$$F(u) = \frac{1}{\alpha_0} \int_{u-\Delta_0}^u F(u') \frac{\sigma_{s0}}{\sigma_t} du' + \sigma_{s1} \frac{e^{-u}}{E_1} . \quad (2.13)$$

In the heterogeneous case, we assume a lattice of absorber lumps--again, index 0--imbedded in a moderating medium--again, index 1--and refer all quantities to single absorber nuclei. For instance, the moderator scattering cross section per absorber nucleus is

$$\sigma_{s1} = (\sigma_{s1})_{\text{actual}} \frac{N_1 V_1}{N_0 V_0} . \quad (2.14)$$

With this notation, we can write the integral equation for the average collision densities in the two media, following Chernick⁽¹³⁾ and Rothenstein,⁽⁹⁾

in the form

$$F_0 = (1 - P_0) \frac{1}{\alpha_0} \int_{u-\Delta_0}^u F_0 \frac{\sigma_{s_0}}{\sigma_{t_0}} du' + P_1 \frac{1}{\alpha_1} \int_{u-\Delta_1}^u F_1 \frac{\sigma_{s_1}}{\sigma_{t_1}} du' , \quad (2.15a)$$

$$F_1 = (1 - P_1) \frac{1}{\alpha_1} \int_{u-\Delta_1}^u F_1 \frac{\sigma_{s_1}}{\sigma_{t_1}} du' + P_0 \frac{1}{\alpha_0} \int_{u-\Delta_0}^u F_0 \frac{\sigma_{s_0}}{\sigma_{t_0}} du' . \quad (2.15b)$$

Here, the P_i are the escape probabilities, that is, the probabilities that a neutron scattered into the lethargy, u , in one medium will make its next collision in the other medium. The asymptotic solutions, valid in a region where

$$\sigma_{t_0} = \sigma_{s_0} = \sigma_{p_0} \quad \text{and} \quad \sigma_{t_1} = \sigma_{s_1} , \quad (2.16)$$

are easily verified to be (under the reciprocity condition (2.19), below)

$$F_0 \text{ as } = \sigma_{p_0} \frac{e^u}{E_1} , \quad F_1 \text{ as } = \sigma_{s_1} \frac{e^u}{E_1} , \quad (2.17)$$

and the resonance integral remains of the form (2.12), that is,

$$I = E_1 \int F_0 \frac{\sigma_{a_0}}{\sigma_{t_0}} e^{-u} du . \quad (2.18)$$

Generalizations to mixtures of materials are obvious.

Equations (2.15a) and (2.15b) represent an empty form unless the escape probabilities are specified. It is the basic assumption in all current theories of resonance absorption that a sufficient approximation is achieved by calculating these functions for a flat source in the respective media. The results of the present work show that this procedure yields results in quantitative agreement with experience. This must be due in part to

compensation of errors. The actual source distribution in the absorber will be peaked at the surface and the actual escape probability will be larger than P_o . On the other hand, an error of opposite sign is introduced by the fact that the flux in the moderator will be depressed near the interface. It would seem to be important that this compensation be studied in more detail.

With the flat-source assumption, several results from transport theory are available. The most important relation is

$$P_o \sigma_{t_o} = P_l \sigma_{t_l}, \quad (2.19)$$

which follows from the reciprocity theorem, as has been shown under very general conditions by Rothenstein.⁽⁹⁾ The functions P_o then become for isolated lumps (that is, with a spacing of several mean free paths) functions of $\bar{r}/\lambda$, where

$$\bar{r} = \frac{4V_o}{S_o} \quad (2.20)$$

is the mean chord length in the absorber. These functions have been determined for simple geometries by Case, de Hoffmann, and Placzek.⁽¹⁴⁾ The case of closely packed assemblies is discussed below under "The Dancoff Correction."

With relation (2.19) and using the narrow-resonance approach for moderator scattering, that is, the $F_{l \text{ as}}$ from (2.17), we obtain an equation for F_o , which does not contain any reference to the moderator,

$$F_o(u) = (1 - P_o) \frac{1}{\alpha_o} \int_{u-\Delta_o}^u F_o(u') \frac{\sigma_{s_o}}{\sigma_{t_o}} du' + P_o \sigma_{t_o} \frac{e^u}{E_1}. \quad (2.21)$$

An obvious generalization for the case that some scatterer of cross section σ_m per absorber atom is mixed in with the absorber yields

$$F(u) = (1 - P_o) \left[\frac{1}{\alpha_o} \int_{u-\Delta_o}^u F(u') \frac{\sigma_{s_o}}{\sigma_{t_o} + \sigma_m} du' + \frac{1}{\alpha_m} \int_{u-\Delta_m}^u F(u') \frac{\sigma_m}{\sigma_{t_o} + \sigma_m} du' \right] + P_o (\sigma_{t_o} + \sigma_m) \frac{e^u}{E_1} . \quad (2.22)$$

If the energy loss in scattering by the admixture is large compared with the line width, the narrow-resonance approximation can be employed and (2.22) simplified to

$$F(u) = (1 - P_o) \frac{1}{\alpha_o} \int_{u-\Delta_o}^u F(u') \frac{\sigma_{s_o}}{\sigma_{t_o} + \sigma_m} du' + [P_o \sigma_{t_o} + \sigma_m] \frac{e^u}{E_1} . \quad (2.23)$$

The asymptotic solution in both cases is

$$F_{as} = (\sigma_{p_o} + \sigma_m) \frac{e^u}{E_1} \quad \text{for} \quad u \leq 0 . \quad (2.24)$$

The homogeneous case is regained from (2.22) or (2.23) by simply putting $P_o = 0$ (no escape from the medium). The resonance integral is always given by Eq. (2.18).

Our program consists now in a direct numerical solution of equations of the type (2.22) or (2.23). We actually admit up to three integrals for different substances, one of which is the absorber. The integrations are carried out stepwise by Simpson's rule. The necessary details will be discussed in the following section.

In former times, the starting point was either the narrow-resonance or the infinite-mass approximation. In the former, the asymptotic form of $F(u)$ is also inserted in the absorber integral, which yields

$$\text{NR: } F(u) = [\sigma_{p_o} + \sigma_m + P_o(\sigma_{t_o} - \sigma_{p_o})] \frac{e^u}{E_1}, \quad (2.25)$$

$$I = \int \frac{\sigma_{a_o}}{\sigma_{t_o} + \sigma_m} [\sigma_{p_o} + \sigma_m + P_o(\sigma_{t_o} - \sigma_{p_o})] du.$$

In the latter, the limit $\alpha_o \rightarrow 0$ is taken, which makes the absorber integral a δ function, yielding

$$\text{IM: } F(u) = (1 - P_o)F(u) \frac{\sigma_{s_o}}{\sigma_{t_o} + \sigma_m} + (P_o \sigma_{t_o} + \sigma_m) \frac{e^u}{E_1}, \quad (2.26)$$

$$I = \int \frac{\sigma_{a_o}}{\sigma_{t_o} + \sigma_m} \frac{\sigma_{t_o} (P_o \sigma_{t_o} + \sigma_m)}{\sigma_{t_o} - (1 - P_o) \sigma_{s_o}} du.$$

Chernick and Vernon⁽⁷⁾ and Rothenstein⁽⁹⁾ have sought to improve these results by recycling the collision densities from (2.25) and (2.26) through the integral Eq. (2.21). This can be done analytically only with neglect of the Doppler broadening. Such a procedure is obviated here, since we solve the integral equation directly. Rothenstein⁽⁹⁾ starts from the analytic expression in the absence of Doppler broadening, and with the rational approximation for P_o , and adds then, as already mentioned, a large number of corrections, obtained approximately, for the above recycling, the Doppler effect, the interference scattering, and the rational approximation. All these effects are included in our calculations.

There is one correction introduced by Rothenstein which is not included in our treatment. For the wide resonances, he uses in (2.15b) the IM approximation for the absorber integral and the NR approximation for the moderator integral. The resultant expression for F_1 is then introduced into Eq. (2.15b) to produce a correction for the IM approximation.

The result obtained with all approximations cited above is

$$\Delta I_m = - \frac{I_2^2}{2\sigma_{s1}\alpha_1} \cong - \frac{I_2^2}{4\xi\sigma_s}, \quad (2.27)$$

to be applied only to the wide resonances. I_2 is the IM resonance integral itself. This correction is normally quite small and could be added to our result. It is doubtful, however, whether this correction is a real one. It does not occur when the NR approximation is used for the absorber, and since the integral equation describes an intermediate behavior, only an uncertain fraction of the correction would be applicable.

3. THE DETAILS OF THE CALCULATION

A. Method of Integration

The equations for the collision density in the absorber are of the general form

$$F(u) = A(u) \int_{u-\Delta_0}^u F(u')R(u') du' + B(u), \quad (3.1)$$

where A , B , and R are known functions of the lethargy, u , and where $F(u)$ is assumed to have its known asymptotic form (compare with (2.24)) for $u \leq 0$. We introduce a mesh equally spaced in u , so that

$$\epsilon n = \Delta_0 = \log \frac{1}{1 - \alpha_0}, \quad (3.2)$$

where n is an even integer. The integral in Eq. (3.1) is then evaluated by Simpson's rule as follows:

$$\begin{aligned} \int_{u_i - \epsilon n}^{u_i} F(u')R(u') du' = & \frac{\epsilon}{3} \left[F_{i-n} R_{i-n} + 4 \sum_{\ell=0}^{(n-2)/2} F_{i-n+1+2\ell} R_{i-n+1+2\ell} \right. \\ & \left. + 2 \sum_{m=0}^{(n-4)/2} F_{i-n+2+2m} R_{i-n+2+2m} + F_i R_i \right]. \quad (3.3) \end{aligned}$$

Insertion of Eq. (3.3) into Eq. (3.1) leads to the recurrence formula

$$F_i \left(1 - \frac{\epsilon}{3} A_i R_i \right) = \frac{\epsilon}{3} A_i \left[F_{i-n} R_{i-n} + 4 \sum_{\ell=0}^{(n-2)/2} F_{i-n+1+2\ell} R_{i-n+1+2\ell} + 2 \sum_{m=0}^{(n-4)/2} F_{i-n+2+2m} R_{i-n+2+2m} \right] + B_i, \quad (3.4)$$

which permits a step-by-step evaluation of F_i .

In the event that there is more than one such integral, as in Eq. (2.22), a mesh has to be introduced so that

$$\epsilon n = \Delta_0, \quad \epsilon m = \Delta_1, \quad (3.5)$$

where both n and m are even integers. If the two intervals are not commensurate, one replaces, with a minimal loss of accuracy, α_1 and σ_1 with nearby values, so that their product, which represents the slowing-down power of the material, has the correct value.

The two-integral procedure permits an exact evaluation of Eq. (2.10) for homogeneous mixtures. For practical reasons, the number of back intervals ($u_1 < 0$) has been limited to 1000. In the case of light moderators and high-energy resonances, the prescription (3.5) may lead to values larger than this number. The code will then indicate this fact and will not perform any calculation. However, under these circumstances, the narrow-resonance approximation will be sufficient. This approximation will, of course, always have to be applied in the case of hydrogen as moderator or scatterer.

B. Computation of the Cross Sections

The proper definition of the Maxwell average for the Doppler-broadened cross sections is

$$\overline{\sigma(E)} = \frac{1}{\sqrt{\pi E} \Gamma_D} \int_0^\infty dE_r \sqrt{E_r} \sigma(E_r) e^{-(E_r - E)^2 / \Gamma_D^2}, \quad (3.6)$$

where

$$\Gamma_D = \sqrt{\frac{4EkT}{A}} \quad (3.7)$$

is the Doppler width, E_r the relative velocity between neutron and target nucleus, and E the neutron energy in the lab system. The Breit-Wigner one-level absorption and scattering cross sections are

$$\sigma_a = \sigma_o \frac{\Gamma_r}{\Gamma} \sqrt{\frac{E_o}{E}} \frac{1}{4(E - E_o)^2/\Gamma^2 + 1}, \quad (3.8a)$$

$$\sigma_s = \sigma_o \frac{\Gamma_{n_o}}{\Gamma} \frac{1}{4(E - E_o)^2/\Gamma^2 + 1} + \left(\sigma_o \sigma_{p_o} g \frac{\Gamma_n^o}{\Gamma} \right)^{1/2} \frac{2(E - E_o)/\Gamma}{4(E - E_o)^2/\Gamma^2 + 1} + \sigma_p \quad (3.8b)$$

The three terms in (3.8b) represent resonance, interference, and potential scattering, respectively. Γ_n^o is the neutron width at resonance,

$$\sigma_o = g 4\pi \lambda_o^2 \frac{\Gamma_n^o}{\Gamma} \quad (3.9)$$

is the cross section at resonance, and

$$g = \frac{2J + 1}{2(2I + 1)}, \quad (3.10)$$

the statistical factor due to nuclear spin, I , with J being the channel spin.

The introduction of (3.7) (with E_r) into (3.6) and the change of variables to

$$x = 2(E - E_o)/\Gamma, \quad y = 2(E_r - E)/\Gamma \quad (3.11)$$

yields, with minor neglects, the customary formulas

$$\overline{\sigma}_a = \frac{\Gamma_r}{\Gamma} \sqrt{\frac{E_o}{E}} \sigma_o \psi(\zeta, x), \quad (3.12a)$$

$$\overline{\sigma}_s = \frac{\Gamma_o}{\Gamma} \sigma_o \psi(\zeta, x) + \left(\sigma_o \sigma_{p_o} g \frac{\Gamma_o}{\Gamma} \right)^{1/2} \chi(\zeta, x) + \sigma_{p_o}, \quad (3.12b)$$

where

$$\zeta = \frac{\Gamma}{\Gamma_D} = \sqrt{\frac{A \Gamma^2}{4EkT}} \quad (3.13)$$

is the ratio of natural to Doppler width and

$$\psi = \frac{\zeta}{\sqrt{4\pi}} \int_{-\infty}^{+\infty} dy \frac{e^{-\zeta^2(x-y)^2/4}}{1+y^2}, \quad (3.14a)$$

$$\chi = \frac{\zeta}{\sqrt{4\pi}} \int_{-\infty}^{+\infty} \frac{2ydy}{1+y^2} e^{-\zeta^2(x-y)^2/4} = 2x\psi - \frac{4}{\zeta^2} \frac{d\psi}{dx}. \quad (3.14b)$$

Introduction of the variable $y = \tan u$ gives

$$\psi = \frac{\zeta}{\sqrt{4\pi}} \int_{-E/2}^{+E/2} e^{-\zeta^2(x-\tan u)^2/4} du. \quad (3.15)$$

The cross-section program uses the form (3.15), which is evaluated by a Gaussian quadrature. The function χ is evaluated by the expression on the right side in Eq. (3.14b). This procedure loses accuracy when $\zeta < 0.1$, whereas, on the other hand, the effect of interference scattering becomes very small. Therefore, interference scattering is neglected by the code whenever $\zeta < 0.1$ for $T = 273^\circ\text{K}$.

The cross sections are stored on tape for reuse. Thus, they have to be calculated only once for given resonance parameters and a given temperature.

C. Selection of the Mesh Size

The fastest-varying factor in the cross sections is the one due to Doppler broadening. The mesh size ϵ_1 in lethargy is, therefore, taken as

a fraction r of the Doppler width at 273°K :

$$\epsilon_1 = \frac{\Gamma_D(273^\circ)}{rE_o} = \frac{0.01723}{r} \sqrt{\frac{273}{AE_o}}. \quad (3.16)$$

The value

$$r = 5 + \frac{0.25}{\zeta} \quad (3.17)$$

was found to be suitable for all resonances in U^{238} and Th^{232} . With this choice, the cross sections at neighboring points differ always by less than a factor of two, and halving the mesh size introduces changes in the resonance integral only of the order of 10^{-4} . Expression (3.17) has therefore been built into the code. As an option, it can, however, be replaced by an arbitrary number.

The number of mesh points in the absorber integral is

$$n_1 = \frac{\Delta_o}{\epsilon_1}.$$

This will, of course, not automatically be an even integer. The procedure is then to take the next larger such integer, n , and to redefine a new ϵ as the actual mesh to be used, i. e.,

$$\epsilon = \frac{\Delta_o}{n}. \quad (3.18)$$

D. Integration Interval

The numerical integration has to be started at an energy E_1 above the resonance and to be terminated at an energy E_2 below it. Since the cross section in the wings of the resonance drops as $(E - E_o)^{-2}$, their contribution to the resonance integral decreases only as $(E_1 - E_o)^{-1}$, and a correction has to be found for the finite interval size. In the treatment of this problem, our aim has been to choose an interval large enough that the end correction can be evaluated by simple analytical approximations.

Normally, we take the integration interval as a multiple, s , of the practical width. This number is generally specified as 5, but it can be changed at the option of the user. The energy limits for the integration are thus taken as

$$E_{1,2} = E_o \pm \frac{s\Gamma}{2\sqrt{\beta}} = E_o \left(1 \pm \frac{s\Gamma}{2E_o\sqrt{\beta}} \right) \quad (3.19)$$

where, as usual,

$$\beta = \frac{\sigma_o}{\sigma_{p_o}}.$$

The limit in the variable x_1 is then

$$x_1 = \frac{s}{\sqrt{\beta}}. \quad (3.20a)$$

The lower lethargy limit is $u_1 = 0$, and the upper limit is

$$u_2 = \log \frac{E_1}{E_2} = \log \frac{1 + (s/2E_o\sqrt{\beta})}{1 - (s/2E_o\sqrt{\beta})}. \quad (3.20b)$$

The total number of mesh points over the resonance is

$$N = \frac{u_2}{\epsilon}. \quad (3.21)$$

Specification (3.19) is not sufficient for very large Doppler broadening (small ζ in Eq. (3.13)). Analytical approximations can only be found for energies where the asymptotic temperature-independent form of the cross section is adequate. This asymptotic behavior is

$$\psi(\zeta, x) \cong \frac{1}{1+x^2} \left[1 + \frac{2\zeta^2(3x^2-1)}{(1+x^2)^2} + \dots \right]. \quad (3.22)$$

The first term, $(1 + x^2)^{-1}$, gives a good enough approximation when

$$x_1 \zeta = \frac{2(E_1 - E_0)\zeta}{\Gamma} = \frac{s\zeta}{\sqrt{\beta}} > 20. \quad (3.23)$$

The program checks whether or not this condition is fulfilled. If not, it selects s on the basis of condition (3.23).

E. Outside Correction

For the wing corrections, which should at most amount to a few per cent of the total, drastic simplifications are permitted. With condition (3.23), the natural line shape can be employed. We utilize further the rational approximation for P_0 and either the NR or the IM approximation. For most of the resonances, we also can neglect the $E^{-1/2}$ factor in the absorption cross section.

If the energy interval from E_2 to E_1 is smaller than the maximum energy loss per collision, that is, if

$$E_1 - E_2 = x_1 \Gamma < \frac{4E_0}{A}, \quad (3.24)$$

we use the NR approximation and obtain for the wing correction

$$\Delta I = \left(\int_{E < E_2}^{E_2} + \int_{E > E_1}^{\infty} \right) \frac{\sigma_{a_0} (\sigma_{p_0} + \sigma_M)}{\sigma_{t_0} + \sigma_M} \frac{dE}{E}, \quad (3.25)$$

where

$$\sigma_M = \sigma_m + \sigma_e \quad (\text{heterogeneous case}),$$

$$= \sigma_{s_1} \quad (\text{homogeneous case}).$$

Upon introduction of the unbroadened line form,

$$\psi = \frac{1}{1+x^2}, \quad \chi = \frac{2x}{x^2+1},$$

we obtain

$$\begin{aligned} \Delta I &= \frac{\Gamma \gamma \sigma_o \beta}{E_o} \frac{1}{2} \left(\int_{-\infty}^{+\infty} - \int_{-x_1}^{+x_1} \frac{dx}{1 + 2 + \gamma + \beta(1 + x^2)} \right) \\ &= \frac{\Gamma \gamma \sigma_o \beta}{E_o \sqrt{\beta(1 + \beta^2) - \gamma^2}} \frac{1}{2} \left(\pi - \tan^{-1} \frac{\beta x_1 + \gamma}{\sqrt{\beta(1 + \beta) - \gamma^2}} + \tan^{-1} \frac{-\beta x_1 + 2}{\sqrt{\beta(1 + \beta) - \gamma^2}} \right), \end{aligned} \quad (3.26)$$

where

$$\beta = \frac{\sigma_{p_o} + \sigma_M}{\sigma_o}, \quad \gamma = \left(\frac{\Gamma_n \sigma_{p_o}}{\Gamma_g \sigma_o} \right)^{1/2}. \quad (3.27)$$

If

$$E_1 - E_2 = x_1 \Gamma > \frac{4E_o}{A}, \quad (3.28)$$

the IM approximation is used. This is achieved simply by putting $\gamma = 0$ and replacing β with

$$\beta_1 = \frac{\sigma_M}{\sigma_o} \frac{\Gamma}{\Gamma_\gamma}. \quad (3.29)$$

The above approximations are not sufficient for the lowest resonances, where the $E^{-1/2}$ factor in the absorption cross section cannot be ignored and where some cutoff has to be introduced to eliminate the $1/v$ part of the cross section. In these cases, the IM approximation is always satisfactory (see below), that is,

$$I = \int \frac{\sigma_{a_o} \sigma_M}{\sigma_a + \sigma_M} \frac{dE}{E}. \quad (3.30)$$

With

$$\sigma_a = \frac{\Gamma \gamma \sigma_o}{\Gamma} \sqrt{\frac{E_o}{E}} \frac{1}{1 + x^2}, \quad x = \frac{2(E - E_o)}{\Gamma}, \quad (3.31)$$

we obtain

$$\Delta I = \frac{\sigma_M \Gamma}{E_o} \frac{1}{2} \int_{|x| > x_1} \frac{dx}{[1 + x(\Gamma/2E_o)] [1 + \beta_1(1 + x^2) \sqrt{1 + x\Gamma/2E_o}]}, \quad (3.32)$$

with

$$\beta_1 = \frac{\sigma_M \Gamma}{\sigma_o \Gamma \gamma} > \frac{\sigma_{p_o}}{\sigma_o}, \quad (3.33)$$

where the lower limit will still have to be defined. Now x_1 is defined by (3.11) and (3.19) as

$$x_1 \geq \frac{s\Gamma^2}{\Gamma} = \frac{10}{\sqrt{\beta}} > \frac{10}{\sqrt{\beta_1}}. \quad (3.34)$$

Since, generally, $\beta, \beta_1 \ll 1$ and, according to (3.34), $\beta_1 x_1^2 \cong 100$, we obtain in very good approximation

$$\begin{aligned} \Delta I &= \frac{\sigma_M \Gamma}{E_o \beta_1} \frac{1}{2} \int_{|x| > x_1} \frac{dx}{\left(1 + \frac{x\Gamma}{2E_o}\right)^{3/2} x^2} \\ &= \frac{\sigma_o \Gamma \Gamma \gamma}{4E_o^2} \int_{|z| > z_1} \frac{dz}{(1+z)^{3/2} z^2}, \end{aligned} \quad (3.35)$$

where

$$z = \frac{x\Gamma}{2E_o} = \frac{E - E_o}{E_o}. \quad (3.36)$$

The integral in (3.35) diverges for $z_1 \rightarrow -1$, i. e., $E \rightarrow 0$, owing to the $1/v$ cross section and other approximations made. This region is, of course, physically not wanted and we have to introduce a lower limit, z_o . The choice of z_o is to some extent arbitrary. We select the value for which the

integrand in (3.35) has its minimum, which occurs at $z_0 = -4/7$. The elementary integration of (3.35) then yields

$$\Delta I = \frac{\sigma_0}{4} \frac{\Gamma\Gamma}{E_0^2} (I_- + I_+) , \quad (3.37)$$

where

$$I_- = \frac{1 - 3z_1}{z_1 \sqrt{1 - z_1}} + \frac{3}{2} \log \frac{1 + \sqrt{1 - z_1}}{1 - \sqrt{1 - z_1}} - 0.44055 ,$$

$$I_+ = \frac{1 + 3z_1}{z_1 \sqrt{1 + z_1}} - \frac{3}{2} \log \frac{\sqrt{1 + z_1} + 1}{\sqrt{1 + z_1} - 1} . \quad (3.38)$$

These formulas are used whenever $z_1 = (E - E_0)/E_0 > 0.1 > 2/A$. This guarantees that the IM approximation is applicable. Otherwise, the preceding method is chosen.

A special case arises if $z_1 > z_0 = 4/7$. This means that the interval selected according to the criteria given previously under "Integration Interval" extends below the minimum of the integrand in (3.35). In this case, only the contribution I_+ from above the resonance is taken, and the main integration is carried down only to $E_2 = (3/7)E_0$ or the lethargy

$$u_2^* = \log \frac{1 + (s\Gamma/2E_0 \sqrt{\beta})}{3/7} . \quad (3.39)$$

This actually happens in the 6.7-ev resonance for U^{238} , where the lower cutoff then is taken as $E_2 = 2.87$ ev.

All the above case distinctions are carried out automatically by the program.

The end corrections are shown separately in the printout. With our procedure, they never amount to more than a few per cent of the main part.

F. The Dancoff Correction

The Dancoff correction for tight lattices, where the different absorber lumps shade each other, is incorporated in the form derived in Ref. 12.

It consists in replacement of the escape probability, P_o , by the corrected form

$$P_o^* = P_o \frac{1 - C}{1 - (1 - \sum_t \bar{r} P_o) C}, \quad (3.40)$$

which is a good approximation for lumps of any degree of grayness. The correction C itself has to be supplied by the user. The most useful reference for its evaluation is the report by Pershagen and Carlvik.⁽¹⁵⁾

An alternative form of the correction, also given in Ref. 12, is the simple substitution in the argument in P_o ,

$$P_o^* (\sum_t \bar{r}) = P_o \left(\frac{\sum_t \bar{r}}{1 - C} \right), \quad (3.41)$$

which is only less good for very transparent absorbers. This correction in $\bar{r}$ also has to be used wherever the rational approximation is employed, i. e., in the wing corrections and in the unresolved resonances. In these cases, a corrected escape cross section,

$$\sigma_e^* = \sigma_e (1 - C) = \frac{1 - C}{N_o \bar{r}}, \quad (3.42)$$

is employed.

G. The Unresolved Resonances

Since the resonances in U^{238} and Th^{232} are now resolved up to ~ 1000 ev, the contribution of the unresolved part is generally less than 10% of the total, and considerable simplifications in its evaluation are permissible. The most important one is that we can again use the rational approximation, which makes it unnecessary to introduce a surface term.

The method for s-wave resonances is the same as in Ref. 5, that is, the narrow-resonance approximation is used and an average over the Thomas-Porter distribution of neutron widths is taken. The average of

the function J ,

$$J = \int_0^{\infty} \frac{\psi}{\psi + \beta} dx, \quad (3.43)$$

is then for a given energy

$$\bar{J} = \frac{1}{\sqrt{2\pi G}} \int_B^{\infty} \frac{d\zeta}{\sqrt{\zeta - B}} J(\zeta, \beta) e^{-(\zeta - B)/2G}, \quad (3.44)$$

where

$$G = \langle \Gamma_n^0 \rangle \sqrt{\frac{A}{4kT}}, \quad B = \Gamma_\gamma \sqrt{\frac{A}{4EkT}},$$

$$C = 3.842 \times 10^{-7} (\sigma_p + \sigma_m + \sigma_e) E, \quad \beta = \frac{C\zeta}{\zeta - B}. \quad (3.45)$$

The resonance integral itself is then

$$I_{\text{unres}} = \frac{(\sigma_p + \sigma_m + \sigma_e)}{D} \int_{E_C}^{\infty} \bar{J}(E) dE = \frac{(\sigma_p + \sigma_m + \sigma_e)}{D} \int_0^{\infty} \bar{J}(n) dn, \quad (3.46)$$

$$n = \log \frac{E}{E_C}.$$

$\langle \Gamma_n^0 \rangle$ is the average neutron width at 1 ev, D the level spacing, and E_C the cutoff energy above which the resonances are considered unresolved. The inclusion of the escape cross section, σ_e , takes care of the surface term in heterogeneous geometries. The integrations in (3.44) and (3.46) are carried out numerically by using tables of the J function. It was found necessary to extend the previous tables by Dresner⁽¹⁶⁾ and by Adler, Hinman, and Nordheim⁽⁵⁾ to smaller ζ values in order not to lose accuracy at high temperatures. This has been done recently by Nather and Nordheim,⁽¹⁷⁾ and their values have been incorporated in the present code. The upper limit in the integral (3.44) has been taken at $\zeta = 1$ and that in

(3.46) at $n = 5$. This program for the unresolved resonances is actually separate from the one for the resolved resonances, and thus has to be prepared independently.

Below 30 keV, p-wave resonances have such a small cross section at maximum--further reduced drastically by the Doppler effect--that there is no appreciable self-shielding left and the infinite dilution limit can be taken (compare with Ref. 9). The same applies for all resonances above 30 keV. Both of these contributions will thus be independent of temperature and, to a large extent, of geometry. They will, however, be somewhat dependent on the general disposition of the reactor under consideration, since the neutron spectrum will generally not be $1/E$ and may also be spatially dependent. The p-wave strength function is also not known with any accuracy. Therefore, no generally valid prescription can be given. It is recommended that unshielded, measured, average cross sections be used down to 30 keV, and that for U^{238} and Th^{232} an additive contribution of ~ 1 barn in I be added for the p-wave resonances below 30 keV.

II. NUMERICAL RESULTS: COMPARISON WITH EXPERIMENTS

4. RESONANCE INTEGRALS FOR U^{238}

The final verification of a theory is furnished by its agreement with experimental data. In the case of resonance absorption, a sufficiently accurate knowledge of the resonance parameters is required. It is known that the experimental values obtained by different observers for the resonance integrals and, in particular, their temperature coefficients vary considerably. A good recent summary of the experimental data is given by Dresner⁽¹⁶⁾ and, for the Doppler coefficient, by Pearce.⁽¹⁸⁾

In the work described here, we found that the more refined the calculation became and the better the resonance data that were used, the closer we approached the results of Hellstrand and his group.^(19, 20, 21) For U^{238} , the agreement is now within the remaining uncertainties, and we will, therefore, as far as possible, compare the calculated values with those measured by Hellstrand. For U^{238} , the resonance data have been taken from the Brookhaven National Laboratory compilation.⁽²²⁾ These are shown in Table 1. Table 2 gives the numerical results for homogeneous mixtures with scatterers of total cross section σ_M per uranium nucleus at 300° and 600° K. Table 3 presents the results for widely separated uranium-metal rods as a function of their radius and temperature, and Table 4 presents the same results for UO_2 rods. The data for unresolved resonances cover only the s resonances, and an additive constant independent of temperature and, to some extent, of composition and geometry should be added for higher l resonances.

For the homogeneous mixtures (Table 2), it is interesting to note that the unresolved resonances saturate considerably earlier than the resolved resonances. The Doppler coefficient goes through a maximum at

Table 1
 RESONANCE PARAMETERS FOR U^{238} *
 (In electron volts)

E_o	Γ_n	Γ_γ	E_o	Γ_n	Γ_γ
6.7	1.52×10^{-3}	2.46×10^{-2}	536.0	5.40×10^{-2}	2.46×10^{-2}
21.0	8.90×10^{-3}		557.0	10.00×10^{-4}	
36.9	3.25×10^{-2}		581.0	4.20×10^{-2}	
66.3	2.50×10^{-2}		596.0	6.60×10^{-2}	
81.3	2.10×10^{-3}		605.0	6.00×10^{-4}	
90.0	9.00×10^{-5}		621.0	3.90×10^{-2}	
102.5	6.50×10^{-2}		629.0	9.00×10^{-3}	
116.5	1.50×10^{-2}		662.0	1.25×10^{-1}	
145.6	8.00×10^{-4}		680.0	1.30×10^{-3}	
165.2	3.50×10^{-3}		695.0	5.30×10^{-2}	
189.6	1.35×10^{-1}		710.0	1.70×10^{-2}	
208.5	5.50×10^{-2}		723.0	1.47×10^{-2}	
237.5	3.20×10^{-2}		732.0	4.25×10^{-3}	
264.5	2.30×10^{-4}		766.0	9.00×10^{-3}	
274.0	2.70×10^{-2}		782.0	3.00×10^{-3}	
291.0	1.90×10^{-2}		792.0	1.10×10^{-2}	
311.5	10.00×10^{-4}		825.0	6.00×10^{-2}	
348.0	4.50×10^{-2}		855.0	1.30×10^{-1}	
377.0	1.50×10^{-3}		859.0	6.00×10^{-2}	
398.5	10.00×10^{-3}		867.0	2.20×10^{-3}	
411.0	1.70×10^{-2}		896.0	1.30×10^{-3}	
435.0	1.40×10^{-2}		909.0	9.00×10^{-2}	
455.0	7.00×10^{-4}		928.0	3.70×10^{-2}	
464.0	7.00×10^{-3}		940.0	1.95×10^{-1}	
479.0	4.50×10^{-3}		960.0	1.90×10^{-1}	
490.0	10.00×10^{-4}		983.0	10.00×10^{-4}	
519.0	3.70×10^{-2}		995.0	4.00×10^{-1}	
Unresolved Resonances					
$\Gamma_\gamma = 2.46 \times 10^{-2}$ ev			$D = 18.5$ ev		
$\langle \Gamma_n^o \rangle = 1.74 \times 10^{-3}$ ev			$E_C = 1005$ ev		

* Taken from Ref. 22.

Table 2
 RESONANCE INTEGRALS FOR HOMOGENEOUS MIXTURES
 OF U^{238} WITH MODERATOR OF SCATTERING
 CROSS SECTION σ_M PER ABSORBER ATOM
 (In barns)

	σ_M					
	80 b	200 b	500 b	1250 b	3775 b	9440 b
300°K						
Resolved	21.09	33.39	53.31	84.46	138.81	186.64
Unresolved	1.86	2.24	2.54	2.73	2.84	2.88
Total	22.95	35.63	55.85	87.19	141.65	189.52
600°K						
Resolved	22.49	36.41	59.40	95.03	152.79	199.93
Unresolved	2.01	2.36	2.62	2.78	2.87	2.90
Total	24.50	38.77	62.02	97.81	155.66	202.83
$\frac{I_{600} - I_{300}}{I_{300}}$	0.068	0.088	0.108	0.122	0.099	0.070
$\frac{I_{300}}{\sqrt{10 + \sigma_M}}$	2.42	2.46	2.47	2.47	2.31	1.92

Table 3
 RESONANCE INTEGRALS FOR URANIUM-METAL
 RODS OF RADIUS a AND DENSITY OF 18.7 G CM^{-3}
 AT VARIOUS TEMPERATURES
 (In barns)

	Radius, a				
	0.1055 cm	0.211 cm	0.422 cm	0.844 cm	1.69 cm
300°K					
Resolved	25.29	18.04	12.91	9.31	6.75
Unresolved	1.96	1.67	1.40	1.18	1.03
Total	27.25	19.71	14.31	10.49	7.78
600°K					
Resolved	27.09	19.00	13.45	9.64	6.99
Unresolved	2.10	1.82	1.55	1.33	1.17
Total	29.19	20.82	15.00	10.97	8.16
900°K					
Resolved	28.58	19.80	13.89	9.88	7.13
Unresolved	2.18	1.91	1.65	1.43	1.27
Total	30.76	21.71	15.54	11.31	8.41

Table 4

RESONANCE INTEGRALS FOR UO_2 RODS OF RADIUS a AND
 DENSITY OF 10.2 G CM^{-3} AT VARIOUS TEMPERATURES
 (In barns)

	Radius, a				
	0.125 cm	0.25 cm	0.50 cm	1.00 cm	2.00 cm
300°K					
Resolved	34.40	24.62	18.01	13.59	10.74
Unresolved	2.21	1.94	1.68	1.46	1.30
Total	36.61	26.56	19.69	15.05	12.14
600°K					
Resolved	37.45	26.23	18.95	14.21	11.14
Unresolved	2.33	2.08	1.83	1.61	1.45
Total	39.78	28.31	20.78	15.82	12.59
900°K					
Resolved	40.00	27.75	19.81	14.71	11.50
Unresolved	2.40	2.17	1.92	1.71	1.54
Total	42.40	29.92	21.73	16.42	13.04
1200°K					
Resolved	42.21	28.99	20.50	15.11	11.75
Unresolved	2.45	2.22	1.99	1.78	1.62
Total	44.66	31.21	22.49	16.89	13.37
1500°K					
Resolved	44.23	30.17	21.16	15.52	12.03
Unresolved	2.49	2.27	2.04	1.83	1.67
Total	46.72	32.44	23.20	17.35	13.70

$\sigma_M \sim 1500$ b, and for not too large σ_M ,

$$I \sim \sqrt{\sigma_{p_0} + \sigma_M}$$

as predicted from a strongly simplified theory.⁽¹²⁾ Even at 9440 b, one is still quite a way from the infinite dilution limit of 268 b with our cross sections.

For heterogeneous assemblies, Table 5 gives a comparison of the old calculated values,⁽¹²⁾ the results of the present work, and the results of Hellstrand's empirical formula⁽¹⁹⁾ for $T = 300^\circ\text{K}$. In the new calculated values, the total values from Tables 3 and 4 have been increased by 1 b for the higher ℓ resonances, which value, as in Ref. 12, gives the best over-all fit.

It is seen that the differences between the old and new calculated total values are slight and much less than for individual resonances. The new values give, however, an improved fit with the experimental values for very thin rods, where the theory should be most accurate. Hellstrand⁽¹⁹⁾ estimates his errors to be within $\pm 2\%$. The actual agreement is everywhere better than this.

The temperature coefficient of the resonance integral is much more sensitive than its absolute value to the details of the calculation, and great accuracy is required in calculating this coefficient. Our new values are systematically smaller, by up to 20%, than those reported in Ref. (12). The temperature dependence is very well given by

$$I(T) = I_{300} [1 + \beta(\sqrt{T} - \sqrt{300})] . \quad (4.1)$$

Such a representation is preferable to listings of dI/dT , since the maximum calculated temperature swing can be utilized. The temperature coefficient, β , is also listed in Table 5. It is definitely nonlinearly dependent on the S/M ratio. As was already mentioned, experimental values scatter rather widely.⁽¹⁸⁾ Quantitative agreement is achieved, however, with the newest

Table 5

COMPARISON OF OLD AND NEW CALCULATED VALUES AND
VALUES FROM HELLSTRAND'S EMPIRICAL FORMULAS
FOR THE RESONANCE INTEGRALS OF URANIUM PLUS
VALUES OF THE TEMPERATURE COEFFICIENT, β

Uranium Metal (Density of 18.7)					
	Radius, a				
	0.1055 cm	0.211 cm	0.422 cm	0.844 cm	1.69 cm
	S/M				
	1.059	0.507	0.254	0.127	0.0634
Calculated, old	29.55	21.26	15.47	11.49	8.78
Calculated, new	28.25	20.71	15.31	11.49	8.78
$2.81 + 24.7 \sqrt{S/M}$	28.21	20.36	15.24	11.62	9.04
$\beta \times 10^2$	0.98	0.75	0.63	0.56	0.57
UO ₂ (Density of 10.2)					
	Radius, a				
	0.125 cm	0.25 cm	0.50 cm	1.0 cm	2.0 cm
	S/M				
	1.570	0.785	0.393	0.196	0.098
Calculated, old	38.06	28.06	20.82	16.09	13.03
Calculated, new	37.61	27.56	20.69	16.05	13.14
$4.45 + 26.6 \sqrt{S/M}$	37.76	27.95	21.10	16.23	12.79
$\beta \times 10^2$	1.26	1.00	0.79	0.67	0.55

measurements by Hellstrand, Blomberg, and Hörner,⁽²⁰⁾ as is shown in Table 6. The quoted limits of errors are those given by Hellstrand and co-workers.

The convergence between experimental and theoretical results for U^{238} strengthens the confidence in both, as well as in the available resonance data. In particular, we believe now that it is generally easier to calculate the Doppler coefficient than it is to measure it. We consider that our goal, a reliable calculation of resonance absorption from resonance data, has been achieved.

5. RESONANCE INTEGRALS FOR Th^{232}

Calculations similar to those for U^{238} have been made for Th^{232} . The resonance parameters used (up to 1000 ev) were those from the Columbia University group⁽²³⁾ modified for the lowest resonance as recommended by the Brookhaven Neutron Cross Section Evaluation Group.⁽²⁴⁾ The values used are shown in Table 7. There are considerable uncertainties left, as discussed below. The results of the calculation are shown in Tables 8 and 9. It is to be noted that again a contribution from the higher ℓ resonances of ~ 1 b should be added to the total. The temperature coefficient, β (see Eq. (4.1)), is also shown. Owing to changes in the resonance parameters, the results differ quite markedly from those given previously.⁽¹²⁾

Previous fairly widely divergent experimental results have been reviewed by Hellstrand and Weitman,⁽²¹⁾ together with their own measurements. They give for thorium metal the following value for the resonance integral at ambient temperatures:

$$\text{Hellstrand and Weitman} \quad I = (1.70 + 15.9 \sqrt{S/M}) \pm 5.5\% . \quad (5.1)$$

Our data from Table 6 for 300°K are well represented by the formula

$$I = I_h + 1.52 + 16.75 \sqrt{S/M} , \quad (5.2)$$

Table 6
 TEMPERATURE COEFFICIENT, $\beta \times 10^2$, FOR URANIUM
 RODS OF RADIUS a

Uranium Metal			
	Radius, a		
	0.4 cm	1.4 cm	
Calculated	0.64	0.55	
Observed	0.64 ± 0.05	0.55 ± 0.05	
UO ₂			
	Radius, a		
	0.4 cm	0.85 cm	1.4 cm
Calculated	0.84	0.69	0.63
Observed	0.82 ± 0.06	0.69 ± 0.05	0.65 ± 0.05

Table 7
 RESONANCE PARAMETERS FOR Th^{232*}
 (In electron volts)

E_o	Γ_n	Γ_γ	E_o	Γ_n	Γ_γ
21.84	2.40×10^{-3}	3.00×10^{-2}	456.40	2.82×10^{-2}	4.10×10^{-2}
23.48	4.00×10^{-3}	↓	465.00	4.50×10^{-2}	
59.55	4.60×10^{-3}		491.00	5.00×10^{-2}	
69.20	3.90×10^{-2}	↓	513.00	3.50×10^{-3}	
113.15	1.10×10^{-2}	4.20×10^{-2}	531.50	1.50×10^{-2}	
121.00	1.85×10^{-5}	4.10×10^{-2}	543.00	10.00×10^{-4}	
128.50	10.00×10^{-3}	↓	573.00	2.50×10^{-2}	
129.40	3.10×10^{-5}		581.00	1.60×10^{-3}	
146.20	10.00×10^{-4}	↓	601.50	1.10×10^{-2}	
154.60	2.20×10^{-2}	4.80×10^{-2}	621.50	5.00×10^{-3}	
170.80	5.80×10^{-2}	5.00×10^{-2}	660.50	3.20×10^{-2}	
193.00	1.40×10^{-4}	4.10×10^{-2}	669.00	1.70×10^{-2}	
196.80	1.30×10^{-3}	↓	679.50	1.25×10^{-1}	
199.80	9.00×10^{-2}	4.60×10^{-2}	692.00	3.80×10^{-2}	
203.00	1.88×10^{-2}	4.20×10^{-2}	705.00	1.80×10^{-2}	
221.80	2.30×10^{-2}	4.10×10^{-2}	717.50	2.50×10^{-1}	
252.30	2.40×10^{-2}	5.00×10^{-2}	746.00	1.60×10^{-3}	
264.00	1.50×10^{-2}	4.10×10^{-2}	783.00	10.00×10^{-1}	
286.80	2.10×10^{-2}	5.30×10^{-2}	810.00	1.25×10^{-2}	
306.50	2.00×10^{-2}	4.10×10^{-2}	848.00	2.30×10^{-3}	
330.40	5.50×10^{-2}	4.10×10^{-2}	872.00	10.00×10^{-2}	
343.30	3.00×10^{-2}	↓	896.00	3.00×10^{-2}	
366.70	3.50×10^{-2}		950.00	4.00×10^{-3}	
371.00	2.40×10^{-3}		970.00	7.50×10^{-2}	
402.80	9.00×10^{-2}		990.00	2.40×10^{-2}	
413.40	2.68×10^{-2}	↓	998.00	7.00×10^{-2}	
Unresolved Resonances					
$\Gamma_\gamma = 4.0 \times 10^{-2} \text{ ev}$			$D = 20.1 \text{ ev}$		
$\langle \Gamma_n^0 \rangle = 1.27 \times 10^{-3} \text{ ev}$			$E_C = 1008 \text{ ev}$		

* Taken from Ref. 23 and modified according to Ref. 24.

Table 8

RESONANCE INTEGRALS FOR THORIUM-METAL RODS OF RADIUS a
 AND DENSITY OF 11.7 G CM^{-3} AT VARIOUS TEMPERATURES,
 AND THE TEMPERATURE COEFFICIENT, β
 (In barns)

	Radius, a				
	0.138 cm	0.275 cm	0.55 cm	1.1 cm	2.2 cm
	S/M				
	1.24	0.623	0.311	0.155	0.078
300°K					
Resolved	18.80	13.16	9.32	6.815	5.148
Unresolved	2.46	2.15	1.85	1.602	1.428
Total	21.26	15.31	11.17	8.417	6.576
600°K					
Resolved	21.47	14.85	10.36	7.434	5.535
Unresolved	2.55	2.26	1.97	1.722	1.544
Total	24.02	17.11	12.33	9.156	7.079
900°K					
Resolved	23.37	16.10	11.10	7.825	5.782
Unresolved	2.58	2.30	2.01	1.769	1.590
Total	25.95	18.40	13.11	9.594	7.372
$\beta \times 10^2$	1.65	1.49	1.26	1.10	0.96

Table 9

RESONANCE INTEGRALS FOR ThO_2 RODS OF RADIUS a AND
 DENSITY OF 7.1 G CM^{-3} AT VARIOUS TEMPERATURES,
 AND THE TEMPERATURE COEFFICIENT, β
 (In barns)

	Radius, a			
	0.25 cm	0.50 cm	1.0 cm	2.0 cm
	S/M			
	1.125	0.564	0.282	0.141
300°K				
Resolved	19.60	14.00	10.31	8.00
Unresolved	2.54	2.25	1.98	1.77
Total	22.14	16.25	12.29	9.77
600°K				
Resolved	22.35	15.82	11.50	8.80
Unresolved	2.63	2.36	2.10	1.90
Total	24.98	18.18	13.60	10.70
900°K				
Resolved	24.33	17.17	12.38	9.39
Unresolved	2.65	2.39	2.14	1.94
Total	26.98	19.56	14.52	11.33
$\beta \times 10^2$	1.66	1.64	1.32	1.14

where I_h is the contribution of the $\ell > 0$ resonances and should be of the order of ~ 1 b.

The deviations between (5.1) and (5.2) are not very large, but seem definitely to lie outside the limits of error. However, good reasons for these discrepancies can be given from our imperfect knowledge of the cross section.

From the measured resonance integrals, the $1/v$ contribution at low energies has to be subtracted for comparison with theory. Since self-shielding in this region is very weak, this correction is generally taken as

$$-\Delta I_{1/v} = - \int_{E_C} \sigma_a \frac{dE}{E} = -\sigma_o \int_{E_C} \frac{\sqrt{E_o} dE}{E^{3/2}} = -2 \sigma_o \sqrt{\frac{E_o}{E_C}}. \quad (5.3)$$

In this formula, the capture cross section is taken as

$$\sigma_a = \sigma_o \sqrt{\frac{E_o}{E}}, \quad (5.4)$$

where σ_o is the capture cross section at the standard energy $E_o = 0.0253$ ev. In order to eliminate the thermal part of the absorption, the samples are generally wrapped in cadmium sheets and E_C is the effective cutoff energy of the order of 0.5 to 0.6 ev. With $\sigma_o = 7.45$ b and $E_C = 0.6$ ev, the correction (5.3) amounts to ~ -3 b. For this value, it is assumed, however, that the cross section is given by (5.4). On the other hand, the value of σ_o in thorium cannot be explained as being due to the tails of the positive energy resonances, the lowest of which are at 21.8 and 23.5 ev. One has, therefore, to invoke negative energy resonances to explain the measured value of σ_o . In this case, the capture cross section will fall faster than $E^{-1/2}$ and the value of the correction (5.3) will be decreased. This change can easily amount to ~ 1 b,* to explain the difference between the constant

*J. Garrison has recently fitted the measured total cross section with the help of a negative energy resonance (private communication). The correction (5.3) then comes out to be -1.4 b, in place of -3 b, at a cutoff at 0.6 ev. This would raise the constant term in (5.1) to about 3.1 b, which would seem to be quite reasonable.

terms in (5.1) and (5.2).

A check on the resonance parameters themselves is furnished by the infinite dilution resonance integral, which has been measured independently. The newest measurement by Johnston, Halperin, and Stoughton⁽²⁵⁾ gives 82 ± 8 b. The data in Table 7 give ~ 95 b. The change in the total resonance integral with self-shielding will be roughly proportional to a corresponding change in the infinite-dilution integral, and the 5% to 6% difference between the $\sqrt{S/M}$ terms in (5.1) and (5.2) can easily be due to inaccuracies in the resonance data. There is, altogether, very good reason to believe that as good an agreement for Th^{232} will be reached as for U^{238} when the cross-section data are known with the same accuracy.

6. DANCOFF-CORRECTION CALCULATIONS

The results of the two preceding discussions on resonance integrals for U^{238} and Th^{232} refer to the case of widely separated absorbers, which do not shade each other appreciably. Not many experimental data exist on the effect of interaction on the resonance integral. However, the treatment proposed in Ref. (12) and described here under "The Dancoff Correction" is theoretically very well founded.

It seemed interesting, however, to compare the results of our methods with those obtained by Rothenstein,⁽⁹⁾ which in their physical content are practically equivalent with ours. Table 10 shows the results of this comparison. Column 2 gives the Dancoff correction and column 3 Rothenstein's values. In the latter column, the contributions of high energies and p-wave resonances (2.12 b) have been omitted, as has been the doubtful, but not very large, moderator correction ΔI_m (see Eq. (2.27)), since these are not included in our treatment. Columns 4 and 5 give our own results, obtained using the formulas for the escape probabilities indicated in the top row.

It is first to be noted that the differences between (3.40) and (3.41) are quite small. They are largest for small-sized rods and large C . In

Table 10
 RESONANCE INTEGRALS OF URANIUM-METAL RODS IN WATER
 AT 300°K AT DIFFERENT WATER-TO-METAL
 VOLUME RATIOS (W/M)
 (In barns)

W/M	C	Rothenstein	Eq. (3. 40)	Eq. (3. 41)
Rods of 0.25-in. Diameter				
∞	0	16.09	16.28	16.28
4:1	0.119	15.11	15.27	15.36
3:2	0.174	14.67	14.80	14.87
2:1	0.280	13.66	13.83	14.00
1:1	0.464	11.41	12.00	12.25
Rods of 0.60-in. Diameter				
∞	0	10.67	10.94	10.94
4:1	0.016	10.58	10.85	10.86
3:2	0.032	10.50	10.77	10.79
2:1	0.080	10.29	10.51	10.55
1:1	0.208	9.57	9.80	9.86

such cases, the formulation (3.40) seems preferable, but otherwise the simpler procedure (3.41) should be entirely adequate.

There is also reasonable agreement between Rothenstein's results and our own, the only sizable deviation being for the largest C encountered. We believe that our results are much more accurate. Rothenstein has compared his values with those measured by Koutz and Sher⁽²⁶⁾ for 0.60-in. rods. There are considerable uncertainties in their values. They are somewhat (1 to 1.5 b) smaller than the values given by Rothenstein. However, this is probably due to a too-large contribution for the high energy resonances assumed by Rothenstein. The differences in the resonance integral at various water-to-metal ratios for the 0.60-in. rods are not dramatic and in general accord with the trend of the measured values.

7. INTEGRAL TREATMENT OF ADMIXED SCATTERERS

The present code permits the full integral treatment of admixed scatterers, as shown in Eq. (2.22), in place of the usual NR approximation (2.23). This feature makes it possible to calculate the resonance integrals in homogeneous mixtures without any neglects except interference between different resonances.

Owing to lack of time, the only test cases run were for the oxygen in UO_2 in heterogeneous geometry at 300°K. The results are shown in Table 11. The values of the resonance integrals are always reduced by the full treatment. The correction is quite small for thin rods, but is sizable in the larger thicknesses. We have, therefore, given the new calculated values in Table 11, together with Hellstrand's values, the same as in Table 5. The new calculated values seem to fall below the observed ones. However, agreement will be fully restored if the assumed contribution of the high ℓ and the high-energy resonances is increased by about 0.3 b, making their total contribution 1.3 b. This is entirely reasonable. The difference introduced by the integral treatment of the oxygen is thus at the limit of

Table 11

REDUCTION, Δ , OF THE RESONANCE INTEGRALS FOR UO_2 RODS
DUE TO INTEGRAL TREATMENT OF THE OXYGEN, AND
A COMPARISON WITH HELLSTRAND'S VALUES

	Radius, a				
	0.125 cm	0.25 cm	0.50 cm	1.0 cm	2.0 cm
	$-\Delta$				
	0.082	0.142	0.247	0.426	0.684
Calculated (revised)	37.53	27.24	20.35	15.62	12.46
Hellstrand	37.76	27.95	21.10	16.23	12.79

experimental verification. Theoretically, the treatment in this section is, of course, the more accurate.

Introduction of this refinement increases considerably the running time of the program. It is important only for the low-lying wide resonances and should, therefore, only be used for these. In U^{238} , in fact, the 6.7-ev resonance gives 68% of the correction and the next two resonances (21 and 36.9 ev) another 28%. They are thus the only ones which warrant the full treatment for oxygen. The situation may be less favorable for large admixtures of heavy scatterers--such as iron, molybdenum, tungsten, or lead--and a systematic study of their effect with the help of our code would seem to be highly desirable.

8. COMPARISON BETWEEN NR, IM, AND INTEGRAL METHODS

The basic philosophy of this work has been to obviate the distinction between narrow and wide resonances, and also to take into account such finer effects as interference scattering. It is instructive, therefore, to compare the effects of the usual approximations for selected cases. Such a comparison is shown in Table 12.

The upper part of the table gives the resonance data used (not exactly the same as those used previously in the report), inclusive of the practical width, the maximum energy loss in a collision, $\alpha_o E_o$, and the ratio, ζ , of natural width to Doppler width. The lower part shows the results from the NR, IM, and present (denoted by INT) treatments. The bracketed numbers give the values when interference scattering is neglected. For the 6.68-ev resonance, the IM value is satisfactory (as expected), the effect of interference scattering being small owing to the small value of Γ_n . In the wide 103-ev resonance, $\Gamma_n > \Gamma_\gamma$ and the effect of interference scattering is quite large, as are the differences between the values obtained with the three procedures. It is interesting to note that the results from the IM method are not too different from those obtained with the INT method with

Table 12

RESONANCE INTEGRALS FOR URANIUM-METAL RODS OF 0.422-CM
RADIUS AT 300°K FOR SELECTED RESONANCES OBTAINED
FROM VARIOUS APPROXIMATIONS, AND RESONANCE
DATA EMPLOYED

Resonance Data Employed				
	E_o			
	6.68 ev	103.0 ev	81.0 ev	475.0 ev
Γ_γ , ev	0.024	0.024	0.024	0.024
Γ_n , ev	0.00148	0.072	0.0021	0.005
Γ_p , ev	1.26	3.98	0.76	0.26
$\alpha_o E_o$, ev	0.11	1.73	1.36	8.0
ζ	0.474	0.455	0.139	0.0639
Resonance Integrals				
NR		0.613	0.259	0.432
	(5.40)	(0.601)	(0.258)	(0.432)
IM		0.555	0.226	
	(4.75)	(0.554)	(0.226)	
INT	4.94	0.518	0.259	0.434
	(4.84)	(0.424)	(0.251)	(0.431)

interference included, which fact explains to some extent the good results obtained with the older theories. The 81- and 475-ev resonances are narrow compared with the maximum energy loss. The NR approximation thus gives good results, and the effect of interference scattering is quite small owing to the predominance of Doppler broadening.

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