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RESONANCE ABSORPTION OF NEUTRONS IN NUCLEAR REACTORS

L. Dresner

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Erratum to ORNL-2659

Page 21, Eq. (18-2) second line should read

$$\Delta_\ell = \frac{x^2(\ell - \Delta_{\ell-1})}{(\ell - \Delta_{\ell-1})^2 + s_\ell^2} - \ell; \quad \Delta_o = 0$$

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Neutron Physics Division

RESONANCE ABSORPTION OF NEUTRONS IN NUCLEAR REACTORS*

Lawrence Dresner

Date Issued
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*A Dissertation presented to the Faculty of Princeton University in candidacy for the Degree of Doctor of Philosophy

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PREFACE

This preface refers to some purely technical aspects of the manuscript concerning the enumeration of equations, etc. Equations, figures, tables, and appendices are denoted with two numbers: the first gives the order of appearance in their respective chapters, and the second gives their chapter number. Thus the fifth equation of Chapter 6 is denoted by "Eq. (5-6)." The only exception to this rule is the enumeration of equations, etc. in appendices. For example, the fifth equation of Appendix (2-11) is denoted by "Eq. (5-11.2)." References appear in the text as parentheses including the first author's initial and the year of publication. In cases where several references would be denoted by the same symbol a small Roman letter has been appended. The collected references appear following the main text. Occasionally complete references appear in parenthetic insertions in the text.

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RESONANCE ABSORPTION OF NEUTRONS IN NUCLEAR REACTORS

Lawrence Dresner

ABSTRACT

The problem of resonance absorption of neutrons in nuclear reactors is considered. Formulae for the effective resonance integral of single resonances are given in the "narrow resonance" approximation in homogeneous media, and in the "narrow resonance" and "infinite mass absorber" approximation in heterogeneous media. It is shown that the Doppler effect in homogeneous media can be expressed through a certain function of two variables, $J(\xi,\beta)$. The properties of this function are studied in detail, and a tabulation given. The effect of interference between resonance and potential scattering on the effective resonance integral is studied. In heterogeneous media in the "narrow resonance" case it is shown that the Doppler effect can again be expressed through the same function, $J(\xi,\beta)$, as in the homogeneous case if a rational approximation for the average escape probabilities due to Wigner is introduced. Furthermore, it is shown that then a formal identity exists between the homogeneous and heterogeneous cases for "narrow" resonances. The error caused by Wigner's rational approximation is studied in detail, and in the case of no Doppler broadening and no interference scattering an improved formula is suggested. In heterogeneous media in the "infinite mass absorber" case an approximate expression for the albedo of an absorber lump is suggested on the basis of heuristic arguments. Precise calculations of the albedo based on a variational method of solving the monoenergetic transport equation are

compared with this approximation, and show it to be quite accurate. Use of the approximate albedo again permits expression of the Doppler effect through the function $J(\xi,\beta)$. The effect of interference between potential and resonance scattering is also studied in the "infinite mass absorber" approximation. These results are applicable to calculating the absorption in low energy resolved resonances for which the widths and energy are known. In the region beyond the experimental limit of resolution statistical considerations are employed. The formulae for single resonances are averaged over the probability distributions of the partial widths. The theory is then applied to the calculation of the effective resonance integrals of uranium and thorium rods, and good agreement is obtained for uranium and fair agreement for thorium.

At high energies resonance absorption cross sections fall sufficiently low to permit neglect of flux depression effects, and attention is focussed on average reaction cross sections. A study of the effect of fluctuations in the partial widths on average reaction cross sections is given. Some general theorems are derived independent of the probability distributions of the widths. If the widths are distributed in member distributions of the chi-squared family, it is shown that the multiple integrals over these distributions which express the averages $\langle \Gamma_s \Gamma_t / \Gamma \rangle$ can be reduced to a single infinite integral. This integral is evaluated in the eighteen simplest cases of interest. A Monte Carlo program for the electronic computer ORACLE for evaluating these averages is described. It is shown that enough experimental data on neutron reactions in U^{238} exists below 500 kev to overdetermine the s-, p-, d-, and f-wave strength functions. Analysis of the data including the important effects of fluctuations in the widths yields consistent values for

the strength functions, in support of the theory. Finally, the statistical formalism of Hauser and Feshbach is transformed from the channel spin representation to another which is more convenient in the presence of spin-orbit coupling. The effect of small amounts of spin-orbit coupling in the analysis of the U^{238} reaction data is found to be unimportant. Finally, it is proven that the total, the compound nucleus formation, and under certain circumstances, the radiative capture cross sections are independent in first order of spin-orbit coupling in the neutron-nucleus interaction.

CHAPTER 1. INTRODUCTION; HISTORICAL SURVEY OF PREVIOUS WORK; SCOPE OF PRESENT WORK

1. In chain reactions in which thermal neutrons are employed as the chain carriers it is necessary to slow down the energetic neutrons from fission, a process accomplished by allowing elastic collisions of the fast neutrons with the nuclei of some suitable material, called a moderator. During this process of moderation the neutrons are subject to removal from the chain by nuclear reaction with any material present in the assembly (excepting those reactions which yield neutrons as their products, e.g., inelastic scattering). Because, historically, the (n,γ) reaction in the sharp nuclear resonance lines of U^{238} was the first such parasitic reaction considered, the entire process has been named resonance absorption, even when the responsible cross section does not have the typical sharp line appearance.

2. The importance of the resonance absorption problem was appreciated even in the short time which intervened between the discovery of fission and the successful establishment of a natural uranium fueled, self-sustaining chain reaction. Turner (T40) writing in January, 1940 concluded after examination of an experiment of Anderson, Fermi, and Szilard (A39), that, except for the then unknown extent of resonance absorption, the chances for establishing such a self-sustaining chain reaction seemed good. Even before any reliable data was available on the resonance absorption process, it was recognized that disposing the uranium in the form of lumps, rather than mixing it homogeneously with the moderator, would substantially decrease the amount of resonance absorption. Fermi and Szilard are credited

with this observation in regard to research carried out in this country; but the suggestion of lumping the uranium was also made by Harteck in Germany, and by Halban, Kowarski, and Joliot in France (C55a). The USSR also claims independent discovery (F55).

3. The lumping of the uranium, however, is not without disadvantages. In addition to decreasing the parasitic capture of resonance neutrons in the uranium, it also decreases the fission-producing capture of thermal neutrons in the uranium. Thus, the early problem of reactor design was the choice of an optimum lattice of uranium lumps and moderating material in which the multiplication constant was a maximum. The first experimental work done on the resonance absorption of uranium in bulk was carried out by activation techniques by E. C. Creutz, R. R. Wilson, and collaborators, at the Princeton University cyclotron in 1941 (S46). This work was finally reported in the open literature in the third and fourth of a series of four articles published in the Journal of Applied Physics (C55b, c). The first of these four articles (C55a) is a review of the work which preceded the Princeton work; since such a comprehensive review already exists we shall merely allude to it and not mention further any of the prior works it cites. The second of these four articles (W55) is a pioneering theoretical paper of Wigner et al., in which nearly all of the basic physical phenomena which play important roles in the resonance absorption process are mentioned, and, in most cases, their effects studied. The rationale in Wigner's work, as in all subsequent theoretical work, was to relate the absorption in bulk to the nuclear properties of the individual absorbing nuclei. The measurement of the uranium resonance

parameters was first accomplished by Anderson (A50), and it was his data that Wigner used.

4. The necessity of obtaining experimental data on heterogeneous resonance absorption was also apparent in other countries in the early 1940's. Creutz et al. (C55a) mention a considerable number of British and French workers, whose reports, at the time of the writing of C55a, were still classified. Their works bear dates from 1942-1944. The earliest Russian experimental work on heterogeneous resonance absorption known to the author is a measurement of Popov and Shapiro (P55) done by activation techniques in the exponential assembly presumably used in the design of the first Soviet uranium graphite reactor. The date of this research is not known and the issue is further complicated by the fact that it is not known when the first Soviet reactor went critical, although it is thought by some to be between 1944 and 1947 (R56). After it went critical further measurements of the activation type, also of uncertain date, were made by Egiazarov et al. (E55). Further work on D_2O exponential assemblies was done by Burgov (B55). Burgov also mentions measurements by Rudek on the uranium-D_2O reactor of the Soviet Academy of Sciences, which went critical in April 1949 (R56). The resonance absorption in both these works was studied indirectly through a knowledge of all the other factors in the four factor formula. According to Burgov, who compared his results with earlier Soviet experiments, the method is unsatisfactory. Beginning in 1943 Soviet theoretical research on the resonance absorption problem was actively pursued (G55). The Soviet work, while instructive, suffers the defect of ignoring moderation by

the uranium nuclei. This particular issue is complicated and will be dealt with at greater length in Chapters 6, 7, and 9.

5. Interest in the resonance absorption problems in the United States was not abated by the very successful beginning made by the Princeton group. In 1944 activation measurements at the Indiana University cyclotron were made on homogeneous mixtures of uranium and various moderators by A. C. G. Mitchell et al. (M44). Nearly simultaneously with this experimental work, Dancoff and Ginsburg (D44) completed a very detailed theoretical study. Experimental work similar to Mitchell's on homogeneous systems was reported for uranium by Hughes and Goldstein (H46) in 1946, and for thorium by Hughes and Eggler (H45) in 1945. In 1949 Muehlhause and Untermyer (M49) obtained further experimental data on lumped uranium by the pile oscillator technique. In 1951 Risser et al. (R51) performed activation experiments on uranium rods in the X-10 graphite reactor; in late 1950 Untermyer and Eggler (E50) reported danger coefficient studies on thorium rods.

6. At the time of the International Conference at Geneva three experimental, one theoretical, and one survey paper on resonance absorption were presented. A Russian experimental paper (S55) by Spivak et al. mentioned only results on the resonance absorption of very thin foils, which, while interesting, is not germane to the study of absorption by uranium in bulk. Similar results of research in the United States are given in the survey paper of Macklin and Pomerance (M55). This paper also mentions much of United States research on bulk absorption already cited in previous paragraphs. An experimental paper (C55d) was presented by V. S. Crocker of

the United Kingdom who used self-indication techniques in a collimated neutron beam. A third experimental paper (E55a) was presented by Eriksen et al. of JENER describing interesting work done on lumped uranium by the pile oscillator technique. A theoretical paper, which suffered considerably from the insufficiency of the available nuclear data, was presented by van der Held (H55) of the Netherlands.

7. Since the Geneva conference several very excellent experiments on resonance absorption have been reported. One, by Hellstrand in Sweden (H57), was done by activation techniques in the Swedish heavy water reactor. Hellstrand considered not only rods of uranium and uranium oxide, but also a variety of more complex fuel assemblies consisting of hollow tubes and bundles of cylindrical pins. These more complex shapes were studied in response to the questions raised by the increasing sophistication evident in fuel element design. Rods of uranium and thorium were studied by Davis (D57) in the Hanford Test Pile by danger coefficient techniques. A similar reactivity change technique was used by Dayton and Pettus (D57a) in the Pennsylvania State swimming pool with thorium and thorium oxide rods and plates. A technique of the activation type, but somewhat more complicated than the usual Cd-covered rod plus monitor foil, has been employed by Niemuth at Hanford (N56).

8. Excellent measurements, basically of the activation type, have been made on slightly enriched uranium rods of two sizes in a water moderated critical assembly by Klein et al. (K56) at Bettis; and by Sher (S57) in several exponential assemblies at Brookhaven. These measurements are complicated somewhat by the fact, originally noted by

Dancoff (D44a), that the rods are close enough to partially shield one another from the resonance flux in the moderator. Sher has tried to turn this fact to advantage in the following manner: A functional dependence of the resonance absorption on the rod size suggested by the theory of Wigner is assumed, with three disposable constants. With the data for the two available rod sizes, for thin foils, and for the dependence of resonance absorption on the lattice spacing through Dancoff's effect, the disposable constants can be determined. Results obtained in this manner have been reported by Sher for both uranium and thorium rods (S57).

9. Another avenue of approach to the problem is through the theoretical analysis of lattice experiments both of the critical and exponential type. Such an approach was taken in the USSR by Burgov (B55) as we have already noted. Work of this sort was undertaken in 1951 in the United Kingdom and culminated in a series of papers by Davey (D55) and Mummery (M56). A similar, somewhat later, analysis, including data from many published United States, British, and Russian exponential experiments, was reported recently by Kouts and Sher (K56a).

10. A considerable burgeoning of the theory of resonance absorption has occurred since Geneva, largely along three rather distinct lines. Firstly, there has been a renewal of effort on the problem of homogeneous resonance absorption, largely because it is felt to be tractable. Papers have been published by Spinney (S56), Weinberg and Wigner (W56), and Corngold (C57). Secondly, there has been an attempt to understand resonance capture in realistic heterogeneous situations by numerical methods, especially the Monte Carlo method, which require the use of

electronic computers. Papers along this line have been written by Richtmyer (R56a), Sampson (S56a), St. John (J56), Chernick (C56), and Stein (S56b). The last approach, to which the present author adheres is based on the hope of solving the combined slowing-down transport problem of resonance absorption approximately in analytic terms. That such a hope is reasonable is indicated by Wigner's original analysis (W55), where several basic approximations are exhibited which considerably reduce the complexity of the problem. Some preliminary efforts following this approach have already been published by the author and by others (D55a, D56, D56a, K58), and it is felt that the present work successfully continues these beginnings.

11. The history of resonance absorption in bulk presented in the previous paragraphs shows the problem to have originated largely in the early attempt to achieve maximum possible neutron multiplication. As enriched uranium became available for reactor purposes and reactor design became more sophisticated, emphasis in the resonance absorption problem broadened. With interest in reactors of intermediate or fast spectrum came interest in the process of resonance absorption in the energy range from about 10 kev to fission energies. The significant differences of this high energy problem from the classical resonance absorption problem are four, viz.:

(i) The resonances in the high energy problem are unresolved, so that statistical models must be employed in relating the absorption to the nuclear properties. This problem exists partially in the classical problem because of the necessity of estimating the effect of the unresolved resonances on the absorption.

(ii) Higher partial waves (i.e., p-, d-, f-, etc. waves) contribute to the absorption effects.

(iii) Other nuclear reactions, notably inelastic scattering and sometimes fission, appear at high energies. These reactions are important to the absorption process both because they compete with it directly, and because their cross sections are related.

(iv) Often, but not always, the problems introduced by the distribution of uranium in bulk simplify considerably.

12. Points (i)-(iv) above indicate that the high energy resonance absorption problem is largely a problem of pure nuclear physics, whereas the classical problem is largely, but not entirely, a problem of neutron transport theory. Until very recently our information on neutron reactions was not really adequate for a treatment of the resonance absorption problem including points (i), (ii), and (iii) above. A summary sketch of our knowledge, for example, at the close of 1950 can be obtained from the "Final Report of the Fast Neutron Data Project" (F51). In the past few years our knowledge has increased enormously, and we are presently in an excellent position to successfully attack the problem of high energy neutron cross sections.

13. From an experimental point of view the most impressive achievement of the last five years is the development of higher resolution instrumentation, largely based on the time-of-flight technique, for investigating neutron resonance cross sections in the 0-1 kev energy range. A wealth of such resonance data exists and nearly all of it has been carefully

studied and tabulated in BNL-325 and BNL-325 Sup. 1 (H55a, H57a). Several other reviews exist, among them two papers by Harvey et al. (H56, H57a, E56). Tables of resonance parameters are available in these references. In addition these references, especially BNL-325 and BNL-325 Sup. 1, contain nearly all available information concerning high energy neutron cross sections. It is not possible nor is it purposeful to review this literature; we shall cite it as needed, and content ourselves at present with noting the existence of considerable data on neutron total, radiative capture, inelastic scattering, and fission cross sections.

14. In regard to progress in theory, the last few years have seen the emergence of four important ideas concerning nuclear structure, viz.:

(i) From a study of neutron total cross sections, Feshbach, Porter, and Weisskopf (F54) were led to introduce the notion of a complex potential to describe the neutron-interaction with the nucleus. Their discovery precipitated an avalanche of analysis of data in terms of complex potentials, with some small but still significant improvement over the original work.

(ii) Wigner, Lane, and Thomas (L55) found a satisfactory interpretation of the complex potential model on the basis of the dispersion theory of nuclear reactions.

(iii) Following intuitive arguments Porter and Thomas (P56) discovered excellent statistical distributions for the neutron and radiative widths of nuclear resonances.

(iv) Hill and Wheeler (H53), and independently Bohr and Mottelson (B53), call attention to the non-spherical shape of many nuclei, and to the consequences of this fact.

15. These developments make possible the approach taken in this work to the resonance absorption problem at high energies. This approach is a phenomenological one; in it the dispersion theory of nuclear reactions [suitably including points (i), (ii), and (iii) above] is used to obtain forms for the cross sections for various reactions involving only a limited number of constants. These constants are then found by comparison with experiment, and the resulting expressions used to predict unmeasured quantities wherever possible. Such a phenomenological approach has been tried in the past to compute the capture-to-fission ratio in U^{235} in the epithermal range by Wigner (W55a) and by Oleksa (O56). Hurwitz and Greebler (G57) have attempted the phenomenological calculation of fission product capture cross sections in the epithermal range. All three of these calculations were largely based on experimentally known resonance parameters for several resonances. Recently, Lane and Lynn (L57) and Cameron (C57a) have done phenominological calculations of radiative capture cross sections at high energies.

16. Having completed this brief history of contributions to the problem of resonance absorption, we shall close this chapter with an outline of the scope of this work and a summary of the innovations it contains. For this purpose it is convenient to consider the problem in three parts, viz.: (i) Resolved resonances - low energy; (ii) Unresolved resonances, only s-waves - intermediate energy; and (iii) High energy.

Let us consider (i) first. In problems of heterogeneous resonance absorption results are only possible, at this writing, either by assuming the absorber to have infinite mass, or to have absorbing lines very much

narrower than the energy lost by a neutron in a single collision. In both these approximations it is necessary to incorporate the Doppler effect, as suggested originally by Wheeler (W55). In both approximations the Doppler effect can be described by a certain function of two variables, which has been tabulated by the author (D56), and whose properties are studied in this work in great detail. It has also been studied by Dancoff and Ginsburg (D44) and by Roe (R54). An effect which has not been considered before, but which is considered in this work, is the interference between potential and resonance scattering, which gives rise to the clearly discernible dips just preceding the high peaks of the low energy s-wave resonances in most nuclides. Among the results of this analysis is the fact that the effective absorption cross section of the nuclei in an absorbing lump can be written as the product of two factors, one of which depends only on the lump size and not on the resonance parameters, and the other of which depends on the resonance parameters and not at all on the lump size. This very important separation was first noted by the author (D56a) on a much more restricted basis than is derived in this report. It implies a sort of universal geometric dependence of the resonance integral, largely independent of the details of the resonance structure.

18. In the intermediate case (ii) the main problem which is considered and solved is that of averaging the formulae for the effective absorption cross section derived in case (i) over the statistical distribution of the reaction widths. Serious statistical consideration of the unresolved resonances was not previously possible because of lack of precise knowledge of the statistical distribution of the reaction widths. Finally because

of its practical importance, the statistically averaged absorption cross section for a thin foil was integrated with a $\frac{1}{E}$ Fermi spectrum. The resulting formula is very useful in comparing thin foil data such as reported by Spivak (S55) or Macklin and Pomerance (M55) with the predictions made from measured resonance parameters.

19. In the high energy range the transport aspect of the problem has been ignored, and the main effort devoted to the reaction cross sections themselves. In the first place, the statistical formalism of Feshbach and Hauser (H52) [actually the neutron one-level formalism of Blatt and Biedenharn (B52) with the statistical assumptions of Feshbach and Hauser] has been generalized to include the effects of fluctuations in the reaction widths. Some general theorems have been derived independent of the precise statistical distribution of the widths. A large number of cases have been investigated analytically under the assumption that the statistical distributions of the widths belonged to the chi-squared family. Finally, a novel machine code has been written for the ORACLE electronic computer, which analyzes the effect of the fluctuations on the cross sections. Secondly, the statistical formalism has been rewritten in another representation convenient for situations in which spin-orbit coupling is present.

20. With the results mentioned in paragraphs 17, 18, and 19 above a detailed comparison of theory and experiment was made for all the data on resonance absorption in U^{238} rods, and for all the available data on U^{238} neutron reaction cross sections. The above summary of the content of this work is, of course, a barest outline and omits mention of much important

work to be found in the text. It serves, however, to orient the reader and is so intended.

CHAPTER 2. SUMMARY OF NECESSARY RESULTS OF NUCLEAR THEORY

1. The purpose of this chapter is to summarize a wealth of background material on which we shall have to draw frequently in subsequent chapters. In discussing those points in this summary that can be found in the literature we shall employ the utmost economy of expression; we shall, however, deal fully with new material.

2. In their review article Blatt and Biedenharn (B52) have explicitly related the differential and total scattering and reaction cross sections to the elements of the scattering matrix. They describe a number of simple situations in which explicit expressions for the scattering matrix are available. Two of these situations are of interest to us here, viz.:

(i) Scattering and reaction cross sections associated with a single s-wave resonance level of the compound nucleus.

(ii) Averaged reaction cross sections, in general, under the statistical assumptions of Feshbach and Hauser (H52).

3. Let us consider situation (i) first. Insofar as s-wave reactions are concerned it follows from Eqs. (5.9) and (4.5) of B52 that

$$\sigma(\alpha s,\alpha' s') = \pi \lambda\!\!\!^{-2}_{\alpha} \cdot \frac{2J+1}{2s+1} \cdot \frac{\Gamma_{\alpha s}\,\Gamma_{\alpha' s'}}{(E-E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} \qquad \alpha' s' \neq \alpha s \qquad (1\text{-}2)$$

The meaning of the symbols is as follows:

$\sigma(\alpha s,\alpha' s')$ is the cross section for reaction from channel α with channel spin s, to channel α' with channel spin s'. $\lambda\!\!\!^{-}_{\alpha}$ is the reduced neutron wave length (neutron wave length divided by 2π) in channel α. J is the total angular momentum of the compound state formed. E is the center of mass energy of the system; E_o is the resonance energy. $\Gamma_{\alpha s}$ are physical parameters

called partial reaction widths; the ones appearing in Eq. (1-2) refer to s-waves only. There is one such width for each distinguishable mode of decay of the compound nucleus. Γ, the total width, is the sum of all the partial reaction widths, including even in the s-wave case, all those which refer to modes of decay of higher angular momentum than zero. Note that Eq. (1-2) describes spin-flip elastic scattering, i.e., $\alpha = \alpha'$; but $s \neq s'$.

4. For s-wave scattering the formula is somewhat more complicated. From Eqs. (6.1), (6.2), (6.3), (6.4), (5.9), and (4.5) of B52 it follows that

$$\sigma(\alpha s, \alpha s) = \pi \lambda\!\!\!^{-}{}_{\alpha}^{2} \cdot \frac{2J+1}{2s+1} \cdot \frac{(\Gamma_{\alpha s})^2}{(E - E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} + 4\pi \lambda\!\!\!^{-}{}_{\alpha}^{2} \sin^2 \xi_\alpha$$

$$- \pi \lambda\!\!\!^{-}{}_{\alpha}^{2} \cdot \frac{2J+1}{2s+1} \cdot \frac{\left\{4(E - E_o) \sin \xi_\alpha \cos \xi_\alpha + 2\Gamma \sin^2 \xi_\alpha\right\} \Gamma_{\alpha s}}{(E - E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} \qquad (2\text{-}2)$$

ξ_α is the s-wave hard sphere scattering phase shift in channel α and is given by

$$\xi_\alpha = - \frac{R_\alpha}{\lambda\!\!\!^{-}{}_\alpha} \qquad (3\text{-}2)$$

where R_α is the channel radius in channel α. At low energies, where $\lambda\!\!\!^{-}{}_\alpha$ is large, $\xi_\alpha << 1$. The trigonometric functions can be approximated by the first terms in their Maclaurin series; secondly, the last term in $\sin^2 \xi_\alpha$ can be neglected. This is because it is only for E very nearly equal to E_o that it is larger than the $\sin \xi_\alpha \cos \xi_\alpha$ term, and under this circumstance it is almost always negligible compared to the first term in Eq. (2-2). With these changes Eq. (2-2) can be written

$$\sigma(\alpha s,\alpha s) = \pi\lambda\!\!\!^{-2}_{\alpha} \cdot \frac{2J+1}{2s+1} \cdot \frac{(\Gamma_{\alpha s})^2}{(E-E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} + 4\pi R_\alpha^2$$

$$+ 4\pi\lambda\!\!\!^{-}_{\alpha} R_\alpha \cdot \frac{2J+1}{2s+1} \cdot \frac{(E-E_o)\,\Gamma_{\alpha s}}{(E-E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} \qquad (4\text{-}2)$$

The three terms on the right hand side of Eq. (4-2) are called resonance, potential, and interference scattering, respectively. Differential cross sections are unnecessary in the case of s-wave reactions since the angular distributions are isotropic.

5. For situation (ii) we proceed as follows: The differential cross section for reaction from channel αs to channel $\alpha' s'$ averaged over an energy interval including many states of the compound nucleus can be written, according to Eq. (4.5) of B52, as

$$\frac{d\sigma(\alpha s,\alpha' s')}{d\Omega} = (2s+1)^{-1}\,\lambda\!\!\!^{-2}_{\alpha} \sum_{L=0}^{\infty} \langle B_L(\alpha s,\alpha' s')\rangle\, P_L(\cos\theta) \qquad (5\text{-}2)$$

The brackets stand for an average over many resonances of the compound nucleus. If we perform this average in Eq. (4.6) of B52 and assume, as do Hauser and Feshbach (H52), that interference terms between levels of different total spin, J, or channels of different orbital angular momentum, ℓ, sum to zero, we obtain

$$\langle B_L(\alpha s,\alpha' s')\rangle = (-)^{s'-s} \cdot \frac{1}{4} \cdot \sum_{J=0}^{\infty} \sum_{\ell=|J-s|}^{J+s} \sum_{\ell'=|J-s'|}^{J+s'} Z(\ell J \ell J; sL)\, Z(\ell' J \ell' J; s' L)$$

$$\left\langle \left| \delta_{\alpha\alpha'}\delta_{ss'}\delta_{\ell\ell'} - S^{J\pi}_{\alpha s\ell,\alpha' s'\ell'} \right|^2 \right\rangle \qquad (6\text{-}2)$$

Here the Z's are the Z-coefficients mentioned in reference B52, and are related to the Racah coefficients. The last term in Eq. (6-2) is the averaged element of the scattering matrix connecting channel $\alpha s \ell$ with channel $\alpha' s' \ell'$ through compound states of total angular momentum J and total parity π. If the scattering matrix for neutrons is given by the one-level formula, Eq. (4.6) of B52, viz.:

$$S^{J\pi}_{\alpha\ell s, \alpha'\ell's'} = e^{i(\xi_{\alpha\ell}+\xi_{\alpha'\ell'})}\left[i \frac{g_{\alpha s\ell} g_{\alpha' s'\ell'}}{E_o - E - i\frac{\Gamma}{2}} + \delta_{\alpha\alpha'}\delta_{ss'}\delta_{\ell\ell'}\right] \quad (7\text{-}2)$$

then the average in Eq. (6-2) becomes for $\alpha' s' \neq \alpha s$

$$\left\langle \left| S^{J\pi}_{\alpha s\ell, \alpha' s'\ell'} \right|^2 \right\rangle = \frac{2\pi}{D_{J\pi}} \left\langle \frac{\Gamma_{\alpha s\ell}\Gamma_{\alpha' s'\ell'}}{\Gamma} \right\rangle \quad (8\text{-}2)$$

In Eq. (7-2) $g_{\alpha s\ell} = \pm\sqrt{\Gamma_{\alpha s\ell}}$. The sign is uncertain. The calculation of this average involves an integration over the resonance line shape and it is assumed in carrying out this integration that the energy dependence of the widths can be neglected. The braces on the right hand side of Eq. (8-2) now represent an average to be taken over the statistical distributions of the reaction widths. As a final point it is worth noting that separation of $\alpha s\ell$ and $\alpha' s'\ell'$ given in Eq. (8-2) does not depend on the assumption of the one-level formula but follows from the general Bohr assumption of independence of formation and decay of the compound nucleus, and the reciprocity laws for nuclear reactions (B52a).

The formulae (5-2) must be averaged over initial polarizations and summed over final polarizations to obtain cross sections for unpolarized beams and unpolarized detectors. The result of this procedure gives

$$\frac{d\sigma(\alpha,\alpha')}{d\Omega} = \frac{\lambda\!\!\!^{-2}_{\alpha}}{2(2I+1)} \sum_{L=0}^{\infty} \left\langle B_L(\alpha,\alpha') \right\rangle P_L(\cos\theta) \tag{9-2}$$

where

$$\left\langle B_L(\alpha,\alpha') \right\rangle = \sum_{s=\left|I-\frac{1}{2}\right|}^{I+\frac{1}{2}} \sum_{s'=\left|I'-\frac{1}{2}\right|}^{I'+\frac{1}{2}} \left\langle B_L(\alpha s,\alpha' s') \right\rangle \tag{10-2}$$

and I and I' are the nuclear spins of the target and residual nuclei, respectively.

6. The formulae presented in the last paragraph have all been derived in a representation in which the neutron spin σ, the nuclear spin I, and the orbital angular momentum are coupled as follows: First σ and I are coupled to form the channel spin, s. Then s and I are coupled to give the total angular momentum, J. Such a representation is convenient for most purposes. However, for the study of reactions in the presence of spin-orbit coupling such a representation may prove inconvenient because s is no longer a good quantum number. Instead, it is better to couple σ and ℓ to a sum j, and then to couple j to I to form J.

The transformation of the scattering matrix from the $\sigma I(s)\ell J$ representation to the $\sigma\ell(j)IJ$ representation can be accomplished with the Racah coefficients as the transformation coefficients (B52b). In particular,

$$S^{J\pi}_{\alpha s\ell,\alpha' s'\ell'} = \sum_{j=|\ell-\sigma|}^{\ell+\sigma} \sum_{j'=|\ell'-\sigma'|}^{\ell'+\sigma'} (2s+1)^{\frac{1}{2}}(2j+1)^{\frac{1}{2}} W(I\sigma J\ell;sj) \cdot S^{J\pi}_{\alpha jI,\alpha' j' I'}$$

$$(2s'+1)^{\frac{1}{2}}(2j'+1)^{\frac{1}{2}} W(I'\sigma' J\ell';s'j') \tag{11-2}$$

The W's are related to the Racah coefficients and discussed, along with the Z's, in B52b. Substitution of Eq. (11-2) into Eq. (9-2) and rearrangement gives

$$\left\langle B_L(\alpha,\alpha')\right\rangle = \frac{1}{4}\sum_{J=0}^{\infty}\sum_{j=|J-I|}^{J+I}\sum_{j'=|J-I'|}^{J+I'}\sum_{\ell=|j-\sigma|}^{j+\sigma}\sum_{\ell'=|j'-\sigma'|}^{j'+\sigma'}\left\langle\left|\delta_{\alpha\alpha'}\delta_{jj'}\delta_{II'}-S^{J\pi}_{\alpha jI,\alpha' j' I'}\right|^2\right\rangle$$

$$\times\ (2j+1)\sum_{s=|I-\sigma|}^{I+\sigma}(-)^{-s}(2s+1)Z(\ell J\ell J;sL)W^2(I\sigma J\ell;sj)$$

$$\times\ (2j'+1)\sum_{s'=|I'-\sigma'|}^{I'+\sigma'}(-)^{s'}(2s'+1)Z(\ell' J\ell' J;s'L)W^2(I'\sigma' J\ell';s'j') \qquad (12\text{-}2)$$

The reduction of the quantities in the second and third lines of Eq. (12-2) can be accomplished as follows:

$$(2j+1)\sum_{s=|I-\sigma|}^{I+\sigma}(-)^{-s}(2s+1)Z(\ell J\ell J;sL)W^2(I\sigma J\ell;sj)$$

$$=(2j+1)(2\ell+1)(2J+1)i^L(-)^{L-J-\ell}(\ell\ell 00|\ell\ell L0)\sum_{s=|I-\sigma|}^{I+\sigma}(2s+1)W(\ell sLJ;J\ell)$$

$$\times\ W(Isj\ell;\sigma J)W(\ell sjI;J\sigma)$$

$$=(2j+1)(2\ell+1)(2J+1)i^L(-)^{L-J-\ell}(\ell\ell 00|\ell\ell L0)W(JLIj;Jj)W(\ell L\sigma j;\ell j)$$

$$=(2J+1)(-)^{-L-I-\sigma}Z(\ell j\ell j;\sigma L)W(JjJj;IL) \qquad (13\text{-}2)$$

The passage from the first line to the second is accomplished using the definition of Z in terms of W (Eq. 23 of B52b), and the symmetry relations for W (Eq. 14 of B52b). Using a sum rule for the products of three W's (Eq. 17 of B52b) enables us to pass to the third line, and again using the symmetry relations and the definition of Z in terms of W we obtain the last line. Taking the complex conjugate of Eq. (13-2) gives an equation whose extreme right hand side and left hand side are identical with those of Eq. (13-2) except that the exponents of - 1 are changed in sign. Substituting Eq. (13-2) and its complex conjugate into Eq. (12-2) gives

$$\left\langle B_L(\alpha,\alpha')\right\rangle = \frac{1}{4} \sum_{J=0}^{\infty} \sum_{j=|J-I|}^{J+I} \sum_{j'=|J-I'|}^{J+I'} \sum_{\ell=|j-\sigma|}^{j+\sigma} \sum_{\ell'=|j'-\sigma'|}^{j'+\sigma'} \left\langle \left|\delta_{\alpha\alpha'}\delta_{jj'}\delta_{II'} - S^{J\pi}_{\alpha jI;\alpha' j' I'}\right|^2 \right\rangle$$

$$\times (-)^{I'+\sigma'-I-\sigma}(2J+1)^2 Z(\ell j \ell j;\sigma L) W(JjJj;IL) Z(\ell' j' \ell' j';\sigma' L) W(Jj'Jj';I'L) \tag{14-2}$$

It can easily be shown now that in the one-level case $S^{J\pi}_{\alpha jI,\alpha' j' I'}$ have the form given in Eq. (7-2). Such a form is possible if we note that the g's transform like wave functions, i.e.,

$$g_{\alpha jI} = \sum_{s=|I-\sigma|}^{I+\sigma} (2s+1)^{\frac{1}{2}}(2j+1)^{\frac{1}{2}} W(I\sigma J\ell;sj) g_{\alpha s\ell} \tag{15-2}$$

and assume the same potential scattering phase shifts, $\xi_{\alpha\ell}$, in both representations. Substituting Eq. (15-2) in Eq. (11-2) will result in an identity (using Eq. 15 of B52b) only if the total width in both representations is the same. But this is insured by the equality

$$\sum_j g^2_{\alpha jI} = \sum_s g^2_{\alpha s\ell} \tag{16-2}$$

easily demonstrable from Eq. (15-2) and the W-coefficient orthogonality relation, Eq. (15) of B52b.

7. In this next paragraph our present knowledge about the partial reaction widths will be summarized. It follows from the work of Wigner and Eisenbud on the dispersion theory of nuclear reactions (see for an excellent resume of this work reference S53) that the partial reaction width for neutrons, Γ_n, in the channel spin representation, can be written

$$\Gamma_{s\ell} = 2 \cdot s_\ell \cdot \gamma^2_{s\ell} \tag{17-2}$$

where γ^2 is called the reduced neutron width, and s_ℓ the penetration function. An exactly similar relation holds in the j-representation, since the γ transform exactly like the g, according to Eq. (15-2). The penetration function depends on the orbital angular momentum, ℓ, and the neutron bombarding energy. It can be expressed in terms of the spherical Bessel and Neumann functions, but it is more conveniently generated by the following recurrence relations:

$$\left.\begin{aligned} s_\ell &= \frac{x^2 s_{\ell-1}}{(\ell - \Delta_{\ell-1})^2 + s^2_{\ell-1}} \; ; \; s_o = x \\ \Delta_\ell &= \frac{x^2(\ell - \Delta_{\ell-1})}{(\ell - \Delta_{\ell-1})^2 + s^2_{\ell-1}} - \ell \; ; \; \Delta_o = 0 \end{aligned}\right\} \tag{18-2}$$

where $x = \frac{R}{\lambda\!\!\!^-}$ for neutrons.

The penetration function measures the attenuation of the neutron waves by the centrifugal barrier of the nucleus; the reduced width measures the probability of appearance of neutrons in the particular channel at the

* See errata

surface of the compound nucleus. The energy and orbital angular momentum variation of the reduced neutron width is not expected to be very rapid, nor is the order of magnitude expected to change profoundly. The complex potential model of Feshbach, Porter, and Weisskopf (F54) obtains a mildly oscillatory behavior for γ^2 in x and ℓ due to multiple reflection phenomena in the nuclear interior. Similar behavior is predicted by the Wigner-Lane-Thomas model (L55) and originates from essentially the same cause. More will be said about these models in a later chapter, and further discussion is deferred until then.

Porter and Thomas (P56) argued on inituitive grounds that the square roots of the reduced widths of neighboring resonances, $\gamma_{s\ell}$, should be normally distributed. Since the transformation connecting the γ_{jI} to the $\gamma_{s\ell}$ is linear, by a theorem of De Moivre (C56a), so also should the γ_{jI} be normally distributed. This implies a chi-squared distribution of one degree of freedom for the reduced widths themselves (C56). Statistical analysis of a considerable amount of resonance data available to Porter and Thomas showed this distribution to be excellent. Another conclusion verified by Porter and Thomas is the near constancy of the radiative width, both from resonance to resonance in the same nucleus, and in neighboring nuclei.

8. This last paragraph will summarize our present knowledge concerning the spacing, $D_{J\pi}$, of levels of the same spin, J, and parity, π. Two recent studies principally are important, one by Lang and LeCouteur (L54) and one by Newton (N56a). Both of these authors emphasize a spin dependence proportional to $(2J + 1)^{-1}$, and both predict a similar and very rapid

decrease of $D_{J\pi}$ with excitation energy. Both formulae are semi-empirical, using forms suggested by theory, and constants determined from experiment.

The statistical distribution of the level spacing has been discussed by Wigner (W56a) in terms of a very elementary model. Wigner's distribution has the virtue of predicting the observed low probability of levels being very close together. This "level repulsion" effect has also been studied by Gurevich and Pevsner (G56). There is at this writing insufficient evidence to conclusively obtain a good statistical distribution for the level spacing.

CHAPTER 3. SLOWING DOWN THEORY IN HOMOGENEOUS MEDIA

1. This third chapter has three purposes: (i) to introduce the few fundamental results of slowing down theory necessary for the discussion of the resonance absorption problem, (ii) to augment the historical survey of low energy resonance absorption in homogeneous media begun in Chapter 1, and (iii) to serve as a vehicle for introducing certain conventional terms, e.g., flux, macroscopic cross section, resonance escape probability, effective resonance integral, etc.

2. In this paragraph let us consider the process of moderation of neutrons by elastic collision with nuclei of mass A; let the unit of mass be the neutron mass. Further, let us consider only s-wave interaction which will nearly always be appropriate for energies less than 100 kev. This restriction has the consequence of causing the scattering to be isotropic in the center of mass coordinate system. In this coordinate system before collision the neutron and nucleus move toward one another along a line parallel to the direction of motion of the incident neutron in the laboratory. The laws of energy and momentum conservation in the center of mass system require that the <u>speeds</u> of the neutron and the nucleus be the same after collision as before, and that their velocities continue to point in opposite directions. With this fact appreciated the dynamics of the collision can be explained with the help of Fig. (1-3).

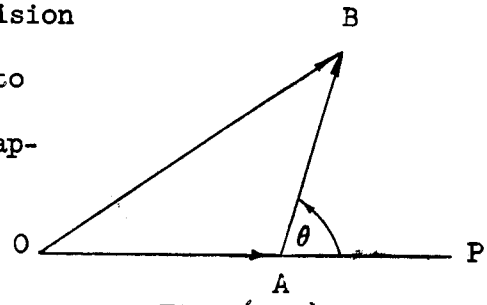


Fig. (1-3)

In this figure OP is the direction of incidence of a neutron of speed v on a nucleus of mass A. $\vec{OA}$ represents the center of mass velocity, of magnitude $\frac{v}{A+1}$. $\vec{AB}$ is the velocity of

the neutron in the center of mass system after collision, its magnitude is the same as before collision, viz.: $\frac{Av}{A + 1}$. θ is the angle of scattering in the center of mass system and $\vec{\mathfrak{B}}$ is the velocity of the neutron in the laboratory after collision. From the law of cosines it follows that

$$\frac{E'}{E} = \frac{v'^2}{v^2} = \left(\frac{1}{A + 1}\right)^2 + \left(\frac{A}{A + 1}\right)^2 + \frac{2A}{(A + 1)^2} \cos\theta \qquad (1\text{-}3)$$

Here E' is the final neutron energy and E the initial neutron energy in the laboratory. It is clear from Eq. (1-3) that E' has the limits

$$E \geq E' \geq \left(\frac{A - 1}{A + 1}\right)^2 E \equiv \alpha E \qquad (2\text{-}3)$$

From the statistical distribution of θ a distribution of E' can be found. For isotropic scattering in the center of mass system

$$P(E') = P(\cos\theta) \left| \frac{d(\cos\theta)}{dE'} \right| = \frac{1}{(1 - \alpha)E} \qquad (3\text{-}3)$$

Thus the scattered neutrons are distributed uniformly in the interval given by Eq. (2-3). For future reference let us express the distribution of scattered neutrons in terms of a variable, u, called lethergy, and defined by the relation $u = \ln\left(\frac{E_o}{E}\right)$, where E_o is some reference energy.

$$P(u') = P(E') \left| \frac{dE'}{du'} \right| = \frac{e^{u-u'}}{1 - \alpha} \qquad (4\text{-}3)$$

3. The scattering distribution (4-3) can be made the basis of an integral equation to describe resonance absorption. This equation can be solved explicitly for the case of moderation by hydrogen; the solution was first given by Bethe (B37). The integral equation can be written as in this case as

$$\Sigma_t(u)\phi(u) = \int_0^u \Sigma_s(u')\phi(u')e^{u'-u}\,du' + S(u) \qquad (5\text{-}3)$$

The symbols mean the following: ϕ is the flux of neutrons as a function of lethargy, defined as the product of density per unit lethargy and velocity. Σ_s is the macroscopic scattering cross section at lethargy u, defined as $N\sigma_s(u)$, where N is the atomic density of scatters and $\sigma_s(u)$ their microscopic scattering cross section. Σ_s is the reciprocal of the scattering mean free path. A similar definition applies to Σ_t, the macroscopic total cross section. If the absorption is due to some heavy, non-moderating material the macroscopic total cross section is given, by the usual rules for composing mean free paths, as $\Sigma_t = N\sigma_s(u) + N_a\sigma_a(u)$ where N_a is the absorber atomic density, and σ_a the microscopic absorption cross section. The product of a macroscopic cross section and a flux per unit lethargy gives a reaction rate per unit volume per unit lethargy. S(u) is the neutron source strength function. The situation becomes very much simpler and no less general, if we consider a unit monoenergetic source of neutrons at the reference energy $E_o(u = 0)$. Let us then take for S(u) the source of once-collided neutrons, which for hydrogen is, from Eqs. (2-3) and (4-3),

$$S(u) = e^{-u}, \quad 0 \leq u \leq \infty \qquad (6\text{-}3)$$

With this choice, differentiation of Eq. (5-3) leads at once to the differential equation

$$\frac{d(\Sigma_t\phi)}{du} + \frac{\Sigma_a}{\Sigma_t}(\Sigma_t\phi) = 0 \qquad (7\text{-}3)$$

A suitable boundary condition can be obtained by setting u = 0 in Eq. (5-3). This procedure gives

$$(\Sigma_t \phi)_{u=0} = S(o) = 1 \tag{8-3}$$

The unique solution of Eqs. (7-3) and (8-3) is

$$\Sigma_t(u)\phi(u) = \exp\left(-\int_o^u \frac{\Sigma_a}{\Sigma_t}\, du'\right) \tag{9-3}$$

4. A measure of the extent of resonance absorption is given directly by the slowing down density at u, q(u), defined as the number of neutrons slowing down past lethargy u per unit volume per unit time. It is given, in the case we are concerned with, by the expressions,

$$q(u) = \int_o^u \Sigma_s(u')\phi(u')du' \cdot \int_u^\infty e^{u'-u''}\, du'' + \int_u^\infty e^{-u'}\, du' \tag{10-3}$$

The u" integral simply represents the probability that a neutron scattered at u' will be slowed down to a lethargy $u'' \geq u$. The first term on the right hand side of Eq. (10-3) is the slowing down density of already collided neutrons, the second term is the slowing down density due to first collisions. If we perform the u" integral, and substitute Eq. (9-3) for the flux, we obtain

$$q(u) = \int_0^u \frac{\Sigma_s}{\Sigma_t} \exp\left(- \int_0^{u''} \frac{\Sigma_a}{\Sigma_t} du''\right) e^{u'-u} du' + \int_0^u e^{-u'} du'$$

$$= e^{-u} \left\{ \int_0^u \frac{\Sigma_s}{\Sigma_t} \exp\left(\int_0^{u'} \frac{\Sigma_s}{\Sigma_t} du''\right) du' + 1 \right\} \qquad (11\text{-}3)$$

The integrand in Eq. (11-3) is a perfect differential. Performing the integral finally gives

$$q(u) = \exp\left(- \int_0^u \frac{\Sigma_a}{\Sigma_t} du'\right). \qquad (12\text{-}3)$$

q(u), normalized to a unit source, as it is here, is called the resonance escape probability, p(u), at lethargy u. It directly measures the fraction of source neutrons surviving resonance absorption to lethargy u.

5. The problem just solved above is the only one in which the slowing down problem with absorption can be exactly solved at all lethargies. There is another very important problem, however, which can be solved at lethargies considerably above source lethargy (u = 0). Let us consider slowing down from a monoenergetic source at u = 0 in a medium of nuclear mass, A, and with a constant ratio, β, of scattering to total cross section. If we use the symbol F(u) for the total collision density, $\Sigma_t(u)\phi(u)$, the slowing down integral equation can be written, far from source lethargy, as

$$F(u) = \beta \int_{u-\epsilon}^{u} F(u') \frac{e^{u'-u}}{1-\alpha} du' \qquad (13\text{-}3)$$

where $\epsilon = \ln\left(\frac{1}{\alpha}\right)$ and is the maximum lethargy loss in a collision with a nucleus of mass A. Let us take as an ansatz an exponential form for F(u), viz., $e^{\lambda u}$. If we substitute in Eq. (13-3) we get the following equation for determining λ:

$$1 + \lambda = \beta \cdot \frac{1 - \alpha^{1+\lambda}}{1 - \alpha} \tag{14-3}$$

The slowing down density is now given by the expression

$$q(u) = \int_{u-\epsilon}^{u} \beta F(u')du' \cdot \int_{u}^{u'+\epsilon} \frac{e^{u'-u''}}{1 - \alpha} du'' \tag{15-3}$$

If we substitute $e^{\lambda u}$ for F(u), integrate, and simplify using Eq. (14-3), we obtain

$$q(u) = - \frac{1 - \beta}{\lambda} e^{\lambda u} \tag{16-3}$$

Some well known conclusions follow from these equations in the case $\beta = 1$, i.e., pure scattering. It is possible to expand λ in powers of $\beta - 1$; the first two terms of the series are

$$\lambda = \frac{1}{\xi} (\beta - 1) - \frac{\xi - \gamma}{\xi^2} (\beta - 1)^2 + \ldots \tag{17-3}$$

where $\xi = 1 - \frac{\alpha\epsilon}{1 - \alpha}$ and $\gamma = 1 - \frac{\frac{1}{2}\alpha\epsilon^2}{(1 - \alpha)\xi}$. ξ is the average lethargy change per collision, and $2\xi\gamma$ is the average squared lethargy change per collision. When $\beta = 1$,

$$F(u) = 1 \text{ and } q(u) = \xi. \tag{18-3}$$

These equations represent the well known asymptotic solution to the slowing down problem without absorption. The scattering density and slowing down density are both constant and in the ratio ξ.

6. An important application of this problem is to an approximate solution of the slowing down problem for slowly varying absorption to scattering ratio. The procedure is a WKB type approach developed by Hurwitz (H51). Let us write the integral slowing down equations as

$$\frac{G(u)}{\beta(u)} = \int_{u-\epsilon}^{u} G(u') \frac{e^{u'-u}}{1-\alpha} du' \tag{19-3}$$

where G(u) is the scattering density. Let us choose a solution of the form

$$G(u) = H(u)\, e^{\int_0^u \lambda(u')du'} \tag{20-3}$$

where $\lambda(u)$ is given in terms of $\beta(u)$ by Eq. (14-3). Let us approximate $G(u')$ in the integral on the right hand side by writing

$$H(u') = H(u) + \frac{dH}{du}(u' - u)$$

and

$$e^{\int_0^u \lambda(u'')du''} = e^{\int_0^u \lambda(u'')du'' + \lambda(u)(u'-u) + \frac{1}{2}\frac{d\lambda}{du}(u'-u)^2}$$

$$= e^{\int_0^u \lambda(u'')du'' + \lambda(u)(u'-u)} \left(1 + \frac{1}{2}\frac{d\lambda}{du}(u' - u)^2\right). \tag{21-3}$$

If we substitute Eq. (21-3) into Eq. (19-3) and keep only terms linear in the first derivatives we obtain, using Eq. (20-3),

$$\frac{G(u)}{\beta(u)} = G(u) \int_{u-\epsilon}^{u} \frac{e^{[\lambda(u)+1](u'-u)}}{1-\alpha} du' + G(u) \cdot \frac{1}{2}\frac{d\lambda}{du} \cdot \int_{u-\epsilon}^{u} \frac{e^{[\lambda(u)+1](u'-u)}}{1-\alpha} (u'-u)^2 du'$$

$$+ G(u) \cdot \frac{1}{H}\frac{dH}{du} \int_{u-\epsilon}^{u} \frac{e^{[\lambda(u)+1](u'-u)}}{1-\alpha} (u'-u) du' \qquad (22\text{-}3)$$

It follows from Eq. (14-3) that

$$\int_{u-\epsilon}^{u} \frac{e^{[\lambda(u)+1](u'-u)}}{1-\alpha} du' = \frac{1}{\beta(u)} \qquad (23\text{-}3)$$

Hence, Eq. (22-3) can be written, after rearrangement, and cancellation of some terms as

$$\frac{1}{2}\frac{d\lambda}{du} \cdot \frac{d^2}{d\lambda^2}\left(\frac{1}{\beta}\right) = -\frac{d\ln H}{du}\frac{d}{d\lambda}\left(\frac{1}{\beta}\right) \qquad (24\text{-}3)$$

or

$$\frac{d\ln H}{du} = -\frac{1}{2}\frac{d}{du}\ln\left(\left|\frac{d\left(\frac{1}{\beta}\right)}{d\lambda}\right|\right) \qquad (25\text{-}3)$$

since $d(\ln y) = d\ln(-y) = d\ln(|y|)$. Finally, then,

$$H(u) = \left|\frac{d}{d\lambda}\left(\frac{1}{\beta}\right)\right|^{-\frac{1}{2}} \qquad (26\text{-}3)$$

The solution (26-3) is unique up to a constant. An important situation in which the constant can easily be related to the source strength and an explicit expression for the resonance escape probability obtained is the case of an absorption cross section which is zero for some distance from source lethargy, then rises slowly and then falls slowly again to zero.

When $\beta = 1$, $F(u) = \xi^{-1/2}$ from Eqs. (26-3) and (17-3). If we wish to normalize to a unit source at low lethargy, before there is any absorption, we must multiply the value of $H(u)$ given by Eq. (26-3) by $\xi^{-1/2}$. After we have passed through the region of absorption, $F(u)$ is given by

$$F(u) = \frac{1}{\xi} e^{\int_0^u \lambda(u')du'} \tag{27-3}$$

and the slowing down density, which with the normalization chosen equals the resonance escape probability, is given by

$$q(u) = p(u) = \xi F(u) = e^{\int_0^u \lambda(u)du} \tag{28-3}$$

7. Formula (28-3) takes a particularly simple form and one very reminiscent of Eq. (12-3) for hydrogen if β is near 1. We can then write, according to Eq. (17-3)

$$\lambda = -\frac{\Sigma_a}{\xi\Sigma_t} \qquad \text{(correct to first order in } \beta - 1) \tag{29-3}$$

$$\lambda = -\frac{\Sigma_a}{\xi\Sigma_s + \gamma\Sigma_a} \qquad \text{(correct to second order in } \beta - 1) \tag{30-3}$$

Equation (29-3) is known as Wigner's approximation, Eq. (30-3) as the Goertzel-Greuling approximation.

8. Formula (29-3) or (30-3) can be used, for example, to calculate the resonance absorption in a homogeneous mixture of uranium and graphite, even though the absorption in the uranium takes place in high sharp resonances, if the uranium atomic density, N_a, is low enough. For $\frac{d\beta}{du}$ is proportional to N_a and will be small if N_a is sufficiently small. On the other hand, if the uranium is present in high density, the WKB approximation of Hurwitz is inapplicable because of the narrowness of the resonances. However, Wigner (W55) has indicated how this circumstance can be turned to advantage. Let us consider an absorbing resonance whose extent in lethargy is very much less than ξ, the average lethargy decrement per collision. This restriction has two important consequences: (i) no neutron can make more than one collision in the region of significant absorption, and (ii) neutrons which make a collision in the region of significant absorption made their last collisions at lethargies far from the resonance. But this last statement implies that the rate of supply of neutrons to each infinitesimal lethargy interval in the range of significant absorption is independent of whether there is a resonance or not. But, at steady state, the rate of supply of neutrons at a lethargy equals the collision density at that lethargy. Hence

$$\Sigma_t(u)\ \phi(u) = \frac{1}{\xi} \tag{31-3}$$

Here $\frac{1}{\xi}$ is the collision density without the resonance, normalized to a

unit source, $\phi(u)$ is the true flux in the resonance. The total absorption rate in the resonance is then

$$A = \int \Sigma_a(u)\phi(u)du = \int \frac{\Sigma_a(u)}{\xi\Sigma_t(u)}\,du \tag{32-3}$$

The integrals extend over the entire resonance. The escape probability through the resonance, p, equal to 1 - A, is given by

$$p = 1 - \int \frac{\Sigma_a(u)}{\xi\Sigma_t(u)}\,du \tag{33-3}$$

If the integral is small compared to unity, as frequently happens, we can write, approximately,

$$p = \exp\left(- \int \frac{\Sigma_a(u)}{\xi\Sigma_t(u)}\,du\right) \tag{34-3}$$

9. Equation (34-3) also applies for a mixture of elements for all of which ξ is very much larger than the range of significant absorption. In such a case Eq. (31-3) still holds but with the right hand side replaced by $\frac{1}{\bar{\xi}}$ where $\bar{\xi}$ is the average lethargy decrement per collision with the mixture and is given by

$$\bar{\xi} = \sum_i \xi_i C_i; \quad C_i = \frac{\Sigma_{si}}{\sum_i(\Sigma_{si})} \tag{35-3}$$

where ξ_i is the average lethargy decrement of element i, and Σ_{si} is its macroscopic scattering cross section.

The collision density we seek obeys the equation

$$F(u) = \sum_i \int_{u-\epsilon_i}^{u} C_i F(u') \frac{e^{u'-u}}{1 - \alpha_i} du' \tag{36-3}$$

and the slowing down density related to it is

$$q(u) = \sum_i \int_{u-\epsilon_i}^{u} C_i F(u') du' \cdot \int_{u}^{u'+\epsilon_i} \frac{e^{u'-u''}}{1 - \alpha_i} du'' \tag{37-3}$$

It is easy to show that setting F(u) equal to a constant, a, solves Eq. (36-3). Inserting the constant in Eq. (37-3) gives, after integration,

$$q(u) = \sum_i C_i \xi_i a = \bar{\xi} a \tag{38-3}$$

Thus if $q = 1$, $a = F(u) = \frac{1}{\bar{\xi}}$.

CHAPTER 4. HOMOGENEOUS RESONANCE INTEGRALS

1. By far the most frequently occurring problem in the calculation of resonance absorption is that dealt with in paragraphs (8-3) and (9-3). It is conventional in this problem to discuss not the resonance escape probability itself, but rather a related quantity, the so-called effective resonance integral, I. Let the macroscopic scattering cross section in the absence of the resonance be Σ_p, let the density of absorbing nuclei be N_a. Let us then define I by the equation

$$\exp\left(-\frac{N_a I}{\bar{\xi}\Sigma_p}\right) = p = \exp\left(-\frac{1}{\bar{\xi}}\int \frac{\Sigma_a}{\Sigma_t}\,du\right) \tag{1-4}$$

The integral on the right hand side now only extends over the resonance. It now follows that

$$I = \int_{\text{res.}} \frac{\Sigma_p}{\Sigma_t}\,\sigma_a\,du \tag{2-4}$$

2. The resonance cross sections involved in Eq. (2-4) are given in Eqs. (1-2) and (4-2). The total absorber cross section, summed over final channel spins and averaged over initial channel spins, is given by (dropping the channel index α)

$$\sigma_t = \pi\lambda\!\!\!^{-2}\cdot g_J\cdot\frac{\Gamma_n\Gamma}{(E-E_o)^2+\left(\frac{\Gamma}{2}\right)^2} + 4\pi\lambda\!\!\!^{-}R\cdot g_J\cdot\frac{(E-E_o)\Gamma_n}{(E-E_o)^2+\left(\frac{\Gamma}{2}\right)^2} + 4\pi R^2 \tag{3-4}$$

Here Γ_n is the neutron width, $\Gamma_{\alpha s}$, summed over channel spins, and $g_J = \frac{2J+1}{2(2I+1)}$. The resonance absorption cross section, averaged over

initial channel spins, is given by Eq. (1-2)

$$\sigma_a = \pi\lambda\!\!\!^{-2} \cdot g_J \cdot \frac{\Gamma_n \Gamma_\gamma}{(E - E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} \tag{4-4}$$

Γ_γ is the radiative width. It is assumed that radiative capture is the only reaction possible, which is nearly always true at low bombarding energies. If this is not so Γ_γ must be replaced by $\Gamma - \Gamma_n$. In any event $\Gamma_n + \Gamma_\gamma = \Gamma$.

It is important to note that all the equations of Chapter 1 apply to the center of mass coordinate system. Frequently widths and resonance energies are quoted in the laboratory system of coordinates, in which case they are larger by a factor $\frac{A + 1}{A}$. $\lambda\!\!\!^{-}$, however, must always be computed in the center of mass coordinate system.

If we define the auxiliary quantities

$$\sigma_o = 4\pi\lambda\!\!\!^{-2} \cdot g_J \cdot \frac{\Gamma_n}{\Gamma} \tag{5a-4}$$

$$\sigma_{pa} = 4\pi R^2 \tag{5b-4}$$

$$x = \frac{E - E_o}{\frac{\Gamma}{2}} \tag{5c-4}$$

we can write succinctly,

$$\sigma_t = \sigma_o(1 + x^2)^{-1} + (\sigma_o \sigma_{pa} g_J \frac{\Gamma_n}{\Gamma})^{\frac{1}{2}} 2x(1 + x^2)^{-1} + \sigma_{pa} \tag{6a-4}$$

$$\sigma_a = \sigma_o \frac{\Gamma_\gamma}{\Gamma} (1 + x^2)^{-1} \tag{6b-4}$$

With this notation we can write

$$\Sigma_p = N_a \sigma_{pa} + \Sigma_m \tag{7a-4}$$

and

$$\Sigma_t = N_a \sigma_t + \Sigma_m \tag{7b-4}$$

where Σ_m is the macroscopic scattering cross section of the moderator. As our final three definitions let us write

$$\sigma_p = \frac{\Sigma_p}{N_a} \tag{8-4}$$

$$\gamma = g_J \cdot \frac{\Gamma_n}{\Gamma} \cdot \frac{\sigma_{pa}}{\sigma_p} \tag{9-4}$$

$$\beta = \frac{\sigma_p}{\sigma_o} \tag{10-4}$$

Some of these new symbols have the following physical significance: σ_o is the total resonance cross section at exact resonance ($x = 0$), σ_{pa} is the potential scattering of the absorber nuclei, and σ_p is the total energy independent (potential) scattering cross section per absorbing nucleus.

3. If we substitute equations (6a- 6b-, 7a-, 8-, 9-4) in Eq. (2-4) we can write finally,

$$I = \int_{res.} \frac{\sigma_p \left\{ \sigma_o \frac{\Gamma_\gamma}{\Gamma} (1 + x^2)^{-1} \right\}}{\sigma_o (1 + x^2)^{-1} + (\sigma_o \sigma_p \gamma)^{1/2} 2x (1 + x^2)^{-1} + \sigma_p} dx \frac{\Gamma}{2E} \qquad (11\text{-}4)$$

Here we have used $- du = \frac{dE}{E} = \frac{\Gamma}{2E} dx$. Because the nuclear resonances are very narrow, i.e., because, generally, $\Gamma << E$, it is a very good approximation to ignore the energy dependence of σ_o, Γ, and E over the range of integration and simply evaluate them at E_o. Moreover, the limits of integration on x can be extended to $\pm \infty$. With some minor rearrangement, Eq. (11-4) can then be written

$$I = \frac{\sigma_p \Gamma_\gamma}{2E_o} \int_{-\infty}^{+\infty} \frac{dx}{1 + (\beta\gamma)^{1/2} 2x + \beta(1 + x^2)} \qquad (12\text{-}4)$$

This integral can easily be evaluated and leads to the following result for I:

$$I = \frac{\frac{\pi}{2} \cdot \sigma_p \cdot \frac{\Gamma_\gamma}{E_o}}{\sqrt{\beta(1 + \beta - \gamma)}} \qquad (13\text{-}4)$$

If $\beta << 1 - \gamma$ as often happens in the low energy resonances of uranium or thorium or other absorbers in fairly concentrated mixtures, I is proportional to $\sqrt{\sigma_p}$. This rule is roughly verified by Mitchell's data (M44) and by the data of Hughes and Eggler (H45). There is, however, a good reason why the rule ought not to be exact, as we shall see in the next paragraph. If $\beta >> 1 - \gamma$ as often happens when the mixture is very dilute

$$I = I_{\infty} = \frac{\pi}{2}\,\sigma_o\,\frac{\Gamma_\gamma}{E_o}\,(\qquad \propto(\sigma_p \to \infty) \tag{14-4}$$

This is the so-called "infinite dilution" resonance integral. The sum of I_{∞} over all resonances has been measured for many materials (M55, S55).

4. The results presented in the last paragraph, with the exception of Eq. (14-4), are not directly comparable with experiment because they have been derived on the basis of stationary absorber nuclei. In actual fact, the absorber nuclei are in thermal motion and this motion strongly affects the absorption of neutrons by them. The effective cross section for neutrons of laboratory velocity v for any resonance process involving moving nuclei is given by

$$v \cdot \sigma_{eff}(v) = \int |\vec{v} - \vec{V}|\ \sigma(|\vec{v} - \vec{V}|)P(\vec{V})d^3V \tag{15-4}$$

where $P(\vec{V})$ is the distribution of target laboratory velocities, $\vec{V}$. The definition of σ_{eff} has been chosen to give the correct reaction rate. $\frac{V}{v} \sim \left(\frac{kT}{AE}\right)^{1/2}$ where kT is the absorber temperature in energy units, A is the absorber nuclear mass and E is the neutron energy. Usually this ratio is $<<1$ (for U^{238} at $300^{o}K$ it is 0.004 for the 6.7 ev resonances), and the first factor in the integrand varies very little from v as V varies. Equating $|\vec{v} - \vec{V}|$ and v we have

$$\sigma_{eff}(v) = \int \sigma(|\vec{v} - \vec{V}|)P(\vec{V})d^3V \tag{16-4}$$

The relative energy, E', associated with the velocity $\vec{v} - \vec{V}$ in the center of mass system is given by

$$E' = \frac{1}{2}\mu \left|\vec{v} - \vec{V}\right|^2 \tag{17-4}$$

where μ is the neutron reduced mass equal to $\frac{A}{A+1}$. In view of the smallness of $\frac{V}{v}$ we can expand E' in the powers of $\frac{V}{v}$. Choose for the z-axis the direction of v. Then to first order

$$E' = \frac{1}{2}\mu v^2 - \mu v V_z \tag{18a-4}$$

$$= E - (2\mu E)^{\frac{1}{2}} V_z \tag{18b-4}$$

where $E = \frac{1}{2}\mu v^2$ is the relative energy for stationary nuclei. If we take $\left|\vec{v} - \vec{V}\right|$ to be only a function of V_z, as indicated above, we can perform the V_x and V_y integrals, and replace the three dimensional probability distribution $P(\vec{V})$ by a one dimensional distribution $P(V_z)$. Using Eqs. (17-4) and (18b-4) we can write

$$\sigma_{eff}(E) = \int \sigma(E') \cdot P\left(\frac{E - E'}{\sqrt{2\mu E}}\right) \cdot \frac{dE'}{\sqrt{2\mu E}} \tag{19-4}$$

where P is the statistical distribution of V_z.

The question of what the correct distribution P for V_z is has been discussed (L39); for most solid materials a Maxwellian distribution is appropriate and we shall accordingly choose it. Thus

$$P(V_z) = \left(\frac{A}{2\pi kT}\right)^{1/2} \cdot \exp\left(-\frac{AV_z^2}{2kT}\right) \tag{20-4}$$

5. If we choose for $\sigma(E')$ Eq. (4-4) and substitute Eq. (4-4) and (20-4) into Eq. (19-4) we obtain after simplification the result

$$\sigma_{a\ eff}(E) = \sigma_o \frac{\Gamma_\gamma}{\Gamma} \cdot \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \frac{\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]}{1+y^2}\, dy \qquad (21\text{-}4)$$

where as before $x = \dfrac{(E - E_o)}{\frac{\Gamma}{2}}$ and where $y = \dfrac{(E' - E_o)}{\frac{\Gamma}{2}}$ and

$$\xi = \frac{\Gamma}{\Delta}\ ;\ \Delta = \left(\frac{4\mu kTE}{A}\right)^{1/2} \qquad (22\text{-}4)$$

Δ is called the Doppler width of the resonance. In taking σ_o and Γ outside the y-integral use has again been made of the thinness of the resonance.

If we rewrite Eq. (21-4) in terms of laboratory system widths and energies its form remains unchanged. In the expression for σ_o, $\lambda\!\!\!^-$ must still be calculated in the center of mass system. ξ remains unchanged in both definition and numerical value but Δ is given by

$$\Delta = \left(\frac{4kTE}{A}\right)^{1/2} \qquad (23\text{-}4)$$

where E is the neutron laboratory energy.

6. The second factor on the right hand side of Eq. (21-4) is called the Doppler broadened line shape and is denoted by $\psi(\xi, x)$. It is the counterpart of the natural line shape, $(1 + x^2)^{-1}$, in Eq. (6b-4). This section will be devoted to a detailed analysis of its properties.

In the first place when $kT \rightarrow 0$, $\xi \rightarrow \infty$ and

$$\frac{\xi}{2\sqrt{\pi}} \exp\left[-\frac{\xi^2}{4}(x - y)\right] \rightarrow \delta(x - y) \tag{24-4}$$

Here δ is the Dirac delta function. Hence

$$\psi(\infty, x) = (1 + x^2)^{-1} \tag{25-4}$$

Another important property of $\psi(\xi, x)$ is that its integral over all x is independent of ξ. It is easy to show that

$$\int_{-\infty}^{+\infty} \psi(\xi, x)dx = \pi \tag{26-4}$$

by first performing the x-integration and then the y-integration.

An asymptotic series valid for large values of x has been derived by several authors (B33, M54). (M54) obtained this series by using the Fourier integral expansion of the integrand in Eq. (21-4). Since

$$\xi\sqrt{\pi}\, e^{-\frac{\xi^2}{4}x^2} = \int_{-\infty}^{+\infty} e^{i\omega x} \cdot e^{-\frac{\omega^2}{\xi^2}} d\omega \tag{27a-4}$$

and

$$(1 + x^2)^{-1} = \int_{-\infty}^{+\infty} \frac{1}{2} e^{-|\omega|} e^{i\omega x} d\omega \tag{27b-4}$$

we can write

$$\psi(\xi,x) = \int_{-\infty}^{+\infty} dx \cdot \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{i\omega(x-y)} e^{-\frac{\omega^2}{\xi^2}} d\omega \cdot \frac{1}{2} \int_{-\infty}^{+\infty} e^{-|\omega'| + i\omega' x} d\omega' \qquad (28\text{-}4)$$

If we note that

$$\int_{-\infty}^{+\infty} e^{i\lambda x}\, dx = 2\pi\delta(\lambda) \qquad (29\text{-}4)$$

we can perform the x and ω' integrations in that order, and obtain

$$\psi(\xi,x) = \frac{1}{2} \int_{-\infty}^{+\infty} e^{-\frac{\omega^2}{\xi^2} - |\omega| + i\omega x}\, d\omega \qquad (30\text{-}4)$$

By completing the square in the exponent and rearranging we can obtain

$$\psi(\xi,x) = \frac{\sqrt{\pi}}{2}\, \xi \cdot \mathrm{Re} \left\{ \exp\left[\frac{(1+ix)\xi}{2}\right]^2 \mathrm{Erfc}\left[\frac{(1+ix)^{\xi}}{2}\right] \right\} \qquad (31\text{-}4)$$

Finally, the complementary error function has an asymptotic expansion, viz.:

$$\frac{\sqrt{\pi}}{2}\, \mathrm{Erfc}(s) \sim \frac{e^{-s^2}}{2s} \left[1 - \frac{1}{2s^2} + \frac{1 \cdot 3}{(2s^2)^2} - \frac{1 \cdot 3 \cdot 5}{(2s^2)^3} + \ldots \right] \qquad (32\text{-}4)$$

In this way the authors of (M54) obtain the following asymptotic series

$$\psi(\xi,x) \sim \frac{1}{1+x^2} \left[1 - \frac{2}{\xi^2} \frac{1-3x^2}{(1+x^2)^2} + \frac{12}{\xi^4} \frac{1-10x^2+5x^4}{(1+x^2)^4} - \ldots \right] \qquad (33\text{-}4)$$

It is evident from Eq. (33-4) that sufficiently far in the wings of a resonance the natural line shape is correct; the condition for this is $\frac{6}{\xi^2 x^2} << 1$. The authors of (M54) also derive a series valid for small ξx by employing the power series for the complementary error function. It will be less useful to us in what follows than Eq. (33-4) and we will not note it down. It follows, however, trivially from Eq. (31-4) that

$$\psi(\xi,0) = \frac{\sqrt{\pi}}{2}\,\xi e^{\xi^2/4}\,\mathrm{Erfc}\left(\frac{\xi}{2}\right) \tag{34-4}$$

When $\xi << 1$, Wigner (W55) has indicated that, at least near the center of the line, we can approximate ψ by setting $y = 0$ in the exponential, since then the natural line shape $(1 + y^2)^{-1}$ will be narrow compared to the exponential. This procedure gives

$$\psi(\xi,x) = \frac{\sqrt{\pi}}{2}\,\xi e^{-\frac{\xi^2}{4}x^2} \tag{35-4}$$

Numerical tables and graphs of $\psi(\xi,x)$ are available from a variety of sources (M54, R54a, M53).

7. The generalization of the interference scattering line shape, $2x(1 + x^2)^{-1}$, in the case of Doppler broadening, can be written similarly to Eq. (21-4) as

$$\chi(\xi,x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{\xi^2}{4}(x - y)^2\right] \frac{2y}{1 + y^2}\,dy \tag{36-4}$$

$\chi(\xi,x)$ is related to $\psi(\xi,x)$ by the relation

$$\chi(\xi,x) = 2x\psi(\xi,x) + \frac{4}{\xi^2} \cdot \frac{d\psi(\xi,x)}{dx} \tag{37-4}$$

From Eq. (37-4) it is immediately obvious that

$$\chi(\infty,x) = 2x(1 + x^2)^{-1} \tag{38-4}$$

$$\int_{-\infty}^{+\infty} \chi(\xi,x)dx = 0 \tag{39-4}$$

$$\chi(\xi,x) \sim 2x(1 + x^2)^{-1} \text{ if } \xi^2x^2 >> 6 \tag{40-4}$$

$$\chi(\xi,0) = 0 \tag{41-4}$$

8. Now let us consider the generalization of Eq. (11-4) for I to the case of Doppler broadening. Let us first consider the case $\gamma = 0$, and defer consideration of interference effects until later. γ will be near zero for (i) a purely absorbing resonance ($\Gamma_n << \Gamma$) or (ii) a dilute mixture ($\sigma_{pa} << \sigma_p$). The latter case is the most frequent in practical situations. The correct generalization of Eq. (11-4) is then obtained by replacing $(1 + x^2)^{-1}$ by $\psi(\xi,x)$; it can be written as

$$I = \sigma_p \frac{\Gamma_\gamma}{E_o} \cdot \int_0^\infty \frac{\psi(\xi,x)}{\psi(\xi,x) + \beta} dx \tag{42-4}$$

The integral on the right hand side of Eq. (42-4) will be denoted as $J(\xi,\beta)$ and the next few paragraphs are devoted to studying its properties.

9. It follows either from Eq. (13-4) or from Eqs. (42-4) and (25-4) that

$$J(\infty,\beta) = \frac{\frac{\pi}{2}}{\sqrt{\beta(1+\beta)}} \tag{43-4}$$

It is furthermore the case that for very small β, in particular $\beta << \frac{1}{6}\xi^2$ $J(\xi,\beta)$ is asymptotic to $J(\infty,\beta)$, i.e.,

$$J(\xi,\beta) \sim J(\infty,\beta) \text{ if } \beta << \frac{1}{6}\xi^2 \tag{44-4}$$

To prove this let us first note that if β is very small the integrand in Eq. (42-4) is virtually unity until $\psi(\xi,x) \cong \beta$. If the value of x at which this happens is sufficiently large, $\psi(\xi,x)$ may be replaced by $(1+x^2)^{-1}$ not only for large x but for small x as well. For the integrand is virtually unity for small x whether $\psi(\xi,x)$ or $(1+x^2)^{-1}$ is used. If this replacement of the Doppler broadened line shape is valid for all x, then Eq. (44-4) must hold. If when $\psi(\xi,x) \cong \beta$, $\psi(\xi,x) \cong (1+x^2)^{-1}$ then x is determined to be approximately $\beta^{-1/2}$. The approximation of replacing $\psi(\xi,x)$ by $(1+x^2)^{-1}$ will be a good one only if $6\beta/\xi^2 << 1$, as can be seen from the discussion following Eq. (33-4).

If on the other hand $\beta > \psi(\xi,0)$, we can prove that

$$\frac{\pi}{2\beta} > J(\xi,\beta) > \frac{\pi}{2\beta}\left[1 - \frac{\psi(\xi,0)}{\beta}\right] \tag{45-4}$$

For

$$J(\xi,\beta) = \int_0^\infty \frac{\psi(\xi,x)}{\psi(\xi,x)+\beta}\,dx = \int_0^\infty \sum_{k=0}^{\infty} (-)^k \left[\frac{\psi(\xi,x)}{\beta}\right]^{k+1} \tag{46-4}$$

If $\beta > \psi(\xi,0) \geq \psi(\xi,x)$ the series will converge uniformly and can be integrated term-by-term. Since the terms alternate we can write

$$\int_0^\infty \frac{\psi(\xi,x)}{\beta}\,dx > J(\xi,\beta) > \int_0^\infty \left\{\frac{\psi(\xi,x)}{\beta} - \frac{\psi^2(\xi,x)}{\beta^2}\right\} dx > \left[1 - \frac{\psi(\xi,0)}{\beta}\right] \int_0^\infty \frac{\psi(\xi,x)}{\beta}\,dx \quad (47\text{-}4)$$

Comparing Eq. (47-4) with Eq. (26-4) gives Eq. (45-4). One can easily see from Eq. (45-4) and Eq. (43-4) that as β becomes very large compared to unity

$$J(\xi,\beta) \sim \frac{\pi}{2\beta} \sim J(\infty,\beta) \quad (48\text{-}4)$$

A simple physical way of understanding Eq. (48-4) is simply that if β is sufficiently large compared to ψ only the area under $\psi(\xi,x)$ is significant in evaluating the integral. Since this area is the same as for the natural line shape we are immediately led to Eq. (48-4). It is for this reason that Eq. (14-4) for the resonance integral at infinite dilution is correct even in the presence of Doppler broadening.

10. Another important general property of $J(\xi,\beta)$ is that it increases as ξ decreases. We prove this as follows: First note that

$$\frac{\partial J}{\partial \xi} = \frac{\partial}{\partial \xi} \int_0^\infty \frac{\psi(\xi,x)}{\psi(\xi,x) + \beta}\,dx = \int_0^\infty \frac{\beta \frac{\partial \psi}{\partial \xi}}{(\psi + \beta)^2}\,dx \quad (49\text{-}4)$$

Now from Eq. (21-4) or Eq. (30-4) it follows that

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{\xi^3}{2} \cdot \frac{\partial \psi}{\partial \xi} \quad (50\text{-}4)$$

Hence, substituting Eq. (50-4) into Eq. (49-4) and integrating by parts we have

$$\frac{\partial J}{\partial \xi} = -\frac{2\beta}{\xi^3}\int_0^\infty \frac{\frac{\partial^2 \psi}{\partial x^2}}{(\psi+\beta)^2} = \frac{2\beta}{\xi^3}\int_0^\infty \frac{\partial \psi}{\partial x}\cdot\frac{\partial}{\partial x}(\psi+\beta)^{-2}\,dx \tag{51-4}$$

since $\frac{\partial \psi(\xi,x)}{\partial x} = 0$ at $x = 0$ and $x = \infty$. Performing the indicated differentiation gives

$$\frac{\partial J}{\partial \xi} = -\frac{4\beta}{\xi^3}\int_0^\infty \left(\frac{\partial \psi}{\partial x}\right)^2 (\psi+\beta)^{-3}\,dx \tag{52-4}$$

Since the integrand in Eq. (52-4) is positive, $\frac{\partial J}{\partial \xi} < 0$ which is what we wished to prove. It is also true that $\frac{\partial J}{\partial \beta} < 0$, and this is very easy to prove. These inequalities imply that the resonance absorption increases with increasing temperature.

11. In addition to being able to evaluate $J(\xi,\beta)$ exactly in the case of no Doppler broadening Eq. (43-4), we can also evaluate $J(\xi,\beta)$ accurately (although not exactly) in what may be termed the case of extreme Doppler broadening. By this we mean $\xi \ll 1$ and also $\psi(\xi,0) \gg \beta \gg \frac{1}{6}\xi^2$. If the sense of any of these inequalities is reversed we have seen that $J(\xi,\beta)$ is given by Eq. (43-4) or Eq. (48-4). If these inequalities are satisfied we can use Eq. (35-4) for $\psi(\xi,x)$. It is true that this expression for $\psi(\xi,x)$ is incorrect in the wings where ψ is asymptotic to the natural line shape, but under the stated conditions the wings contribute little to the integral. That is to say, the region where $x^2 \gg \frac{6}{\xi^2}$ and $\psi \sim (1+x^2)^{-1}$,

γ is of the order of $\frac{\xi^2}{6}$ which is $<<\beta$. Thus the contribution to the integral is small. Indeed it is easily shown for the natural line shape that

$$\int_x^\infty \frac{\gamma(\infty,x)}{\gamma(\infty,x)+\beta}\,dx = J(\infty,\beta)\left[1-\frac{2}{\pi}\arctan\left(x\sqrt{\frac{\beta}{1+\beta}}\right)\right] \tag{53-4}$$

Since $J(\xi,\beta) > J(\infty,\beta)$ the fractional contribution to the integral from the region of $x > \frac{\sqrt{6}}{\xi}$ is less than $1-\frac{2}{\pi}\arctan\left(\sqrt{\frac{6\beta/\xi^2}{1+\beta}}\right)$ which is approximately equal to $\frac{2}{\pi}\sqrt{\frac{\xi^2}{6\beta}}$ under the conditions $1 >> \beta >> \frac{\xi^2}{6}$. By hypothesis this last quantity is $<< 1$. Thus we can write with good accuracy under the stated conditions:

$$J(\xi,\beta) = \int_0^\infty \frac{\frac{\sqrt{\pi}\,\xi}{2}\,e^{-\frac{\xi^2}{4}x^2}}{\frac{\sqrt{\pi}\,\xi}{2}\,e^{-\frac{\xi^2}{4}x^2}+\beta}\,dx \tag{54-4}$$

If the parameter $\frac{\xi\sqrt{\pi}}{2\beta} >> 1$ we can approximately evaluate the integral in Eq. (54-4) by a method suggested by Wigner (W55). The integrand will be nearly unity until $x \cong \frac{2}{\xi}\sqrt{\ln\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)}$, and then fall rapidly to zero. But then, approximately

$$J(\xi,\beta) \cong \frac{2}{\xi}\sqrt{\ln\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)} \tag{55-4}$$

On the other hand if the parameter $\frac{\xi\sqrt{\pi}}{2\beta} < 1$ we can obtain a power series for $J(\xi,\beta)$. $J(\xi,\beta)$ can be written

$$J(\xi,\beta) = \frac{\sqrt{\pi}\,\xi}{2\beta} \int_0^\infty e^{-\frac{\xi^2}{4}x^2} \left(1 + \frac{\sqrt{\pi}\,\xi}{2\beta} e^{-\frac{\xi^2}{4}x^2}\right)^{-1} dx \tag{56a-4}$$

$$= \frac{\sqrt{\pi}\,\xi}{2\beta} \int_0^\infty e^{-\frac{\xi^2}{4}x^2} \sum_{k=0}^{\infty} (-)^k \left(\frac{\sqrt{\pi}\,\xi}{2\beta}\right)^k e^{-k\frac{\xi^2}{4}x^2} dx \tag{56b-4}$$

$$= \frac{\sqrt{\pi}}{\beta} \sum_{k=0}^{\infty} (-)^k \left(\frac{\sqrt{\pi}\,\xi}{2\beta}\right)^k \int_0^\infty e^{-(k+1)y^2} dy \tag{56c-4}$$

$$= \frac{\pi}{2\beta} \cdot \sum_{k=0}^{\infty} \frac{(-)^k}{\sqrt{k+1}} \left(\frac{\sqrt{\pi}\,\xi}{2\beta}\right)^k \tag{56d-4}$$

Equations (55-4) and (56d-4) are not entirely adequate for the computation of $J(\xi,\beta)$ because they provide no information when the parameter $\frac{\xi\sqrt{\pi}}{2\beta}$ is only somewhat larger than unity. It is possible to remedy the situation by analytically continuing the power series (56d-4) by the following artifice: Let us abbreviate the series in Eq. (56d-4) by $\sum_{k=0}^{\infty} A_k x^k$. If we define $y = \frac{x}{1+x}$ then

$$x = \sum_{\ell=0}^{\infty} y^{\ell+1} \tag{57-4}$$

If we substitute Eq. (57-4) in the series $\sum_{k=0}^{\infty} A_k x^k$ and collect coefficients of the powers of y we obtain a series $\sum_{k=0}^{\infty} B_k y^k$. The relation of the B's to the A's is given by

$$B_o = A_o \; ; \quad B_k = \sum_{\ell=1}^{k} C_{\ell-1}^{k-1} A \tag{58-4}$$

where the C_ℓ^k are the binomial coefficients. For the series in Eq. (56d-4) the B_k decrease and hence the y-series converges rapidly even for values of y corresponding to $x > 1$. For future reference we note that if $A_k = (-)^k(k + 1)^{-1/2}$, the first few B's are:

$$\begin{aligned} B_o &= 1.00000 & B_4 &= -\ 0.02784 \\ B_1 &= -\ 0.70711 & B_5 &= -\ 0.01710 \\ B_2 &= -\ 0.12976 & B_6 &= -\ 0.01150 \\ B_3 &= -\ 0.05241 & B_7 &= -\ 0.00823 \end{aligned} \tag{59-4}$$

If we note from Eq. (55-4) that $J(\xi,\beta) \cdot \frac{2\beta}{\pi}$ approaches zero as $\frac{\xi\sqrt{\pi}}{2\beta}$ approaches infinity we see that $\sum_{k=o}^{\infty} B_k = 0$. If all the B_k are negative, except B_o, then the error in taking K + 1 terms of the series is less than

$\left(-\sum_{k=o}^{K} B_k\right) y^{K+1}$. For K = 7, $\sum_{k=o}^{K} B_k = 0.04605$.

12. The properties studied in paragraphs 8, 9, 10, and 11 tell us much about the general behavior of $J(\xi,\beta)$, but in order to have accurate numerical values available a tabulation of the function was carried out by the author (D56) using the Oak Ridge National Laboratory electronic computer, ORACLE. $J(\xi,\beta)$ was calculated in the form

$$J(\xi,\beta) = \sum_{k=1}^{N} \int_{(k-1)\Delta}^{k\Delta} \frac{\psi(\xi,x)}{\psi(\xi,x) + \beta}\, dx + \frac{\frac{\pi}{2} - \arctan\left(N\Delta \sqrt{\frac{\beta}{1+\beta}}\right)}{\sqrt{\beta(1+\beta)}} \tag{60-4}$$

$\psi(\xi,x)$ in the form

$$\psi(\xi,x) = \frac{\xi}{2\sqrt{\pi}} \int_{x-\frac{2a}{\xi}}^{x+\frac{2a}{\xi}} \frac{\exp\left[-\frac{\xi^2}{4}(x-y)^2\right]}{1+y^2}\, dy \tag{61-4}$$

and the arctangent in the form

$$\arctan x = \int_0^x \frac{dy}{1+y^2}\,. \tag{62-4}$$

The integrals were evaluated using Gauss' integration rule (143), which as is well known is very accurate. In Eq. (60-4) 64 points of integration were used per interval Δ, in Eq. (61-4) 16×2^n points were used, in Eq. (61-5) 16×2^m points were used. The parameters Δ, N, a, n, and m must now be fixed; their determination involves striking a balance between computing time and accuracy.

Let us first consider the parameter a. It can easily be shown that the error involved in the use of Eq. (61-4) is given by

$$\psi(\xi,x) - \psi_{approx}(\xi,x) < \frac{\xi}{2\sqrt{\pi}}\, e^{-a^2}\left[\pi - \arctan\left(\frac{2a}{\xi} + x\right) - \arctan\left(\frac{2a}{\xi} - x\right)\right] \tag{63a-4}$$

$$< \frac{\sqrt{\pi}\,\xi}{2}\, e^{-a^2}. \tag{63b-4}$$

From Eq. (63a-4)
we see that at $x = 0$ the relative error in ψ will be

$$\frac{\psi(\xi,0) - \psi_{approx}(\xi,0)}{\psi(\xi,0)} < \frac{1}{\pi} \cdot \frac{\xi e^{-\left(\frac{\xi}{2}\right)^2}}{\mathrm{Erfc}\left(\frac{\xi}{2}\right)} \cdot \frac{e^{-a^2}}{a} \tag{64-4}$$

At $x = N\Delta$, the relative error will be

$$\frac{\psi(\xi,N\Delta) - \psi_{approx}(\xi,N\Delta)}{\psi(\xi,N\Delta)} < \frac{\xi\sqrt{\pi}}{2} \cdot \left[1 + (N\Delta)^2\right]^{-1} e^{-a^2} \tag{65-4}$$

since at $N\Delta = x$, ψ is supposed to be accurately given by the natural line shape.

The value of $N\Delta$ also affects the error involved in using Eq. (53-4) to evaluate the contribution from the wings. If we define

$$J'(\xi,\beta,N\Delta) = \int_{N\Delta}^{\infty} \frac{\psi(\xi,x)}{\psi(\xi,x) + \beta}\, dx \tag{66-4}$$

then

$$\delta J' = \int_{N\Delta}^{\infty} \frac{\beta\, \delta\psi(\xi,x)}{\left[\psi(\xi,x) + \beta\right]^2}\, dx < \left[\frac{\delta\psi(\xi,x)}{\psi(\xi,x)}\right]_{\substack{\mathrm{Max} \\ x \geq N\Delta}} \cdot \left[\frac{\beta}{\psi(\xi,x) + \beta}\right]_{\substack{\mathrm{Max} \\ x \geq N\Delta}} J' \tag{67-4}$$

Thus the fractional error in J' is less than the maximum fractional error in ψ for $x \geq N\Delta$. From Eq. (33-4) it follows that $\delta J'/J'$ approximately equals

$\dfrac{6}{\xi^2 \left\{ (N\Delta)^2 + \beta^{-1} \right\}}$ if the latter quantity is small. Thus according to Eq. (53-4) the total relative error in J from the natural line shape approximation to the wings is

$$\frac{\delta J'}{J} = \frac{\delta J'}{J'} \cdot \frac{J'}{J} < (N\Delta\sqrt{\beta})^2 \frac{1 - \frac{2}{\pi}\arctan\left(N\Delta\sqrt{\frac{\beta}{1+\beta}}\right)}{1 + (N\Delta\sqrt{\beta})^2} \cdot \frac{6}{\xi^2(N\Delta)^2} \tag{68-4}$$

The maximum value of the first factor occurs for $N\Delta\sqrt{\beta} \sim \frac{3}{2}$ and is about $\frac{1}{4}$. In the tabulation carried out only values of ξ were considered between $\frac{1}{10}$ and 1; N was taken equal to 256. The maximum error in J is then about $\frac{1}{4}$ % and occurs for $\xi = 0.1$ and $\beta \sim 4 \times 10^{-5}$.

A much better estimate of this error can be obtained by setting

$$\delta\psi(\xi, x) = \frac{6}{\xi^2} \cdot \frac{x^2}{(1 + x^2)^3} \tag{69-4}$$

in Eq. (67-4) (cf. Eq. 33-4). The resulting integral can easily be carried out and gives for $\frac{\delta J'}{J}$ the estimate

$$\frac{\delta J'}{J} < (N\Delta\sqrt{\beta})^2 \left[(\beta + \tfrac{1}{2})\left[1 - \frac{2}{\pi}\arctan\left(N\Delta\sqrt{\frac{\beta}{1+\beta}}\right) - \sqrt{\beta(1+\beta)}\left(1 - \frac{2}{\pi}\arctan(N\Delta)\right)\right]\right.$$
$$\left. - \frac{1}{\pi}\frac{N\Delta\sqrt{\beta(1+\beta)}}{1 + (N\Delta\sqrt{\beta})^2 + \beta}\right]\left[1 - \frac{2}{\pi}\arctan\left(N\Delta\sqrt{\frac{\beta}{1+\beta}}\right)\right] \cdot \frac{6}{\xi^2(N\Delta)^2} \tag{70-4}$$

Evaluating Eq. (70-4) for the choice of parameters $N\Delta = 256$, $N\Delta\sqrt{\beta} = \frac{3}{2}$ gives $\frac{\delta J'}{J} < 3.4 \times 10^{-4}$. Hence the error from the choice $N\Delta = 256$ is negligible.

Insofar as the value of a is concerned it was taken to be 4 in tabulation actually carried out. e^{-a^2} is then close to 10^{-7}, and the resulting error in ψ is very small whether calculated from Eq. (64-4) or Eq. (65-4). A reduction of a to 3 halves the computing time, but costs

about a factor of 1000 in the error: hence the choice a = 4.

13. When β is very large compared to $\frac{1}{N\Delta}$ the relative error involved in choosing N = 256, given by Eq. (68-4), say, is very small; for $\xi = 0.1$ k = 26 (β = 671.1) it is of the order of 10^{-5}. Thus the errors are due to the choice of n, Δ β and m. In all cases these errors are worst for large β for the following reasons. First

$$\frac{\delta\left(\frac{\gamma}{\gamma+\beta}\right)}{\left(\frac{\gamma}{\gamma+\beta}\right)} = \left(\frac{\beta}{\gamma+\beta}\right)\frac{\delta\gamma}{\gamma} \tag{69-4}$$

Thus the larger β the more nearly a relative error in γ will reflect itself in a relative error in the integrand of J. Secondly, the smaller β the more nearly constant the integrand of J is, and the more accurate the integration rule will be for a fixed number of points. Hence the largest error occurs for large β. Finally, the density of integration points is least for the arctangent for large β. Clearly, also, the relative error one expects will rise to a constant value as β increases, and will already be achieved when $\beta >> 1 \geq \gamma(\xi, x)$.

To determine this relative error let us note that for the very largest β ($\gtrsim$ 800, roughly) Eqs. (45-4) and (34-4) imply that $J = \frac{\pi}{2\beta}$ to at least four significant figures for $\xi = 0.1$. Presented in Table (1-4),* calculated by the author in 1956 (D56), are values of $J(\xi, \beta)$ calculated for $\xi = 0.1\ (0.1)\ 1.0$ and $\beta = 2^k \times 10^{-5}$, k = 0 (1) 31 with the parameters N = 4, n = 3, m = 5. Comparing $J(0.1, \beta)$ with $\frac{\pi}{2\beta}$ for $k \geq 26$ ($\beta \gtrsim 670$) gives agreement within one unit in the fourth decimal place, indicating a combined error due to our choice of Δ, n, a and m of at most about one part

* See Errata

TABLE 1.4 THE FUNCTION $J(\xi,\beta)$ FOR $\xi = 0.1\ (0.1)\ 1.0$ AND $\beta = 2^k \times 10^{-5}$

k	$J(\xi,\beta)$									
	$\xi = 0.1$	$\xi = 0.2$	$\xi = 0.3$	$\xi = 0.4$	$\xi = 0.5$	$\xi = 0.6$	$\xi = 0.7$	$\xi = 0.8$	$\xi = 0.9$	$\xi = 1.0$
0	4.979(2)*	4.970(2)	4.969(2)	4.968(2)	4.968(2)	4.968(2)	4.967(2)	4.967(2)	4.967(2)	4.967(2)
1	3.532	3.517	3.514	3.513	3.513	3.513	3.513	3.513	3.513	3.513
2	2.514	2.491	2.487	2.485	2.485	2.484	2.484	2.484	2.484	2.484
3	1.801	1.767	1.761	1.759	1.758	1.757	1.757	1.757	1.757	1.757
4	1.307	1.257	1.248	1.245	1.244	1.243	1.243	1.243	1.242	1.242
5	9.667(1)	8.993(1)	8.872(1)	8.831(1)	8.812(1)	8.802(1)	8.796(1)	8.792(1)	8.790(1)	8.788(1)
6	7.355	6.501	6.335	6.278	6.252	6.238	6.230	6.225	6.221	6.218
7	5.773	4.777	4.562	4.485	4.450	4.430	4.419	4.412	4.407	4.403
8	4.647	3.589	3.328	3.230	3.183	3.158	3.143	3.133	3.126	3.121
9	3.781	2.759	2.471	2.354	2.297	2.265	2.245	2.232	2.223	2.217
10	3.045	2.153	1.867	1.741	1.675	1.638	1.614	1.598	1.587	1.579
11	2.367	1.676	1.423	1.301	1.235	1.194	1.168	1.151	1.138	1.129
12	1.730	1.268	1.074	9.718(0)	9.119(0)	8.739(0)	8.484(0)	8.304(0)	8.174(0)	8.077(0)
13	1.164	9.081(0)	7.815(0)	7.087	6.629	6.322	6.107	5.950	5.833	5.744
14	7.172(0)	6.014	5.342	4.914	4.624	4.419	4.268	4.154	4.066	3.997
15	4.088	3.658	3.371	3.169	3.022	2.911	2.826	2.759	2.706	2.663
16	2.204	2.067	1.966	1.889	1.829	1.781	1.743	1.712	1.687	1.666
17	1.148	1.109	1.078	1.053	1.033	1.016	1.002	9.904(−1)	9.805(−1)	9.722(−1)
18	5.862(−1)	5.757(−1)	5.671(−1)	5.599(−1)	5.539(−1)	5.488(−1)	5.445(−1)	5.408	5.376	5.348
19	2.963	2.936	2.913	2.894	2.877	2.863	2.851	2.840	2.831	2.823
20	1.490	1.483	1.477	1.472	1.468	1.464	1.461	1.458	1.455	1.453
21	7.468(−2)	7.452(−2)	7.437(−2)	7.424(−2)	7.413(−2)	7.403(−2)	7.395(−2)	7.388(−2)	7.381(−2)	7.375(−2)
22	3.739	3.735	3.732	3.728	3.726	3.723	3.721	3.719	3.718	3.716
23	1.871	1.870	1.869	1.868	1.868	1.867	1.867	1.866	1.866	1.865
24	9.358(−3)	9.356(−3)	9.355(−3)	9.352(−3)	9.350(−3)	9.349(−3)	9.348(−3)	9.346(−3)	9.345(−3)	9.344(−3)
25	4.680	4.680	4.679	4.679	4.678	4.678	4.678	4.677	4.677	4.677
26	2.340	2.340	2.340	2.340	2.340	2.340	2.340	2.340	2.340	2.340
27	1.170	1.170	1.170	1.170	1.170	1.170	1.170	1.170	1.170	1.170
28	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)	5.851(−4)
29	2.925	2.926	2.926	2.926	2.926	2.926	2.926	2.926	2.926	2.926
30	1.463	1.463	1.463	1.463	1.463	1.463	1.463	1.463	1.463	1.463
31	7.314(−5)	7.314(−5)	7.315(−5)	7.315(−5)	7.315(−5)	7.315(−5)	7.314(−5)	7.314(−5)	7.314(−5)	7.314(−5)

*Numbers in parentheses are powers of 10, which multiply the entry next to which they stand and all unmarked entries below it.

in 2000 (0.05%). The computing time for this calculation is about $N2^{n+1}$ minutes for each ξ and all β, or about ten hours for the entire calculation. Recently, Nordheim (N57) has recalculated $J(\xi,\beta)$ for $\xi = 0.05\ (0.05)\ 0.5$ and $k = 4.0\ (0.5)\ 20.0$; agreement with the author's earlier paper is always to one unit in the fourth decimal place.

14. Plotted in Figs (1-4) and (2-4) is the function $J(\xi,\beta)$ vs β with ξ as a parameter. As we can see, it has the general shape we might have predicted from its properties already derived. In particular, J decreases with increasing β or ξ; and it is asymptotic to $J(\infty,\beta)$ for either β very large or very small. In this connection it is worth noting that $J(\xi,\beta)$ for $\xi = 1.0$ is quite close to $J(\infty,\beta)$ for all β. Finally, we note that J assumes a $\frac{\pi/2}{\beta}$ behavior for smaller β the smaller ξ is, in accordance with Eqs. (45-4) and (34-4).

The table may be used to check the validity of Eqs. (54-4), (55-4), and (56-4). In Fig. (3-4) $\frac{2\beta}{\pi} J(\xi,\beta)$ has been plotted versus $\frac{\xi\sqrt{\pi}}{2\beta}$ using these equations. The dotted region is a graphical interpolation between the series on the left and the logarithmic asymptotic expression on the right. Plotted also are exact values for $\xi = 0.1$ and 0.2. The agreement is good in general shape and magnitude. For $\xi = 0.1$ the agreement is within 5% or less for $\frac{\xi\sqrt{\pi}}{2\beta}$ less than about 20; the margin of error then increases somewhat, being about 30% near $\frac{\xi\sqrt{\pi}}{2\beta} = 100$. Also plotted in Fig. (3-4) is a curve based on the following rational approximation to $J(\xi,\beta)$

$$J(\xi,\beta) = \frac{\pi}{2\beta + \sqrt{\frac{\pi}{2}}\ \xi} \tag{70-4}$$

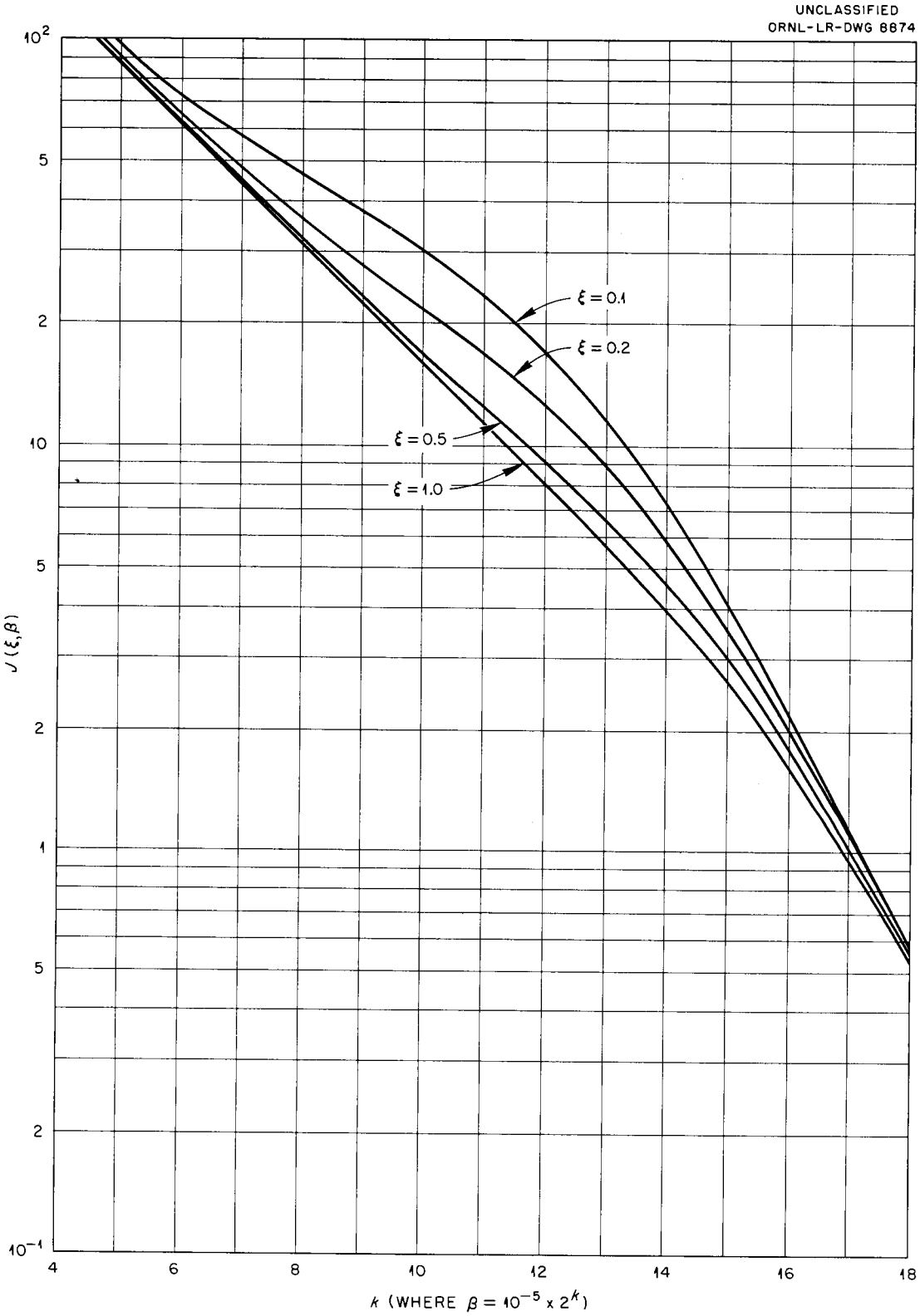


Fig. 1-4. $J(\xi, \beta)$ vs k for $\xi = 0.1-1.0$.

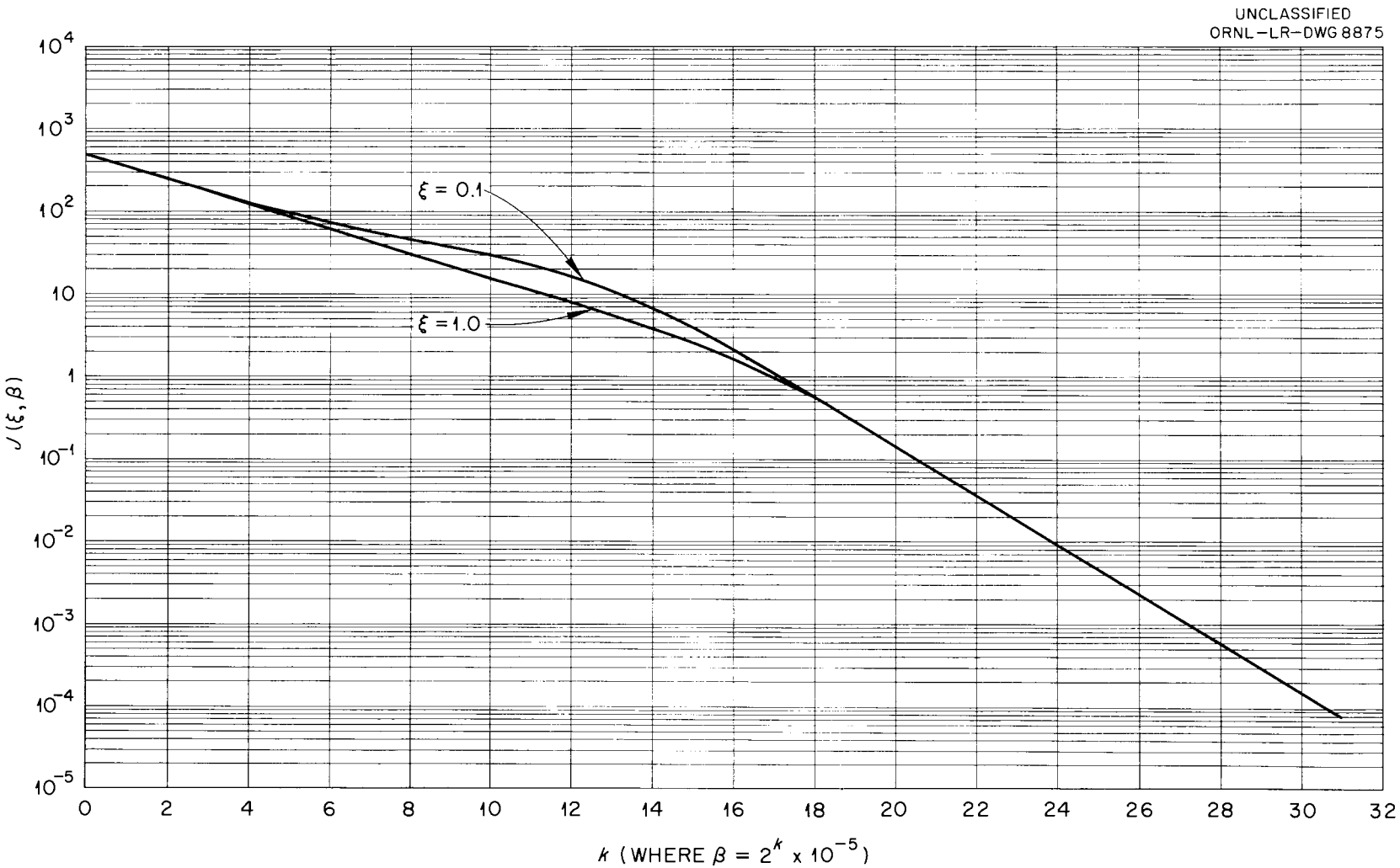

UNCLASSIFIED
ORNL-LR-DWG 8875
10^4
10^3
10^2
10
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
$J(\xi, \beta)$
$\xi = 0.1$
$\xi = 1.0$
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28
30
32
k (WHERE $\beta = 2^k \times 10^{-5}$)

Fig. 2-4.

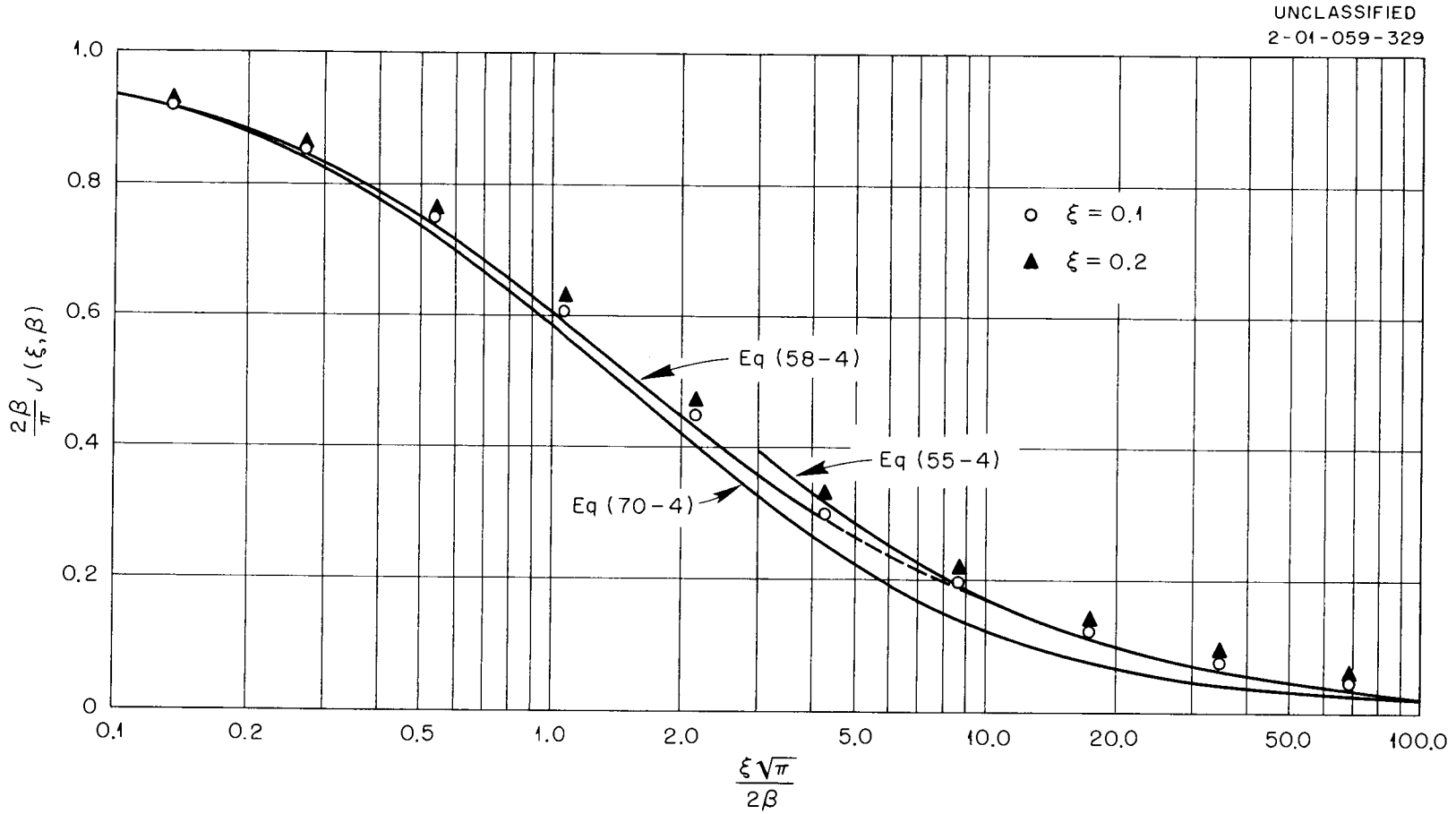

UNCLASSIFIED
2-01-059-329
1.0
0.8
0.6
0.4
0.2
0
$\frac{2\beta}{\pi} J(\xi,\beta)$
0.1
0.2
0.5
1.0
2.0
5.0
10.0
20.0
50.0
100.0
$\frac{\xi\sqrt{\pi}}{2\beta}$
o $\xi = 0.1$
▲ $\xi = 0.2$
Eq (58-4)
Eq (55-4)
Eq (70-4)

Fig. 3-4.

This rational approximation has the property that the first two terms in the Maclaurin series in $\xi\sqrt{\pi}/2\beta$ are the same as the first two terms of Eq. (56a-4). It should only be good for $\xi\sqrt{\pi}/2\beta << 1$, but as one can see from Fig. (3-4) it is quite good for much larger $\xi\sqrt{\pi}/2\beta$.

15. In paragraph 8 we began the study of the effect of Doppler broadening of resonance lines on the effective resonance integral in the case $\gamma = 0$. When $\gamma \neq 0$, Eq. (42-4) for I must be replaced by

$$I = \sigma_p \frac{\Gamma_\gamma}{E_o} \cdot \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\xi,x)}{\psi(\xi,x) + (\beta\gamma)^{1/2}\chi(\xi,x) + \beta} dx \tag{71-4}$$

Let us first consider the case $\beta << \frac{1}{6}\xi^2$. For the natural line shapes one can easily show that the maximum fractional contribution of the interference term to the total denominator occurs when $x = -\sqrt{\frac{1+\beta}{\beta}}$ and is equal to $\frac{\sqrt{\gamma}}{1-\sqrt{\gamma}}$. If $\frac{6\beta}{\xi^2} << 1$, then this will also be true for the Doppler broadened line shape, because for $x \approx \frac{1}{\sqrt{\beta}} >> \frac{6}{\sqrt{\xi}}$, the Doppler broadened line shape is very close to the natural line shape. In the center of the line, on the other hand, the interference term can be neglected. It is easy to prove, for example, from Eq. (37-4) that

$$\frac{|\chi(\xi,x)|}{\psi(\xi,x)} \leq 2|x| \tag{72-4}$$

We simply note that the two terms in Eq. (37-4) have opposite sign, and that $\chi(\xi,x)$ has the sign of the first. Thus in the center of the line the interference term makes a fractional contribution to the denominator of the integrand of less than $2|x|(\beta\gamma)^{1/2}$. Thus if $\frac{6\beta}{\xi^2} << 1$ we can find a

constant C between $\frac{6}{\sqrt{\xi}}$ and $\frac{1}{\sqrt{\beta}}$ such that for $|x| \leq C$ the interference term is negligible, and for $|x| \geq C$ the effects of Doppler broadening are negligible. If we call the integral in Eq. (71-4) $2J(\xi,\beta,\gamma)$ we can write:

$$2J(\xi,\beta,\gamma) = \int_{-C}^{C} \frac{\psi(\xi,x)}{\psi(\xi,x) + \beta}\, dx + \left(\int_{C}^{\infty} + \int_{-\infty}^{-C} \right)$$

$$\times \frac{(1 + x^2)^{-1}}{(1 + x^2)^{-1} + (\beta\gamma)^{1/2} 2x(1 + x^2)^{-1} + \beta}\, dx \qquad (73\text{-}4)$$

We can furthermore write

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

$$\times \frac{(1 + x^2)^{-1}}{(1 + x^2)^{-1} + (\beta\gamma)^{1/2} 2x(1 + x^2)^{-1} + \beta}\, dx \qquad (74\text{-}4)$$

and

$$2J(\xi,\beta) = \int_{-C}^{C} \frac{\psi(\xi,x)}{\psi(\xi,x) + \beta}\, dx + \left(\int_{C}^{\infty} + \int_{-\infty}^{-C} \right) \frac{(1 + x^2)^{-1}}{(1 + x^2)^{-1} + \beta}\, dx \qquad (75\text{-}4)$$

By subtracting Eqs. (74-4) and (75-4) from Eq. (73-4) we obtain

$$J(\xi,\beta,\gamma) - J(\infty,\beta,\gamma) - J(\xi,\beta) + J(\infty,\beta) = 0 \qquad (76\text{-}4)$$

Comparing Eq. (76-4) with Eq. (13-4) we have

$$J(\xi,\beta,\gamma) = \frac{\frac{\pi}{2}}{\sqrt{\beta(1 + \beta - \gamma)}} + J(\xi,\beta) - J(\infty,\beta) \qquad (77\text{-}4)$$

Equation (77-4) is a quantitative expression of the fact that when $\beta << \frac{6}{\xi^2}$, the effect of Doppler broadening of resonance lines is caused mainly by alteration of the line center, while the effect of interference between potential and resonance scattering is caused mainly by alteration of the wings. Since Eq. (77-4) was derived on the assumption that $\frac{6\beta}{\xi^2} << 1$, the last two terms will nearly cancel, as we can see from Eq. (44-4).

When β is sufficiently large it is again possible to prove inequality (45-4). We again proceed by noting that

$$J(\xi,\beta,\gamma) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\xi,x)}{\beta} \left[1 + \frac{\psi(\xi,x) + (\beta\gamma)^{1/2}\chi(\xi,x)}{\beta} \right]^{-1} dx \quad (78a\text{-}4)$$

$$= \frac{1}{2} \sum_{k=0}^{\infty} (-)^k \int_{-\infty}^{+\infty} \frac{\psi(\xi,x)}{\beta} \left[\frac{\psi(\xi,x) + (\beta\gamma)^{1/2}\chi(\xi,x)}{\beta} \right]^k dx \quad (78b\text{-}4)$$

Now all the integrals in this series are positive, since only products of even powers of χ (which must be positive) and any power of ψ (positive) survive. Hence, since the series alternates, and

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\xi,x)}{\beta} dx > J(\xi,\beta,\gamma) > \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\xi,x)}{\beta}$$

$$\times \left[1 - \frac{\psi(\xi,x) + (\beta\gamma)^{\frac{1}{2}}\chi(\xi,x)}{\beta} \right] dx \quad (79\text{-}4)$$

This immediately becomes Eq. (45-4) if we note that the χ-integral vanishes.

16. If $\xi << 1$ and $\chi(\xi,0) >> \beta >> \frac{1}{6}\xi^2$ we can make the approximation which leads to Eq. (35-4) in Eq. (36-4) or substitute Eq. (35-4) in Eq. (37-4). In either case we get $\chi(\xi,x) \approx 0$. This conclusion simply means that in the line center the thermal motion of the moderator atoms averages the interference cross section over its positive and negative parts with nearly equal weight. Hence, under the stated conditions it is a very good approximation to write

$$J(\xi,\beta,\gamma) = J(\xi,\beta) \tag{80-4}$$

17. We have made no tabulation of $J(\xi,\beta,\gamma)$ comparable to that for $J(\xi,\beta)$. The reasons for this are threefold:

(i) The first, and controlling reason, is that for practical homogeneous situations the ratio $\frac{\sigma_{pa}}{\sigma_p}$, which always exceeds γ, is very much less than unity. For example, for an aqueous solution of uranium salts containing as much as 500 grams of U per kilogram of water, the ratio $\frac{\sigma_{pa}}{\sigma_p}$ is of the order of 0.0085.

(ii) Nearly all of the resonances of absorbing materials have values of $\xi << 1$ at room temperature or at the higher temperatures at which power producing reactors are run. Unless β is very small, $J(\xi,\beta,\gamma) = J(\xi,\beta)$.

(iii) The most conspicuous resonances for which (ii) above fails are the resonances which occur at fairly low energies (e.g., the 6.7 ev resonance in U^{238}). In such resonances it is frequently the case that $\frac{\Gamma_n}{\Gamma} << 1$ (e.g. $\sim$ 0.04 in the example mentioned).

CHAPTER 5. TRANSPORT THEORY FUNDAMENTALS

1. In the following two chapters we shall study the resonance absorption problem in heterogeneous media. As a necessary aid to this study we shall develop in this chapter certain special results of neutron transport theory. These theorems all concern the transport of neutrons in situations in which a convex lump is embedded in an infinite purely absorbing medium. In the next two chapters these theorems will be applied to the resonance absorption problem by interpreting the convex lump as the absorber, and the surrounding medium as the moderator. That the moderator can be considered in these applications as a purely absorbing medium depends on the following considerations:

Since moderators are nearly always materials of small mass number, the average lethargy change per collision with a moderator nucleus is assumed to be very much larger than the extent of the resonance in lethargy. This assumption is valid in the vast majority of situations, although exceptions are possible (e.g., the 0.3 ev resonance in Pu^{239}). The assumption has consequences similar to those mentioned in Chapter 3 in connection with Eq. (34-3), viz.: (i) Neutrons which appear in the moderator at the resonance lethargy due to last collisions in the moderator made those last collisions at lower lethargies at which the resonance cross section was substantially zero. (ii) If such moderator neutrons at the resonance lethargy collide with a moderator nucleus before reaching the lump, they will be moderated from the lethargy interval of significant absorption, and need not be considered further for the calculation of absorption in this particular resonance. (iii) A neutron leaking out of the lump in the resonance lethargy interval cannot return to it in the same interval since at least one moderator collision must intervene. Hence, such neutrons also need not be considered further.

Consequences (ii) and (iii) imply that insofar as absorption in the particular resonance is concerned, the moderator appears to be purely absorbing. Consequence (i) implies that the collision source density in the moderator at the resonance lethargy interval is spatially uniform, since it originates from last collisions at lethargies where there is no absorption.

In Chapter 6 moderation by the absorbing nuclei is also assumed to cause an average lethargy change per collision very much larger than the resonance lethargy interval. In such a case, the so-called narrow resonance case, scattering by the absorber nuclei in the resonance interval can also be treated as absorption. The details of this treatment are given in the next chapter, but in the next three paragraphs, (5-2), (5-3), and (5-4), some necessary theorems of transport theory applicable in purely absorbing media are proven.

2. Let us consider a finite mass of purely absorbing material in the shape of a convex body, V, immersed in a medium also purely absorbing in which a spatially uniform, isotropic neutron source of strength Q exists. Let us calculate the neutron current into the body at each point of its surface, and the angular distribution of these neutrons about the normal.

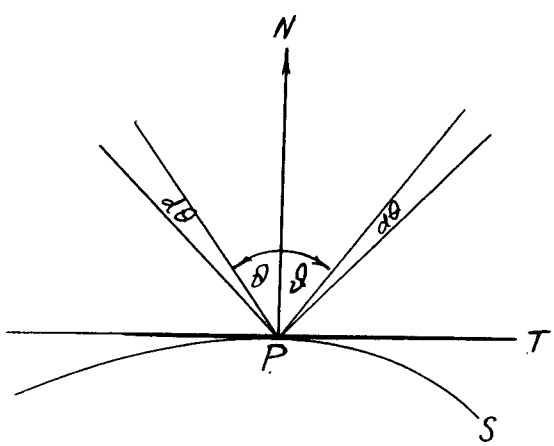


Fig. (1-5)

In Fig. (1-5) S represents the convex absorber surface, T the tangent plane at some point P, and $\overline{PN}$ the normal pointing into the source medium. The inward current at P is clearly azimuthally symmetric around $\overline{PN}$. The inward current in the differential cone between polar angles θ and $\theta + d\theta$ is given by

$$j(\cos\theta)d(\cos\theta)dS = \int_{\phi=0}^{\phi=2\pi} \int_{r=0}^{r=\infty} Q\cdot r^2 dr \sin\theta \, d\theta \, d\phi \cdot \frac{dS \cos\theta}{4\pi r^2} \cdot e^{-\Sigma_a^* r} \qquad (1\text{-}5)$$

The first factor on the right is the isotropic source strength, the second factor the infinitesimal source volume, the third factor the fraction of source neutrons oriented in direction so as to cut S in an infinitesimal

area dS at P, and the last factor the probability of reaching P without collision in the source medium. Σ_a^* is the macroscopic absorption (total) cross section of the source medium. Carrying out the integral immediately gives

$$j(\cos\theta) = \frac{1}{2} \cdot \frac{Q}{\Sigma_a^*} \cdot \cos\theta \tag{2-5}$$

The total inward current is given by

$$J = \int_{\theta=0}^{\theta=\frac{\pi}{2}} j(\cos\theta)\, \sin\theta\, d\theta = \frac{1}{4} \cdot \frac{Q}{\Sigma_a^*} \tag{3-5}$$

3. The next theorem which we shall prove is that flux at any point, $\vec{r}$, of the body, V, due to the uniform, isotropic source, Q, <u>outside V</u>, is given by $\frac{Q}{\Sigma_a} P(\vec{r})$, where $P(\vec{r})$ is the probability that neutrons from an isotropic source at $\vec{r}$ <u>in V</u> will escape from V without collision. The theorem is a special case of a general reciprocity theorem for the neutron transport equation proven by Case, Placzek, and deHoffmann (C53).

To prove it, let us first derive a general expression for the flux at $\vec{R}$ due to a unit isotropic source at the origin in a purely absorbing medium. It is given by

$$\Sigma_a(\vec{R})\phi(\vec{R}) \cdot R^2 dR d\Omega = \frac{d\Omega}{4\pi} \cdot d\left(e^{-\int_0^R \Sigma_a ds}\right) \tag{4-5}$$

The left hand side is the collision rate in an infinitesimal volume at $\vec{R}$, the right hand side is the product of the probability of the source neutrons

being properly oriented to intersect the volume at $\vec{R}$, and the probability that they will reach R, but not R + dR, uncollided. The exponent is the so-called optical path length from the origin to $\vec{R}$, and is defined as the <u>positive</u> line integral of Σ_a over a straight line connecting the end points. From Eq. (4-5) it follows that

$$\phi(\vec{r}) = \frac{e^{-\int_0^R \Sigma_a ds}}{4\pi R^2} \tag{5-5}$$

The escape probability of neutrons born at $\vec{r}$ in V can now be obtained by integrating the absorption density over the volume outside of V, V*. Thus

$$P(\vec{r}) = \Sigma_a^* \int_{V^*} \frac{e^{-\int_{\vec{r}'}^{\vec{r}} \Sigma_a \, ds}}{4\pi |r - r'|^2} \, d^3r' \tag{6-5}$$

Here Σ_a^* is the absorption cross section of V*. The flux at $\vec{r}$ due to a uniform source Q in V* can be written as

$$\phi(\vec{r}) = Q \int_{V^*} \frac{e^{-\int_{\vec{r}'}^{\vec{r}} \Sigma_a ds}}{4\pi |r - r'|^2} \, d^3r' \tag{7-5}$$

Thus

$$\phi(\vec{r}) = \frac{Q}{\Sigma_a^*} P(\vec{r}) \tag{8-5}$$

as we wished to prove. As we shall see in the next two chapters Eq. (8-5) occupies a central role in the problem of resonance absorption in heterogeneous media.

4. A quantity useful in what follows is the average of P(r) over V, i.e.,

$$P \equiv \frac{1}{V} \int_V P(\vec{r}) d^3r \tag{9-5}$$

It is possible to get a simple expression for P using Eq. (8-5) as follows:

The total absorption rate of neutrons in V can be written in two equivalent ways, viz.:

$$\Sigma_a \left(\frac{Q}{\Sigma_a^*} P \right) V = \int dS \int d\Omega \left(\frac{1}{4\pi} \frac{Q}{\Sigma_a^*} \cos\theta \right) \left(1 - e^{-\Sigma_a \ell} \right) \tag{10-5}$$

The term in parenthesis on the left hand side is the average flux in V, as can be readily seen from Eqs. (8-5) and (9-5). The first term in the integrand on the right is the inward current into the solid angle $d\Omega = \sin\theta \, d\theta \, d\phi$ at dS. ℓ is the length of the chord proceeding from the infinitesimal area dS in the direction $d\Omega$. The last parenthesis on the right hand side in Eq. (10-5) is the capture probability of neutrons entering dS in direction $d\Omega$. Σ_a is the absorption cross section in V. Equation (10-5) can be rewritten as

$$P = \frac{1}{\Sigma_a} \cdot \frac{S}{4V} \cdot \frac{1}{S} \int dS \int d\Omega \frac{\cos\theta}{\pi} \left(1 - e^{-\Sigma_a \ell}\right) \tag{11a-5}$$

$$= \frac{1}{\Sigma_a} \cdot \frac{S}{4V} \cdot \frac{1}{S} \int dS \int d\Omega \, \delta(\ell - \ell') d\ell' \frac{\cos\theta}{\pi} \left(1 - e^{-\Sigma_a \ell'}\right) \tag{11b-5}$$

$$= \frac{1}{\Sigma_a} \cdot \frac{S}{4V} \cdot \int f(\ell') d\ell' \left(1 - e^{-\Sigma_a \ell'}\right) \tag{11c-5}$$

where

$$f(\ell') = \frac{1}{S} \int dS \int d\Omega \frac{\cos\theta}{\pi} \cdot \delta(\ell - \ell'). \tag{12-5}$$

$f(\ell')$ is a particular distribution of chord lengths in V, weighted with the element of surface, the element of solid angle, and the cosine of the angle with the normal appropriate to the chord. It is clear that Eq. (12-5) for $f(\ell')$ is normalized.

When $\Sigma_a \rightarrow 0$, it is obvious that $P \rightarrow 1$, in view of its definition as an average escape probability. From Eq. (11c-5) we obtain

$$\lim_{\Sigma_a \rightarrow 0} P = 1 = \frac{S}{4V} \int f(\ell) d\ell \lim_{\Sigma_a \rightarrow 0} \left(\frac{1 - e^{-\Sigma_a \ell}}{\Sigma_a} \right) \tag{13a-5}$$

$$= \frac{S}{4V} \int f(\ell) \cdot \ell \, d\ell = \frac{S}{4V} \cdot \bar{\ell} \tag{13b-5}$$

Thus $\bar{\ell}$, the average chord length with the distribution (12-5), is given by $\frac{4V}{S}$. This theorem is originally due to Gauss. Wigner (W55) has suggested a rational approximation for P, viz.:

$$P = (1 + \Sigma_a \bar{\ell})^{-1} \tag{14-5}$$

By comparison of Eqs. (11c-5) and (14-5) it can be seen that the rational approximation has the correct value for very large and very small values of $\Sigma_a \bar{\ell}$. It has the twofold advantage of being easy to handle in calculation, and of being independent of the details of the shape of the body, but it has the disadvantage, as we shall see in the next chapter, of introducing a fairly sizeable inaccuracy in some calculations.

5. In Chapter 7 collision of the neutrons with the absorbing nuclei is treated as producing a negligible energy change. The conditions under which this approximation (wide resonance approximation) and the approximation of Chapter 6 (narrow resonance approximation) are valid are discussed in detail in Chapter 9. In the wide resonance case the interior of the absorbing lump can be treated by monoenergetic transport theory, and multiple collision phenomena must be taken into account. The moderator, for the same reasons as before, can be treated as purely absorbing. Many of the results of Chapter 7 will be obtained from a simple approximation to monoenergetic transport theory called diffusion theory. In the remainder of this chapter the diffusion approximation will be discussed, and the remaining analysis of the wide resonance case deferred until Chapter 7.

The diffusion approximation can be derived as follows: for a medium with isotropic scattering the relation between flux and current across a particular plane, T, is given by an equation similar to Eq. (3-5), viz.:

$$j = \int_{\phi=0}^{\phi=2\pi} \int_{\theta=0}^{\theta=\frac{\pi}{2}} \int_{r=0}^{r=\infty} \Sigma_s \phi(\vec{r}) \cdot r^2 dr \sin\theta \, d\theta \, d\phi \cdot \frac{\cos\theta}{4\pi r^2} \cdot e^{-\Sigma_t r} \qquad (15\text{-}5)$$

Here Σ_s is the scattering cross section of the medium and Σ_t its total cross section, r, θ, and ϕ are polar coordinates with the point at which j is being calculated as origin, and with the normal to the reference plane T which points

toward the source neutrons as polar axis. $\phi(\vec{r})$ is the flux at point $\vec{r}$. Because of the exponential attenuation of the contribution from radius r, only points within a few total mean free paths of the origin are important. If $\phi(\vec{r})$ varies slowly in a total mean free path we can express it approximately as

$$\phi(\vec{r}) = \phi(0) + \vec{r} \cdot \nabla\phi(0) \tag{16-5}$$

Equation (16-5) is the essence of the diffusion approximation. If (θ_o, ϕ_o) are the polar angles of a unit vector pointing in the direction of $\nabla\phi$, this can be rewritten as

$$\phi(\vec{r}) = \phi(0) + r\left|\nabla\phi(0)\right| \left\{\cos\theta \cos\theta_o + \sin\theta \sin\theta_o \cos(\phi - \phi_o)\right\} \tag{17-5}$$

If we insert Eq. (17-5) into Eq. (15-5) and carry out the integrals we find that

$$j = \frac{1}{4} \cdot \frac{\Sigma_s}{\Sigma_t} \cdot \phi(0) + \frac{1}{6} \frac{\Sigma_s}{\Sigma_t^2} \cos\theta_o \left|\nabla\phi(0)\right| \tag{18a-5}$$

$$= \frac{\Sigma_s}{\Sigma_t} \left(\frac{1}{4} \phi(0) + \frac{1}{6\Sigma_t} \vec{n} \cdot \nabla\phi(0) \right) \tag{18b-5}$$

where $\vec{n}$ is the normal to T pointing <u>toward</u> the source medium. Equation (16-5) will not be a good approximation in general unless $\Sigma_a << \Sigma_t$. In this latter event Eq. (18b-5) can be written

$$j = \frac{1}{4} \phi(0) + \frac{1}{6\Sigma_s} \vec{n} \cdot \nabla\phi(0) \tag{19-5}$$

The net current in the direction of n is clearly

$$j_{net} = \left(\frac{1}{4} \phi(0) - \frac{1}{6\Sigma_s} \vec{n} \cdot \nabla\phi\right) - \left(\frac{1}{4} \phi(0) + \frac{1}{6\Sigma_s} \vec{n} \cdot \nabla\phi(0)\right)$$

$$= - \frac{1}{3\Sigma_s} \vec{n} \cdot \nabla\phi(0) \tag{20-5}$$

From Eq. (20-5) a second order differential equation for the flux can be obtained by writing a neutron balance over an arbitrary volume V with surface S. If the neutron source density at $\vec{r}$ is $Q(\vec{r})$ then

$$-\frac{1}{3\Sigma_s}\int_S \vec{dS}\cdot\nabla\phi(\vec{r}) + \int_V \Sigma_a\phi(\vec{r})dV = \int_V Q(\vec{r})dV \qquad (21\text{-}5)$$

Using the divergence theorem to convert the surface integral to a volume integral and noting the arbitrariness of V we have

$$-\frac{1}{3\Sigma_s}\nabla^2\phi(\vec{r}) + \Sigma_a\phi(\vec{r}) = Q(\vec{r}) \qquad (22\text{-}5)$$

The boundary condition most frequently used at an interface between two media is the continuity of the partial currents in both directions across the surface. From Eq. (19-5) one can see that these conditions are equivalent to the continuity of flux, $\phi(\vec{r})$, and net current, $-\frac{1}{3\Sigma_s}\vec{n}\cdot\nabla\phi(\vec{r})$, across the surface.

6. Let us now consider the problem of the albedo of a convex body in the diffusion approximation. The albedo is defined as the probability that a neutron entering the lump will leave again without being absorbed. Instead of looking for an exact solution for each possible geometric shape, we shall, in this paragraph, look for a universal, approximate expression, like Eq. (14-5), for example, which does not depend on the <u>details</u> of the shape but just on some mean linear dimension.

If the body is very large it appears locally as an infinite half space bounded by its tangent plane. From Eq. (22-5) in one dimension with $Q = 0$, we see that the solution for the flux must be

$$\phi(x) = Ae^{-\chi x} \tag{23-5}$$

where A is a constant, $\chi = \sqrt{3\Sigma_s\Sigma_a}$, and x is a distance measured normal to the plane bounding the half-space ($x = 0$) and measured positively into the medium whose albedo we want. From Eqs. (23-5) it follows that

$$\frac{1}{\phi}\frac{\partial\phi}{\partial n} = \chi \tag{24-5}$$

where n is the outward normal to the absorbing medium at its surface.

If the lump is small we can assume that both the flux and its outward normal derivative are independent of position on the surface of the lump, and that the surface flux equals the volume averaged flux. Then from Eq. (21-5) with $Q = 0$, it follows that

$$\frac{1}{\phi}\frac{\partial\phi}{\partial n} = \frac{1}{4}\chi^2\bar{\ell} \tag{25-5}$$

An expression for $\frac{1}{\phi}\frac{\partial\phi}{\partial n}$ which has Eq. (24-5) for its limit when $\chi\bar{\ell} >> 1$ and Eq. (25-5) for its limit when $\chi\bar{\ell} << 1$ is

$$\frac{1}{\phi}\frac{\partial\phi}{\partial n} = \frac{\chi^2\bar{\ell}}{\chi\bar{\ell} + 4} \tag{26-5}$$

From Eqs. (19-5) and (26-5) it follows that the albedo is given by

$$\delta = \frac{1 + \frac{\sqrt{3}}{4}\bar{\ell}(\Sigma_a\Sigma_s)^{\frac{1}{2}} - \frac{1}{2}\Sigma_a\bar{\ell}}{1 + \frac{\sqrt{3}}{4}\bar{\ell}(\Sigma_a\Sigma_s)^{\frac{1}{2}} + \frac{1}{2}\Sigma_a\bar{\ell}} \tag{27-5}$$

which is the expression we have been seeking. Equation (27-5) has the same advantages and disadvantages as Eq. (14-5).

CHAPTER 6. HETEROGENEOUS RESONANCE INTEGRALS - NARROW RESONANCES

1. In this chapter we shall consider the problem of calculating the effective resonance integral for a heterogeneous arrangement of absorber and moderator. We shall restrict ourselves in this chapter to the narrow resonance approximation, i.e., we shall assume ξ for both the moderator and absorber is very much larger than the lethargy extent of the resonance under consideration.

Let us consider a lump of absorber in the shape of a convex body surrounded by an infinite moderating region. Let us calculate the absorption of neutrons by this lump in a single narrow resonance. For this purpose let us divide the neutrons which make a collision in the lump in the vicinity of resonance energy into two classes according to whether their last collisions were made in the lump or in the moderator. In any case, their last collisions were made at energies far above the resonance, where the flux, ϕ, is uniform spatially and lethargy wise in both lump and moderator. Let us consider the neutrons whose last collision was in the lump. The rate at which these neutrons appear per unit lethargy in the resonance is independent of whether there is a resonance or not because these neutrons came from collisions far above the resonance energy. If there is no resonance this rate is equal to the collision density of the lethargy in question, since the spatial uniformity of the flux then prohibits any net transport of neutrons. Thus the source density per unit lethargy in the resonance in the lump is just $\Sigma_p\phi$, where Σ_p is the potential scattering cross section of the lump material. If the lump is a chemical compound of the absorber, e.g., UO_2, or a mixture, Σ_p may consist of two parts, Σ_{pa} and Σ_m, as

in Chapter 4. Since at the lethargy of last collision the flux was spatially uniform and equal to ϕ, the source, $\Sigma_p\phi$, is also spatially uniform.

In the presence of the resonance the flux near resonance is not spatially uniform and neutron transport can occur. Since the source density, $\Sigma_p\phi$, is uniform in the lump, the total collision rate in the lump of neutrons whose last collision was in the lump is

$$\Sigma_p\phi \left[1 - P(\Sigma_t)\right] V \tag{1-6}$$

where P is the average escape probability defined by Eq. (9-5), but evaluated for a lump cross section equal to Σ_t, the total cross section in the lump including the resonance contribution. Any source neutron which escapes the lump is lost for, by hypothesis, a single moderator collision is sufficient to moderate the neutrons well below the resonance energy. Similarly, any source neutron which makes a scattering collision in the lump is lost for precisely the same reason. Hence, the total absorption rate in the lump of neutrons whose last collision was in the lump is

$$\Sigma_p\phi \left[1 - P(\Sigma_t)\right] V \cdot \frac{\Sigma_a}{\Sigma_t} \tag{2-6}$$

3. Let us now consider neutrons whose last collisions were in the moderator. By precisely similar reasoning as employed in paragraph 2 we see that the flux per unit lethargy in the moderator at resonance energy is just ϕ. By the theorem of paragraph 3-5, the density of first collisions of these neutrons in the lump is

$$\phi\, P(\Sigma_t) V \Sigma_t \tag{3-6}$$

Again the fraction of these collisions which are scattering collisions cause the neutrons involved to become unavailable for absorption. Hence, the total absorption rate in the lump of neutrons whose last collision was in the moderator is

$$\phi\, P(\Sigma_t) V \Sigma_t \cdot \frac{\Sigma_a}{\Sigma_t} \tag{4-6}$$

4. From the definition of the effective resonance integral given in Eq. (1-4) it is clear that it is the lethargy integral of the effective absorption cross section, i.e., that cross section which when multiplied by the flux which would exist in the absence of the resonance gives the true absorption rate. In the heterogeneous case being considered here the same quantity, I, is defined by the equation

$$NI\phi V = \int \Sigma_p \phi \left[1 - P(\Sigma_t)\right] V \frac{\Sigma_a}{\Sigma_t}\, du + \int \phi P(\Sigma_t) V \Sigma_t \frac{\Sigma_a}{\Sigma_t}\, du \tag{5-6}$$

which can be simplified to

$$NI = \int \frac{\Sigma_p \Sigma_a}{\Sigma_t}\, du + \int \frac{(\Sigma_t - \Sigma_p)\Sigma_a}{\Sigma_t} P(\Sigma_t)\, du \tag{6-6}$$

Here N is the atomic density of absorber nuclei in the lump.

5. If for $P(\Sigma_t)$ one substitutes Wigner's rational approximation, Eq. (14-5), the expression for I can be rewritten as

$$I = \left(1 + \frac{1}{\Sigma_p \bar{\ell}}\right) \int \frac{\Sigma_p}{\Sigma_t + (\bar{\ell})^{-1}} \sigma_a\, du \tag{7-6}$$

Now according to Eqs. (6-4) and (7-4)

$$\Sigma_t = N\sigma_t + \Sigma_m = N(\sigma_s + \sigma_a) + \Sigma_p \tag{8-6}$$

where σ_s and σ_a are the resonance scattering and absorption cross section respectively. But then

$$\Sigma_t + (\bar{\ell})^{-1} = N(\sigma_s + \sigma_a) + \Sigma_p\left(1 + \frac{1}{\Sigma_p\bar{\ell}}\right) \tag{9-6}$$

Hence if we define $b = 1 + (\Sigma_p\bar{\ell})^{-1}$ Eq. (7-6) can be rewritten in precisely the same form as Eq. (2-4) except that we must replace σ_p by $b\sigma_p$ everywhere. <u>Thus we have reduced the heterogeneous case to the homogeneous one in the narrow resonance approximation, and all the results of Chapter 4 apply mutatis mutandis.</u>

6. The conclusion reached in the previous paragraph gives rise to two very interesting and practical rules. The first of these is the following: Let us consider lumps containing a particular absorbing material and various amounts of other moderating materials. All such lumps with the same value of $\sigma_p + (N\bar{\ell})^{-1}$ have the same effective resonance integral, I. The proof of this is trivial; it consists in noting that in Eq. (71-4) that σ_p only occurs in the combination $b\sigma_p = \sigma_p + (N\bar{\ell})^{-1}$. It is worth noting explicitly that the coefficient of the interference line shape, $(\beta\gamma)^{1/2}$, is actually independent of σ_p as can be seen from Eqs. (9-4) and (10-4). An example of the significance of the rule we have just proven is that if one knows the resonance integral for a series of Th rods one can immediately obtain the value for a related series of ThO_2 rods (or spheres, or any other shape for that matter).

The second rule, proven in exactly the same way, states that the effective resonance integral for a lump is the same as that for a homogeneous mixture of moderator and some absorber in which the potential scattering cross section per absorbing nucleus equals $\sigma_p + (N\bar{\ell})^{-1}$, where σ_p refers to the lump. It is of considerable importance to note that these rules do not depend on any knowledge whatever of the resonance parameters. They can be used both for predictive purposes and as a check on the theory.

7. Another very interesting rule of a more approximate nature than those just considered, but which also has the advantageous feature of not depending on the resonance parameters, concerns the dependence of the effective resonance integral on geometry. Let us first consider only the natural line shape. The effective resonance integral is then given by Eq. (13-4) appropriately modified, viz.:

$$I = \frac{\frac{\pi}{2}(b\sigma_p)\frac{\Gamma_\gamma}{E_o}}{\sqrt{\beta b\left(1 + \beta b - \frac{\gamma}{b}\right)}} \approx \frac{\pi}{2}\sigma_p \frac{\Gamma_\gamma}{E_o}\beta^{-\frac{1}{2}} \cdot \frac{b}{\sqrt{b - \gamma}} \qquad (10\text{-}6)$$

The approximate equality is based on the requirement that $\beta b << 1$, a condition nearly always fulfilled for the important resonances in most materials. Plotted in Fig. (1-6) is the second factor on the right hand side of Eq. (10-6) for all b and several values of γ. As we can see from the figure all these curves are asymptotic to the value $\sqrt{b}$. Thus with increasing b the dependence of the effective resonance integral on the interference between potential and resonance scattering disappears. For

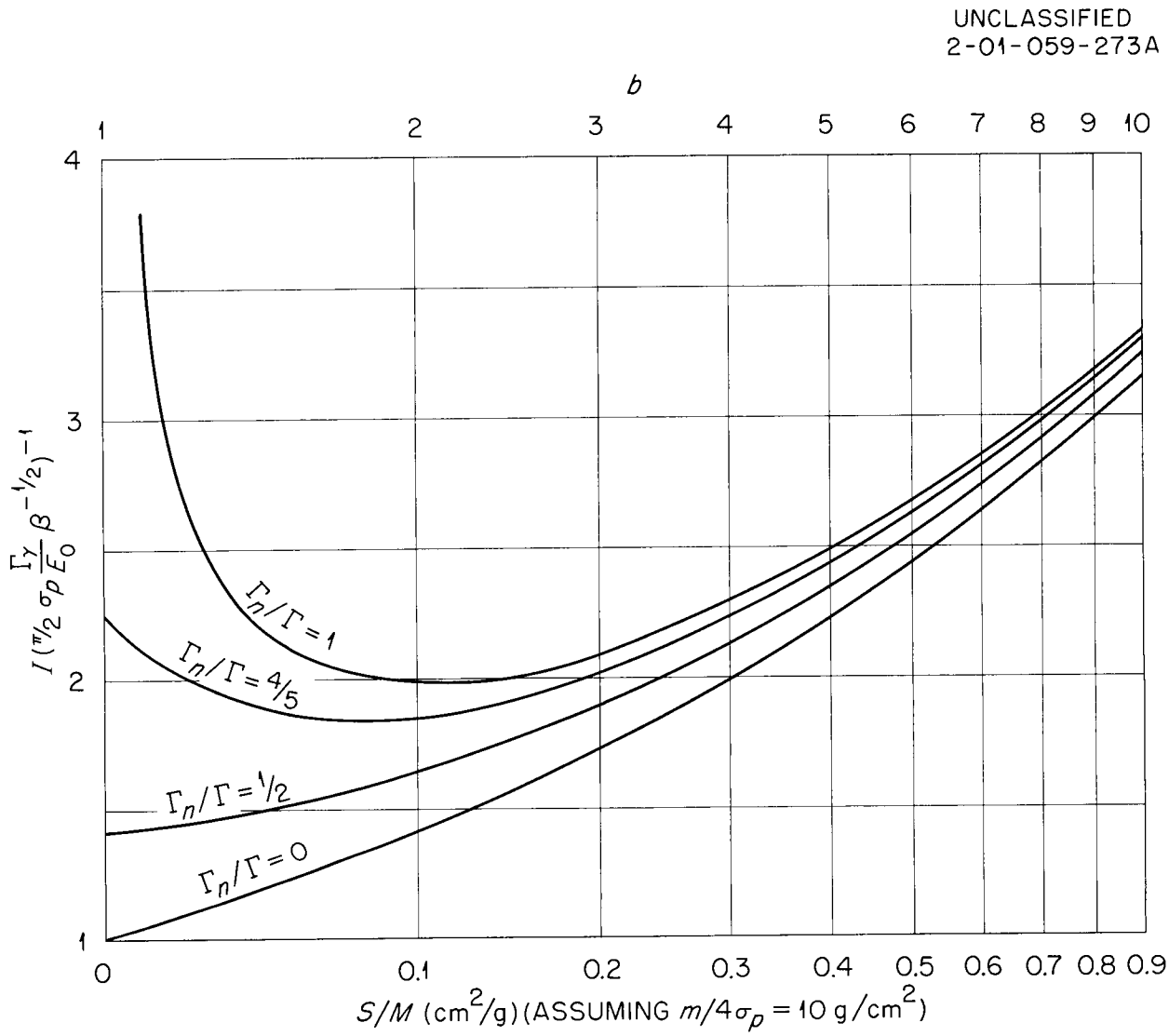


Fig. 1-6. Geometric Dependence of Resonance Integral.

any absorbing material in which the resonances responsible for the bulk of the absorption are narrow, the dependence of I on geometry for not too small b should be proportional to $\sqrt{b}$. This geometric dependence was previously noted by the author (D56a) in the case $\gamma = 0$, and an attempt was made to exploit its independence of the resonance parameters. As we shall see later, however, the strongly absorbing resonances are frequently not narrow.

The effect of Doppler broadening of resonance lines on this geometric dependence ought not to be too great for the following reasons: Most heterogeneous arrangements contain the absorber in relatively pure form (e.g., U, UO_2, Th, ThO_2). Usually, then, $\sigma_p \sim$ 10-20 barns. σ_o for the low energy, strongly absorbing resonance lines, on the other hand, is usually of the order of 1-2 x 10^4 barns, so that $\beta \sim 10^{-3}$. For these low energy resonances ξ is usually $\sim$ 0.3 or more. Hence, $\frac{6\beta}{\xi^2}$ is generally of the order of 0.1. Thus we are never very far from the natural line shape limit.

The $\sqrt{b}$ geometric dependence for heterogeneous systems is equivalent to the $\sqrt{\sigma_p}$ law for homogeneous systems mentioned in paragraph (3-4). This is an immediate corollary of the second rule of paragraph (6-6). The rules we have discussed in this and the last paragraph are of vital practical importance. They make it possible, for example, to obtain the effective resonance integral for a considerable range of heterogeneous and homogeneous arrangements from a measurement on a single lump or a single homogeneous system.

8. All of the preceding work depends on the use of the rational approximation (14-5) for the escape probability. The rest of this chapter will be devoted to an analysis of the error involved in the use of this approximation. Average escape probabilities for slabs, cylinders, and spheres have been tabulated by Case, Placzek, and deHoffmann (C53). Plotted in Fig. (2-6) are their results along with a plot of Eq. (14-5). As it happens, the exact average escape probabilities for sphere and cylinder never differ by more than 2% for any value of $\Sigma\bar{\ell}$, and are essentially the same for $\Sigma\bar{\ell} \gtrsim 3$. The average escape probability for a slab is about 10% at most below that for a sphere for $\Sigma\bar{\ell} \sim 1$, and is essentially the same as that for a sphere (or cylinder) for $\Sigma\bar{\ell} \gtrsim 3$. The rational approximation, on the other hand, is consistently low, often by as much as 23% near $\Sigma\bar{\ell} \sim 2$.

In order to discover the effects of these differences on the effective resonance integral, let us consider absorption by lumps in the absence of Doppler broadening and of interference between resonance and potential scattering. Under these conditions the term in the expression for I involving the average escape probabilities can be written

$$I' \equiv \int \frac{\sigma_a(\sigma_a + \sigma_s)}{\sigma_t} P(\Sigma_t)du = \frac{1}{N\bar{\ell}} \cdot \frac{\Gamma_\gamma}{E_o} \cdot \int f(\ell)d\ell \cdot \int_0^\infty \frac{dx}{\left[1 + \beta(1 + x^2)\right]^2}$$

$$\times \left(1 - e^{-\frac{N\ell\sigma_o}{1 + x^2} - N\ell\sigma_p}\right) \qquad (11\text{-}6)$$

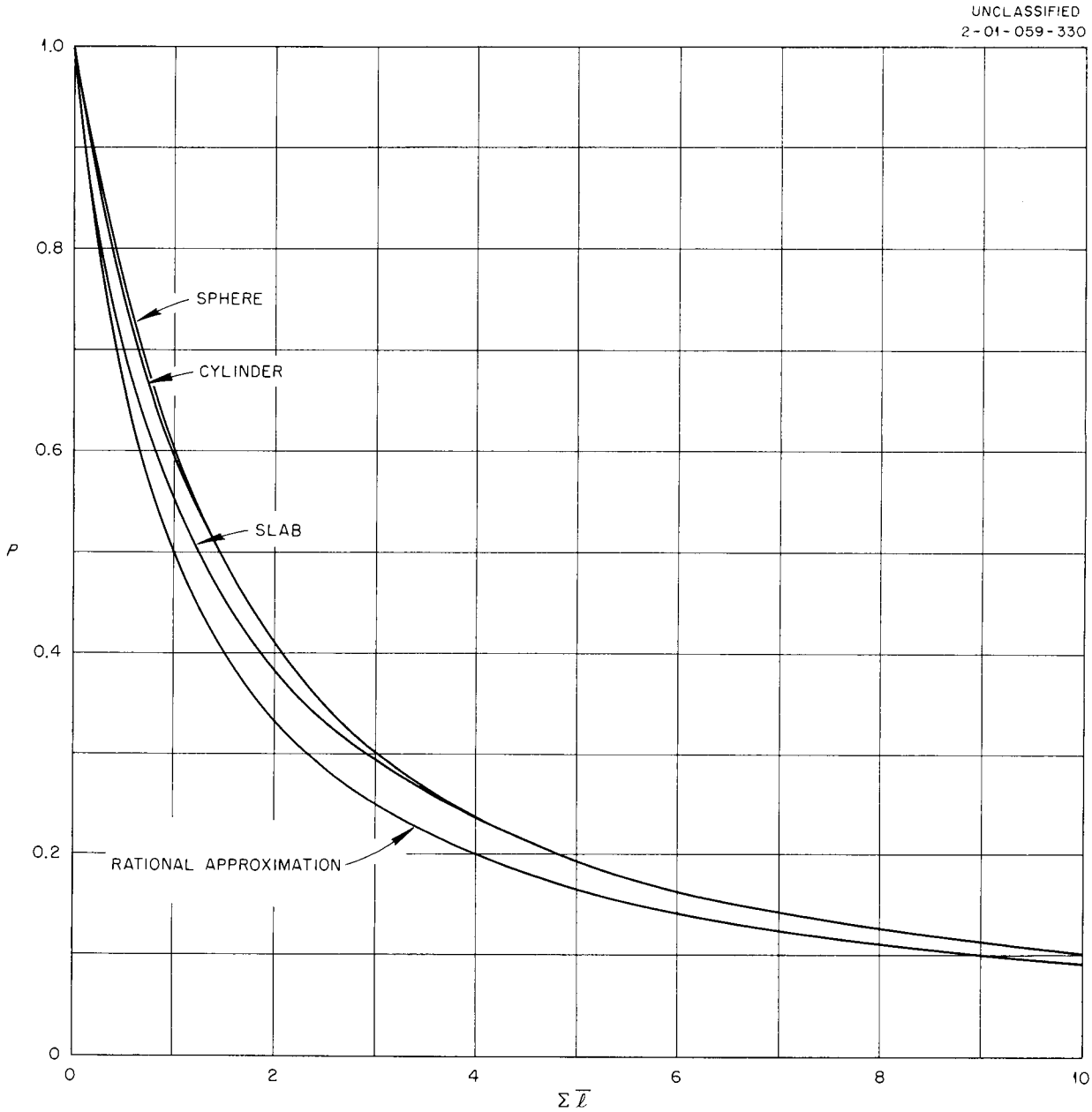

UNCLASSIFIED
2-01-059-330
1.0
0.8
0.6
0.4
0.2
0
P
SPHERE
CYLINDER
SLAB
RATIONAL APPROXIMATION
0
2
4
6
8
10
$\Sigma \bar{\ell}$

Fig. 2-6.

Here we have used Eq.(11c-5) for P and interchanged the order of the x and ℓ integrations. x is defined as usual by Eq. (5c-4). The x-integral can be done approximately employing an artifice due to Gurevich and Pomeranchouk (G55). If $N\bar{\ell}\sigma_o >> 1$, $1 + x^2$ can be replaced by x^2 in the exponent; for the exponential is only significant when $x^2 \sim N\bar{\ell}\sigma_o >> 1$. If we make this replacement and then make the substitution $y = (N\ell\sigma_o)^{1/2}/x$ we obtain, after rearrangement

$$I' = (N\bar{\ell})^{-\frac{1}{2}} \frac{(\sigma_o \Gamma_\gamma^2)^{\frac{1}{2}}}{E_o} \int f(\ell)d\ell \sqrt{\frac{\ell}{\bar{\ell}}} \int_o^\infty \frac{y^2 dy}{(y^2 + N\ell\sigma_p)^2} \left(1 - e^{-N\ell\sigma_p - y^2}\right) \quad (12\text{-}6)$$

In arriving at Eq. (12-6) we have also neglected β in comparison with unity.

9. Let us consider the two functions, L(a) and K(a), defined by

$$L(a) = \int_o^\infty e^{-y^2} \frac{y^2 dy}{(y^2 + a^2)^2} \quad (13a\text{-}6)$$

and

$$K(a) = \int_o^\infty \frac{y^2 dy}{(y^2 + a^2)^2} \quad (13b\text{-}6)$$

in terms of which I' can be calculated. To evaluate L in terms of tabulated functions we proceed as follows: We note first that

$$L(a) = \frac{d}{d(a^2)} \cdot a^2 \int_o^\infty \frac{e^{-y^2}}{y^2 + a^2} dy = \frac{d}{d(a^2)} a \cdot \int_o^\infty \frac{e^{-a^2 z^2}}{1 + z^2} dz \quad (14\text{-}6)$$

The second equality follows from the substitution $y = az$. If we denote by $F(a)$ the infinite z-integral on the extreme right hand side, it can easily be shown that it obeys the following first order linear differential equation and boundary condition

$$\frac{dF}{d(a^2)} - F = -\frac{\sqrt{\pi}}{2a} \; ; \; F(0) = \frac{\pi}{2} \tag{15-6}$$

The unique solution to this system is then

$$F(a) = e^{a^2}\left(\frac{\pi}{2} - \frac{\sqrt{\pi}}{2}\int_0^{a^2} e^{-x}\frac{dx}{\sqrt{x}}\right) \tag{16-6}$$

By substituting $x = y^2$ in Eq. (16-6) one can obtain the result

$$F(a) = \frac{\pi}{2}\, e^{a^2}\, \mathrm{Erfc}(a) \tag{17-6}$$

where $\mathrm{Erfc}(a)$ is the complementary error function. Substituting this expression in Eq. (14-6) gives for $L(a)$

$$L(a) = \frac{\pi}{4a}\left\{(1 + 2a^2)\, e^{a^2}\, \mathrm{Erfc}(a) - \frac{2}{\sqrt{\pi}}\, a\right\} \tag{18-6}$$

By integration by parts it is easy to prove

$$K(a) = \frac{\pi}{4a} \tag{19-6}$$

Using Eqs. (18-6) and (19-6) one can write Eq. (12-6) as

$$I' = (N\bar{\ell})^{-\frac{1}{2}} \frac{(\sigma_o \Gamma_\gamma^2)^{1/2}}{E_o} \cdot \frac{\frac{\pi}{4}}{\sqrt{N\bar{\ell}\sigma_p}}$$

$$\times \left\langle 1 - (1 + 2N\ell\sigma_p)\mathrm{Erfc}\left(\sqrt{N\ell\sigma_p}\right) + \frac{2}{\sqrt{\pi}}\sqrt{N\ell\sigma_p}\; e^{-N\ell\sigma_p}\right\rangle \tag{20-6}$$

where the bracket denotes an average with respect to the distribution of chord lengths. If to I' we add Eq. (13-4) with $\gamma = 0$ and β neglected in comparison with unity, we obtain the appropriate total effective resonance integral. It is possible to rearrange Eq. (13-4) as follows

$$\frac{\pi}{2}\,\sigma_p\,\frac{\Gamma_\gamma}{E}\,\beta^{-1/2} = (N\bar{\ell})^{-1/2}\,\frac{(\sigma_o\Gamma_\gamma^2)^{1/2}}{E_o}\cdot\frac{\pi}{2}\,\sqrt{N\bar{\ell}\sigma_p} \tag{21-6}$$

Thus I can be written as

$$I = (N\bar{\ell})^{-1/2}\,\frac{(\sigma_o\Gamma_\gamma^2)^{1/2}}{E_o}\left[\frac{\pi}{2}\sqrt{N\bar{\ell}\sigma_p} + \frac{\frac{\pi}{4}}{\sqrt{N\bar{\ell}\sigma_p}}\right.$$

$$\left.\left\langle 1 - (1 + 2N\ell\sigma_p)\,\mathrm{Erfc}\left(\sqrt{N\ell\sigma_p}\right) + \frac{2}{\sqrt{\pi}}\sqrt{N\ell\sigma_p}\;e^{-N\ell\sigma_p}\right\rangle\right] \tag{22-6}$$

The corresponding expression in the rational approximation can be written, similarly to Eq. (21-6), as

$$I = (N\bar{\ell})^{-1/2}\,\frac{(\sigma_o\Gamma_\gamma^2)^{1/2}}{E_o}\cdot\frac{\pi}{2}\sqrt{1 + N\bar{\ell}\sigma_p} \tag{23-6}$$

10. Since the average escape probability is nearly the same for cylinders as for spheres, the respective values of I will be nearly equal. Hence, if we evaluate the average indicated in Eq. (22-6) for spheres we may also apply the results to cylinders with good accuracy. In order to carry this program through we must first calculate the distribution of chord lengths from Eq. (12-5). Since all points on a sphere's surface are equivalent the surface integral disappears, and since there is azimuthal symmetry about the normal the integration is trivial. Noting then that $\ell = 2R\cos\theta$ where θ is the angle of the chord to the normal, we have from Eq. (12-5)

$$f(\ell) = \int_0^{\pi/2} \sin\theta \, d\theta \cdot 2\cos\theta \cdot \delta(\ell - 2R\cos\theta) \tag{24a-6}$$

$$= \frac{1}{2R^2} \int_0^{2R} d(2R\cos\theta) \cdot 2R\cos\theta \cdot \delta(\ell - 2R\cos\theta) \tag{24b-6}$$

$$= \frac{\ell}{2R^2} \qquad 0 \leq \ell \leq 2R \tag{24c-6}$$

Now the quantity in the braces in Eq. (22-6) can be written as the following power series:

$$\frac{4}{\sqrt{\pi}} \left[(N\ell\sigma_p)^{1/2} - \frac{\sqrt{\pi}}{2} N\ell\sigma_p + \frac{1}{3}(N\ell\sigma_p)^{3/2} - \frac{1}{30}(N\ell\sigma_p)^{5/2} + \frac{(N\ell\sigma_p)^{7/2}}{210} - \frac{(N\ell\sigma_p)^{9/2}}{1512} + \ldots \right] \tag{25-6}$$

This series can be averaged with respect to the distribution (24c-6) by noting that

$$\int_0^{2R} \frac{\ell}{2R^2} \cdot \ell^{k+\frac{1}{2}} \, d\ell = \frac{4(2R)^{k+\frac{1}{2}}}{2k+5} = \frac{4\left(\frac{3}{2}\right)^{k+\frac{1}{2}}}{2k+5} \, (\bar{\ell})^{k+\frac{1}{2}} \tag{26-6}$$

If we write a for $N\bar{\ell}\sigma_p$ we can then write for the square brackets in Eq. (22-6) the series

$$\sqrt{\pi}\left[\frac{4}{5}\left(\frac{3}{2}\right)^{\frac{1}{2}} + \frac{1}{3}\cdot\frac{4}{7}\cdot\left(\frac{3}{2}\right)^{\frac{3}{2}} a - \frac{1}{30}\cdot\frac{4}{9}\cdot\left(\frac{3}{2}\right)^{\frac{5}{2}} a^2 + \frac{1}{210}\cdot\frac{4}{11}\cdot\left(\frac{3}{2}\right)^{\frac{7}{2}} a^3 - \frac{1}{1512}\right.$$

$$\left.\cdot\frac{4}{13}\cdot\left(\frac{3}{2}\right)^{\frac{9}{2}} a^4 + \ldots\right] = \sqrt{\pi}\left[0.9798 + 0.3499a - 0.04082a^2\right.$$

$$\left. + 0.007158a^3 - 0.001262a^4 + \ldots\right] \qquad (27\text{-}6)$$

The corresponding expression in the rational approximation is $\frac{\pi}{2}\sqrt{1 + a}$. Presented below in Table (1-6) are values of the relative error incurred through the use of the rational approximation for the escape probability. The exact values to which these errors are referred are correct for spheres and cylinders. It is clear from Fig. (1-6) that the difference between the exact results for cylinders and spheres is very small. The difference cannot exceed 2%, and is surely very much less. For curves which differ as much

Table (1-6). Error Due to the Rational Approximation for Spheres and Cylinders

$a = N\bar{\ell}\sigma_p$	0	0.25	0.50	0.75	1.00	∞
% Error	- 10.6%	- 7.5%	- 5.5%	- 4.2%	- 3.3%	0%

as the extreme upper and lower curves in Fig. (1-6) the errors are given in Table (1-6). The escape probability curves for sphere and cylinder have a relative difference which is always better than 10 times smaller than the extreme curves, and consequently, lead to insignificant differences in the effective resonance integrals. The errors for slabs will be smaller than the values in Table (10-6) since the escape probability for slabs lies between that for spheres and the rational approximation.

The values in Table (1-6) are correct for $\beta << 1$, and overestimates for larger values of β. This can be seen as follows: The error due to the use of the rational approximation is mainly due to the wings of the resonance where $\Sigma_t \bar{l} \lesssim 1$. In the center of the line, where $\Sigma_t \bar{l} >> 1$, the rational approximation is correct. The relative contribution of the center of the resonance is least when $\beta << 1$; then the flux suffers a depression in the neighborhood of the resonance. As β increases the depression in the flux decreases and the relative importance of the center of the resonance increases. When $\beta >> 1$ the resonance integral given by Eq. (10-6) approaches the infinite dilution value which is correct for no flux depression at all.

CHAPTER 7. HETEROGENEOUS RESONANCE INTEGRALS - WIDE RESONANCES

1. In this chapter we shall consider heterogeneous resonance absorption in the case that the width of the resonance in lethargy greatly exceeds the average lethargy decrement per collision, ξ, of the absorbing material. We shall specifically exclude, at first, lumps in which any strong moderator is included, e.g., UO_2. These conditions suggest the idealization of taking the absorber mass infinite, in which case monoenergetic neutron transport theory is applicable to the interior of the lump. The resonance is narrow, on the other hand, with respect to the lethargy decrement per collision in the moderator surrounding the lump. The flux in the moderator, ϕ, is therefore uniform spatially and lethargy-wise for reasons similar to those mentioned in the previous chapter. The effective resonance integral, I, defined as in the last chapter, is then related to the lethargy integral of the albedo by the following equation:

$$NVI\phi = \frac{\phi}{4} S \int (1 - \delta)du \qquad (1\text{-}7)$$

Both sides of Eq. (1-7) represent the absorption rate in the lump by the resonance being considered; the left hand side expresses it as the volume and lethargy integral of the product of the flux and effective cross section, the right hand side expresses it as the difference of the incident and excident currents. It follows from Eq. (1-7) that

$$I = (N\bar{\ell})^{-1} \int (1 - \delta)du \qquad (2\text{-}7)$$

2. The remainder of this chapter will proceed according to the following plan: First, an approximate expression for the albedo will be proposed. Secondly, the integral in Eq. (2-7) will be evaluated, and I expressed

explicitly in terms of the parameters of the resonance and the lump size. Finally, the accuracy of the proposed approximation for the albedo will be studied.

The approximate expression we propose for $1 - \delta$ is

$$1 - \delta = \frac{\Sigma_a \bar{\ell}}{1 + \frac{\sqrt{3}}{4} \bar{\ell} (\Sigma_a \Sigma_t)^{1/2} + \left(1 - \frac{\sqrt{3}}{4}\right) \Sigma_a \bar{\ell}} \tag{3-7}$$

In the event that $\Sigma_t \bar{\ell} >> 1$ and $\Sigma_a << \Sigma_t \sim \Sigma_s$ we anticipate that diffusion theory would be applicable. But under the circumstances mentioned Eqs. (3-7) and (27-6) are essentially the same. The only differences are the replacement of Σ_s by Σ_t and $\frac{1}{2}$ by $1 - \frac{\sqrt{3}}{4}$. The first replacement is surely valid if $\Sigma_a << \Sigma_t$. The second replacement can never cause more than 7% error (when $\Sigma_s = 0$ and $\Sigma_a \bar{\ell} = \Sigma_t \bar{\ell} >> 1$) and under the condition $\Sigma_a << \Sigma_t$ will clearly cause much less.

When $\Sigma_s = 0$, Eq. (3-7) gives

$$1 - \delta = \Sigma_a \bar{\ell} \, (1 + \Sigma_a \bar{\ell})^{-1} \tag{4-7}$$

We can prove this to be correct as follows: Since the flux, ϕ, outside the lump is spatially uniform the absorption rate in the lump is given by $\phi P(\Sigma_a)\Sigma_a V$, according to the theorem of paragraph (3-5). If we equate this quantity to the right hand side of Eq. (1-7) we immediately obtain

$$1 - \delta = \Sigma_a \bar{\ell} \cdot P(\Sigma_a) \tag{5-7}$$

If we use the rational approximation for P Eqs. (5-7) and (4-7) are identical.

If $\Sigma_t \bar{\ell} << 1$, we need only consider absorption on the first collision, since second and higher collisions are very unlikely. Hence, by a precisely similar analysis as that leading to Eq. (5-7) we obtain

$$1 - \delta = \Sigma_a \bar{\ell}\, P(\Sigma_t) \approx \Sigma_a \bar{\ell}\, (1 + \Sigma_t \bar{\ell})^{-1} \approx \Sigma_a \bar{\ell} \qquad (6\text{-}7)$$

since $\Sigma_t \bar{\ell} << 1$. The limit (6-7) is indeed the limiting value of Eq. (3-7) for very small lumps. The expression (3-7) for the albedo thus has the correct limiting value for either very black or very transparent lumps, and very large and very small lumps. As we shall see later it is quite an excellent approximation to the albedo presented by a medium to a uniform source outside.

3. If we insert Eq. (3-7) into Eq. (2-7), and make use of the definitions given in Eqs. (5 to 10-4) we can write for I the result

$$I = \frac{1}{2}\sigma_p \frac{\Gamma_\gamma}{E_o} \beta^{-\frac{1}{2}} \cdot \int_{-\infty}^{+\infty} dy \left[y^2 + \frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{\frac{1}{2}} \left\{ y^2 + 2\sqrt{\gamma}\; y + 1 + \beta \right\}^{\frac{1}{2}} \right.$$

$$\left. + \left(1 - \frac{\sqrt{3}}{4}\right) a \frac{\Gamma_\gamma}{\Gamma} + \beta \right]^{-1} \qquad (7\text{-}7)$$

Here we have used the variable $y = x\sqrt{\beta}$, with x given by Eq. (5c-4). Finally, a is defined in Chapter 6 as $N\bar{\ell}\sigma_p$. Since we have excluded any diluent in the lump, $\sigma_{pa} = \sigma_p$, and $\gamma = g_J \frac{\Gamma_n}{\Gamma}$.

If $\frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2} << 1$, it is relatively easy to evaluate the integral in Eq. (7-7) approximately. When $y^2 >> \frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2}$ the first term in the

integrand greatly exceeds the second, and little error is incurred by replacing the curly bracket by unity. When $y^2 << \frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2}$ the curly bracket is essentially unity (if $\beta << 1$ is assumed). Replacing the curly bracket by unity gives an easy integrand of the form

$\left[y^2 + \frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2} + (1 - \frac{\sqrt{3}}{4}) a \frac{\Gamma_\gamma}{\Gamma} + \beta\right]^{-1}$. I can then be written

$$I = \frac{\pi}{2} \sigma_p \frac{\Gamma_\gamma}{E_o} \beta^{-1/2} \cdot \left[\frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2} + \left(1 - \frac{\sqrt{3}}{4}\right) a \frac{\Gamma_\gamma}{\Gamma} + \beta\right]^{-1/2} \qquad (8\text{-}7)$$

4. In case $\frac{\Gamma_n}{\Gamma} << 1$ and $\beta << 1$ it is possible to evaluate the integral in Eq. (7-7) exactly, and test the accuracy of Eq. (8-7). This is probably the most important case in which the infinite mass absorber approximation will be used, for wide resonances occur only at low energy, where, usually $\Gamma_n << \Gamma$. If $\frac{\Gamma_n}{\Gamma} << 1$, so is γ; let us set $\gamma = 0$, $\frac{\Gamma_\gamma}{\Gamma} = 1$, and ignore β compared to unity in the square root. Then the integral, $\mathcal{I}$, in Eq. (7-7) can be written

$$\mathcal{I} = 2 \int_0^\infty dy \left[y^2 + u\sqrt{1 + y^2} + v\right]^{-1} \qquad (9\text{-}7)$$

where $u = \frac{\sqrt{3}}{4} a$ and $v = \left(1 - \frac{\sqrt{3}}{4}\right) a + \beta$. If we make the change of variables $y = \frac{2w}{1 - w^2}$, Eq. (9-7) can be rewritten as

$$\mathcal{I} = 4 \int_0^1 dw \left\{1 + w^2\right\} \left\{w^4 (v - u) + w^2 (4 - 2v) + (u + v)\right\}^{-1} \qquad (10\text{-}7)$$

If β^2 and α^2 are the <u>negative</u> roots of the equation

$$x^2 + \frac{4 - 2v}{v - u} x + \frac{v + u}{v - u} = 0 \tag{11-7}$$

we can rewrite $\mathcal{J}$ as

$$\left(\frac{v - u}{4}\right)\mathcal{J} = \frac{1}{\beta^2 - \alpha^2} \int_0^1 dw \left\{\frac{1 - \alpha^2}{w^2 + \alpha^2} - \frac{1 - \beta^2}{w^2 + \beta^2}\right\} \tag{12a-7}$$

$$= \frac{1}{\beta^2 - \alpha^2}\left\{\frac{1 - \alpha^2}{\alpha} \arctan\left(\frac{1}{\alpha}\right) - \frac{1 - \beta^2}{\beta} \arctan\left(\frac{1}{\beta}\right)\right\} \tag{12b-7}$$

Presented in Table (1-7) is the relative error in percent for several values of a.

Table 1-7. Relative Error in Eq. (8-7) vs a

a	1.76	1.00	0.50	0.20
Relative Error	+ 8.7%	+ 5.9%	+ 3.3%	+ 1.6%

For fixed a, the error in using Eq. (8-7) may be expected to decrease as $\frac{\Gamma_\gamma}{\Gamma}$ decreases. When $\frac{\Gamma_\gamma}{\Gamma}$ is very small compared to unity, we may take $\gamma = 1$ (if the nucleus has zero spin so that $g_J = 1$). In this case we can also find $\mathcal{J}$ exactly. Again ignoring β in the square root we can write

$$\mathcal{J} = \int_{-\infty}^{+\infty} dy \left[y^2 + u\left|y + 1\right| + v\right]^{-1} \tag{13-7}$$

where u and v now mean $\frac{\sqrt{3}}{4} a \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2}$ and $\left(1 - \frac{\sqrt{3}}{4}\right) a \frac{\Gamma_\gamma}{\Gamma} + \beta$, respectively. The absolute value signs arise because the square root is proportional to the inverse diffusion length, $\mathcal{K} = \sqrt{3\Sigma_a\Sigma_s}$, which is always positive. Writing $z = y + 1$, we have

$$\mathcal{J} = \int_0^\infty dz \left[z^2 + (u - 2)z + (1 + v)\right]^{-1} + \int_0^\infty dz \left[z^2 + (u + 2)z + (1 + v)\right]^{-1} \tag{14-7}$$

An explicit expression for $\mathcal{J}$ in terms of tabulated functions can be obtained with the standard integral

$$\int_0^\infty \frac{dx}{x^2 + 2Ax + B^2} = \begin{cases} (B^2 - A^2)^{-1/2} \arccos\left(\frac{A}{B}\right) & B > A \\ (A^2 - B^2)^{-1/2} \operatorname{arccosh}\left(\frac{A}{B}\right) & B < A \end{cases} \tag{15-7}$$

Taylor's series expansion of $\mathcal{J}$ from Eq. (14-7) gives

$$\mathcal{J} = \pi(u + v)^{-1/2} + \frac{\pi}{8} u^2(u + v)^{-3/2} - \frac{u}{3} + \frac{3\pi}{128} u^4(u + v)^{-5/2} - \frac{4}{5} uv + \ldots \tag{16-7}$$

Using the first term in this expansion corresponds to using Eq. (8-7) for I. As we see the fractional error in this procedure is of the order $\frac{u^2}{8(u + v)}$. Choosing the case a = 1, corresponding to the second entry in Table (1-7), and choosing $\frac{\Gamma_\gamma}{\Gamma} = 0.1$, we find the error estimated from the second term of series (16-7) to be about 1.2%, while that calculated exactly from Eq. (15-7) is about 0.7%.

Thus for not too large a, Eq. (8-7) is a good approximation, being worst for a purely absorbing resonance and improving with decreasing $\frac{\Gamma_\gamma}{\Gamma}$. Then, if $\beta \ll 1$, the geometric dependence of Eq. (8-7) is proportional to $a^{-1/2}$, which when expressed in terms of the variable b is $\sqrt{b - 1}$. This variation asymptotically approaches a $\sqrt{b}$ - law. Hence, for not too small b the very same geometric dependence applies asymptotically in the infinite-mass-absorber case as in the narrow resonance case.

5. Equation (8-7) has the following very interesting property, viz.: that it is independent of σ_p and is the correct result obtained for I if we first let σ_p approach zero in Eq. (7-7) and then perform the integration. In order to take the limit of Eq. (7-7) as $\sigma_p \longrightarrow 0$, we must first transform the integral $\mathcal{J}$ back to the variable $x = y\sqrt{\beta}$. Doing so and then letting $\sigma_p \longrightarrow 0$ we obtain

$$I = \frac{\sigma_o \Gamma \gamma}{2E_o} \int_{-\infty}^{+\infty} dx \left[x^2 + 1 + \frac{\sqrt{3}}{4} N\bar{\ell}\sigma_o \left(\frac{\Gamma\gamma}{\Gamma}\right)^{1/2} + \left(1 - \frac{\sqrt{3}}{4}\right) N\bar{\ell}\sigma_o \frac{\Gamma\gamma}{\Gamma} \right]^{-1} \qquad (17a\text{-}7)$$

$$= \frac{\sigma_o \Gamma \gamma}{2E_o} \pi \left[\frac{\sqrt{3}}{4} N\bar{\ell}\sigma_o \left(\frac{\Gamma\gamma}{\Gamma}\right)^{1/2} + \left(1 - \frac{\sqrt{3}}{4}\right) N\bar{\ell}\sigma_o \frac{\Gamma\gamma}{\Gamma} + 1 \right]^{-1/2} \qquad (17b\text{-}7)$$

It is very easy to show that Eq. (17b-7) and Eq. (8-7) are identical.

This possibility of neglecting σ_p has the following explanation: In the line center resonance processes far outweigh potential scattering, since $\sigma_o >> \sigma_p$. In the wings of the line where $\sigma_o << \sigma_p$, very few absorptions at all occur if $a = N\bar{\ell}\sigma_p$ is not too large, for even the likelihood of collision is small. Hence σ_p is never very important. The error in letting $\sigma_p \longrightarrow 0$ as a function of lump size is given by Table (1-7).

6. The observations made in the last paragraph simplify the infinite-mass-absorber approximation sufficiently to allow inclusion of the Doppler effect. If we set $\sigma_p = 0$, but use the Doppler broadened line shape, Eq. (7-7) is replaced by the equation:

$$I = \frac{1}{N\bar{\ell}} \cdot \frac{\Gamma}{2E_o} \int_{-\infty}^{+\infty} \frac{N\sigma_o \bar{\ell} \frac{\Gamma_\gamma}{\Gamma} \psi(\xi,x)}{1 + N\sigma_o \bar{\ell} \left\{ \frac{\sqrt{3}}{4} \left(\frac{\Gamma_\gamma}{\Gamma}\right)^{1/2} + \left(1 - \frac{\sqrt{3}}{4}\right) \frac{\Gamma_\gamma}{\Gamma} \right\} \psi(\xi,x)} \, dx \tag{18a-7}$$

$$= \sigma_o \frac{\Gamma_\gamma}{E_o} \int_{o}^{\infty} \frac{\psi(\xi,x)}{1 + \left(\frac{u+v}{\beta}\right) \psi(\xi,x)} \, dx \tag{18b-7}$$

$$= \sigma_p \frac{\Gamma_\gamma}{E_o} (u+v)^{-1} \cdot J\left[\xi, \beta(u+v)^{-1}\right] \tag{18c-7}$$

where u and v are defined as in Eq. (13-7). Again the Doppler effect enters through the function $J(\xi,\beta)$ which has been studied in Chapter 4. Finally since the resonances we shall be concerned with in this approximation occur at low energies, they will be very high and narrow, and $6\beta << \xi^2$. The effect of Doppler broadening will be slight, especially on the $\sqrt{b-1}$ geometric dependence.

7. The entire procedure on which our final result, Eq. (18c-7), is based depends on the accuracy of the expression (3-7) for the complementary albedo, $1 - \delta$. The next portion of this chapter will be devoted to studying the accuracy of Eq. (3-7). Let us first consider the case $\Sigma_t \bar{\ell} \lesssim 1$, applicable to either very small lumps or in the wings of the resonance. We can find the complementary albedo accurately and easily by use of a variational technique. It will be convenient in the calculations which are described below to choose the total mean free path in the lump as the unit of length, and to set $C = \frac{\Sigma_s}{\Sigma_t}$ = number of secondary neutrons produced per collision in the lump. Finally let the flux outside the lump be spatially uniform, and of unit magnitude. The analogue of Eq. (1-7) for $1 - \delta$ is then

$$(1 - \delta)\,\frac{1}{4}\,S = \int_V P(\vec{r})\,d^3r - C\int_V \phi(\vec{r})P(\vec{r})\,d^3r \qquad (19\text{-}7)$$

Here both sides represent the absorption rate in the lump. The left hand side represents the difference of incident and excident current through the surface, S, of the lump. The first term on the right hand side is the density of first collisions in the lump. Here $P(\vec{r})$ is the escape probability function defined in paragraph 3 of Chapter 5. The second term on the right hand side is the rate of escape of collided neutrons from the lump; $\phi(\vec{r})$ is the collision density in the lump.

$\phi(\vec{r})$ is determined by the integral transport equation, viz.:

$$\phi(\vec{r}) = C\int_V \phi(\vec{r}\,')\,\frac{\exp\left(-\left|\vec{r} - \vec{r}\,'\right|\right)}{4\pi\left|\vec{r} - \vec{r}\,'\right|^2}\,d^3r' + P(\vec{r}) \qquad (20\text{-}7)$$

The two terms on the right hand side represent the contributions to the collision density at $\vec{r}$ from previously collided and previously uncollided neutrons, respectively. The kernel in the integral is essentially that of Eq. (5-5). It is very easy to show that the function $J\left[\phi\right]$ written below is stationary for the solution of Eq. (20-7)

$$J\left[\phi\right] = C\int_V d^3r \int_V d^3r'\,\phi(\vec{r})\,\frac{\exp\left(-\left|\vec{r} - \vec{r}\,'\right|\right)}{4\pi\left|\vec{r} - \vec{r}\,'\right|^2}\,\phi(\vec{r}\,') - \int_V \phi^2(\vec{r})\,d^3r$$

$$+\,2\int_V \phi(\vec{r})P(\vec{r})\,d^3r \qquad (21\text{-}7)$$

Moreover, the stationary value is just the second integral on the right hand side of Eq. (19-7), i.e.,

$$J\left[\phi^*\right] = \int_V \phi^*(\vec{r})P(\vec{r})\, d^3r \tag{22-7}$$

where ϕ^* is a solution of Eq. (20-7). From Eqs. (19-7), (21-7), and (22-7) it then follows that

$$1 - \delta = \bar{\ell}\left\{\frac{1}{V}\int_V P(\vec{r})\, d^3r - \frac{C}{V} J\left[\phi(\vec{r})\right]\right\} \tag{23a-7}$$

$$= \bar{\ell}\left\{\frac{1}{V}\int_V P(\vec{r})\, d^3r - \frac{C^2}{V}\int_V d^3r \int_V d^3r'\, \phi(\vec{r})\, \frac{\exp\left(-\left|\vec{r} - \vec{r}'\right|\right)}{4\pi\left|\vec{r} - \vec{r}'\right|^2}\, \phi(\vec{r})\right.$$

$$\left. + \frac{C}{V}\int_V \phi^2(\vec{r})\, d^3r - \frac{2C}{V}\int_V \phi(\vec{r})P(\vec{r})\, d^3r\right\} \tag{23b-7}$$

This equation has the very important advantage that the error in the complementary albedo, $1 - \delta$, is of <u>second order</u> in the error in a trial function for the collision density. In general, the integrals are difficult; but with a constant trial function they can be expressed in terms of the average escape probabilities, P, which have been tabulated (C53). Let us choose $\phi(\vec{r}) = A$. Then

$$J\left[A\right] = CA^2V(1 - P) - VA^2 + 2AVP \tag{24-7}$$

Use has been made here of the identity

$$\int_V d^3r \int_V d^3r' \frac{\exp\left(-\left|\vec{r} - \vec{r}'\right|\right)}{4\pi \left|\vec{r} - \vec{r}'\right|^2} = 1 - P \tag{25-7}$$

which is clear, since both sides represent the collision probability averaged over the lump volume. The best value for A is now determined from the requirement that dJ/dA vanish; it is

$$A = \frac{P}{1 - C(1 - P)} \tag{26-7}$$

Substituting Eq. (26-7) into Eq. (24-7) and this result into Eq. (23a-7) one obtains

$$1 - \delta = \frac{\bar{\ell}(1 - C)P}{1 - C(1 - P)} \tag{27-7}$$

This expression has the interesting property that it can be derived from a successive generations approach, assuming all generations to have a spatially uniform collision density. The absorption rate is then calculated for each generation, and the result is a geometric series

$$\frac{1}{4} S (1 - \delta) = \frac{1}{4} S \left[P(1 - C) + PC\cdot(1 - P)(1 - C) + PC(1 - P)C\cdot(1 - P)(1 - C) + \ldots\right] \tag{28a-7}$$

$$= \frac{1}{4} S P(1 - C) \left[1 + (1 - P)C + (1 - P)^2C^2 + \ldots\right] \tag{28b-7}$$

which when summed gives Eq. (27-7). The latter equation was suggested by Pershagen (P57) on the successive approximations basis. He applied it to the calculation of thermal utilization and noted, by comparison with numerical solution of the linear Boltzmann equation, that it was very accurate.

It is now apparent that the high accuracy is due to the variational nature of the equation.*

8. A precisely similar variational procedure can be followed in the alternative case $\Sigma_t \bar{\ell} >> 1$. In this case the surface of the lump can be treated as a plane, and the albedo will be nearly that of an infinite half-space. (In the limit $\bar{\ell} \longrightarrow \infty$ the infinite half-space results will be exact.) Hence we shall consider the albedo of the Milne problem for a cosine current at the interface. A cosine current at the interface is equivalent to a uniform source strength outside the reflecting medium [cf Eq. (2-5)].

Before proceeding with the development of the variational equations it will be necessary to derive two integral kernels analogous to that of Eq. (5-5), but appropriate in plane geometry. Let us first consider the <u>uncollided</u> current at one plane due to a source of unit strength and angular distribution $G(\cos\theta)$ on a parallel plane removed a distance x (see Fig. 1-7). Let us again take the unit of length as the total mean free path. Then

$$j(x)dS = \int_{\theta=0}^{\theta=\frac{\pi}{2}} d\left[\pi(x\tan\theta)^2\right] \cdot \frac{dS\cos\theta}{(x\sec\theta)^2} \cdot \frac{G(\cos\theta)}{2\pi} \cdot e^{-x\sec\theta}$$

The first term in the integrand is the source strength of a ring source on the source plane, the second term is the infinitesimal solid angle the infinitesimal area dS subtends, the third term is the probability of a source neutron <u>being oriented in</u> velocity so as to intersect dS if

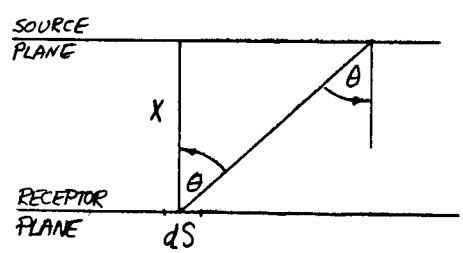


Fig. (1-7)

*Some time after completion of this work it came to the author's attention that the variational treatment of the albedo problem in the case treated in paragraph (7-7)($\Sigma_t \bar{\ell} << 1$) had been suggested by G. W. Stuart (Nuc. Sci. Eng. 2 617, 1957).

it remains uncollided, and the fourth term is the non-collision probability. Writing $\mu = \cos\theta$, Eq. (29-7) can be simplified to

$$j(x) = \int_0^1 e^{-x/\mu}\, G(\mu)\, d\mu \tag{30-7}$$

$G(\mu)$ is normalized on the μ-interval (-1, +1). The corresponding collision density at the receptor plane is given by

$$\phi(x) = -\frac{dj(x)}{dx} = \int_0^1 e^{-x/\mu}\, G(\mu)\, \frac{d\mu}{\mu} \tag{31-7}$$

For isotropy $G(\mu) = \frac{1}{2}$, and

$$j(x) = \frac{1}{2} \int_1^\infty e^{-\zeta x} \frac{d\zeta}{\zeta^2} \equiv \frac{1}{2} E_2(x) \tag{32a-7}$$

$$\phi(x) = \frac{1}{2} \int_1^\infty e^{-\zeta x} \frac{d\zeta}{\zeta} \equiv \frac{1}{2} E_1(x) \tag{32b-7}$$

where $\zeta = \mu^{-1}$. The E_n-functions, defined by $\int_1^\infty e^{-\zeta x} \frac{d\zeta}{\zeta^n} = E_n(x)$, have been studied extensively; a tabulation and bibliography are given in reference C53. For a cosine distribution $G(\mu) = |\mu|$, and

$$j(x) = \int_1^\infty e^{-\zeta x} \frac{d\zeta}{\zeta^3} \equiv E_3(x) \tag{33a-7}$$

$$\phi(x) = \int_1^\infty e^{-\zeta x} \frac{d\zeta}{\zeta^2} \equiv E_2(x) \tag{33b-7}$$

9. With these preliminaries established we shall now derive the variational expression for the albedo. The analogue of Eq. (19-7) for a semi-infinite reflecting medium located to the right of the plane x = 0 is

$$\frac{1}{4}(1 - \delta) = (1 - C)\int_0^\infty \phi(x)\,dx \tag{34-7}$$

where $\phi(x)$ is the collision density. The flux to the left of the plane x = 0 is taken spatially uniform, and of unit magnitude. The integral transport equation corresponding to Eq. (20-7) is

$$\phi(x) = \frac{C}{2}\int_0^\infty \phi(x')E_1(|x - x'|)dx' + \frac{1}{2}E_2(x) \tag{35-7}$$

The inhomogeneous term, the density of first collisions, is proportional to $E_2(x)$, as follows from Eq. (33b-7). The factor of $\frac{1}{2}$ is to normalize the incident current, j(0), to the value $\frac{1}{4}$, rather than $\frac{1}{2}$ as follows from Eq. (33b-7).

If we integrate Eq. (35-7) over x we obtain after rearrangement

$$(1 - C)\int_0^\infty \phi(x)dx = \frac{1}{4} - \frac{C}{2}\int_0^\infty E_2(x)\phi(x)dx \tag{36-7}$$

Here we have made use of the following properties of the E_n-functions

$$E_n(0) = \frac{1}{n - 1}\ ; \quad E_n(\infty) = 0 \tag{37a-7}$$

$$\int_0^x E_n(x)dx = \frac{1}{n} - E_{n+1}(x) \tag{37b-7}$$

to show that

$$\int_0^\infty E_1(|x - x'|)dx = 2 - E_2(x') \tag{38-7}$$

Thus from Eq. (36-7) and Eq. (34-7) we can write

$$\delta = 2C \int_0^\infty E_2(x)\phi(x)dx \tag{38-7}$$

A functional which is stationary for the solution of Eq. (35-7) is

$$J\left[\phi\right] = \frac{C}{2} \int_0^\infty dx \int_0^\infty dx'\, \phi(x)E_1(|x - x'|)\phi(x')$$

$$- \int_0^\infty \phi^2(x)dx + \int_0^\infty \phi(x)E_2(x)dx \tag{40-7}$$

Finally the stationary value of J is

$$J\left[\phi^*\right] = \frac{1}{2} \int_0^\infty \phi^*(x)E_2(x)dx \tag{41-7}$$

where ϕ^* solves Eq. (35-7). Combining Eqs. (41-7) and (39-7) gives a variational expression for δ whose error is of second order in the error in the trial function for ϕ, viz.:

$$\delta = 4CJ\left[\phi\right] \tag{42a-7}$$

$$= 2C^2 \int_0^\infty dx \int_0^\infty dx'\, \phi(x)E_1(|x - x'|)\phi(x') - 4C \int_0^\infty \phi^2(x)dx$$

$$+ 4C \int_0^\infty \phi(x)E_2(x)dx \tag{42b-7}$$

10. If C is not too small, suitable trial functions are suggested by the spherical harmonics approximations to the linear Boltzmann equation (D57b). These solutions are always of the form of sums of negative exponentials. In order to evaluate the integrals in Eq. (42b-7) explicitly we will first of all need to know the integral

$$\mathcal{F}(k,k') = \int_0^\infty dx \int_0^\infty dx' \, e^{-kx-k'x'} \, E_1(|x - x'|) \tag{43-7}$$

We can write $\mathcal{F}(k,k')$ as

$$\mathcal{F}(k,k') = \mathcal{D}(k,k') + \mathcal{D}(k',k) \tag{44-7}$$

where

$$\mathcal{D}(k,k') = \int_0^\infty dx \int_0^x dx' \, e^{-kx-k'x'} \, E_1(x - x') \tag{45a-7}$$

$$= \int_0^\infty dx \int_0^x dx' \, e^{-kx-k'x'} \int_1^\infty \frac{d\zeta}{\zeta} \, e^{-\zeta(x-x')} \tag{45b-7}$$

$$= \int_1^\infty \frac{d\zeta}{\zeta} \int_0^\infty dx \, e^{-(k+\zeta)x} \int_0^x e^{-(k'-\zeta)x'} \, dx' \tag{45c-7}$$

$$= \int_1^\infty \frac{d\zeta}{\zeta(k' - \zeta)} \int_0^\infty dx \left\{ e^{-(k+\zeta)x} - e^{-(k+k')x} \right\} \tag{45d-7}$$

$$= \frac{1}{k + k'} \int_1^\infty \frac{d\zeta}{\zeta(k + \zeta)} = \frac{\ln(1 + k\ )}{k(k + k')} \tag{45e-7}$$

The second integral which we need is

$$\int_0^\infty E_2(x)e^{-kx}\,dx = \int_0^\infty dx\; e^{-kx} \int_1^\infty \frac{d\zeta}{\zeta^2}\, e^{-\zeta x} \tag{46a-7}$$

$$= \int_1^\infty \frac{d\zeta}{\zeta^2(k + \zeta)} \tag{46b-7}$$

$$= \frac{k - \ln(1 + k)}{k^2} \tag{46c-7}$$

11. Let us now consider a trial function of the form suggested by diffusion theory. According to diffusion theory

$$\phi(x) = Ae^{-\gamma x} \tag{47a-7}$$

where

$$\gamma = \sqrt{3(1 - c)} \tag{47b-7}$$

The constant A can be determined from the condition that the partial current into the medium be $\frac{1}{4}$; but we shall not do this, but instead choose A to make δ stationary in accordance with Eq. (42a-7). As it happens, the difference is very small where this trial function is expected to be valid. In principle the same procedure can be used for η, but it becomes tedious, and we shall see in practice unnecessary.

From Eqs. (47a-7), (46c-7), (45e-7), and (42b-7) one finds that

$$\delta = - M(\gamma)\, A^2 + 2N(\gamma)\, A \tag{48a-7}$$

where

$$M(\gamma) = 2C \cdot \frac{\gamma - C\ln(1 + \gamma)}{\gamma^2} \tag{48b-7}$$

and

$$N(\gamma) = 2C \cdot \frac{\gamma - \ln(1 + \gamma)}{\gamma^2} \tag{48c-7}$$

The value of A which makes δ stationary is $\frac{N(\varkappa)}{M(\varkappa)}$. The corresponding value of δ is

$$\delta = \frac{N^2(\varkappa)}{M(\varkappa)} \tag{49-7}$$

A similar result applies for the case of a P_3-approximation to the Boltzmann equation, in which case

$$\phi(x) = A_1 e^{-\varkappa_1 x} + A_2 e^{-\varkappa_2 x} \tag{50-7}$$

The values of $\varkappa_1$ and $\varkappa_2$ depend only on the medium, and are the positive roots of the equation

$$9\varkappa^4 - \left[35 + 55(1 - C)\right]\varkappa^2 + 105(1 - C) = 0 \tag{51-7}$$

These roots have been tabulated by Davison (D57b). The values of A_1 and A_2 are again chosen to make δ stationary. The final result is

$$\delta = \frac{M(\varkappa_1)N^2(\varkappa_2) + M(\varkappa_2)N^2(\varkappa_1) + 2Q(\varkappa_1,\varkappa_2)N(\varkappa_1)N(\varkappa_2)}{M(\varkappa_1)M(\varkappa_2) - Q^2(\varkappa_1,\varkappa_2)} \tag{52-7}$$

where M and N are defined in Eq. (48-7) and

$$Q(\varkappa_1,\varkappa_2) = \frac{2C}{\varkappa_1 + \varkappa_2}\left[C\,\frac{\ln(1 + \varkappa_1)}{\varkappa_1} + C\,\frac{\ln(1 + \varkappa_2)}{\varkappa_2} - 2\right] \tag{53-7}$$

12. The results expressed in Eq. (48-7) or Eq. (52-7) are only useful when diffusion theory of P_3-theory are at least approximately true, i.e., if C is not too small. In the opposite extreme of very small C we can obtain a very useful expression for the albedo by considering only the neutrons which escape the medium after one collision. As in Eq. (35-7) the density of

first collisions is $\frac{1}{2} E_2(x)$. Since the scattering is isotropic, the reflected current originating from first collision at x is given by Eq. (32a-7). But the reflected current is $\frac{\delta}{4}$; thus

$$\delta = C \int_0^\infty E_2^2(x)\, dx \tag{54a-7}$$

$$= C \int_0^\infty dx \int_1^\infty \frac{dv}{v^2} e^{-vx} \int_1^\infty \frac{du}{u^2} e^{-ux} \tag{54b-7}$$

$$= C \int_1^\infty \frac{dv}{v^2} \int_1^\infty \frac{du}{u^2} \frac{1}{u + v} \tag{54c-7}$$

$$= C \int_1^\infty \frac{dv}{v^2} \left\{ \frac{v - \ln(1 + v)}{v^2} \right\} \tag{54d-7}$$

$$= C \cdot \frac{2}{3} (1 - \ln 2) \tag{54e-7}$$

The transition from step (c) to step (d) employed the partial fractions expansion

$$\frac{1}{u^2(u + v)} = \frac{1}{u^2 v} - \frac{1}{v^2 u} + \frac{1}{v^2(u + v)} \tag{55-7}$$

The logarthmic integral in step (d) can be done by parts. Equation (54e-7) always underestimates δ as is clear from its definition.

13. Presented in Table (2-7) are values of the albedo calculated in several different ways for three different values of C. It follows from these results, in the first place, that the variational results for the diffusion theory and P_3 trial functions never differ by more than 0.2%. Thus

Table (2-7). Albedo of a Half Space

Method	C = 0.7	C = 0.5	C = 0.3
First Collision - Eq. (54e-7)	0.1432	0.1022	0.06137
Diffusion Theory	0.2252	0.1010	0.01723
P_3 Approximation	0.2443	0.1370	-
Variational-Diffusion Theory Trial Function - Eq. (49-7)	0.2560	0.1461	0.07413
Variational-P_3 Trial Function - Eq. (52-7)	0.2565	0.1464	0.07423

the P_3 trial function will then give nearly exact results, while the diffusion theory trial function will give results accurate to the order of tenths of a percent. In the second place, neither diffusion theory nor the P_3 approximation will give very accurate results except for $1 - C \ll 1$. Their respective errors are -14% and -5% at C = 0.7 and -45% and -7% at C = 0.5. As a matter of fact for C as high as 0.95 the error in the diffusion theoretic albedo is already -1%. Thirdly, it appears that the variational result approaches the exact result from below. Plotted in Fig. (2-7) is the albedo calculated with the variational method with a diffusion theory trial function, with ordinary diffusion theory, and with the one collision approximation. The variational calculation was carried out for $C \gtrsim 0.3$ and graphically extrapolated to C = 0, using the slope and value at the origin given by Eq. (54e-7). Also included in the figure is a curve for $C \geq 0.5$ marked "P_3-approximation." It is based on the two points in Table (2-7) and a graphical extrapolation in the direction of C = 1. Its absolute accuracy is not great and it is only meant to indicate what a considerable improvement

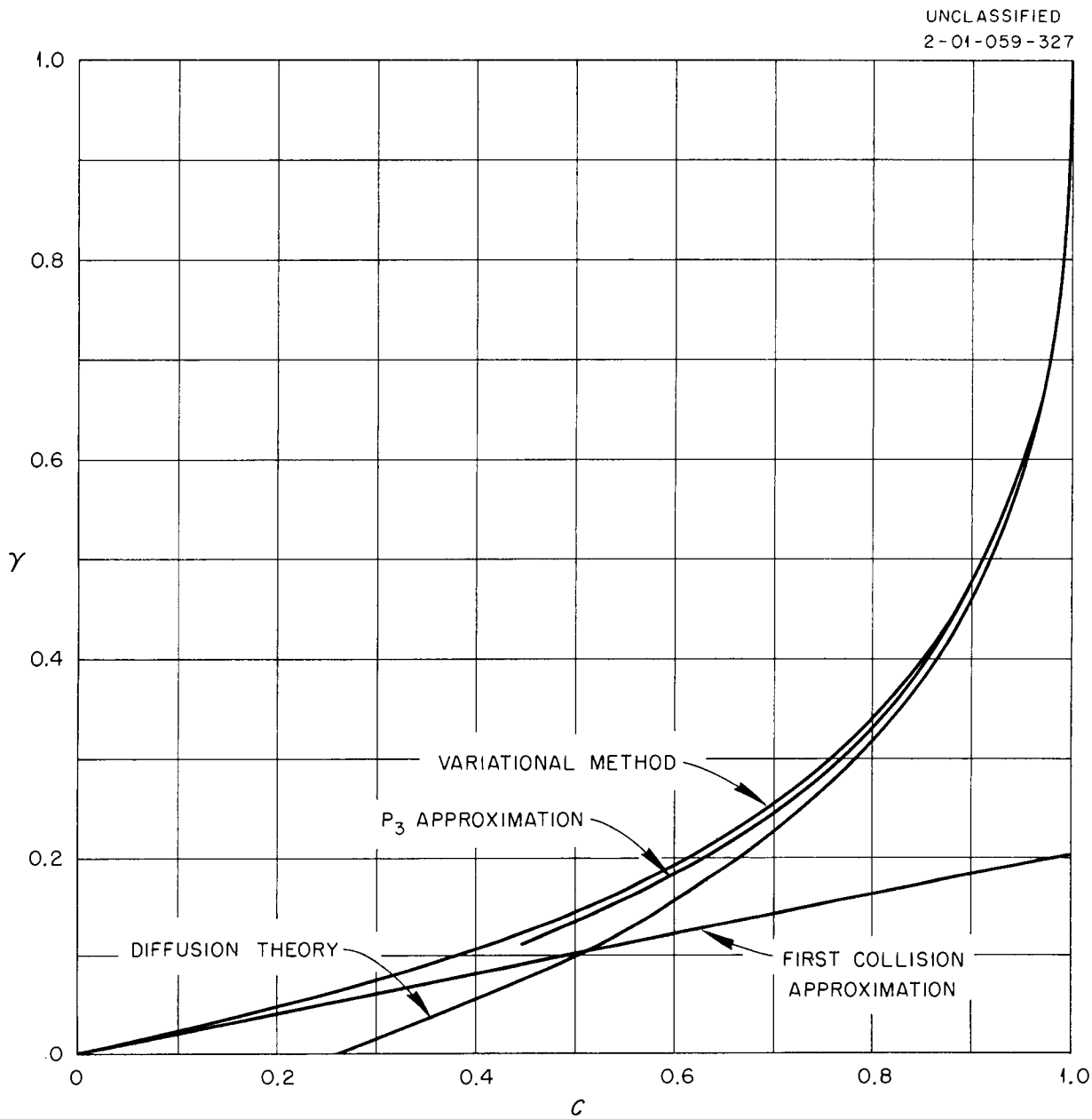


Fig. 2-7. Albedo of a Half Space with a Plane Boundary to a Uniform Isotropic Source Outside the Boundary.

one can make passing from diffusion theory to the P_3 approximation.

Table (3-7) shows a comparison between the complementary albedo, $1 - \delta$, derived from Eq. (3-7), and that calculated from the variational method with a diffusion theory trial function. The error in Eq. (3-7) in the limit $\bar{\ell} \longrightarrow \infty$ is less than about 1% for all C.

14. Let us now consider small $\bar{\ell}$. Let us first note that the variational expression (27-7) is exact in the limits C = 0 or C = 1. In the limit C = 1, Eq. (3-7) is also exact. In the limit C = 0, Eq. (27-7) gives $\bar{\ell}$ P for the complementary albedo, and Eq. (3-7) gives the same thing except that P is replaced by Wigner's rational approximation [cf Eq. (4-7) noting that for comparison with Eq. (27-7) the unit of length must be chosen as the total mean free path.] Thus for C = 1, Eq. (3-7) is exact, and for C = 0 it is an underestimate, the amount being given in Fig. (2-6). Given in Table (4-7) are values of $1 - \delta$ calculated from Eq. (27-7) and Eq. (3-7) for

Table (3-7). Error in Eq. (3-7) When $\bar{\ell} \rightarrow \infty$

C	$1 - \delta$ Approximate	$1 - \delta$ Exact	% Error
0	1.0000	1.0000	0%
0.1	0.9771	0.9770*	0%
0.2	0.9514	0.9525*	- 0.11%
0.3	0.9221	0.9259	- 0.41%
0.4	0.8881	0.8931	- 0.57%
0.5	0.8479	0.8539	- 0.70%
0.6	0.7990	0.8058	- 0.85%
0.7	0.7366	0.7440	- 1.00%
0.8	0.6513	0.6587	- 1.13%
0.9	0.5165	0.5183	- 0.34%
1.0	0.0000	0.0000	0%

*Graphical estimate.

for cylinders with $\bar{\ell}$ = 1, 2 for all C. The error in these two examples is always about the same as it is when C = 0, except when 1 - C is quite small.

Table (4-7). Error in Eq. (3-7) When $\bar{\ell}$ = 1,2

	$\bar{\ell}$ = 1			$\bar{\ell}$ = 2		
C	Eq. (27-7)	Eq. (3-7)	% Error	Eq. (27-7)	Eq. (3-7)	% Error
1.0	0	0	0%	0	0	0%
0.8	0.1761	0.1530	-15%	0.3098	0.2478	-25%
0.6	0.3147	0.2665	-18%	0.5055	0.3998	-26%
0.4	0.4265	0.3579	-19%	0.6405	0.5104	-25%
0.2	0.5187	0.4346	-19%	0.7390	0.5966	-24%
0.0	0.5960	0.5000	-19%	0.8143	0.6667	-22%

Since Eq. (3-7) is nearly correct in the line center, where much of the resonance absorption takes place, the error in I will not be as large as the error in 1 - δ. It is possible to calculate this error exactly in the case C = 0 (pure absorption), since in this case we must compare the integral

$$I = \frac{1}{N\bar{\ell}}\int \Sigma_a \bar{\ell} \cdot P \, du = \int \sigma_a P \, du \qquad (56\text{-}7)$$

with the corresponding one when P is replaced by the rational approximation. But integral (56-7) is the same as integral (11-6) when we set $\sigma_s = \sigma_p = 0$. According to Table (1-6) the approximate value of the integral is 10.6% lower than the exact value. Finally, it should be remarked that the error induced by the use of Eq. (3-7) is largest when C = 0, for the wings give the largest

relative contribution for a purely absorbing line. The reason for this is as follows: When $\Sigma_t \bar{\ell} << 1$, the flux in the lump is nearly flat. If we keep Σ_t constant but increase the proportion of scattering, the flux will be flattened by the increased diffusion but the relative change cannot be much. In the center of the line where $\Sigma_t \bar{\ell} >> 1$ the flux falls very steeply and an increase in the proportion of scattering will cause the greatest relative change there.

15. The last thing we will consider in this chapter is absorption in lumps composed of a chemical compound or mixture of a resonance absorber which alone may be treated in the infinite-mass-absorber approximation, and a non-resonant moderating material. E.g., let us consider absorption by a lump of UO_2 embedded in a block of graphite in a resonance which in pure U metal may be correctly treated in the infinite-mass-absorber approximation. Let us furthermore assume that the resonance is narrow in the sense of Chapter 6 with respect to collisions in the graphite or oxygen. It is difficult to solve this problem directly, but we can get some information by the arguments given below. Let us denote the macroscopic cross section of the oxygen by Σ_m and define $\sigma_m = \Sigma_m/N_a$. Let us divide the neutrons which make collisions in the lump in the vicinity of the resonance energy according to whether their last moderating collision was in the graphite or the oxygen. First, consider neutrons which made their last moderating collision in the graphite, and let their contribution to the integrated effective cross section (effective resonance integral) by I_1. Then

$$I_1' \geq I_1 \geq I_1''$$

where I_1' is calculated assuming the oxygen does not moderate, and I_1'' is calculated

by counting only absorptions on the first resonance energy collision. Now consider neutrons which have made their last moderating collision in the oxygen; let their contribution to the effective resonance integral be I_2. Then

$$I_2' \geq I_2 \geq I_2'' \tag{58-7}$$

where I_2' is calculated assuming no leakage from the lump and I_2'' is calculated

counting only absorptions on the first resonance energy collision.

The sum $I_1'' + I_2''$ can easily be calculated by the methods of Chapter 6, e.g., the analogue of Eq. (5-6) is

$$N_a(I_1'' + I_2'') = \int \Sigma_m \left[1 - P(\Sigma_t)\right] \frac{\Sigma_a}{\Sigma_t} du + \int \Sigma_a P(\Sigma_t) du \qquad (59\text{-}7)$$

The total cross section Σ_t includes the moderator cross section Σ_m, as well as the absorber resonance absorption, resonance scattering, and potential scattering cross sections. If we employ the rational approximation for the escape probability, Eq. (59-7) can be written

$$I_1'' + I_2'' = \frac{b - 1 + \frac{\sigma_m}{\sigma_p}}{b} \cdot \int \frac{\sigma_a(b\sigma_p)}{\sigma_a + \sigma_s + (b\sigma_p)} du \qquad (60\text{-}7)$$

where $b = 1 + (\Sigma_p \bar{\ell})^{-1}$ and σ_p is the sum of the moderator cross section and the potential scattering cross section of the absorber, i.e., $\sigma_{pa} + \sigma_m$. The integral in Eq. (60-7) is identical with that of Eq. (7-6), and the results of Chapters 6 and 4 apply <u>mutatis mutandis</u>.

I_2' can also be calculated as in Chapter 6, for by hypothesis the only way neutrons can leave the resonance is by absorption or moderation by σ_m. Thus

$$N_a I_2' = \int \Sigma_m \cdot \frac{\Sigma_a}{\Sigma_a + \Sigma_m} du \qquad (61\text{-}7)$$

or

$$I_2' = \int \frac{\sigma_m \sigma_a}{\sigma_a + \sigma_m} du \qquad (62\text{-}7)$$

I_2' has exactly the same form as Eq. (11-4) with $\gamma = 0$ and $\sigma_p = \sigma_m \frac{\Gamma}{\Gamma_\gamma}$. Hence again the results of Chapter 4 apply <u>mutatis mutandis</u>.

I_1' is precisely the quantity considered in this chapter, except that we must generalize σ_p to $\sigma_{pa} + \sigma_m$ instead of σ_{pa} as was its meaning in the first part of this chapter. γ is again defined as in Eq. (10-4).

As a practical illustration of these inequalities let us consider the case of a purely absorbing resonance, i.e., $\frac{\Gamma_n}{\Gamma} << 1$ and $\gamma = 0$. Then $I = I_1 + I_2$ obeys the inequality

$$\sigma_p \frac{\Gamma}{E_o} (b - 1) J\left[\xi, \beta(b - 1)\right] + \sigma_m \frac{\Gamma}{E_o} J(\xi, \beta \frac{\sigma_m}{\sigma_p}) \geq I$$

$$\geq \left[b - 1 + \frac{\sigma_m}{\sigma_p}\right] \sigma_p \frac{\Gamma}{E_o} J(\xi, \beta b) \tag{58-7}$$

In case $J(\xi, \beta) \sim J(\infty, \beta)$ this equation can be written

$$\sqrt{b - 1} + \left(\frac{\sigma_m}{\sigma_p}\right)^{1/2} \geq I\left(\frac{\pi}{2} \sigma_p \frac{\Gamma}{E_o} \beta^{-1/2}\right)^{-1} \geq \frac{b - 1 + \left(\frac{\sigma_m}{\sigma_p}\right)}{\sqrt{b}} \tag{59-7}$$

For sufficiently large b both sides of Eq. (59-7) are asymptotic to $\sqrt{b}$.

CHAPTER 8. THE STATISTICAL ESTIMATION OF RESONANCE ABSORPTION

1. In paragraph (16-1) the problem of resonance absorption was divided into three parts. The first part, dealing with resonance absorption in resolved s-wave resonances, was treated in Chapters 3, 4, 5, 6, and 7. The second part, which will be dealt with in this chapter, is concerned with estimating resonance absorption in the unresolved, but nonoverlapping, s-wave resonances. The first problem we shall consider along these lines is the case of infinite dilution in homogeneous media ($\sigma_p \longrightarrow \infty$), or equivalently the case of heterogeneous absorption in very small lumps ($b \longrightarrow \infty$), e.g., thin foils. In both these cases the effective resonance integral of a single resonance is given by the formula

$$I = \frac{\pi}{2} \sigma_o \frac{\Gamma_\gamma}{E_o} \tag{1-8}$$

The contribution to the total resonance integral, I^*, from all the resonances of the same spin and parity in a small energy interval ΔE about E_o is then

$$\Delta I^* = \frac{\pi}{2E_o} \left\langle \sigma_o \Gamma_\gamma \right\rangle \frac{\Delta E}{D_J} \tag{2-8}$$

where D_J is the average spacing of levels of the given spin and parity. The braces denote an average to be taken with respect to the statistical distribution of the reaction widths. The total contribution to the resonance integral from resonances above some cutoff energy E^* is then

$$I^* = \frac{\pi}{2D_J} \int_{E^*}^{\infty} \left\langle \sigma_o \Gamma_\gamma \right\rangle \frac{dE}{E} \tag{3-8}$$

It has been assumed that in the energy range of significant absorption no change in D_J need be considered. The important energy range usually does not extend beyond several tens of kilovolts, so that this assumption is justified. We can write Eq. (3-8) in a somewhat more explicit form by using Eq. (5a-4) for σ_o, and using a chi-squared distribution for the distribution of reduced neutron widths, and choosing Γ_γ constant for all resonances. For the sake of convenience in this rewriting let us define a new quantity, Γ_n^o, also conventionally called the reduced neutron width, and defined by $\Gamma_n^o = \Gamma_n E_o^{-1/2}$. By reference to Eq. (17-2) for s-waves we can see that Γ_n^o is proportional to γ^2 with an energy independent factor of proportionality. Γ_n^o is anticipated to be energy independent and to be distributed in a chi-squared distribution of one degree of freedom, viz.:

$$P(\Gamma_n^o)d\Gamma_n^o = \left(\frac{2\pi\Gamma_n^o}{\langle\Gamma_n^o\rangle}\right)^{-1/2} \exp\left(-\frac{\Gamma_n^o}{2\langle\Gamma_n^o\rangle}\right)\frac{d\Gamma_n^o}{\langle\Gamma_n^o\rangle} \tag{4-8}$$

With these preliminaries Eq. (3-8) can be rewritten as

$$I^* = \frac{\pi}{2}\sigma_o^*\frac{\Gamma_\gamma}{D_J}\int_{E^*}^{\infty}\frac{dE}{E}\cdot\frac{E^*}{E}\int_0^{\infty}P(\Gamma_n^o)d\Gamma_n^o\,\frac{\sqrt{\frac{E}{E^*}}}{\sqrt{\frac{E}{E^*}}+\frac{\Gamma_\gamma}{\sqrt{E^*}\,\langle\Gamma_n^o\rangle}\cdot\frac{\langle\Gamma_n^o\rangle}{\Gamma_n^o}} \tag{5-8}$$

If we employ the variables of integration $y^2 = \frac{E}{E^*}$ and $w = \frac{\Gamma_n^o}{\langle\Gamma_n^o\rangle}$, and define the parameter $B = \frac{\Gamma_\gamma}{\langle\Gamma_n^o\rangle\sqrt{E^*}}$ we can interchange the Γ_n^o and E integrations and write

$$I^* = \frac{\pi}{2}\,\sigma_o^*\,\frac{\Gamma_\gamma}{D_J}\int_0^\infty P(w)dw \int_1^\infty 2\,\frac{dy}{y^2\left(y + \frac{B}{w}\right)} \tag{6-8}$$

where

$$P(w)dw = (2\pi w)^{-1/2}\, e^{-w/2}\, dw \tag{7-8}$$

The y-integration can be carried out using the partial fractions expansion

$$\frac{1}{y^2\left(y + \frac{B}{w}\right)} = \frac{w}{B}\left[\frac{1}{y^2} - \frac{w^2}{B^2 y} + \frac{w^2}{B^2\left(y + \frac{B}{w}\right)}\right] \tag{8-8}$$

The result is

$$I^* = \pi\,\sigma_o^*\,\frac{\Gamma_\gamma}{D_J}\int_0^\infty P(w)dw \cdot \frac{\frac{B}{w} - \ln\left(1 + \frac{B}{w}\right)}{\left(\frac{B}{w}\right)^2} \tag{9-8}$$

2. The evaluation of the integral in Eq. (9-8) is relatively difficult and a rough result can be obtained by choosing a delta function distribution around w = 1 (the mean of distribution 7-8). This procedure gives immediately

$$I^* = \pi\,\sigma_o^*\,\frac{\Gamma_\gamma}{D_J} \cdot \frac{B - \ln(1 + B)}{B^2} \tag{10-8}$$

This result was previously obtained by the author (D55a) and used by him as the basis of a rough systematics of resonance integrals. The value of the integral I in Eq. (9-8) was calculated by Kuhn and Dresner (K58); it is their method we now describe.

3. If B >> 1 we can obtain an asymptotic expansion for the integral in Eq. (9-8). First we can rewrite

$$I' = \int_0^\infty \frac{\frac{B}{w} - \ln\left(1 + \frac{B}{w}\right)}{\left(\frac{B}{w}\right)^2} \cdot (2\pi w)^{-1/2} e^{-w/2} dw$$

$$= (2\pi)^{-1/2} B^{-1} \int_0^\infty e^{-w/2} w^{1/2} dw - (2\pi)^{-1/2} B^{-2} \ln\left(\frac{B}{2}\right) \int_0^\infty e^{-w/2} w^{3/2} dw$$

$$+ (2\pi)^{-1/2} B^{-2} \int_0^\infty w^{3/2} e^{-w/2} \ln\left(\frac{w}{2}\right)$$

$$- (2\pi)^{-1/2} B^{-2} \int_0^\infty w^{3/2} e^{-w/2} \ln\left(1 + \frac{w}{B}\right) dw \qquad (11\text{-}8)$$

It can easily be shown that

$$\int_0^\infty w^{1/2} e^{-w/2} dw = 2\sqrt{2}\,\Gamma\left(\frac{3}{2}\right) = (2\pi)^{1/2} \qquad (12a\text{-}8)$$

$$\int_0^\infty w^{3/2} e^{-w/2} dw = 4\sqrt{2}\,\Gamma\left(\frac{5}{2}\right) = 3(2\pi)^{1/2} \qquad (12b\text{-}8)$$

$$\int_0^\infty w^{3/2} e^{-w/2} \ln\left(\frac{w}{2}\right) dw = 4\sqrt{2}\,\Gamma'\left(\frac{5}{2}\right) = (2\pi)^{1/2} (8 - 3C + 6\ln 2) \qquad (12c\text{-}8)$$

Here Γ is the gamma function, C is the Euler-Mascheroni constant (= 0.577 216 ...), and the prime denotes differentiation of the gamma function. Using Eq. (12-8) the first three terms in Eq. (11-8) may be evaluated. To evaluate the last term we proceed as follows:

Maclaurin's series for any function can be written

$$f(x) = \sum_{k=o}^{u} f^{(k)}(0)\,\frac{x^k}{k!} + f^{(u+1)}(\theta x)\,\frac{x^{u+1}}{(u+1)!} \qquad (13\text{-}8)$$

If for f(x) it happens that $\left|f^{(k)}(x)\right| \leq \left|f^{(k)}(0)\right|$ and that $f^{(k)}(x)$ is of one sign for all x, then the error in using only the first n terms of Eq. (13-8) is less than the term neglected in magnitude, and of the same sign. For $f(x) = \ln\left(1 + \frac{x}{B}\right)$, $f^{(k)}(x) = (-)^{k+1}(k-1)!(x+B)^{-k}$, which does fulfill the stated conditions. Hence

$$\int_0^\infty w^{3/2}\, e^{-w/2}\, \ln\left(1 + \frac{w}{B}\right) dw = \int_0^\infty w^{3/2}\, e^{-w/2} \sum_{k=1}^{u} (-)^{k+1} \frac{w^k}{kB^k}\, dw \qquad (14a\text{-}8)$$

$$= \sum_{k=1}^{u} 4\sqrt{2} \cdot (-)^{k+1} \cdot \frac{\Gamma\left(k + \frac{5}{2}\right)}{k\left(\frac{B}{2}\right)^k} \qquad (14b\text{-}8)$$

$$= (2\pi)^{1/2} \sum_{k=1}^{u} (-)^{k+1} \frac{(2k+3)!!}{kB^k} \qquad (14c\text{-}8)$$

where the double factorial is derived by $x! = x(x-2)(x-4)\ldots 2$ or 1, and the error is less than the (u + 1) term of the series (i.e., the first term neglected). The series (14c-8) is asymptotic, since for any value of B it is clear that the terms first decrease but ultimately begin to increase. Combining all these results we obtain for the integral in Eq. (9-8) the asymptotic series

$$I' = \frac{1}{B} + \frac{8 - 3(\ln B + C + \ln 2)}{B^2} + \sum_{k=1}^{u} (-)^k \frac{(2k+3)!!}{k\,B^{k+2}} \qquad (15\text{-}8)$$

4. If $B << 1$ a power series for I' in powers of $\sqrt{B}$ can be derived as follows:

First let us rewrite I' using the variable ω defined by $\omega^2 = \frac{W}{B}$. Then

$$I' = \left(\frac{2B}{\pi}\right)^{1/2} \int_0^\infty \left\{\omega^2 - \omega^4 \ln\left(\frac{1+\omega^2}{\omega^2}\right)\right\} e^{-\frac{B}{2}\omega^2} d\omega \qquad (16\text{-}8)$$

The limiting value of the quantity in the curly braces as $\omega \to \infty$ is $\frac{1}{2}$, so it, by itself, is not integrable. If we add and subtract $\frac{1}{2}$ to it we can then write I' as

$$I' = \left(\frac{2B}{\pi}\right)^{1/2} \int_0^\infty \frac{1}{2} e^{-\frac{B}{2}\omega^2} d\omega$$

$$- \left(\frac{2B}{\pi}\right)^{1/2} \int_0^\infty \left\{\frac{1}{2} - \omega^2 + \omega^4 \ln\left(\frac{1+\ \ 2}{\omega^2}\right)\right\} e^{-\frac{B}{2}\omega^2} d\omega \qquad (17\text{-}8)$$

The quantity in the curly braces, $\psi_0(\omega)$, now vanishes like ω^{-2} as $\omega \to \infty$ and is integrable. Hence we can integrate the second term in Eq. (17-8) by parts. It can readily be verified by

$$\int \psi_0(\omega) d\omega = \int \left\{\frac{1}{2} - \omega^2 + \omega^4 \ln\left(\frac{1+\omega^2}{\omega^2}\right)\right\} d\omega$$

$$= \frac{\omega^5}{5} \ln\left(\frac{1+\omega^2}{\omega^2}\right) - \frac{\omega^3}{5} + \frac{\omega}{10} + \frac{2}{5} \arctan \omega \qquad (18\text{-}8)$$

Now using the formula of partial integration in the form

$$\int_0^\infty \gamma_o(\omega) e^{-\frac{B}{2}\omega^2} d\omega = -\int_0^\infty d\left(\int_\omega^\infty \gamma_o(v)dv\right) e^{-\frac{B}{2}\omega^2} \tag{19a-8}$$

$$= \int_0^\infty \gamma_o(\omega)d\omega - B\int_0^\infty \omega e^{-\frac{B}{2}\omega^2} d\omega \int_\omega^\infty \gamma_o(v)dv \tag{19b-8}$$

we can write for I' the result:

$$I' = \frac{1}{2} - \frac{(2\pi)^{\frac{1}{2}}}{5} B^{\frac{1}{2}} + \left(\frac{2}{\pi}\right)^{\frac{1}{2}} B^{\frac{3}{2}} \int_0^\infty d\omega . \omega . e^{-\frac{B}{2}\omega^2}$$

$$\left\{\frac{\pi}{5} - \frac{\omega^5}{5} \ln\left(\frac{1+\omega^2}{\omega^2}\right) + \frac{\omega^3}{5} - \frac{\omega}{10} - \frac{2}{5}\arctan\omega\right\} \tag{20-8}$$

This procedure can be repeated by adding and subtracting $\frac{1}{3}$ to the curly bracket in the last integral. The details are tedious and similar to those presented. The result is

$$I' = \frac{1}{2} - \frac{(2\pi)^{\frac{1}{2}}}{5} B^{\frac{1}{2}} + \frac{1}{3} B - \frac{(2\pi)^{\frac{1}{2}}}{14} B^{\frac{3}{2}} + \ldots \tag{21-8}$$

It is of interest to note that the integrated term in Eq. (19b-8), $\int_0^\infty \gamma_o(\omega)d\omega$, is just what one would obtain by setting B = 0 in the integral in Eq. (17-8). It is clearly an overestimate in magnitude. Hence, the error in using Eq. (21-8) is less than the first <u>even order</u> term neglected. In both Eq. (21-8) and Eq. (15-8) one can improve the magnitude of the

error by at least a factor of two, and often by much more by adding half the first term ordinarily neglected. This procedure has the disadvantage of rendering the sign of the error unknown.

Using Eq. (21-8), Eq. (15-8), and three numerical integrations of Eq. (16-8) near B = 1, the curve of Fig. (1-8) was calculated for the ratio of Eq. (9-8) to Eq. (10-8). As one can see, the correction to Eq. (10-8) introduced by the statistical fluctuations of the neutron width is never more than 30%, so that Eq. (10-8) is suitable for rough estimation.

5. The infinite dilution case is the only case in which the integration over energy and the average over the distribution of neutron widths can be carried out explicitly. In all other cases we shall indicate how to obtain results for the effective absorption cross section (corresponding to $E_o \frac{\Delta I^*}{\Delta E}$), and rely on a numerical integration to obtain the effective resonance integral (corresponding to I*). Our main problem in calculating these cross sections will be averaging the function $J(\xi,\beta)$ over the distribution of neutron widths.

In finding the average of a function f(x,y), a very useful approximate formula is

$$\langle f(x,y)\rangle = f(\langle x\rangle, \langle y\rangle) + \frac{1}{2}\,\mathrm{var}(x)\left(\frac{\partial^2 f}{\partial x^2}\right)_{\langle x\rangle,\ \langle y\rangle} + \frac{1}{2}\,\mathrm{var}(y)\left(\frac{\partial^2 f}{\partial y^2}\right)_{\langle x\rangle,\ \langle y\rangle} \tag{22-8}$$

This formula can be derived by expanding of f(x,y) in a Taylor's series around $\langle x\rangle$, $\langle y\rangle$, and dropping all but the first two nonvanishing

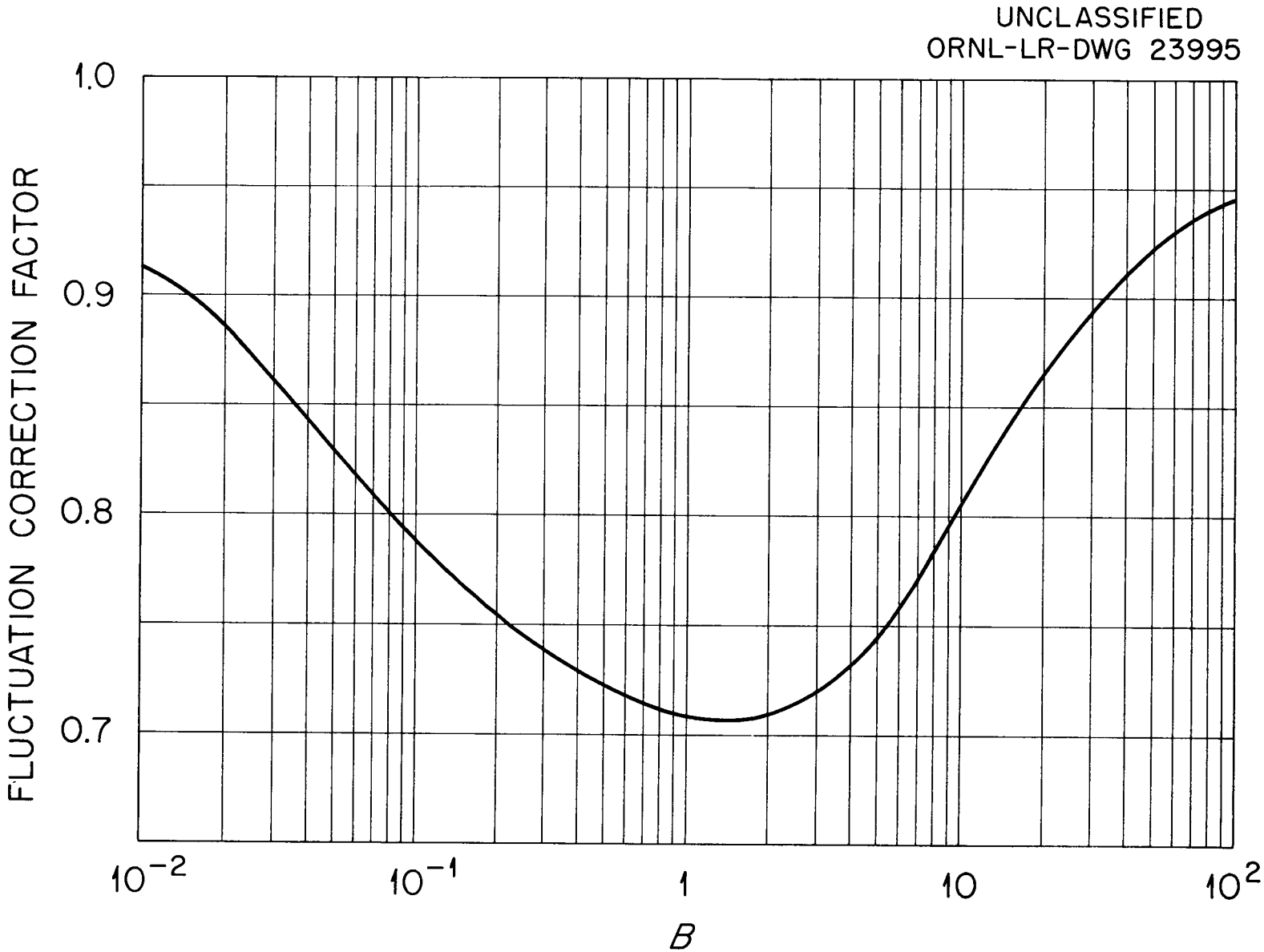


Fig. 1-8. Reduction in the Resonance Integral Due to Fluctuations in the Neutron Width for Infinite Dilution.

terms. In calculating $\left\langle J(\xi,\beta)\right\rangle$ we shall use Eq. (22-8); however, we shall not use the obvious variables ξ and β, but rather the variables ξ^{-1} and $\beta^{-1/2}$. As we shall see immediately below, $J(\xi,\beta)$ varies roughly linearly with these variables over considerable ranges and this will tend to make the second derivatives in Eq. (22-8) small. Then the series of which Eq. (22-8) is the first two terms will converge rapidly.

If $\xi << 1$, $\psi(\xi,0) >> \beta >> \frac{1}{6}\xi^2$, and $\frac{\xi\sqrt{\pi}}{2\beta} >> 1$, $J(\xi,\beta)$ is given approximately by Eq. (55-4) which, excepting the very slowly varying square root term, indicates a ξ^{-1} dependence on ξ. On the other hand, if any of the inequalities above has its sense reversed in the ξ-dependence of J disappears, and again the curvature of J in the variable ξ^{-1} disappears. In the transition region between these behaviors there is some curvature of J in the variable ξ^{-1} but it is small if $\xi << 1$ as we shall presently see.

Let us now consider the β-dependence of J. If $\xi << 1$, $\psi(\xi,0) >> 6\beta >> \xi^2$, and $\frac{\xi\sqrt{\pi}}{2\beta} >> 1$, J is again given by Eq. (55-4). On a log J-log β plot, such as is given by Figs. (1-4) and (2-4), this equation gives the slope of log J as $-\frac{1}{2}\left[\ln \frac{\xi\sqrt{\pi}}{2\beta}\right]^{-1}$. Hence, if $\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)$ is not too large the slope will be near $-\frac{1}{2}$. For example, if $\frac{\xi\sqrt{\pi}}{2\beta} \sim 7$, the slope is $\sim -\frac{1}{4}$. The curve $\beta^{-1/4}$ when plotted vs $\beta^{-1/2}$ <u>for $\beta << 1$</u>, looks like $\sqrt{x}$ plotted vs x for $x >> 1$. The latter function varies linearly with x over quite large ranges of x for large x. A scrutiny of the log J-log β plot for small β substantiates these considerations by revealing a strong similarity in shape between $J(0.1,\beta)$, for example, and $J(\infty,\beta)$, which latter function is proportional to $\frac{1}{\sqrt{\beta}}$ in this range. Furthermore, from Table (1-4)

it is possible to find linear relations between $J(0.1,\beta)$ and $J(\infty,\beta)$, which hold quite accurately over considerable ranges of β. One such example is given below. The slope and value are correct at the point k = 10, and have been obtained from Table (1-4). Such linear laws imply a linear relation between J and $\frac{1}{\sqrt{\beta}}$ over quite large ranges of β.

	$k = \ln_2(10^5\ \beta)$	8	9	10	11	12
	$J(0.1,\beta)$	46.47	37.81	30.45	23.67	17.30
1.301	$J(\infty,\beta) + 9.907$	50.51	38.75	30.45	24.59	20.41

In the foregoing discussion we have added another condition, viz., $\beta << 1$. This condition implies high, narrow resonances and is always fulfilled in the situations where this analysis is intended to apply.

If either $\xi >> 1$ <u>or</u> $6\beta << \xi^2$ J takes the value appropriate to the natural line shape, and if $\beta << 1$ is proportional to $\frac{1}{\sqrt{\beta}}$. Finally, if $\xi << 1$, $6\beta >> \xi^2$, and $\frac{\xi\sqrt{\pi}}{2\beta} << 1$, the β-dependence of J is proportional to $\frac{1}{\beta}$; however, in the cases where this occurs the corresponding term in Eq. (22-8) will be small. Consequently, the use of the variable $\frac{1}{\sqrt{\beta}}$ is justified in all cases.

6. Equation (22-8) can now be written in the form

$$\langle J(\xi,\beta)\rangle = J(\xi^*,\beta^*) + \frac{1}{2}\left(\left\langle\frac{\xi_o^2}{\xi^2}\right\rangle\Big/\left\langle\frac{\xi_o}{\xi}\right\rangle^2 - 1\right)\left(\frac{1}{\xi^2}\ \frac{\partial^2 J}{\partial(\xi^{-1})^2}\right)_{\xi^*,\beta^*}$$
$$+ \frac{1}{2}\left(\left\langle\frac{\beta_o}{\beta}\right\rangle\Big/\left\langle\sqrt{\frac{\beta_o}{\beta}}\right\rangle^2 - 1\right)\left(\frac{1}{\beta}\ \frac{\partial^2 J}{\partial(\beta^{-1/2})^2}\right)_{\xi^*,\beta^*} \qquad (23\text{-}8)$$

where $\xi_o = \xi(\langle \Gamma_n^o \rangle)$, $\beta_o = \beta(\langle \Gamma_n^o \rangle)$, $(\xi^*)^{-1} = \langle \xi^{-1} \rangle$, and $(\beta^*)^{-1/2} = \langle \beta^{-1/2} \rangle$. It will now be shown that:

$$\left\langle \frac{\xi_o}{\xi} \right\rangle = (1 + B) \sqrt{\frac{\pi}{2B}}\, e^{B/2}\, \mathrm{Erfc}\left(\sqrt{\frac{B}{2}}\right) \tag{24a-8}$$

$$\left\langle \frac{\xi_o^2}{\xi^2} \right\rangle = \frac{(1 + B)^2}{2B} \sqrt{\frac{\pi}{2B}}\, e^{B/2} \left[(1 - B)\mathrm{Erfc}\left(\sqrt{\frac{B}{2}}\right) + \sqrt{\frac{2B}{\pi}}\, e^{-B/2} \right] \tag{24b-8}$$

$$\left\langle \sqrt{\frac{\beta_o}{\beta}} \right\rangle = \sqrt{1 + B}\; e^{B/2}\, \mathrm{Erfc}\left(\sqrt{\frac{B}{2}}\right) \tag{24c-8}$$

$$\left\langle \frac{\beta_o}{\beta} \right\rangle = (1 + B) \left[1 - \frac{\pi}{2} \sqrt{\frac{2B}{\pi}}\, e^{B/2}\, \mathrm{Erfc}\left(\sqrt{\frac{B}{2}}\right) \right] \tag{24d-8}$$

<u>Case (i) Eq. (24a-8)</u>

$$\xi = \frac{\Gamma}{\Delta} = \frac{\langle \Gamma_n^o \rangle \sqrt{E}\; w + \Gamma_\gamma}{\Delta} = \frac{\langle \Gamma_n^o \rangle \sqrt{E} + \Gamma_\gamma}{\Delta} \cdot \frac{\langle \Gamma_n^o \rangle \sqrt{E}\; w + \Gamma_\gamma}{\langle \Gamma_n^o \rangle \sqrt{E} + \Gamma_\gamma} = \xi_o \cdot \frac{w + B}{1 + B} \tag{25-8}$$

Hence:

$$\left\langle \frac{\xi_o}{\xi} \right\rangle = \int_0^\infty (2\pi w)^{-1/2}\, e^{-w/2} \left(\frac{1 + B}{w + B}\right) dw \tag{26a-8}$$

$$= (1 + B) \sqrt{\frac{2}{\pi B}} \int_0^\infty \frac{e^{-B/2\, y^2}}{1 + y^2}\, dy \tag{26b-8}$$

The second line follows from the substitution $w = By^2$. The integral in Eq. (26b-8) is the same as the integral denoted by F(a) in connection with Eq. (14-6). It has been evaluated in Eq. (17-6); employing this equation and Eq. (26b-8) one readily obtains Eq. (24-8).

Case (ii) Eq. (24b-8)

Proceeding as before we have

$$\left\langle \frac{\xi_o^2}{\xi^2} \right\rangle = \int_o^\infty (2\pi w)^{-1/2} e^{-w/2} \left(\frac{1 + B}{w + B}\right)^2 dw \tag{27a-8}$$

$$= \frac{(1 + B)^2}{B} \cdot \sqrt{\frac{2}{\pi B}} \cdot \int_o^\infty \frac{e^{-B/2\, y^2}}{(1 + y^2)^2} \tag{27b-8}$$

If we denote by G(a) the integral

$$G(a) = \int_o^\infty \frac{e^{-a^2 z^2}}{(1 + z^2)^2} dz \tag{28-8}$$

we can immediately write

$$\frac{dG(a)}{d(a^2)} - G(a) = - F(a) = - \frac{\pi}{2} e^{a^2} \operatorname{Erfc}(a); \; G(0) = \frac{\pi}{4} \tag{29-8}$$

where F(a) is again given by Eq. (17-6) and defined in the text following Eq. (14-6). The solution to the system (29-8) is

$$G(a) = e^{a^2} \left[\frac{\pi}{4} - \frac{\pi}{2} \int_o^{a^2} \operatorname{Erfc}(\sqrt{x})\, dx \right] \tag{30-8}$$

The integral in Eq. (30-8) can be written in terms of tabulated functions as follows: First changing the order of integration we obtain:

$$\int_0^{a^2} \mathrm{Erfc}(\sqrt{x})\, dx = \int_0^{a^2} dx \frac{2}{\sqrt{\pi}} \int_{\sqrt{x}}^{\infty} e^{-y^2}\, dy \tag{31a-8}$$

$$= \frac{2}{\sqrt{\pi}} \int_0^{a} dy\, e^{-y^2} \int_0^{y^2} dx + \frac{2}{\sqrt{\pi}} \int_a^{\infty} dy\, e^{-y^2} \int_0^{a^2} dx \tag{31b-8}$$

$$= \frac{2}{\sqrt{\pi}} \int_0^{a} dy\, y^2 e^{-y^2} + a^2\, \mathrm{Erfc}(a) \tag{31c-8}$$

By partial integration we can show

$$\frac{2}{\sqrt{\pi}} \int_0^{a} y^2 e^{-y^2}\, dy = \frac{1}{2}\, \mathrm{Erf}(a) - \frac{1}{\sqrt{\pi}}\, a\, e^{-a^2} \tag{32-8}$$

Collecting the results of Eqs. (32-8), (31c-8), (30-8), (28-8), and (27b-8) yields Eq. (24b-8).

<u>Case (iii) Eq. (24c-8)</u>

By definition

$$\beta = \frac{\sigma_p}{4\pi\lambda\!\!\!^{-2}} \frac{\Gamma}{\Gamma_n} = \frac{\sigma_p}{4\pi\lambda\!\!\!^{-2}} \frac{\langle \Gamma_n^o \rangle \sqrt{E} + \Gamma_\gamma}{\langle \Gamma_n^o \rangle \sqrt{E}} \cdot \frac{\langle \Gamma_n^o \rangle \sqrt{E}\, w + \Gamma_\gamma}{w(\langle \Gamma_n^o \rangle \sqrt{E} + \Gamma_\gamma)} = \beta_o \cdot \frac{w + B}{w(1 + B)} \tag{33-8}$$

Hence:

$$\left\langle \sqrt{\frac{\beta_o}{\beta}} \right\rangle = \int_0^{\infty} (2\pi w)^{-1/2}\, e^{-w/2} \left[\frac{w(1 + B)}{w + B} \right]^{1/2} dw \tag{34-8}$$

Equation (24c-8) follows immediately from the substitution $w + B = 2y^2$.

Case (iv) Eq. (24d-8)

Proceeding as before we have

$$\left\langle \frac{\beta_o}{\beta} \right\rangle = \int_0^\infty (2\pi w)^{-1/2} e^{-w/2} \frac{w(1 + B)}{w + B} dw \tag{35a-8}$$

$$= 2(1 + B) \sqrt{\frac{B}{2\pi}} \int_0^\infty \frac{y^2 e^{-B/2 y^2}}{1 + y^2} dy \tag{35b-8}$$

if we set $By^2 = w$. But

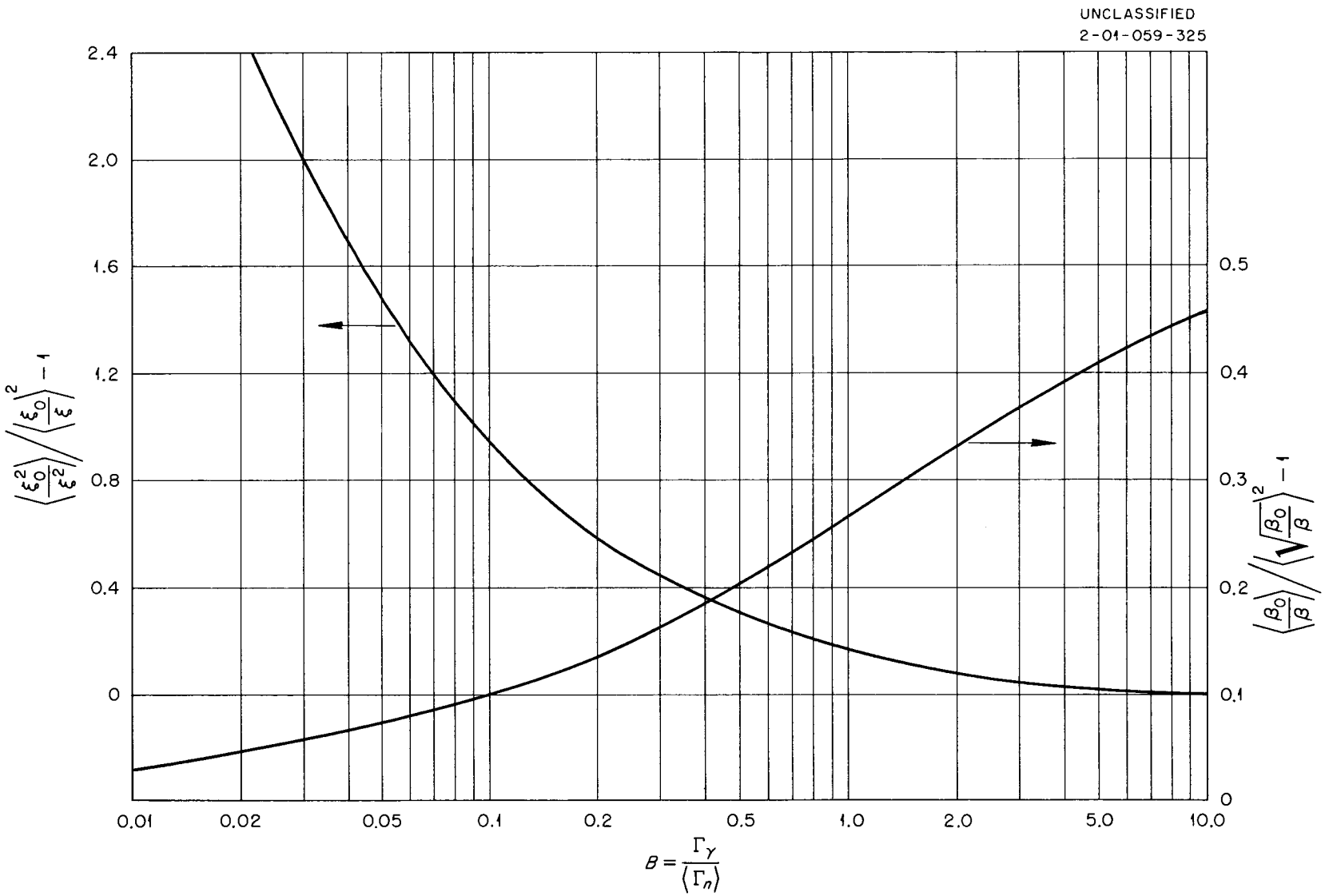
$$\int_0^\infty \frac{y^2 e^{-a^2y^2}}{1 + y^2} dy = \int_0^\infty e^{-a^2y^2} dy - F(a) \tag{36a-8}$$

$$= \frac{\sqrt{\pi}}{2a} - \frac{\pi}{2} e^{a^2} \operatorname{Erfc}(a) \tag{36b-8}$$

Combining Eqs. (36-8) and (35b-8) one obtains Eq. (24d-8).

Using Eqs. (24-8) the quantities $\left\langle \frac{\xi_o^2}{\xi^2} \right\rangle \Big/ \left\langle \frac{\xi_o}{\xi} \right\rangle^2 - 1$ and $\left\langle \frac{\beta_o}{\beta} \right\rangle \Big/ \left\langle \sqrt{\frac{\beta_o}{\beta}} \right\rangle^2 - 1$ have been calculated and are plotted in Fig. (2-8); the quantities $\left\langle \sqrt{\frac{\beta_o}{\beta}} \right\rangle$ and $\left\langle \frac{\xi_o}{\xi} \right\rangle$ are plotted in Fig. (3-8).

7. Next we turn our attention to the calculation of the second derivatives. We restrict ourselves to the case in which ξ is small and β is not very much less than $\frac{\xi^2}{6}$. This is the only case which will arise in practice. If $\frac{\xi\sqrt{\pi}}{2\beta} >> 1$, then differentiation of Eq. (55-4) immediately yields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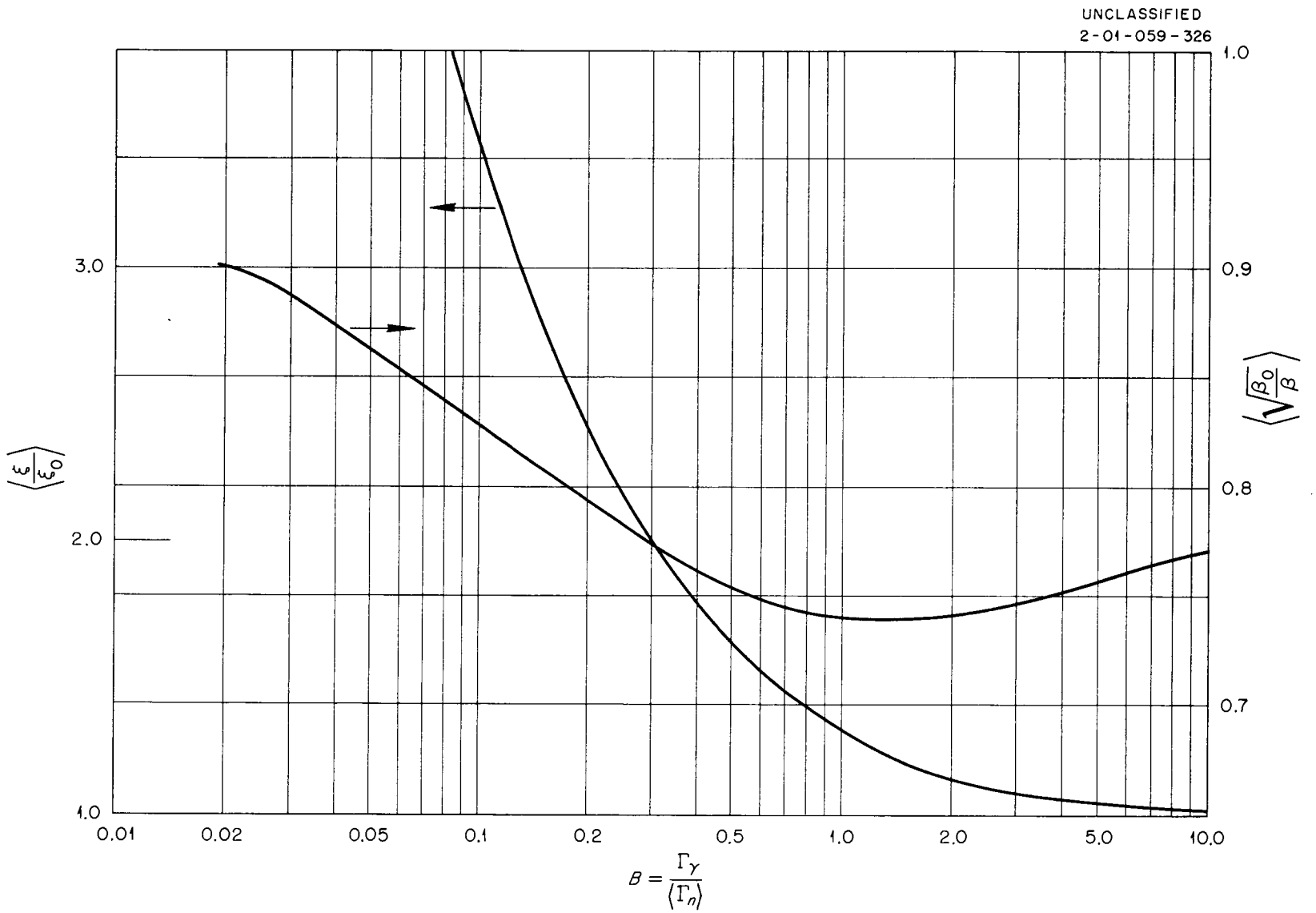
10.0
$\left\langle \frac{\xi_0^2}{\xi^2} \right\rangle \Big/ \left\langle \frac{\xi_0}{\xi} \right\rangle^2 - 1$
$\left\langle \frac{\beta_0}{\beta} \right\rangle \Big/ \left\langle \sqrt{\frac{\beta_0}{\beta}} \right\rangle^2 - 1$
$B = \frac{\Gamma_\gamma}{\langle \Gamma_n \rangle}$

Fig. 2-8.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5.0
10.0
$\left\langle \frac{\sigma_0}{\sigma} \right\rangle$
$\left\langle \sqrt{\frac{\beta_0}{\beta}} \right\rangle$
$B = \frac{\Gamma_\gamma}{\langle \Gamma_n \rangle}$

Fig. 3-8.

$$\frac{\partial^2 J}{\partial(\beta^{-1/2})^2} = -\sqrt{\pi}\,\frac{\ln\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)+1}{\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)\left[\ln\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)\right]^{3/2}} \tag{37a-8}$$

$$\frac{1}{\xi}\,\frac{\partial^2 J}{\partial(\xi^{-1})^2} = -\frac{\ln\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)+\frac{1}{2}}{\left[\ln\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)\right]^{3/2}} \tag{37b-8}$$

If, on the other hand $\frac{\xi\sqrt{\pi}}{2\beta} < 1$, one can differentiate the power series (56d-4) to obtain

$$\frac{\partial^2 J}{\partial(\beta^{-1/2})^2} = \pi \sum_{k=o}^{\infty} (-)^k \sqrt{k+1}\,(2k+1)\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)^k \tag{38a-8}$$

$$\frac{1}{\xi}\,\frac{\partial^2 J}{\partial(\xi^{-1})^2} = \sqrt{\pi}\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)\sum_{k=1}^{\infty} (-)^k\, k\sqrt{k+1}\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)^k \tag{38b-8}$$

It is again possible to extend the radius of convergence of these series by the analytic continuation technique described in connection with Eqs. (56d-4) in Eqs. (57-to 59-4). The B-coefficients for Eq. (38a-8) are

$$\begin{aligned} B_o &= 1 & B_4 &= 0.13725 \\ B_1 &= -\,4.24263 & B_5 &= 0.04750 \\ B_2 &= 4.41762 & B_6 &= 0.02228 \\ B_3 &= -\,0.92213 & B_7 &= -\,0.01218 \end{aligned} \tag{39a-8}$$

The B-coefficients for Eq. (38b-8) are

$$\begin{aligned} B_o &= 0 & B_4 &= -\,0.07763 \\ B_1 &= -\,1.41421 & B_5 &= -\,0.02814 \\ B_2 &= 2.04989 & B_6 &= -\,0.01366 \\ B_3 &= -\,0.48601 & B_7 &= -\,0.00770 \end{aligned} \tag{39b-8}$$

Using Eqs. (37-, 38- and 39-8) the second derivatives have been plotted in Figs. (4-8) and (5-8). The left hand side of the solid curve was obtained with the power series, and the right hand side of the solid curve with Eqs. (37-8). A graphical interpolation (dashed curve) was then performed between them. Since Eq. (37-8) is not accurate unless $\frac{\xi\sqrt{\pi}}{2\beta} >> 1$ the lack of agreement of the dashed and full curves for $4 \leq \frac{\xi\sqrt{\pi}}{2\beta} \leq 10$ is understandable.

8. In the case $\frac{\xi\sqrt{\pi}}{2\beta} << 1$ above it is possible to use Eq. (70-4) for $J(\xi,\beta)$. It follows then from Eqs. (25-8), (33-8), and (7-8) that

$$\left\langle J(\xi,\beta)\right\rangle = \int_0^\infty (2\pi w)^{-\frac{1}{2}} e^{-\frac{w}{2}} \cdot \frac{\pi}{2\beta_o \cdot \frac{w+B}{w(1+B)} + \sqrt{\frac{\pi}{2}} \cdot \xi_o \frac{w+B}{1+B}} dw \qquad (40a\text{-}8)$$

$$= \frac{\pi}{2\beta_o}\,\theta(1+B) \int_0^\infty (2\pi w)^{-\frac{1}{2}} e^{-\frac{w}{2}} \frac{w}{(w+B)(w+\theta)} dw \qquad (40b\text{-}8)$$

where $\theta^{-1} = \frac{1}{\sqrt{2}} \cdot \frac{\xi_o\sqrt{\pi}}{2\beta_o}$. Using a partial fraction expansion of the integrand, we can write at once

$$\left\langle J(\xi,\beta)\right\rangle = \frac{\pi}{2\beta_o} \cdot \frac{\theta(1+\epsilon)}{\theta - B} \cdot \int_0^\infty (2\pi w)^{\frac{1}{2}} e^{-\frac{w}{2}} w \left[\frac{1}{w+B} - \frac{1}{w+\theta}\right] dw \qquad (41\text{-}8)$$

But these integrals are the same as those of case (iv) of paragraph (6-8). Hence, from these results we immediately obtain

$$\left\langle J(\xi,\beta)\right\rangle = \frac{\pi}{2\beta_o}\,\theta(1+B)\,\frac{M(B) - M(\theta)}{\theta - B} \qquad (42a\text{-}8)$$

where

$$M(\zeta) = 1 - \frac{\pi}{2}\sqrt{\frac{2\zeta}{\pi}}\; e^{\frac{\zeta}{2}}\,\mathrm{Erfc}\left(\sqrt{\frac{\zeta}{2}}\right) \qquad (42b\text{-}8)$$

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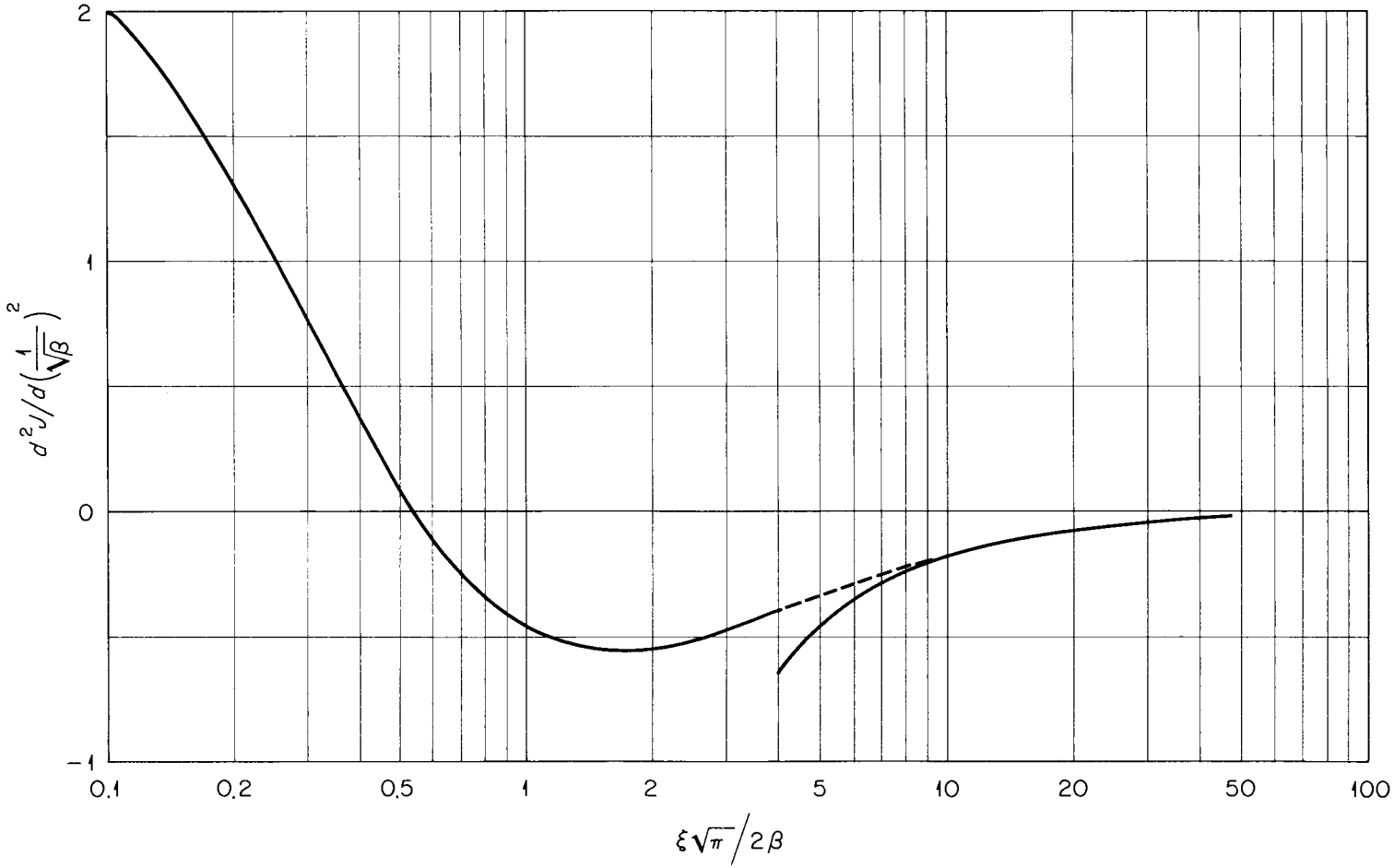

Fig. 4-8. $\dfrac{d^2J}{d\left(\frac{1}{\sqrt{\beta}}\right)^2}$ vs. $\left(\dfrac{\xi\sqrt{\pi}}{2\beta}\right)$ for $\xi \ll 1$

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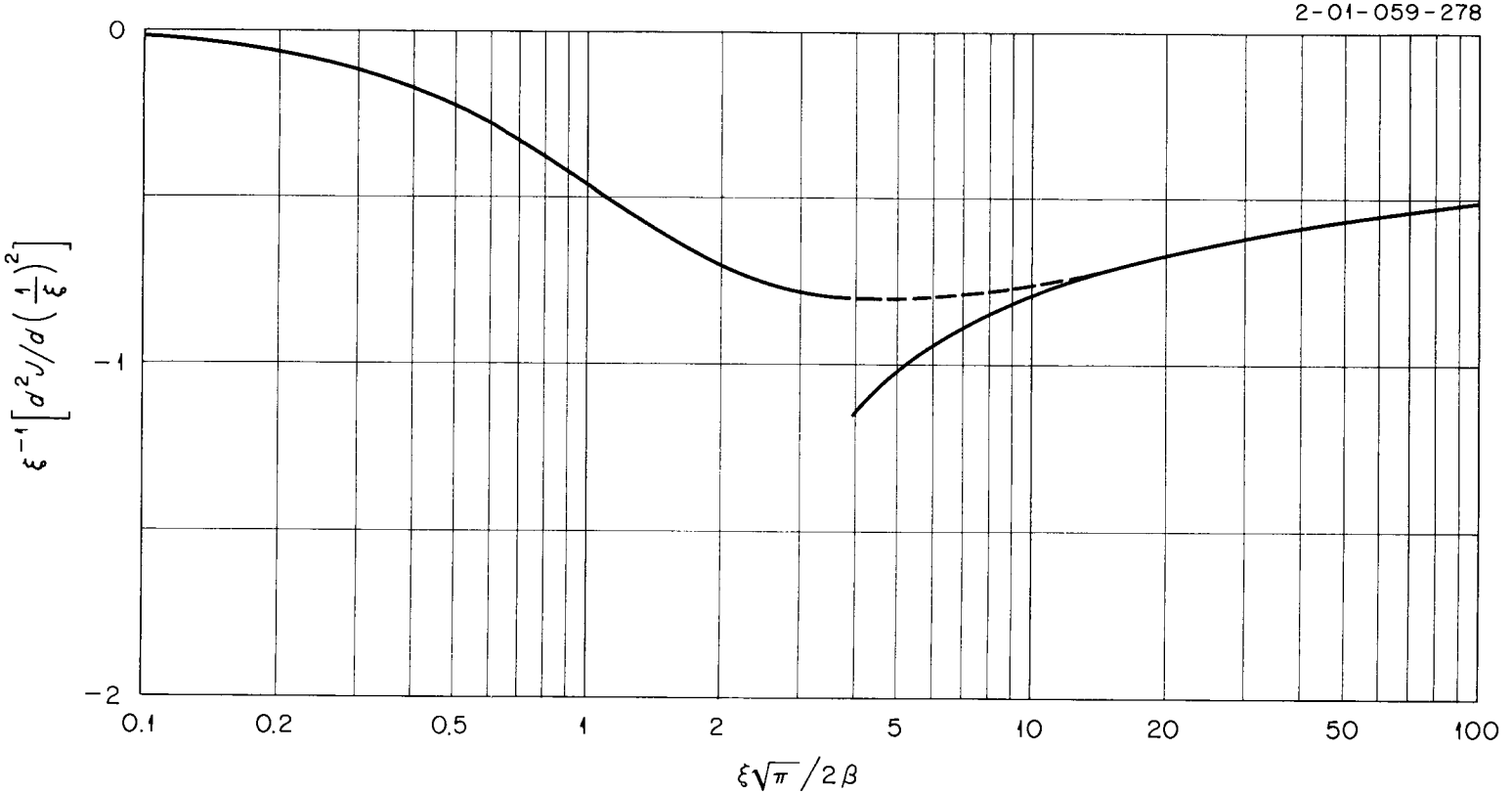

Fig. 5-8. $\frac{1}{\xi}\frac{d^2J}{d\left(\frac{1}{\xi}\right)^2}$ vs. $\left(\frac{\xi\sqrt{\pi}}{2\beta}\right)$ for $\xi << 1$

The results of the last three paragraphs permit the averaging of the function $J(\xi,\beta)$ over the distribution of widths, and allow the calculation of the effective absorption cross section in all cases previously discussed, except that of Eq. (77-4). It yet remains to average the difference of the first and third terms. This difference can be written, when generalized to include heterogeneous media also,

$$J(\infty,\beta b)\left[\sqrt{\frac{1+b\beta}{1+b\beta-\frac{\gamma}{b}}}-1\right]\approx\frac{\pi}{2}(b\beta)^{-\frac{1}{2}}\left[\sqrt{\frac{b}{b-\gamma}}-1\right] \tag{43-8}$$

The approximate equality depends on the assumption $\beta b << 1$. If $b = \gamma = 1$, the right hand side of Eq. (43-8) becomes singular; even the non-singular left hand side becomes equal to the infinite dilution value. However, this situation never arises. In homogeneous media, $b = 1$, γ is usually small, as indicated in paragraph (17-4). On the other hand, in heterogeneous media, when γ can equal unity, b is usually a good bit larger than unity. We shall therefore consider the case in which $\frac{\gamma}{b}$ is at least somewhat less than unity. In such case

$$\frac{\pi}{2}(\beta b)^{-\frac{1}{2}}\left(\sqrt{\frac{b}{b-\gamma}}-1\right)=\frac{\pi}{2}(\beta b)^{-\frac{1}{2}}\left[\frac{1}{2}\frac{\gamma}{b}+\frac{3}{8}\frac{\gamma^2}{b^2}+\frac{5}{16}\frac{\gamma^3}{b^3}+\ldots\right] \tag{44-8}$$

Now $\beta \propto \frac{\Gamma}{\Gamma_n}$ and $\gamma \propto \frac{\Gamma_n}{\Gamma}$. Thus $\beta = \beta_o \cdot \frac{\gamma_o}{\gamma}$ and the average of Eq. (44-8) can be written

$$\left\langle\frac{\pi}{2}(\beta b)^{-\frac{1}{2}}\left(\sqrt{\frac{b}{b-\gamma}}-1\right)\right\rangle=\frac{\pi}{2}(\beta_o b)^{-\frac{1}{2}}\left[\frac{\gamma_o}{2b}\left\langle\frac{\gamma^{3/2}}{\gamma_o^{3/2}}\right\rangle+\frac{3\gamma_o^2}{8b^2}\left\langle\frac{\gamma^{5/2}}{\gamma_o^{5/2}}\right\rangle\right.$$
$$\left.+\frac{5\gamma_o^3}{16\,b^3}\left\langle\frac{\gamma^{7/2}}{\gamma_o^{7/2}}\right\rangle+\ldots\right] \tag{45-8}$$

To complete the evaluation of Eq. (45-8) it is necessary to calculate the quantities $\left\langle \frac{\gamma^{n+1/2}}{\gamma_o^{n+1/2}} \right\rangle$. Now

$$\gamma = \frac{\sigma_{pa}}{\sigma_p} g_J \frac{\Gamma_n}{\Gamma} = \frac{\sigma_{pa}}{\sigma_p} g_J \frac{\left\langle \Gamma_n^o \right\rangle \sqrt{E}\ w}{\left\langle \Gamma_n^o \right\rangle \sqrt{E}\ w + \Gamma_\gamma} = \gamma_o \cdot \frac{(1 + B)w}{w + B} \tag{46-8}$$

Hence

$$\left\langle \frac{\gamma^{n+1/2}}{\gamma_o^{n+1/2}} \right\rangle = \int_o^\infty (2\pi w)^{-\frac{1}{2}} e^{-\frac{w}{2}} \left[\frac{w(1 + B)}{w + B} \right]^{n+1/2} dw \tag{47a-8}$$

$$= (1 + B)^{n+1/2} \sqrt{\frac{2B}{\pi}}\ e^{\frac{B}{2}} \int_1^\infty e^{-\frac{B}{2} y^2} \left(1 - \frac{1}{y^2} \right)^n dy \tag{47b-8}$$

The second line follows from the substitution $w + B = By^2$. Expanding the binomial we can write

$$\left\langle \frac{\gamma^{n+1/2}}{\gamma_o^{n+1/2}} \right\rangle = (1 + B)^{n+1/2} \sqrt{\frac{2B}{\pi}} \sum_{k=o}^{n} (-)^k \frac{n!}{(n - k)!k!} N_k \left(\frac{B}{2} \right) \tag{48a-8}$$

where

$$N_k(\alpha) \equiv e^\alpha \int_1^\infty e^{-\alpha y^2} \cdot y^{-2k} \cdot dy \tag{49a-8}$$

By partial integration we can easily show that

$$(2k + 1)N_{k+1}(\alpha) = 1 - 2\alpha\ N_k(\alpha) \tag{50-8}$$

Finally,

$$N_o(\alpha) = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}}\ e^\alpha \operatorname{Erfc}\left(\sqrt{\alpha} \right) \tag{51-7}$$

CHAPTER 9. NUMERICAL CALCULATIONS

1. In the previous eight chapters a complete theory of resonance absorption has been developed in two extreme approximations, viz.: the narrow resonance approximation and the infinite-mass-absorber (wide resonance) approximation. The first of these extreme approximations corresponds to a small mass absorber, so that neutrons in a single collision with an absorber atom can jump entirely over an absorbing resonance. A simple condition for the validity of this approximation has been stated by Wigner (W55) in terms of a parameter of the resonance called the practical width, Δ. The practical width is defined as the energy interval between the two points at which the resonance cross section (absorption plus scattering) equals the potential scattering cross section. Wigner's definition properly applies to large lumps ($b \sim 1$), and for smaller lumps the replacement of σ_p by $b\sigma_p$ should be made, as previously noted. The practical width Δ is a measure of the interval over which appreciable flux depression takes place. E.g., if we consider a narrow resonance with no interference term (i.e., $\gamma = 0$) and $b\beta \ll 1$ half the absorption takes place inside the practical width and half outside for the natural line shape. The half that occurs outside is equal to almost 80% of the absorption contributed by this part of the resonance line in the infinite dilution case, while the half which occurs inside equals a fraction $\frac{1}{2}\sqrt{\beta b}$ ($\ll 1$) of the corresponding quantity in the infinite dilution case. Hence, if the average energy loss per collision in the absorber, ξE_o, is very much greater than Δ, the narrow resonance approximation will apply.

2. Let us next consider a resonance in which $\xi E_o \ll \Delta$, and for the moment in which $\frac{\Gamma_n}{\Gamma} \ll 1$ (absorption resonance). As we shall see next for

such a resonance the wide resonance (infinite mass) approximation is valid. Let us follow the life history of a neutron which is absorbed in the resonance but outside of the practical width. For the natural line shape and b somewhat larger than unity such absorption in the wide resonance approximation is again about 50% of the total absorption, and about 80% of the corresponding quantity in the infinite dilution case. A neutron entering the resonance in the wings cannot enter the line center by elastic collision with absorber nuclei since $\xi E_o << \Delta$. Indeed the contribution of neutrons moderated by the absorber into the line center to the total absorption is $qV = \xi \Sigma_p \phi V$, where q is the slowing down density associated with a flux ϕ in an infinite medium of absorber material. The contribution of this process to the resonance integral is then only $\xi \sigma_p$ which is of the order of 0.1 b in U^{238} and Th^{232}. Hence neutrons which enter the wings simply diffuse in the lump with small amounts of energy loss. In the wings in the neighborhood of the practical width, Δ is the order of magnitude of energy change required to produce appreciable change in the resonance absorption cross section. If $\xi E_o << \Delta$ and the neutrons do not make too many collisions in the lump the cross sections they experience do not change much and their spatial distribution can be accurately calculated by one velocity transport theory.

Concerning the last point, viz., the average number of collisions a neutron makes in the lump, one can say the following: It can be shown [cf Appendix (1-9)] that in one velocity transport theory the average number of collisions made by neutrons which are incident on a lump, collide in it, and leak out again is given by

$$\langle n \rangle = \frac{C}{\delta - \delta_o} \left(\frac{d\delta}{dC} \right) \tag{1-9}$$

where C is the average number of secondaries per collision, δ is the albedo, and $\delta_o = 1 - \bar{\ell}P$, where P is the escape probability. Again we have used units in which the total mean free path is unity. If δ is given by Eq. (22-7), which is appropriate outside the practical width, then for pure scattering (C = 1)

$$\langle n \rangle = \frac{1}{P} \tag{2-9}$$

For small lumps this number is fairly small; e.g., for cylinders for which $\bar{\ell} = 1$ (b = 2) $\langle n \rangle = 1.67$.

In the center of the line neutrons incident on the lump through the surface are absorbed on their first collision and hence one velocity transport theory is permissible (and trivial) for calculating their spatial distribution. Hence, for not too small ($b \gtrsim 2$), purely absorbing $\left(\frac{\Gamma_n}{\Gamma} << 1\right)$ lumps, for a resonance for which $\xi E_o << \Delta$ the wide resonance formula should be applicable.

3. If we now relax the condition $\frac{\Gamma_n}{\Gamma} << 1$ of the last paragraph and keep everything else the same we can proceed as follows:

By the same arguments as in the last paragraph we can show (i) that the absorption of neutrons moderated into the practical width by the absorber nuclei is very small and (ii) that one-velocity transport theory is applicable outside the practical width. However, some of the neutrons which are incident on the lump with energies near the line center undergo more than one collision in the lump, and the moderation which occurs after the first collision will change the cross section relevant to the second collision unless $\xi E_o << \Gamma$, which is, practically speaking, a condition never realized. However, as we shall next show, even for rather large $\frac{\Gamma_n}{\Gamma}$ the error introduced due to this moderation is small.

First note that deep inside the practical width where the cross section changes most rapidly $C = \frac{\Gamma_n}{\Gamma}$, and is independent of energy. Further note that deep inside the practical width the surface of the lump can be treated as a plane surface. Let us choose for the sake of argument C = 0.3 and roughly calculate effect of moderation by the absorber on the amount of absorption as follows: In the first place, only 30% of the incident neutrons make more than one collision. As shown in Appendix (1-9) in one velocity transport theory the average number of collisions made by neutrons which leak out is 1.20 for C = 0.3. We shall therefore assume that all the leakage occurs between the first and second collisions. This procedure is admittedly rough but it allows us to assess the importance of moderation by the absorber. In the one velocity case, the actual absorption is given by Eq. (52-7) by 92.59%, and in the one-collision-leakage approximation as 93.86%. These two figures are sufficiently close to justify our approximate procedure.

If moderation occurs on the first collision the first collision albedo is given by

$$\delta = C \int_0^\infty E_2(x)\, E_2(\zeta x)\, dx \qquad (3\text{-}9)$$

where ζ is the ratio of the cross section at the lower energy to that at the higher energy. By an exactly similar technique to that used in connection with Eq. (54a-7) we can show that

$$\delta(\zeta) = \frac{C}{3}\left[\frac{1+\zeta}{\zeta} - \left(\frac{1+\zeta^2}{\zeta^2}\right)\log(1+\zeta) + \zeta\log\zeta\right] \qquad (4\text{-}9)$$

It is very important to note that in the line center the line shape is symmetric, so that while a certain number of neutrons are moderated from an energy at which the cross section is σ_1, say, to an energy at which the cross section is σ_2 on the first collision, an equal number are moderated from σ_2 to σ_1. Hence, we must compare $\delta(\rho = 1)$ with $\frac{1}{2}\left[\delta(\rho) + \delta\left(\frac{1}{\rho}\right)\right]$. Since this last quantity is concave upwards when plotted vs ρ it always exceeds $\delta(\rho = 1)$. For moderation in which the cross section changes by a factor of 2 ($\rho = 2$), the absorption in the one-collision-leakage approximation is 89.31%, or about 5% less than if no moderation occurred at all. In the case for C = 0.5 it is about 9% lower. If the cross section changes by a factor of $\frac{3}{2}$ the corresponding percentages are 2% and 3%, respectively. In addition, it must be remembered that these errors really affect only the half of the absorption occurring inside the practical width, and, moreover, that if the change in cross section is a factor of 2, say, near the line center, it will be less far from it. Finally, the Doppler broadening of resonance lines tends to smooth out the line shape and decrease the cross section change in a given energy interval compared to the natural line shape. In sum, if $\xi E_o << \Delta$ but $\sim \Gamma$ and $\frac{\Gamma_n}{\Gamma}$ is not too large we expect the wide resonance approximation to be valid.

Finally, in order to apply the criterion developed in the previous paragraphs explicit expressions are necessary for Δ. For the natural line shape, it can easily be shown that

$$\Delta = \Gamma \cdot \sqrt{\frac{1 + \gamma}{\beta b}} \tag{5-9}$$

This expression is only applicable if <u>in the neighborhood of</u> $x_\Delta = \frac{\Delta}{\Gamma}$ the natural line shape applies, and if $\beta << 1$ this will only be the case if

$\frac{\xi^2 x_\Delta^2}{6} >> 1$, or equivalently, $\beta b << (1 + \gamma) \frac{\xi^2}{6}$. On the other hand, in the case of the extreme Doppler broadened line shape, Eq. (35-4), is given by

$$\Delta = \Gamma \cdot \frac{2}{\xi} \sqrt{\ln\left(\frac{\xi\sqrt{\pi}}{2\beta b}\right)} \tag{6-9}$$

4. Presented in the first two columns of Table (1-9) are the energies and neutron widths of the resolved resonances of U^{238} as reported by Hughes and Schwartz(H57a). The third column is the ratio $\frac{\Gamma_n}{\Gamma}$ and is based on the assumption of a constant radiative width, Γ_γ, of 25 mv. A constant radiative width is indicated in the work of Porter and Thomas (P56), and the numerical value of 25 mv is taken from Hughes and Schwartz(457a). The fourth column, β, is based on a value of σ_p of 10.75 barns, as recommended by Seth(556c). The fifth column, ξ, is based on an absolute temperature of about 300°K (kT = 0.025 ev).

In the first column of Table (2-9) is the parameter $\frac{\xi^2}{6\beta b}$, and in the second column the parameter $\frac{\xi E_o}{\Delta}$. Δ was calculated with either Eq. (5-9) or Eq. (6-9) according as the entry in the first column was greater or less than unity. In the next three columns are values of the resonance integral calculated for b = 4 $\left(\frac{S}{M} = 0.33\ cm^2/gm\right)$ and kT = 0.025 ev, according to (i) the narrow resonance approximation including interference effects, Eq. (71-4), (ii) the narrow resonance approximation without interference effects, Eq. (42-4) and (iii) the wide resonance approximation. For b = 4 and $\frac{\Gamma_n}{\Gamma} \leq 0.5$ approximation (ii) will vary from approximation (iii) by from -17% for $\frac{\Gamma_n}{\Gamma} = 0.5$ to +13% for $\frac{\Gamma_n}{\Gamma} = 0$. This is a fortunate circumstance because in cases in which neither of these extreme approximations is strictly applicable (i.e., when $\frac{\xi E_o}{\Delta} \sim 1$) one may conjecture that neither of them can be in very great error.

Table (1-9). Parameters of Resolved Resonances in Uranium^{238}

Γ_γ = 25 mv
σ_p = 10.75 b
kT = 0.025 ev
D = 18 ev

E_o (ev)	Γ_n (mv)	Γ_n/Γ	$2^k = \beta \times 10^5$	ξ
6.68	1.48	0.05589	49.43	0.4998
21.0	9.0	0.2647	32.80	0.3620
36.8	33	0.5690	26.74	0.4664
66.3	23	0.4792	57.21	0.2876
81.1	2.1	0.07749	432.8	0.1468
90	0.09	0.003587	10370	0.1290
103	72	0.7423	57.36	0.4663
117	17	0.4048	119.5	0.1894
146	0.8	0.03101	1947	0.1042
166	2.8	0.1007	681.7	0.1053
191	138	0.8466	93.32	0.5754
211	41	0.6212	140.4	0.2217
239	35	0.5833	169.4	0.1894
258	1.3	0.04942	2159	0.07989
278	40	0.6154	186.8	0.1902
297	40	0.6154	199.6	0.1840

Table (2-9). Effective Resonance Integrals for Resolved Uranium Resonances for b = 4

$\xi E_o/\Delta$	$\xi^2/6(b\beta)$	kT = .025[a] I (barns)	kT = .025[b] I (barns)	kT = .025[c] I (barns)	kT = 0[a] I (barns)	kT = 0[b] I (barns)	kT = 0[c] I (barns)
0.09422	21.06	5.921	5.882	5.175	5.725	5.686	5.036
0.1879	16.65	2.362	2.286	2.228	2.297	2.220	2.166
0.1743	33.90	1.551	1.439	1.721	1.515	1.403	1.671
0.5550	6.024	0.6107	0.5757	0.6461	0.5674	0.5324	0.5913
1.299	0.2075	0.2746	0.2731	0.2252	0.1598	0.1582	0.1414
∞*	0.01512	0.03940	0.03940	0.03673	0.02913	0.02912	0.02525
0.4272	15.80	0.3915	0.3544	0.5181	0.3793	0.3422	0.4899
1.618	1.251	0.2777	0.2662	0.2852	0.2202	0.2088	0.2206
6.003	0.02324	0.08728	0.08712	0.07874	0.04162	0.04146	0.3635
2.382	0.06775	0.1332	0.1325	0.1173	0.06236	0.06160	0.05559
0.6014	14.78	0.1690	0.1507	0.2642	0.1630	0.1447	0.2473
2.012	1.459	0.1416	0.1321	0.1752	0.1162	0.1068	0.1334
1.768	0.8823	0.1225	0.1155	0.1462	0.09284	0.08580	0.1035
∞**	0.01232	0.04939	0.04927	0.04532	0.02242	0.02228	0.01968
1.939	0.8069	0.1019	0.09582	0.1261	0.07639	0.07026	0.08723
2.033	0.7067	0.09433	0.08879	0.1170	0.06917	0.06362	0.07898
		12.33	11.97	11.90	11.53	11.17	11.43

*Infinite dilution value = 0.04523.

**Infinite dilution value = 0.07581.

a. Narrow, including interference.

b. Narrow, no interference.

c. Wide.

For the most important resonances, i.e., those at 6.68, 21.0, and 36.8 ev, however, the wide resonance approximation is surely preferable, for in none of these cases does $\frac{\xi E_o}{\Delta}$ exceed 20%. These three resonances alone contribute about 75% of the total absorption of the resolved resonances. In addition to the three approximations mentioned above let us define a fourth, the preferred approximation, which consists of selecting one of the first three according as the parameters $\frac{\xi E_o}{\Delta}$ and $\frac{\xi^2}{6\beta b}$ are $\gtrless 1$. For b = 4 and kT = 0.025 ev the preferred approximation gives 11.85 b. To this figure several approximate corrections need to be applied: In the case of wide resonances two errors arise, one due to the fact that Eq. (3-7) does not give quite the right albedo in the wings for small lumps [cf. paragraph (14-7)] and one due to approximating the integral in Eq. (7-7) by neglecting σ_p [cf. paragraph (5-7)]. For b = 4 these corrections combined increase I_W by roughly 8%, according to Table (1-7) and the discussion following Eq. (56-7). For narrow resonances an error is introduced by the use of Wigner's rational approximation for the escape probability [cf. paragraph (8-9) ff.] and according to Table (1-6) increases I_n by about 7%. If we apply a uniform 7.5% correction the preferred approximation we obtain a value for the resonance integral of the resolved resonances of 12.7 barns.

Insofar as the calculational uncertainties in this figure are concerned very little can be said. The main error arises from the inapplicability of one of the extreme approximations (wide or narrow). Let us first consider the resonances at 6.68, 21.0, and 36.8 ev. For these resonances, especially the first two for which $\frac{\Gamma_n}{\Gamma}$ is small, we expect the wide resonance approximation to be quite good. Some corroboration of this point is available from some calculations of Corngold and Chernick on uranium water lattices. Corngold(C56b)

considered an alternating lattice of thin slabs of uranium and light water, with uranium slabs corresponding to a parameter, b, of about 3. He carried out exact calculations of absorption in the uranium resonances by solving the Boltzmann equation for the case $A = \infty$ and $A = 238$. Comparison of these cases showed the former in error by +3% for the 36.8 ev resonance, and +0.5% for the 20.9 ev resonance. No calculation is reported for the 6.68 ev resonance, but we may infer from the above figures a negligible errors since $\frac{\xi E_o}{\Delta}$ and $\frac{\Gamma_n}{\Gamma}$ are smallest for this lowest resonance. In the higher resonances which Corngold considered, in which $\frac{\xi E_o}{\Delta}$ is always about 0.6 or greater, the error in the $A = \infty$ case ranged as high as 25% but fluctuated in sign. A Monte Carlo calculation reported by Chernick (C56) on the 36.8 ev resonance in uranium, in a lattice of cylindrical rods with b = 2, indicated an error in the infinite mass approximation of about +1%. In this connection it is worth noting that, although the statistical accuracy of I is estimated at about 3%, Richtmyer(R56a) has pointed out that differential effects such as we are concerned with may be obtained with higher accuracy than I itself.

All the resonances below 300 ev except the first three contribute only 2.9 barns, and as much as 20% error in this part would produce an error the total of I of about 0.6 barns, which is less than 5%. Actually 20% error is a rather high figure, for since the errors in the contributions of individual resonances fluctuate in sign considerable cancellation can be expected. Such cancellation occurs in Corngold's calculation.

Similar calculations for b = 8 $\left(\frac{S}{M} = 0.76\ cm^2/gm\right)$ are presented in Table(3-9). Quite a similar discussion applies to these results as to the results of Table (2-9). The preferred approximation gives 18.5 barns for I

Table (3-9). Effective Resonance Integrals for Resolved Uranium Resonances for b = 8

$\xi E_o/\Delta$	$\xi^2/6(\beta b)$	kT = 0.025[a] I (barns)	kT = 0.025[b] I (barns)	kT = 0.025[c] I (barns)
0.1332	10.53	8.483	8.455	8.074
0.2657	8.325	3.360	3.306	3.523
0.2465	16.95	2.134	2.059	2.693
0.7849	3.012	0.8779	0.8543	1.063
1.603	0.1038	0.4131	0.4120	0.3971
∞	0.007560	0.04296	0.04295	0.04173
0.6041	7.900	0.5362	0.5120	0.8234
1.310	0.6255	0.4238	0.4161	0.4948
∞	0.01162	0.1090	0.1089	0.1067
3.603	0.03388	0.1896	0.1891	0.1845
0.8505	7.390	0.2292	0.2174	0.4237
1.760	0.7295	0.2052	0.2046	0.2970
1.998	0.4412	0.1829	0.1782	0.2507
∞	0.006160	0.03379	0.03369	0.05809
2.195	0.4035	0.1536	0.1494	0.2153
2.318	0.3534	0.1422	0.1384	0.1987
		17.52	17.28	18.84

a. Narrow, including interference.

b. Narrow, no interference.

c. Wide.

without correction; after a correction of about 9% for the effects previously discussed, I becomes 20.1 barns.

5. In order to complete the calculation of the resonance integral of uranium for b = 4 and 8 an estimate must be made of the contributions from the unresolved resonances above 300 ev. These resonances are described in terms of the following parameters: An average spacing, D, of 18 ev, a reduced neutron width, Γ_n^o, of 2.5 mv and a radiative width, Γ_γ, of 25 mv. These data are consistent with the resonance parameters reported in reference H57a for the resolved uranium resonances. The effective absorption cross section has been calculated according to the narrow resonance approximation, and interference effects have been neglected. This is in view of the fact that the parameters $\frac{\xi^2}{6\beta b}$ and $\frac{\xi E_o}{\Delta}$ are less than and greater than unity, respectively, when evaluated at the point (ξ^*, β^*) $\left[\xi^* \text{ and } \beta^* \text{ are defined in Eq. (23-8)}\right]$. These calculations have been carried out at 300 ev, 1500 ev, 7500 ev, and 37,500 ev. At the first three points the averaging of $J(\xi, \beta)$ over the distribution of neutron widths was accomplished with Eq. (23-8). At the last point Eq. (42-8) was used.

Presented in Table (4-9) are the results of these calculations. Since the tabular entries are at constant intervals in $\ln E$ we can use the "three-eighths" rule of Newton to find the contribution of this energy range to the resonance integral. These figures are written directly below their respective columns. To them one must now apply the correction factors previously discussed, obtaining for the corrected contribution to the resonance integral, 3.4 b and 4.6 b, respectively, for b = 4 and 8.

Presented in Table (5-9) are the values of $J(\xi^*, \beta^* b)$, $\langle J(\xi, \beta b) \rangle$ and $J(\xi_o, \beta_o b)$ employed in the computation of the effective absorption cross

Table (4-9). Effective Absorption Cross Section of Uranium Lumps for b = 4, 8

E_o (ev)	b = 4 σ_a^{eff} (b)	b = 8 $\sigma_{a\ eff}$ (b)
300	1.302	1.943
1500	0.8642	1.160
7500	0.4269	0.4922
37500	0.1017	0.1075
	3.185	4.229

Table (5-9). Effect of Fluctuations on the Resonance Absorption in Uranium for b = 4 and 8

	b = 4			b = 8		
E	$J(\xi^*, \beta^* b)$	$\langle J(\xi, \beta b) \rangle$	$J(\xi_o, \beta_o b)$	$J(\xi^*, \beta^* b)$	$\langle J(\xi, \beta b) \rangle$	$J(\xi_o, \beta_o b)$
300	24.33	21.80	24.25	18.61	16.27	18.91
1500	17.12	14.47	15.96	10.82	9.715	11.51
7500	7.493	7.148	7.466	3.973	4.121	4.518
37500	-	1.703	2.144	-	0.8995	1.131

section. Comparison of the first two quantities found in columns 2 and 3, and 5 and 6 of the table is an index of the rapidity of the convergence of the procedure employed in performing the average over the distribution of neutron widths. The second order terms in Eq. (23-8) are never more than about 20% of the leading term, and for most entries in the table are considerably less, indicating good convergence. Comparison of the last two quantities, found in columns 3 and 4, and 5 and 6 of Table (5-9), indicate that the effect of fluctuations in the neutron width is to reduce the effective absorption cross section. The resultant reduction in the resonance integral from the energy range 300-37500 ev is about 9% for b = 4 and 14% for b = 8.

6. A simple estimate of the remaining contribution from energies above 37500 ev can be made by ignoring the effects of fluctuations entirely. This neglect will be valid if $B \ll 1$ and $\theta \gg 1$. For the first requirement says that $\Gamma_\gamma \ll \langle \Gamma_n \rangle$ and that Γ_n/Γ is nearly unity except with very low probability. The second requirement says that J is given by Eq. (70-4) and that the term in ξ is very small compared to the term in β. It can then be straightforwardly shown that

$$\int_{E_c}^{\infty} \frac{dE'}{E'} J(\xi,\beta) = \frac{\pi}{2} \int_{\beta_c}^{\infty} \frac{d\beta}{\beta} \frac{1}{\beta + \xi\sqrt{\frac{\pi}{8}}} = \frac{\pi}{2\beta_c}\,\theta_c \ln\left(1 + \frac{1}{\theta_c}\right) \qquad (7\text{-}9)$$

Evaluating this quantity in the case $E_c = 37500$ for b = 4 and 8 (and replacing β by $b\beta$) one obtains additional contributions to the resonance integral of 0.14 b in both cases.

Finally then, the calculated total resonance integrals for uranium for $b = 4$ and 8, respectively, are 16.2 b and 24.8 b. Because most of this absorption is due to wide levels a $\sqrt{b - 1}$ law of geometric dependence ought to be good. This proves to be the case; the expression $9.36 \sqrt{b - 1}$ fits the calculated points at $b = 4$ and 8 exactly. Since $b - 1$ is proportional to S/M a $\sqrt{b - 1}$ law of geometric dependence implies a dependence on S/M proportional to $\sqrt{S/M}$. In particular, the expression $9.36 \sqrt{b - 1}$ gives for the resonance integral of uranium lumps in barns

$$I = 28.4 \sqrt{\frac{S}{M}} \qquad (8\text{-}9)$$

when S/M is expressed in cm^2/gm. Equation (8-9) is only valid in the range $4 \leq b \leq 8$ and perhaps slightly outside this range; this range corresponds to a range in S/M of $0.33\ cm^2/gm \leq S/M \leq 0.76\ cm^2/gm$.

7. Precisely similar calculations have been performed for Th^{232} for $b = 4$ and 8, and are summarized in Tables (6-9), (7-9), (8-9), and (9-9). After correction by the 7.5% and 9% previously mentioned in connection with uranium lumps the preferred approximation gives for the resonance integral 11.5 and 17.2 barns for $b = 4$ and 8, respectively. These last figures contain 0.18 b from energies above 37500 ev, in addition to the contributions already noted in the tables. The expression

$$I = 18.6 \sqrt{\frac{S}{M}} \qquad (9\text{-}9)$$

fits the two calculated points within 1%, which is well within the uncertainties of the calculation. Concerning these uncertainties we can only anticipate that they are somewhat larger than in the case of uranium. In that latter

Table (6-9). Parameters of Resolved Resonance in Thorium^{232}

Γ_γ = 30 mv, σ_p = 12.00 b, D = 17 ev, kT = 0.025 ev

E_o (ev)	Γ_n (mv)	Γ_n/Γ	$2^k = \beta \times 10^5$	ξ
22.0	2.0	0.06250	162.5	0.3287
23.7	3.7	0.1098	99.59	0.3335
59.6	4.5	0.1304	210.9	0.2153
70.1	40	0.5714	56.63	0.4027
114	10	0.2500	210.5	0.1805
123	27	0.4737	119.9	0.2476
131	11	0.2683	225.4	0.1726
152	15	0.3333	210.5	0.1758
174	70	0.7000	114.7	0.3652
195	30	0.5000	180.0	0.2070
202	19	0.3878	290.4	0.1661
215	2.3	0.07120	139.4	0.1061
226	41	0.5775	180.6	0.2275
235	1.3	0.04153	261.2	0.09835
256	51	0.6296	187.7	0.2439
269	22	0.4231	293.5	0.1498
290	57	0.6552	204.3	0.2461
310	105	0.778	184.0	0.3693

Table (7-9). Effective Resonance Integrals for Resolved Thorium Resonances for b = 4

$\xi^2/6\beta b$	$\xi E_o/\Delta$	kT = 0.025[a]	kT = 0.025[b]	kT = 0.025[c]
2.770	0.4767	1.464	1.454	1.254
4.654	0.3818	1.683	1.662	1.489
0.9158	0.9059	0.5534	0.5465	0.4882
11.93	0.4099	0.7630	0.7087	0.8588
0.6450	1.289	0.3133	0.3062	0.2939
2.130	1.831	0.3305	0.3132	0.3545
0.5508	1.409	0.2713	0.2649	0.2575
0.6116	1.495	0.2395	0.2323	0.2359
4.845	1.014	0.2284	0.2090	0.2966
0.9921	1.608	0.1890	0.1796	0.2087
0.4479	1.782	0.1765	0.1705	0.1645
0.03365	4.200	0.09651	0.09611	0.08602
2.144	2.327	0.1595	0.1500	0.1870
0.01543	∞	0.06229	0.06213	0.05607
1.320	2.356	0.1368	0.1277	0.1690
0.3185	2.140	0.1300	0.1255	0.1371
1.235	2.592	0.1168	0.1087	0.1494
3.088	1.695	0.1055	0.09582	0.1154

a. Narrow resonances with interference.
b. Narrow resonances with no interference.
c. Wide resonances.

Table (8-9). Effective Resonance Integrals for Resolved Thorium Resonance for b = 8

$\xi^2/6\beta b$	$\xi E_o/\Delta$	kT = 0.025[a]	kT = 0.025[b]	kT = 0.025[c]
1.385	0.6741	2.193	2.186	2.078
2.327	0.5399	2.490	2.475	2.415
0.4579	1.027	0.8524	0.84760	0.8333
5.965	0.5797	1.066	1.030	1.373
0.3225	1.475	0.4829	0.4780	0.5044
1.065	2.589	0.4904	0.4788	0.6005
0.2754	1.622	0.4177	0.4133	0.4412
0.3858	1.712	0.3675	0.3626	0.4038
2.423	1.434	0.3227	0.3100	0.4843
0.4961	1.554	0.2856	0.2793	0.3561
0.2390	2.064	0.2697	0.2656	0.3090
0.01683	∞	0.1266	0.1263	0.1232
1.072	3.291	0.2381	0.2317	0.3190
0.007715	∞	0.07511	0.07500	0.07206
0.6600	0.2029	0.2023	0.1963	0.2854
0.1593	2.532	0.1971	0.1941	0.2301
0.6175	2.148	0.1724	0.1671	0.2508
1.544	2.397	0.1495	0.1432	0.1835

a. Narrow resonances with interference.
b. Narrow resonances with no interference.
c. Wide resonances.

Table (9-9). Effective Absorption Cross Sections of Thorium Lumps for b = 4 and 8

E (ev)	σ_a^{eff}(b) b=4	σ_a^{eff} (b) b=8
300	1.602	2.355
1500	1.082	1.440
7500	0.4973	0.5478
37500	0.1135	0.1360

case fully 60% of the resonance absorption was contributed by only three resonances, for which the wide resonance approximation was anticipated to be quite good. In thorium this is not the case.

8. Presented in Tables (10-9) and (11-9) are comparisons of Eqs. (8-9) and (9-9) with experimentally determined resonance integrals. As is apparent from Table (10-9) agreement among the various experiments for uranium is only fair. In the table the formulae of Creutz (C55b), Risser (R50), Sher (S57), Davis (D57), and Eriksen (E55a) have not been evaluated beyond $S/M = 0.40\ cm^2/gm$, since this limit is well outside the range of these experiments. It is apparent that a linear dependence on S/M predicts a too rapid rise in I for large values of S/M. The experiments of Davis (D57) and Eriksen (E55a) should be ignored in a comparison of theory and experiment because of the apparent presence of systematic errors. Davis' (D57) experiment gives results $\sim$ 20-30% higher than the first five experiments noted in the table; Eriksen's (E55a) experiment is $\sim$20% too high. The agreement of Egiazarov's (E55) results and Hellstrand's (H57) is always within 8% or less, the former lying lower than the latter. Hellstrand (H57) quotes an error of $\pm$2% in his formula, not including errors in I_∞ to which the results were normalized. Agreement of the theory and Hellstrand's (H57) experiment is within 5% in the range $0.30 \leq S/M \leq 1.00$. At low values of S/M the <u>extrapolated</u> theoretical values will be underestimates, since there the extrapolation tends to weight the wide resonances too strongly. For better values another calculation should be attempted. In sum, in the range of applicability of the calculations carried out here, the theory predicts the resonance integral of uranium rods quite well.

Table (10-9). Comparison of Theory and Experiment for Uranium Rods

Reference	Resonance Integral (barns)	Calibration	Approximate Range of Experiments	$\frac{S}{M}$ =0.10	$\frac{S}{M}$ = 0.25	$\frac{S}{M}$ = 0.40	$\frac{S}{M}$ = 0.55	$\frac{S}{M}$ = 0.70	$\frac{S}{M}$ = 0.85	$\frac{S}{M}$ = 1.00
Creutz (C55b)	$8.5+27.4\left(\frac{S}{M}\right)$	I_∞ = 280 barns*	0.05-0.15 cm^2/gm	11.2	15.4	19.5				
Risser (R50)	$8.4+28.0\left(\frac{S}{M}\right)$	A=8.4 barns*	0.02-0.15	11.2	15.4	19.6				
Egiazarov (E55)	$3.85+21.5\left(\frac{S}{M}\right)^{1/2}$	* *	0.40-4.8	10.6	14.6	17.4	19.8	21.8	23.7	25.4
Hellstrand (H57)	$2.81+24.7\left(\frac{S}{M}\right)^{1/2}$	I_∞ = 280 barns	0.07-0.53	10.6	15.2	18.4	21.1	23.5	25.6	27.5
Sher (S57,S57a)	$0.1+33.5\left(\frac{S}{M}\right)^{1/2}$	Unknown	0.18-0.22	10.7	16.9	21.3				
Davis (D57)	$6.0\left\{1+15.6\frac{S}{M}\left[1-2.18\frac{S}{M}+2.19\left(\frac{S}{M}\right)^2\right]\right\}$	Unknown	0.1-0.35	13.5	19.8	23.9				
Eriksen (E55a)	$9.6+31.9\left(\frac{S}{M}\right)$	$I_\infty(In^{115})$= 3200 barns*	0.02-0.13	12.8	17.6	22.4				
Theory	$28.4\left(\frac{S}{M}\right)^{1/2}$	I_∞ = 285 barns***		9.0	14.2	18.0	21.1	23.8	26.2	28.4

*These data have been renormalized to the most recent cross section data by Hellstrand (H57). The original data of Risser were based on a "volume" absorption term of 9.0 barns as measured by Hughes and Goldstein (H46). This measurement is based on certain assumed values for the indium cross sections and the thermal U^{238} cross sections. When renormalized to recent values of these data the "volume" term is 8.4 barns.

**Renormalized by E. P. Wigner, BNL (433)-C24, September, 1956.

***I_∞ = 285 barns for the resonance parameters employed in this calculation (including an estimate of the contribution of the unresolved resonances by the methods of Chapter 8).

Table (11-9). Comparison of Theory and Experiment for Thorium Rods

Reference	Resonance Integral (barns)	Calibration	Approximate Range of Experiments	$\frac{S}{M} = 0.10$	$\frac{S}{M} = 0.30$	$\frac{S}{M} = 0.50$	$\frac{S}{M} = 0.70$	$\frac{S}{M} = 0.90$	$\frac{S}{M} = 1.10$	$\frac{S}{M} = 1.30$
Dayton and Pettus (D57a)	$I=-0.6+24.1\left(\frac{S}{M}\right)^{1/2}$	$\sigma_{th}(B)=769b$	$0.1-1.3\ \frac{cm^2}{gm}$	7.0_2	12.6	16.4	19.6	22.3	24.7	26.9
Davis (D57)	$I=6.11\left\{1+5.0\ \frac{S}{M}\left[1-0.87\left(\frac{S}{M}\right)^2\right]\right\}$	Unknown	0.1-0.3	9.1_4	14.6	18.06				
Sher (S57, S57a)	$I=2.2_4+17.1_3\left(\frac{S}{M}\right)^{1/2}$		~ 0.4		11.6	14.4				
Theory	$I=18.6\left(\frac{S}{M}\right)^{1/2}$			5.8_8	10.2	13.2	15.6	17.6	19.5	21.2

In the case of thorium rods the situation is not nearly so good. Only one experiment, that of Dayton and Pettus (D57a) spans a large range of S/M. In the entire range $0.3 \leq S/M \leq 1.3$ the measurements are larger than the calculated results by $\sim 25\%$. The cause of this discrepancy is not understood.

One can, however, offer a plausible reason why some doubt concerning the experiment may exist. By comparing the results of calculation in the narrow and wide resonance approximations one sees that for the rod sizes corresponding to the range $b \sim 4$ the resonance integral does not depend significantly on the approximation employed. For the resolved resonances in uranium, for example, the sums of columns 4 and 5 of Table (2-9) are essentially equal, and a similar condlusion holds for thorium in Table (7-9). One might then assume that this independence of the approximation made to describe the moderation holds as well for the oxides of uranium and thorium. In such a case, the effective resonance integral of the oxides could be obtained from those of the metals in the narrow resonance approximation, according to the first rule of paragraph (6-6). Hellstrand (H57) has measured the effective resonance of both uranium metal and oxide. The resonance integral of the oxide calculated from that measured for the metal according to the rule of paragraph (6-6) agreed within 5% with those directly measured in the range $0.25 \leq S/M \leq 1.00$ cm^2/gm (corresponding to $3.3 \leq b \leq 10.2$). As expected the error vanished near $b = 4$. Dayton and Pettus have measured the effective resonance integrals of thorium and thorium oxide. The resonance integral obtained for the oxide from that of the metal by the method of paragraph (6-6) exceeded the directly measured one by 20-30% in the range $0.5 \leq S/M \leq 1.3$ ($5 \leq b \leq 11.4$), although

agreement was good for S/M = 0.3 (b = 3.4). This poor agreement raises a doubt which could be settled by further measurements on Th.

APPENDIX (1-9)

The current leaving any lump of material irradiated on the surface by an infinite isotropic spatially uniform source producing unit inward current can be written as $\delta = \sum_{n=0}^{\infty} \delta_n \cdot C^n$, where δ_n is the excident current of neutrons which have experienced n collisions <u>for a purely scattering lump</u>. This form follows from the obvious fact that the absorption probability, 1-C, is independent of position in the lump. Then

$$\frac{C}{\delta - \delta_o}\left(\frac{d\delta}{dC}\right) = \frac{\sum_{n=1}^{\infty} n\delta_n C^n}{\sum_{n=1}^{\infty} \delta_n C^n} = \langle n \rangle \qquad (1\text{-}9.1)$$

where $\langle n \rangle$ is the average number of collisions made by neutrons which collide in the lump and leak out again. δ_o is the current of neutrons which escape collision in the lump, and is clearly given by $1 - \bar{\ell}P$, since $\bar{\ell}P$ is the first collision rate in units where the lump total mean free path is unity. For an infinite lump ($\bar{\ell} \to \infty$), $\delta_o \to 0$. By definition, δ is the lump albedo.

CHAPTER 10. THE EFFECT OF FLUCTUATIONS IN THE WIDTHS ON REACTION CROSS SECTIONS

1. In the previous chapters the problem of resonance absorption in the s-wave resonances of the absorbing material was considered. In treating this problem the simplifying assumption was made that only scattering and radiative capture of neutrons by the absorber are possible. However, the effects of flux depression by the absorber and the associated effects of the Doppler broadening of resonance lines, as well as effects introduced by the spatial distribution of the absorber, were carefully taken into account. At high energies, usually of the order of 100 kev or more, the problem of resonance absorption is peculiarly inverted. Resonance cross sections fall sufficiently low so that flux depression effects and their attendant difficulties become unimportant while the effects of other reactions, e.g., inelastic scattering and fission, and higher angular momenta become important. In the remainder of this work emphasis will be placed on the calculation of resonance integrals with spatial and flux depression effects ignored. This problem is really the same as the problem of calculation of reaction cross sections averaged over many resonances in a small energy band. Since the flux in the 100-kev range and above is generally not a slowing down flux $\left(\frac{1}{E}\right)$, the total resonance integral depends on the form chosen for the flux. Hence, in the remainder of this work we shall calculate only average reaction cross sections as functions of energy.

2. It has been pointed out in Chapter 2 that average reaction cross sections in both the $\alpha s \ell$ and $\alpha j I$ representations are proportional to sums, each term of which contains an average squared S-matrix element, whose form is given in Eq. (8-2). In order to conduct an analysis of experimental data the

properties of such averages must be studied, and rapid means of evaluating them acquired. It is the purpose of this chapter to accomplish this desideratum.

If we restrict ourselves to situations in which fission is unlikely, then for the heavy elements only elastic and inelastic scattering and radiative capture need be considered. In such a case the only widths which appear in Eq. (8-2) are neutron and radiative widths. According to the results of Porter and Thomas (P56) the neutron widths are statistically distributed in chi-squared distributions of one degree of freedom, while the radiative widths are essentially constant. Frequently, in the expressions for total reaction cross sections averages of the type appearing in Eq. (8-2) occur in which one of the neutron widths must be considered as having two degrees of freedom. Such a situation arises as follows:

In schematic theories of nuclear reactions (H57, F54) the assumption is frequently made that the average reduced neutron widths are independent of channel spin, s. If this is the case and if the reduced widths for different channel spins are statistically independent Eq. (10-2) for $B_o(\alpha,\alpha')$ can be written

$$B_o(\alpha,\alpha') = \frac{1}{4}\sum_{J=0}^{\infty}\frac{2\pi}{D_{J\pi}}\sum_{\ell=0}^{\infty}\sum_{\ell'=0}^{\infty}\frac{\epsilon(\ell;I\pi;J\pi)\Gamma_{\alpha\ell}\,\epsilon(\ell';I'\pi';J\pi)\Gamma_{\alpha\ell'}}{\sum_{\ell''I''\pi''}\epsilon(\ell''I''\pi'';J\pi)\Gamma_{\alpha\ell}} \qquad (1\text{-}10)$$

Here $\epsilon(\ell;I\pi;J\pi)$ is the symbol of Hauser and Feshbach, and equals the number of channel spins which can combine with orbital angular momentum ℓ, target spin and parity I and π, to form a compound state of spin J and parity π. For neutrons ϵ can only equal 0, 1, or 2. From the addition theorem for

the member distributions of the chi-squared family (C56a) it follows that $\epsilon\Gamma_{\alpha\ell}$ may be interpreted as a random variable with mean $\epsilon\langle\Gamma_{\alpha\ell}\rangle$ and ϵ degrees of freedom. We shall therefore be interested in the averages of quantities like $\Gamma_s\Gamma_t/(\Gamma_s + \Gamma_t + \Gamma_r + ---)$ where Γ_s, Γ_t, Γ_r, etc. are independently distributed in member distributions of the chi-squared family with 1, 2, or infinitely many degrees of freedom. (Infinitely many degrees of freedom corresponds to a delta function distribution.) In the next part of this paper we shall evaluate explicitly in terms of tabulated functions averages in which there are three or fewer widths. Table (1-10) summarizes the cases done.

Table (1-10)

Γ_s	Γ_t	Γ_r
1	1	absent, 1, 2, ∞
1	2	absent, 1, 2, ∞
2	2	absent, 1, 2, ∞
1	∞	absent, 1, 2
2	∞	absent, 1, 2

The entries in the table represent the number of degrees of freedom in the distribution of the corresponding width. We can find the averages of expressions like $\Gamma_s^2/(\Gamma_s + \Gamma_t + \Gamma_r)$ from the identity:

$$\langle\Gamma_s\rangle = \left\langle\frac{\Gamma_s\Gamma_t}{\Gamma_s + \Gamma_t + \Gamma_r}\right\rangle + \left\langle\frac{\Gamma_s\Gamma_t}{\Gamma_s + \Gamma_t + \Gamma_r}\right\rangle + \left\langle\frac{\Gamma_s^2}{\Gamma_s + \Gamma_t + \Gamma_r}\right\rangle \qquad (2\text{-}10)$$

Reduction of the Multiple Integrals

In general, the averages will be represented by multiple integrals, one integration for each random variable (width) present. For widths distributed in the chi-squared distributions an artifice exists for reducing these multiple integrals to a single integral. The result is general, but we prove it only in detail for the case of three widths.

A normalized chi-squared distribution with 2ρ $(= \nu)$ degrees of freedom is

$$P(x,\rho) = \frac{\rho}{\Gamma(\rho)} (\rho x)^{\rho-1} e^{-\rho x} \tag{3-10}$$

where $\Gamma(\rho)$ is a gamma function. If we let $a_s = \left\langle \Gamma_s \right\rangle$ then

$$\left\langle \frac{\Gamma_s \Gamma_t}{\Gamma_s + \Gamma_t + \Gamma_r} \right\rangle = \int_0^\infty dx_s \int_0^\infty dx_t \int_0^\infty dx_r$$

$$\times\ P(x_s,\rho_s)P(x_t,\rho_t)P(x_r,\rho_r) \frac{a_s x_s \cdot a_t x_t}{a_s x_s + a_t x_t + a_r x_r} \tag{4-10}$$

If we now set

$$\frac{1}{a_s x_s + a_t x_t + a_r x_r} = \int_0^\infty d\lambda\ e^{-\lambda(a_s x_s + a_t x_t + a_r x_r)} \tag{5-10}$$

in the right hand side of Eq. (5-10) and interchange the order of integration so that the λ-integration is last, the x-integrations are independent, and easily carried out. The result after some simple rearrangement, is

$$\left\langle \frac{\Gamma_s \Gamma_t}{\Gamma_s + \Gamma_t + \Gamma_r} \right\rangle = a_s a_t \int_0^\infty \left(1 + \frac{\lambda a_s}{\rho_s}\right)^{-(\rho_s+1)}$$

$$+ \left(1 + \frac{\lambda a_t}{\rho_t}\right)^{-(\rho_t+1)} \left(1 + \frac{\lambda a_r}{\rho_r}\right)^{-\rho_r} d\lambda \qquad (6\text{-}10)$$

When a given ρ_k approaches ∞, the corresponding bracket in Eq. (6-10) approaches $e^{-\lambda a_k}$. For convenience we shall express our results in terms of the ratio R, defined by

$$R = \left\langle \frac{\Gamma_s \Gamma_t}{\Gamma_s + \Gamma_t + \Gamma_r} \right\rangle \frac{a_s + a_t + a_r}{a_s a_t} \qquad (7\text{-}10)$$

4. Let us first consider the two-width cases, i.e., those in which Γ_r is absent.

<u>Case (i): $\rho_s = \rho_t = \frac{1}{2}$</u>

According to Eqs. (6-10) and (7-10) we can write

$$R = (a_s + a_t) \int_0^\infty (1 + 2\lambda a_s)^{-3/2} (1 + 2\lambda a_t)^{-3/2} \, d\lambda \qquad (8\text{-}10)$$

If we set $\mu = 2 \cdot \sqrt{a_s a_t} \cdot \lambda$ we obtain for R the expression

$$R = \frac{a_s + a_t}{2\sqrt{a_s a_t}} \cdot \int_0^\infty (\mu^2 + 2p\mu + 1)^{-3/2} \, d\mu \qquad (9\text{-}10)$$

where $p = \frac{1}{2}\left(\sqrt{\frac{a_s}{a_t}} + \sqrt{\frac{a_t}{a_s}}\right)$. If we change the variable of integration to ζ, defined by $\mu + p = (p^2 - 1)^{1/2}(1 - \zeta^2)^{-1/2}$, the integral in Eq. (9-10) becomes

$$\frac{1}{p^2 - 1} \int_{1/p}^{1} \frac{d\xi}{\xi^2} = \frac{1}{p + 1} \tag{10-10}$$

Combining Eq. (9-10) and (10-10) it is easy to show that

$$R = \frac{a_s + a_t}{(\sqrt{a_s} + \sqrt{a_t})^2} \tag{11-10}$$

<u>Case (ii): $\rho_s = \frac{1}{2}$, $\rho_t = 1$</u>

In this case

$$R = (a_s + a_t) \int_0^\infty (1 + 2a_s\lambda)^{-3/2}(1 + a_t\lambda)^{-2}\, d\lambda \tag{12-10}$$

If we define the auxiliary parameter $r^2 = \frac{2a_s}{a_t} - 1$ and change the variable of integration to θ, defined by $1 + 2a_s\lambda = r^2 \tan^2\theta$ R can be written as

$$R = \frac{4a_s(a_s + a_t)}{a_t^2} \cdot \frac{1}{r^5} \int_{\text{arccot}\, r}^{\pi/2} (\csc^2\theta - 2 + \sin^2\theta)\, d\theta \tag{13-10}$$

These trigonometric integrals can be performed easily, and give after rearrangement

$$R = \frac{3 + r^2}{2} \left(\frac{3 + 2r^2}{r^4} - 3\, \frac{1 + r^2}{r^5} \arctan r \right) \tag{14-10}$$

<u>Case (iii): $\rho_s = \rho_t = 1$</u>

In this case

$$R = (a_s + a_t) \int_0^\infty (1 + \lambda a_s)^{-2}(1 + \lambda a_t)^{-2}\, d\lambda \tag{15-10}$$

Setting $\mu = \sqrt{a_s a_t}\ \lambda$ gives

$$R = \frac{a_s + a_t}{a_s a_t} \int_0^\infty (\mu^2 + 2p\mu + 1)^{-2}\, d\pi \tag{16-10}$$

where p is defined as in case (i). If we set $\mu + p = (p^2 - 1)\zeta^{-1}$ the integral in Eq. (16-10) can be written as

$$(p^2 - 1)^{-3/2} \int_0^{\left(\frac{p^2-1}{p^2}\right)^{\frac{1}{2}}} \frac{\zeta^2 d\zeta}{(1 - \zeta^2)^2} = (p^2 - 1)^{-3/2} \times$$

$$\int_0^{\left(\frac{p^2-1}{p^2}\right)^{\frac{1}{2}}} \left[\frac{1}{(1 - \zeta)^2} + \frac{1}{(1 + \zeta)^2} - \frac{1}{1 - \zeta} - \frac{1}{1 + \zeta}\right] d\zeta \tag{17-10}$$

The integrals are elementary, and when carried out yield after rearrangement:

$$R = \left(\frac{a_s + a_t}{a_s - a_t}\right)^2 \left[1 - \frac{2a_s a_t}{a_s^2 - a_t^2}\ \ln\left(\frac{a_s}{a_t}\right)\right] \tag{18-10}$$

<u>Case (iv): $\rho_s = \frac{1}{2}$, $\rho_t = \infty$</u>

In this case

$$R = (a_s + a_t) \int_0^\infty (1 + 2\lambda a_s)^{-3/2}\, e^{-\lambda a_t}\, d\lambda \tag{19-10}$$

If we change the variable of integration to ζ defined by $\zeta^2 = 1 + 2a_s\lambda$, Eq. (19-10) becomes

$$R = \frac{a_s + a_t}{a_s} \cdot e^{\frac{a_t}{2a_s}} \int_1^{\infty} e^{-\frac{a_t}{2a_s}\zeta^2} \frac{d\zeta}{\zeta^2} \tag{20-10}$$

The integral in Eq. (20-10) is just $N_1\left(\frac{a_t}{2a_s}\right)$, where N_1 is defined in Eq. (49a-7). Using Eqs. (50-7) and (51-7) it can be evaluated and gives for R:

$$R = \frac{a_t + a_s}{a_s}\left[1 - \sqrt{\pi}\sqrt{\frac{a_t}{2a_s}}\; e^{\frac{a_t}{2a_s}} \operatorname{Erfc}\left(\sqrt{\frac{a_t}{2a_s}}\right)\right] \tag{21-10}$$

<u>Case (v): $\rho_s = 1$, $\rho_t = \infty$</u>

In this case

$$R = a_t + a_s \int_0^{\infty} e^{-\lambda a_t} (1 + \lambda a_s)^{-2}\, d\lambda \tag{22-10}$$

If we make the substitution $\zeta = 1 + \lambda a_s$, R becomes

$$R = \frac{a_t + a_s}{a_s} e^{\frac{a_t}{a_s}} \int_1^{\infty} e^{-\frac{a_t}{a_s}\zeta} \frac{d\zeta}{\zeta^2} = \frac{a_t + a_s}{a_s} e^{\frac{a_t}{a_s}} E_2\left(\frac{a_t}{a_s}\right) \tag{23-10}$$

The E_n functions, defined as $\int_1^{\infty} \frac{dz}{z^n} e^{-zx}$, are tabulated in reference (C53).

Corresponding formulae for the three width cases are noted for reference in Appendix (1-10) of this chapter, together with some brief description of their manner of derivation.

5. In Figs. (1-10) and (2-10) the ratio R for the preceding two width cases is plotted vs $\frac{a_s}{a_t}$ in the range $0.03 \leq \frac{a_s}{a_t} \leq 30$. All of the curves have minima in the neighborhood $\frac{a_s}{a_t} = 1$; the symmetric curves (those for which

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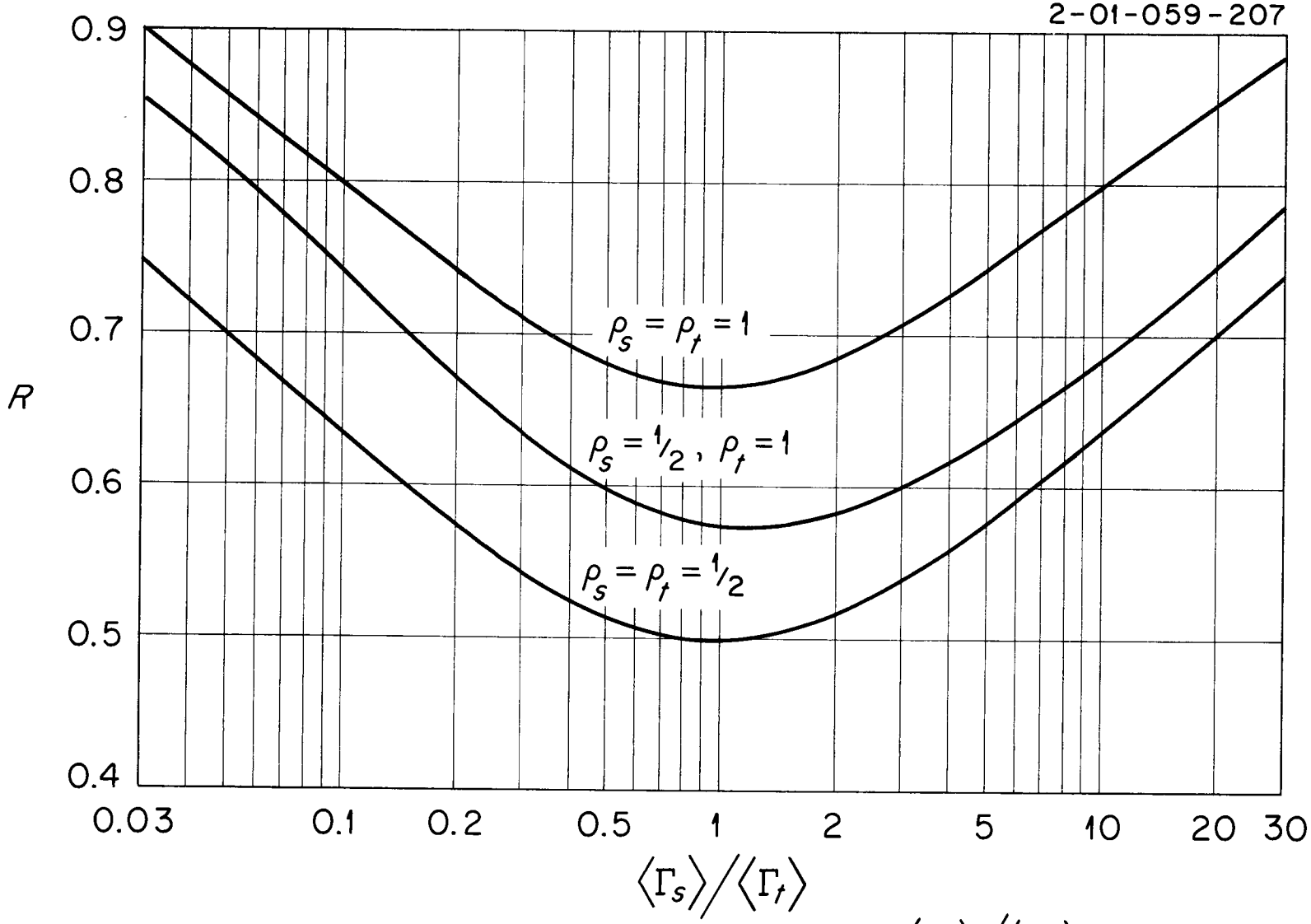

Fig. 1-10. R as a Function of $\langle\Gamma_s\rangle/\langle\Gamma_t\rangle$.

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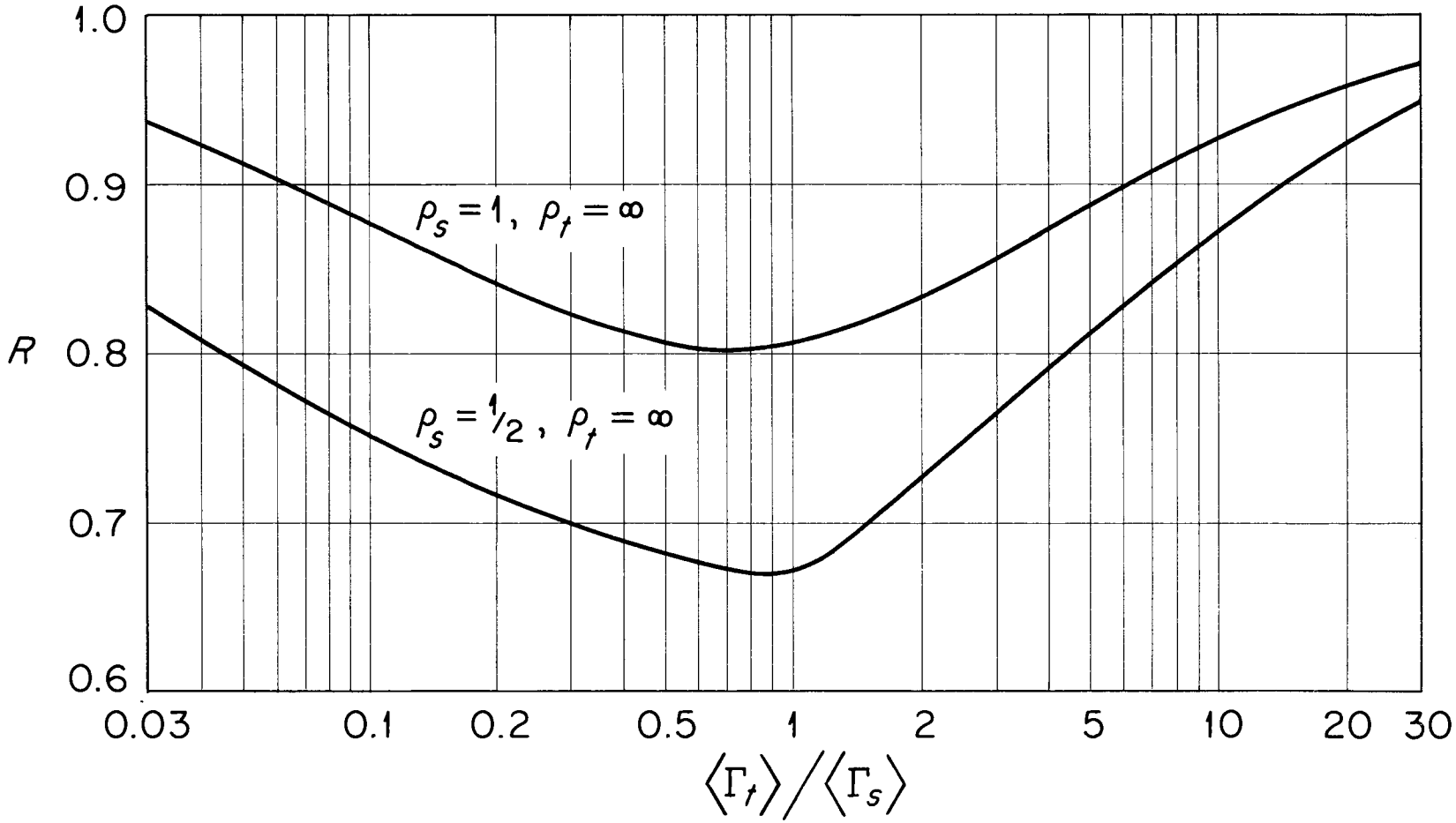

Fig. 2-10. R as a Function of $\langle\Gamma_t\rangle / \langle\Gamma_s\rangle$.

$\rho_s = \rho_t$) have minima exactly as $\frac{a_s}{a_t} = 1$. For the cases plotted in Figs. (1-10) and (2-10) R is always less than unity.

R cannot be less than one for all reactions, however, since the sum of all reaction cross sections equals the cross section for compound nucleus formation, for which R = 1 irrespective of the distribution of widths. Thus if we define $R_{km} = \frac{\sum a_i}{a_k a_m} \left\langle \frac{\Gamma_k \Gamma_m}{\sum \Gamma_i} \right\rangle$, it can easily be shown that

$$\sum_k a_k (R_{km} - 1) = 0 \tag{24-10}$$

Hence, if some of the R_{km} are less than unity, others must be greater. For two width reactions we have seen that $R_{st} \leq 1$ (and consequently R_{ss}, $R_{tt} \geq 1$). For two widths this is a general conclusion and we can establish it as follows:

Let us consider the inequality $\left\langle (\Gamma_s + \lambda \Gamma_t)^2 / (\Gamma_s + \Gamma_t) \right\rangle \geq 0$. By expanding the square it can be shown easily that

$$\lambda^2 \frac{a_t}{a_s} R_{tt} + 2\lambda R_{st} + \frac{a_s}{a_t} R_{ss} \geq 0 \tag{25-10}$$

Since Eq. (25-10) must be true for all real λ the discriminant of the quadratic form must not be positive. Hence

$$R_{st}^2 \leq R_{ss} R_{tt} \tag{26-10}$$

If we define $R_{st} = 1 + D_{st}$ we can rewrite Eq. (26-10) as

$$D_{st}^2 + 2D_{st} \leq D_{ss} D_{tt} + D_{ss} + D_{tt} \tag{27-10}$$

It follows from Eq. (24-10) that

$$- D_{st} = \frac{a_s}{a_t} D_{ss} = \frac{a_t}{a_s} D_{tt} \tag{28-10}$$

Combining Eqs. (27-10) and (28-10) yields

$$D_{st} \leq \frac{1}{2}\left(D_{ss} + D_{tt}\right) \tag{29-10}$$

Since D_{ss} and D_{tt} must have the same sign, and opposite sign to D_{st}, it follows that D_{st} is never positive, and if it vanishes so do D_{ss} and D_{tt}.

It is a general theorem that D_{ss} is never negative, even when there are more than two widths. For the purpose of deriving this inequality we can replace the sum of all the widths which appear in the total width except those for the entrance channels by a single random and variable, Γ_r. Then from the results of the two width case

$$\left\langle \frac{\Gamma_s(\Gamma_t + \Gamma_r)}{\Gamma_s + (\Gamma_t + \Gamma_r)} \right\rangle \leq \frac{a_s \cdot (a_t + a_r)}{a_s + (a_t + a_r)} \tag{30-10}$$

From Eq. (30-10) we can prove that

$$a_t D_{st} + a_r D_{sr} \leq 0 \tag{31-10}$$

Since, however, Eq. (24-10) in this case is written

$$a_s D_{ss} + a_t D_{st} + a_r D_{sr} = 0 \tag{32-10}$$

we must have $D_{ss} \geq 0$ always.

One may inquire, then, whether D_{st} is always ≤ 0? The answer is no as we can see as follows: If $\Gamma_r \geq \Gamma_s + \Gamma_t$ with very small probability D_{st} will be very close to its value for $\Gamma_r = 0$ which is less than one. On the other hand, if $\Gamma_r \leq \Gamma_s + \Gamma_t$ with very small probability D_{st} will be close to the value $\left\langle \Gamma_r^{-1} \right\rangle a_r$, which is greater than one.* These considerations indicate

*We prove this with Schwartz' inequality. If f(x) isanormalized probability distribution,

$$1 = \left(\int \sqrt{\frac{f(x)}{x}}\sqrt{xf(x)}\,dx\right) \leq \left(\int \frac{f(x)}{x}\,dx\right)\left(\int f(x)x\,dx\right) = \langle x^{-1}\rangle\langle x\rangle \quad .$$

that there may be considerable enhancement of a cross section due to fluctuations. The appropriate circumstances may arise, for example, in the radiative capture cross section when there is strong inelastic competition by several excited states. The inelastic width may then greatly exceed the elastic (entrance) and radiative (exit) widths.

6. The analytic formulae derived in the previous paragraphs suffer two defects: (i) The effects of reaction channels competing with the entrance and exit channels must be approximated by a single random variable with 1, 2, or infinitely many degrees of freedom. (ii) The numerical evaluation of R from the three width formulae is tedious and time consuming. For these reasons the computation of R has been coded for the ORACLE. The Monte Carlo method was used for the computation. In this method a large number of values of R are formed by choosing each width from its appropriate distribution, and substituting them in Eq. (7-10). From this sample various moments of the R-distribution can be found; in this coding the first and second moments are calculated. The first moment is the value of R given in Eq. (7-10).

The manner of choosing random numbers from chi-squared distributions of 1 and 2 degrees of freedom is instructive and will be described briefly below. Fundamental to these procedures is the method of choosing numbers distributed uniformly on the interval (0,1). These numbers are generated according to the algorithm $R_n = 5^{15n} \bmod (2^{40}) \times 2^{-39}$. The success of this method is based on the theorem that if $x \equiv 5 \bmod 8$ then $x, x^2, \ldots x^{2^{q-2}}$ are distinct mod (2^q). Thus the algorithm provides one fourth of all possible residues mod (2^q) and furthermore, since they are all powers of 5, only those whose last two binary digits are 01. Clearly these numbers are nearly uniformly distributed.

Let us now consider a chi-squared distribution of 2 degrees of freedom. According to Eq. (5-10) such a distribution is an ordinary exponential, e^{-x}. Random numbers may be drawn from an exponential distribution by the following method due to Von Neumann and described by H. Kahn (K54). Choose random numbers, $x_o, x_1, x_2, \ldots$, uniformly distributed on the interval (0,1), until one exceeds the one before it, i.e.,

$$x_o \geq x_1 \geq x_2 \ldots \geq x_n < x_{n+1} \tag{24-10}$$

Then if n is even keep x_o. (We define this as a success.) If not (a failure) repeat the procedure until an even n is obtained. If the number of repetitions (failures) is k, $k + x_o$ is distributed exponentially. The proof of this is as follows: The probability that x_o will lie between x and dx is dx. The probability that $x_1, \ldots, x_n$ will be less than x_o is x_o^n ; the probability that they will be ordered as in Eq. (24-10) is $\frac{1}{n!}$. The probability for the sequence (24-10) is then

$$\left(\frac{x_o^n}{n!} - \frac{x_o^{n+1}}{(n+1)!} \right) dx \tag{25-10}$$

The probability of a success on the first try with $x \leq x_o \leq x + dx$ is then the sum of (25-10) over all <u>even</u> n, i.e., $\sum_{k=o}^{\infty} \frac{(-)^k}{k!} x_o^k \, dx = e^{-x_o} \, dx$. The probability of a failure on any try is $\int_o^1 (1 - e^{-x}) \, dx = e^{-1}$. Hence, the probability of k failures and a success with $x \leq x_o \leq x + dx$ is just $e^{-(k + x_o)} \, dx$, q.e.d.

The usefulness of this rather oblique method is that when used in conjunction with high speed electronic computing machinery it is very fast,

involving only addition, subtraction, multiplication, and logical decisions.

To choose from a chi-squared distribution of one degree of freedom the following method, due to R. R. Coveyou, is employed. z is chosen as described from an exponential distribution, and two random numbers u and v satisfying the inequality $u^2 + v^2 \leq 1$ are chosen from the uniform distribution. Finally, $w_1 = 2zu^2/(u^2 + v^2)$ and $w_2 = 2zv^2/(u^2 + v^2)$ are formed. It can be shown that w_1 and w_2 are statistically independent and both are drawn from chi-squared distributions of one degree of freedom. The first time the subroutine employed in this calculation (coded by R. R. Coveyou) is used both w_1 and w_2 are calculated, and w_1 is used as output; the second time the subroutine is used w_2 is used as output, and the subroutine returned to its original form.

The code contains the subroutines just described for choosing random numbers from chi-squared distributions of 1 or 2 degrees of freedom. This restriction to $\nu = 1, 2,$ (or ∞) is not essential, however, for if it is desired to compute averages in which one of the partial widths, Γ_s, has, say, $\nu = 3$ the addition theorem for the chi-squared family can be employed to write Γ_s either as the sum of three widths with $\nu = 1$ and mean $\frac{1}{3} \langle \Gamma_s \rangle$, or two widths, one with $\nu = 2$ and mean $\frac{2}{3} \langle \Gamma_s \rangle$, and one with $\nu = 1$ and mean $\frac{1}{3} \langle \Gamma_s \rangle$. As a matter of fact, as we have already seen, even the subroutines used for choosing from the $\nu = 1$ and $\nu = 2$ distributions are related by the addition theorem. Thus the code is quite general and can be used for calculating R for widths with any ν. The only restriction on the code is that there be no more than 20 partial widths. The running time is about $(N + 2)\, 2^{K-13}$ minutes, where N is the number of partial widths, and 2^K is

the number case histories (values of R) computed. Thus for 6 widths and 4096 cases, the running time is 4 minutes.

In the calculations described in the remaining chapters the numerous calculations of R-factors were performed on the ORACLE. Sufficiently many cases were used so that the statistical accuracy was always of the order of 1% or better.

Appendix (1-10). R for the Three Width Cases

Let us first consider cases in which none of the widths have $\rho = \infty$.

Case (i): $\rho_s = \rho_t = \rho_r = \frac{1}{2}$

According to Eqs. (6-10) and (7-10) we have

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}} (1 + 2\lambda a_t)^{-\frac{3}{2}} (1 + 2\lambda a_r)^{-\frac{1}{2}} d\lambda \qquad (1\text{-}10.1)$$

If we set $\mu = 2\lambda \sqrt{a_s a_t}$ we can rewrite R as

$$R = \frac{t + \frac{1}{t} + \frac{1}{2} q}{\sqrt{q}} \int_0^\infty \frac{d\mu}{(\mu + t)(\mu + \frac{1}{t}) \sqrt{(\mu + t)(\mu + \frac{1}{t})(\mu + \frac{1}{q})}} \qquad (2\text{-}10.1)$$

where $t = \text{larger}\left(\sqrt{\frac{a_s}{a_t}}, \sqrt{\frac{a_t}{a_s}}\right)$ and $q = \frac{a_r}{\sqrt{a_s a_t}}$. The integral, I, appearing in Eq. (2-10.1) is elliptic and can be found in the tables of Byrd and Friedman (B54). Three subcases occur:

(Case (i-i): $t > \frac{1}{t} > q$ (B54 - 231.13)

$$I = 2\left(\frac{qt}{t - q}\right)^{5/2} \frac{1}{k^2 k'^4} \left[k'^2 F(\phi,k) + (1 + k^2)E(\phi,k) + k^2 \sin\phi \right.$$

$$\left. \times \left(\frac{\cos\phi}{\Delta(\phi,k)} + \frac{\Delta(\phi,k)}{\cos\phi} \right) \right] \qquad (3\text{-}10.1)$$

where $k = (1 - qt)^{1/2} \left(1 - \frac{q}{t}\right)^{-1/2}$, $\phi = \arccos \left(\frac{q}{t}\right)^{1/2}$, $k'^2 = 1 - k^2$, and $\Delta(\phi,k) = \sqrt{1 - k^2 \sin^2\phi}$. F and E are the incomplete elliptic integrals of first and second kind respectively.

Case (ii-i): $t > \frac{1}{q} > \frac{1}{t}$ (B54 - 231.12)

$$I = 2\left(\frac{t}{t^2 - 1}\right)^{\frac{5}{2}} \frac{1}{k^2 k'^2} \left[(1 - 2k^2)E(\phi,k) - k'^2 F(\phi,k) + k^2 \Delta(\phi,k) \tan\phi\right] \quad (4\text{-}10.1)$$

where $k = \left(t^2 - \frac{t}{q}\right)^{1/2} (t^2 - 1)^{-1/2}$ and $\phi = \arccos\left(\frac{1}{t}\right)$. k', Δ, E, and F are defined as before.

Case (iii-i): $t > \frac{1}{t} > \frac{1}{q}$ (B54 - 231.11)

$$I = 2\left(\frac{q}{qt - 1}\right)^{\frac{5}{2}} \frac{1}{k'^2 k^4} \left[(1 + k'^2)E(\phi,k) - 2k'^2 F(\phi,k) - \frac{k^2 \sin\phi \cos\phi}{\Delta(\phi,k)}\right] \quad (5\text{-}10.1)$$

where $k = (t^2 - 1)^{1/2}(t^2 - \frac{t}{q})^{-1/2}$ and $\phi = \arccos\left(\frac{1}{qt}\right)^{1/2}$.

Case (ii) $\rho_s = \rho_t = \frac{1}{2}$, $\rho_r = 1$

In this case

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}} (1 + 2\lambda a_t)^{-\frac{3}{2}} (1 + \lambda a_r)^{-1} \, d\lambda \quad (6\text{-}10.1)$$

If we again set $\mu = 2\lambda\sqrt{a_s a_t}$ R becomes

$$R = \left[\frac{1}{2}\left(t + \frac{1}{t}\right) + q\right] \int_0^\infty \left[\mu + \left(t + \frac{1}{t}\right)\mu + 1\right]^{-\frac{3}{2}} (1 + q\mu)^{-1} \, d\mu \quad (7\text{-}10.1)$$

where <u>now</u> $t = \sqrt{\frac{a_s}{a_t}}$ and $q = \frac{a_r}{2\sqrt{a_s a_t}}$. The integral in Eq. (7-10.1) can be performed with the aid of Pierce (P29) No. 199, No. 162, and No. 195. The result is:

$$R = \left[\frac{q + \frac{1}{2}\left(t + \frac{1}{t}\right)}{(q - t)\left(q - \frac{1}{t}\right)}\right]\left[\frac{q^2}{\sqrt{(q - t)\left(q - \frac{1}{t}\right)}} \times\right.$$

$$\left.\log\left\{\frac{\frac{q}{2}\left(t + \frac{1}{t}\right) - 1 - \sqrt{(q - t)\left(q - \frac{1}{t}\right)}}{q\left[q - \frac{1}{2}\left(t + \frac{1}{t}\right) - \sqrt{(q - t)\left(q - \frac{1}{t}\right)}\right]}\right\} - \frac{q\left(t + \frac{1}{t} + 1\right) - 1}{1 + \frac{1}{2}\left(t + \frac{1}{t}\right)}\right] \qquad (8\text{-}10.1)$$

<u>Case (iii): $\rho_s = \frac{1}{2}$, $\rho_t = 1$, $\rho_r = \frac{1}{2}$</u>

$$R = (a_s + a_t + a_r)\int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}}(1 + \lambda a_t)^{-2}(1 + 2\lambda a_r)^{-\frac{1}{2}}\, d\lambda \qquad (9\text{-}10.1)$$

If we set $\mu = 2\lambda\sqrt{a_s a_r}$, $t = \sqrt{\frac{a_s}{a_r}}$, $q = \frac{a_t}{2\sqrt{a_s a_r}}$ and $p = \frac{1}{2}\left(t + \frac{1}{t}\right)$

$$R = \left[\frac{1}{2}\left(t + \frac{1}{t}\right) + q\right]\int_0^\infty \left(\mu^2 + \left(t + \frac{1}{t}\right)\mu + 1\right)^{-\frac{1}{2}}(1 + \mu t)^{-1}(1 + \mu q)^{-2}\, d\mu \qquad (10\text{-}10.1)$$

Using the partial fractions identity:

$$\frac{1}{(1 + \mu t)(1 + \mu q)^2} = \frac{t^{-2}(q - t)^{-2}}{1 + \mu t} - \frac{qt(q - t)^{-2}}{1 + \mu q} + \frac{q(q - t)^{-1}}{(1 + \mu q)^2} \qquad (11\text{-}10.1)$$

R can be written as the sum of three integrals which can be performed with the aid of Pierce 195, 196, and 197. The result is

$$R = \left[\frac{q + \frac{1}{2}\left(t + \frac{1}{t}\right)}{(q - t)^2}\right]\left[\frac{t^2(q - 1)}{\frac{q}{2}\left(t + \frac{1}{t}\right) - 1} + \frac{q(q - 1)}{q - \frac{1}{t}} + \frac{q}{\sqrt{(q - t)\left(q - \frac{1}{t}\right)}} \times\right.$$

$$\left.\left\{t + \frac{\frac{q}{2}\left(t + \frac{1}{t}\right) - 1}{q - \frac{1}{t}}\right\}\log\left(\frac{q\left[q - \frac{1}{2}\left(t + \frac{1}{t}\right) - \sqrt{(q - t)\left(q - \frac{1}{t}\right)}\right]}{\frac{q}{2}\left(t + \frac{1}{t}\right) - 1 - \sqrt{(q - t)\left(q - \frac{1}{t}\right)}}\right)\right]$$

$$(12\text{-}10.1)$$

Case (iv): $\rho_s = \frac{1}{2}$, $\rho_t = 1$, $\rho_r = 1$

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}}(1 + \lambda a_t)^{-2}(1 + \lambda a_r)^{-1}\, d\lambda \qquad (13\text{-}10.1)$$

If we set $\mu = \lambda\sqrt{a_r a_t}$, $t = \sqrt{\frac{a_t}{a_r}}$, and $q = \frac{2a_s}{\sqrt{a_r a_t}}$, we have

$$R = \frac{t + \frac{1}{t} + \frac{1}{2}q}{q^{3/2}\, t} \int_0^\infty \left(\mu + \frac{1}{q}\right)^{-\frac{3}{2}}(\mu + t)^{-1}\left(\mu + \frac{1}{t}\right)^{-2} d\mu \qquad (14\text{-}10.1)$$

Using the partial fractions identity:

$$\frac{1}{(\mu + \frac{1}{q})(\mu + t)(\mu + \frac{1}{t})^2} = \frac{1}{(t - \frac{1}{q})(\frac{1}{t} - \frac{1}{q})^2(\mu + \frac{1}{q})} + \frac{1}{(\frac{1}{q} - t)(\frac{1}{t} - t)^2(\mu + t)}$$

$$+ \frac{1}{(\frac{1}{q} - \frac{1}{t})(t - \frac{1}{t})(\mu + \frac{1}{t})^2} + \frac{1}{(\frac{1}{q} - \frac{1}{t})^2(\frac{1}{t} - t)^2(\mu + \frac{1}{t})}$$

(15-10.1)

R can be written as the sum of four integrals which can be performed with Pierce 101, 114, and 119. The result is

$$R = \left[\frac{t + \frac{1}{t} + \frac{1}{2}q}{tq^{3/2}}\right]\left[\frac{2\sqrt{q}}{(t - \frac{1}{q})(\frac{1}{t} - \frac{1}{q})^2} + \frac{\log\left(\frac{1 + \sqrt{1 - qt}}{1 - \sqrt{1 - qt}}\right)}{(\frac{1}{q} - t)^{3/2}(t - \frac{1}{t})^2}\right.$$

$$\left. + \frac{\frac{t}{\sqrt{q}} - \frac{1}{2}\left(\frac{1}{q} - \frac{1}{t}\right)^{-\frac{1}{2}} \log\left(\frac{1 + \sqrt{1 - \frac{q}{t}}}{1 - \sqrt{1 - \frac{q}{t}}}\right)}{(\frac{1}{q} - \frac{1}{t})^2(t - \frac{1}{t})} + \frac{(\frac{2}{t} - t - \frac{1}{q}) \log\left(\frac{1 + \sqrt{1 - \frac{q}{t}}}{1 - \sqrt{1 - \frac{q}{t}}}\right)}{(\frac{1}{q} - \frac{1}{t})^{5/2}(t - \frac{1}{t})^2}\right]$$

(16-10.1)

Case (v): $\rho_s = 1,\ \rho_t = 1,\ \rho_r = \frac{1}{2}$

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + \lambda a_s)^{-2}(1 + \lambda a_t)^{-2}(1 + 2\lambda a_r)^{-\frac{1}{2}}\, d\lambda \qquad (17\text{-}10.1)$$

With the notation $\mu = \lambda\sqrt{a_s a_t}$, $t = \sqrt{\frac{a_s}{a_t}}$, and $q = \frac{2a_r}{\sqrt{a_s a_t}}$,

$$R = \frac{t + \frac{1}{t} + \frac{1}{2}q}{\sqrt{q}} \int_0^\infty (\mu + \tfrac{1}{t})^{-2}(\mu + t)^{-2}(\mu + \tfrac{1}{q})^{-\frac{1}{2}}\, d\mu \qquad (18\text{-}10.1)$$

Using the partial fractions identity

$$\frac{1}{(\mu + \frac{1}{t})^2(\mu + t)^2} = \frac{1}{(t - \frac{1}{t})^2(\mu + \frac{1}{t})^2} + \frac{1}{(t - \frac{1}{t})^2(\mu + t)^2}$$

$$- \frac{2}{(t - \frac{1}{t})^3(\mu + \frac{1}{t})} + \frac{2}{(t - \frac{1}{t})^3(\mu + t)} \qquad (19\text{-}10.1)$$

R can be written in terms of four integrals which can also be evaluated using Pierce 101, 114, and 119. The result is:

$$R = \left[\frac{t + \frac{1}{t} + \frac{1}{2}q}{\sqrt{q}\,(t - \frac{1}{t})^2}\right]\left[\frac{\frac{t}{\sqrt{q}} - \frac{1}{2}\left(\frac{1}{q} - \frac{1}{t}\right)^{-1/2}\log\left(\frac{1 + \sqrt{1 - \frac{q}{t}}}{1 - \sqrt{1 - \frac{q}{t}}}\right)}{(\frac{1}{q} - \frac{1}{t})}\right.$$

$$+ \frac{\frac{1}{t\sqrt{q}} - \frac{1}{2}(\frac{1}{q} - t)^{-1/2}\log\left(\frac{1 + \sqrt{1 - qt}}{1 + \sqrt{1 - qt}}\right)}{(\frac{1}{q} - t)}$$

$$- 2 \frac{\log\left(\dfrac{1 + \sqrt{1 - \frac{q}{t}}}{1 - \sqrt{1 - \frac{q}{t}}}\right)}{(t - \frac{1}{t})(\frac{1}{q} - \frac{1}{t})^{1/2}} + 2 \frac{\log\left(\dfrac{1 + \sqrt{1 - qt}}{1 - \sqrt{1 - qt}}\right)}{(t - \frac{1}{t})(\frac{1}{q} - t)^{1/2}} \Bigg] \tag{20-10.1}$$

<u>Case (vi): $\rho_s = \rho_t = \rho_r = 1$</u>

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + \lambda a_s)^{-2}(1 + \lambda a_t)^{-2}(1 + \lambda a_r)^{-1}\, d\lambda \tag{21-10.1}$$

If we set $\mu = \lambda \sqrt{a_s a_t}$, $t = \sqrt{\dfrac{a_s}{a_t}}$, and $q = \dfrac{a_r}{\sqrt{a_s a_t}}$ we have

$$R = \frac{t + \frac{1}{t} + q}{q} \int_0^\infty (\mu + t)^{-2}(\mu + \tfrac{1}{t})^{-2}(\mu + \tfrac{1}{q})^{-1}\, d\mu \tag{22-10.1}$$

Using Eq. (19-10.1) and Pierce 39 and 42 we have

$$R = \left[\frac{t + \frac{1}{t} + q}{q(t - \frac{1}{t})^2}\right]\left[\frac{\log\left(\frac{q}{t}\right) - 1 + \frac{t}{q}}{(\frac{1}{t} - \frac{1}{q})^2} + \frac{\log(qt) - 1 + \frac{1}{qt}}{(t - \frac{1}{q})^2}\right.$$

$$- 2 \frac{\log\left(\frac{q}{t}\right)}{(t - \frac{1}{t})(\frac{1}{t} - \frac{1}{q})} + 2 \frac{\log(qt)}{(t - \frac{1}{t})(t - \frac{1}{q})} \tag{23-10.1}$$

Let us next turn to cases in which one $\rho = \infty$. There are seven such cases in all; in only two can the ratio R be expressed in terms of tabulated functions. In the remaining cases we must be content with an expansion which will, in general, be a good representation when the radiative width ($\rho = \infty$) is small

compared to the geometric mean of the other two (neutron) widths. This latter requirement is usually fulfilled in practice.

Case (vii): $\rho_s = \rho_t = \frac{1}{2}$, $\rho_r = \infty$

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}} (1 + 2\lambda a_t)^{-\frac{3}{2}} e^{-\lambda a_r} d\lambda \qquad (24\text{-}10.1)$$

Making the substitutions $\mu = 2\lambda \sqrt{a_s a_t}$, $p = \frac{1}{2}\left(\sqrt{\frac{a_s}{a_t}} + \sqrt{\frac{a_t}{a_s}}\right)$, and

$q = \frac{a_r}{\sqrt{a_s a_t}}$, we can write

$$R = (p + \tfrac{q}{2}) \int_0^\infty (\mu^2 + 2p\mu + 1)^{-\frac{3}{2}} e^{-\frac{1}{2} q\mu} d\mu \qquad (25\text{-}10.1)$$

If we integrate twice by parts and add and subtract $\mu + p$ to the integrand of the resulting integral we obtain

$$R(p + \tfrac{q}{2})^{-1} = \frac{1 - \frac{1}{2} q}{1 + p} + \frac{(\frac{1}{2} q)^2}{p^2 - 1} \int_0^\infty (\mu + p) \left[1 - \sqrt{1 - \frac{p^2 - 1}{(\mu + p)^2}}\right] e^{-\frac{1}{2} qu} du \qquad (26\text{-}10.1)$$

If we expand the square root in the integral in the powers of $\frac{p^2 - 1}{(\mu + p)^2}$ and integrate term-by-term we obtain the following series for R:

$$R = \left[p + \tfrac{1}{2} q\right] \left[(1 + p)^{-1} - (\tfrac{1}{2} q)(1 + p)^{-1} + (\tfrac{1}{2} q)^2 e^{\frac{1}{2} pq} \times \right.$$

$$\left. \sum_{n=1}^{\infty} \frac{(|2n - 3|)!!}{(2n)!!} E_{2n-1}(\tfrac{1}{2} pq) \left(\frac{p^2 - 1}{p^2}\right)^{n-1}\right] \qquad (27\text{-}10.1)$$

where the E's are the E_n functions defined in connection with Eq. (23-10). The double factorial notation was defined in paragraph (3-8). The convergence of this series is good if $q << 1$ or $p^2 - 1 << 1$.

Case (viii): $\rho_s = \frac{1}{2}$, $\rho_t = 1$, $\rho_r = \infty$

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}} (1 + \lambda a_t)^{-2} e^{-\lambda a_r} d\lambda \tag{28-10.1}$$

If we set $\mu^2 = 1 + 2a_s\lambda$, $t = \sqrt{\frac{2a_s}{a_t}}$, $q = \frac{a_r}{\sqrt{2a_s a_t}}$, and $r^2 = t^2 - 1$, we can write

$$R = t^2(t^2 + 2 + qt)\, e^{\frac{q}{t}} \int_1^\infty \frac{d\mu}{\mu^2(\mu^2 + r^2)^2} \cdot e^{-\frac{q}{t}\mu^2} \tag{29-10.1}$$

Now

$$\mu^2(\mu^2 + r^2)^{-2} = \sum_{k=o}^{\infty} (-)^k (k + 1) \frac{r^{2k}}{\mu^{2(k + 3)}} \tag{30-10.1}$$

Thus

$$R = t^2(t^2 + 2 + qt) \times \sum_{k=o}^{\infty} (-)^k (k + 1)\, r^{2k}\, N_{k+3}\left(\frac{q}{t}\right) \tag{31-10.1}$$

where N_k is defined in Eq. (49a-7). This series converges rapidly if $r << 1$, but if $r \geq 1$ and q is small it does not. This defect can be remedied as follows:

From Eq. (50-7) it follows that

$$N_{k+1}(\alpha) = \sum_{m=o}^{k} (-)^m \frac{(2k - 2m-1)!!}{(2k + 1)!!} (2\alpha)^m + \frac{(-)^{k+1}(2\alpha)^{k+1}}{(2k + 1)!!} N_o(\alpha) \tag{32-10.1}$$

Inserting this series in Eq. (31-10.1) and interchanging the order of summation one obtains

$$R = t^2(t^2 + 2 + qt)\left[\sum_{n=o}^{\infty} (-)^n \left(\frac{2q}{t}\right)^n \left\{\sum_{k=\max(0,n-2)}^{\infty} (-)^k \frac{(2k + 3 - 2n)!!}{(2k + 5)!!} (k + 1)r^{2k}\right\}\right.$$

$$\left. - N_o \left(\frac{q}{t}\right) \sum_{n=o}^{\infty} \frac{(n + 1)}{(2n + 5)!!} r^{2n} \left(\frac{2q}{t}\right)^{n+3}\right] \qquad (33\text{-}10.1)$$

The curly braces (k-series) can be summed in closed form for the various values of n as follows: For n = 0, it follows from Eq. (30-10.1)

$$\sum_{k=o}^{\infty} (-)^k \frac{k + 1}{2k + 5} r^{2k} = \int_1^{\infty} \frac{d\mu}{\mu^2(\mu^2 + r^2)^2} = \frac{1}{r^5}\left(r - \frac{3}{2} \arctan r + \frac{1}{2} \frac{r}{1 + r^2}\right) \qquad (34\text{-}10.1)$$

Any of the other k-series may be generated from this relation by multiplying by an appropriate power of r and integrating. E.g., the k series for n = 1 can be obtained as follows:

$$\sum_{k=o}^{\infty} (-)^k(k + 1) \frac{r^{2k}}{(2k + 5)(2k + 1)} = r^{-3} \int \frac{dr}{r^3}\left(r - \frac{3}{2} \arctan r + \frac{1}{2} \frac{r}{1 + r^2}\right)$$

$$= \frac{1}{2r^3} - \frac{1}{4r^4} + \frac{3 + r^2}{4r^5} \tan^{-1} r \qquad (35\text{-}10.1)$$

This procedure is particularly useful when q is small and r is not, so that only a few terms need be taken in the n-series, while many must be taken in the k-series.

Case (ix): $\rho_s = \rho_t = 1, \quad \rho_r = \infty$

$$R = (a_s + a_t + a_r) \int_o^{\infty} (1 + \lambda a_s)^{-2}(1 + \lambda a_t)^{-2} e^{-\lambda a_r} d\lambda \qquad (36\text{-}10.1)$$

Substituting $\mu = \lambda\sqrt{a_s a_t}$, $t = \sqrt{\frac{a_s}{a_t}}$, and $q = \frac{a_r}{\sqrt{a_s a_t}}$ we have

$$R = \left(t + \frac{1}{t} + q\right) \int_0^\infty \left(\mu + \frac{1}{t}\right)^{-2} (\mu + t)^{-2} e^{-q\mu}\, d\mu \tag{37-10.1}$$

If we make use of Eq. (19-10.1) and the equality

$$\int_0^\infty \frac{e^{-bx}}{(x + a)^n}\, dx = a^{1-n} e^{ab} E_n(ab) \tag{38-10.1}$$

We can write the final result:

$$R = \left[\frac{t + \frac{1}{t} + q}{\left(t - \frac{1}{t}\right)^2}\right]\left[te^{\frac{q}{t}} E_2\left(\frac{q}{t}\right) + \frac{1}{t} e^{qt} E_2(qt) - \frac{2e^{\frac{q}{t}} E_1\left(\frac{q}{t}\right)}{t - \frac{1}{t}} \quad \frac{2e^{qt} E_1(qt)}{t - \frac{1}{t}}\right] \tag{39-10.1}$$

<u>Case (x): $\rho_s = \frac{1}{2}$, $\rho_t = \infty$, $\rho_r = \frac{1}{2}$</u>

$$R = (a_s + a_t + a_r) \int_0^\infty (1 + 2\lambda a_s)^{-\frac{3}{2}} e^{-\lambda a_t} (1 + 2\lambda a_r)^{-\frac{1}{2}}\, d\lambda \tag{40-10.1}$$

If we set $\mu = 2\lambda\sqrt{a_s a_r}$, $t = \sqrt{\frac{a_r}{a_s}}$, and $q = \frac{a_t}{\sqrt{a_r a_s}}$ then

$$R = \frac{1}{2}\left(t^2 + 1 + qt\right) \int_0^\infty (\mu + t)^{-\frac{3}{2}} \left(\mu + \frac{1}{t}\right)^{-\frac{1}{2}} e^{-\frac{1}{2}q\mu}\, d\mu \tag{41-10.1}$$

An integration by parts gives after some rearrangement

$$R = \frac{1}{2}\left(t^2 + 1 + qt\right)\left[\frac{2}{1 - t^2} + \frac{q}{t - \frac{1}{t}} \int_0^\infty e^{-\frac{1}{2}q\mu} \left(1 - \frac{t - \frac{1}{t}}{\mu + t}\right)^{\frac{1}{2}} d\mu\right] \tag{42-10.1}$$

Expanding the root in powers of $\dfrac{t - \frac{1}{t}}{\mu + t}$ and using Eq. (38-10.1) one obtains

$$R = \frac{1}{2}(t^2 + 1 + qt)\left[\frac{2}{1+t} - qe^{\frac{1}{2}qt}\sum_{k=1}^{\infty}\frac{(|2k-3|)!!}{(2k)!!}E_k\left(\frac{1}{2}qt\right)\left(\frac{t^2-1}{t^2}\right)^{k-1}\right] \tag{43-10.1}$$

<u>Case (xi): $\rho_s = \frac{1}{2}$, $\rho_t = \infty$, $\rho_r = 1$</u>

$$R = (a_s + a_t + a_r)\int_0^{\infty}(1 + 2\lambda a_s)^{-\frac{3}{2}}(1 + \lambda a_r)^{-1}e^{-\lambda a_t}\,d\lambda \tag{44-10.1}$$

Setting $\mu^2 = 1 + 2a_s\lambda$, $t = \sqrt{\dfrac{a_s}{a_r}}$, $q = \dfrac{a_t}{\sqrt{a_s a_r}}$, $r^2 = 2t^2 - 1$, we can write

$$R = 2(1 + t^2 + qt)\cdot e^{\frac{q}{2t}}\int_1^{\infty}\frac{e^{-\frac{q}{2t}\mu^2}\,d\mu}{\mu^2(\mu^2 + r^2)} \tag{45-10.1}$$

Now:

$$\mu^{-2}(\mu^2 + r^2)^{-1} = \sum_{k=0}^{\infty}(-)^k\frac{r^{2k}}{\mu^{2(k+2)}} \tag{46-10.1}$$

Hence:

$$R = 2(1 + t^2 + qt)\sum_{k=0}^{\infty}(-)^k r^{2k} N_{k+2}\left(\frac{q}{2t}\right) \tag{47-10.1}$$

Substituting Eq. (32-10.1) in Eq. (47-10.1) and interchanging the order of summation we obtain

$$R = 2(1 + t^2 + qt) \left[\sum_{n=o}^{\infty} (-)^n \left(\frac{q}{t}\right)^n \left\{ \sum_{k=\max(0,n-1)}^{\infty} (-)^k r^{2k} \frac{(2k + 1 - 2n)!!}{(2k + 3)!!} \right\} \right.$$

$$\left. + N_o \left(\frac{q}{2t}\right) \sum_{n=o}^{\infty} \frac{r^{2n} \left(\frac{q}{t}\right)^{n+2}}{(2n + 3)!!} \right] \qquad (48\text{-}10.1)$$

The k-series can be summed explicitly starting from the n = 0 k-series:

$$\sum_{k=o}^{\infty} (-)^k \frac{r^{2k}}{2k + 3} = \int_1^{\infty} \frac{d\mu}{\mu^2(\mu^2 + r^2)} = \frac{1}{r^2} \left(1 - \frac{1}{r} \arctan r\right) \qquad (49\text{-}10.1)$$

<u>Case (xii): $\rho_s = 1, \rho_t = \infty, \rho_r = \frac{1}{2}$</u>

$$R = (a_s + a_t + a_r) \int_o^{\infty} (1 + \lambda a_s)^{-2} e^{-\lambda a_t} (1 + 2\lambda a_r)^{-\frac{1}{2}} d\lambda \qquad (50\text{-}10.1)$$

If we set $\mu^2 = 1 + 2\lambda a_r$, $t = \sqrt{\frac{a_r}{a_s}}$, $q = \frac{a_t}{\sqrt{a_s a_r}}$, and $r^2 = 2t^2 - 1$, we have:

$$R = 4t^2(1 + t^2 + qt) \int_1^{\infty} \frac{e^{-\frac{q}{2t}\mu^2} d\mu}{(\mu^2 + r^2)^2} \qquad (51\text{-}10.1)$$

Since

$$(\mu^2 + r^2)^{-2} = \sum_{k=o}^{\infty} (-)^k (k + 1) \frac{r^{2k}}{\mu^{2(k + 2)}} \qquad (52\text{-}10.1)$$

$$R = 4t^2(1 + t^2 + qt) \sum_{k=o}^{\infty} (-)^k (k + 1) r^{2k} N_{k+2}\left(\frac{q}{2t}\right) \qquad (53\text{-}10.1)$$

Substituting Eq. (32-10.1) in Eq. (53-10.1) and interchanging the order of summation we obtain

$$R = 4t^2(t^2 + 1 + qt)\left[\sum_{n=o}^{\infty} (-)^n \left(\frac{q}{t}\right)^n \left\{\sum_{k=\max(0,n-1)}^{\infty} (-)^k(k + 1)\, r^{2k} \frac{(2k + 1 - 2n)!!}{(2k + 3)!!}\right\}\right.$$

$$+ N_o \left(\frac{q}{2t}\right) \sum_{n=o}^{\infty} \frac{(n + 1)r^{2n} \left(\frac{q}{t}\right)^{n+2}}{(2n + 3)!!} \qquad (54\text{-}10.1)$$

The k-series can be summed explicitly starting from the n = 0 k-series

$$\sum_{k=o}^{\infty} (-)^k \frac{(k + 1)r^{2k}}{2k + 3} = \int_1^{\infty} \frac{d\mu}{(\mu^2 + r^2)^2} = \frac{1}{2r^2}\left(\frac{1}{r} \arctan r - \frac{1}{1 + r^2}\right) \qquad (55\text{-}10.1)$$

<u>Case (xiii): $\rho_s = 1,\ \rho_t = \infty,\ \rho_r = 1$</u>

$$R = (a_s + a_t + a_r) \int_o^{\infty} (1 + \lambda a_s)^{-2}\, e^{-\lambda a_t}\, (1 + \lambda a_r)^{-1}\, d\lambda \qquad (56\text{-}10.1)$$

If we set $\mu = \lambda\sqrt{a_s a_r}$, $t = \sqrt{\frac{a_s}{a_r}}$, and $q = \frac{a_t}{\sqrt{a_s a_r}}$ R becomes

$$R = \frac{t^2 + qt + 1}{t^2} \int_o^{\infty} \left(\mu + \frac{1}{t}\right)^{-2} (\mu + t)^{-1}\, e^{-q\mu}\, d\mu \qquad (57\text{-}10.1)$$

Using the partial fractions expansion

$$\frac{1}{(\mu + \frac{1}{t})^2(\mu + t)} = \frac{1}{(t + \frac{1}{t})(\mu + \frac{1}{t})^2} - \frac{1}{(t - \frac{1}{t})^2(\mu + \frac{1}{t})} + \frac{1}{(t - \frac{1}{t})^2(\mu + t)} \qquad (58\text{-}10.1)$$

and Eq. (38-10.1) we can write finally

$$R = \left[\frac{t^2 + qt + 1}{t^2 - 1}\right]\left[e^{\frac{q}{t}} E_2\left(\frac{q}{t}\right) - \frac{e^{\frac{q}{t}} E_1(q/t)}{t^2 - 1} + \frac{e^{qt} E_1(qt)}{t^2 - 1}\right] \tag{59-10.1}$$

CHAPTER 11. AN ANALYSIS OF NEUTRON REACTIONS IN U^{238}

1. In the previous chapter a formalism was developed permitting rapid calculation of the effect of fluctuations in the widths on reaction cross sections. With this preparation we can attempt the calculation of average reaction cross sections. The rationale which will be adopted in this chapter is to attempt to deduce the strength functions for the various partial waves from experimental data. As we shall see for U^{238} some rough theoretical considerations together with the low energy resonance data serve to determine the s- and d-wave strength functions. The available reaction data can then be used to determine the p- and f-wave strength functions. As it happens, there are enough reaction data to overdetermine the p-wave strength function, so that agreement among the individual determinations gives the theory a measure of absolute significance.

In order to carry out an analysis of the data it is necessary to know the spins and parities of any states excited in the reaction. A 2+ state has been observed(H54,D55b) at 44 kev, and states have been observed (A57,C57b) at 146 and 306 kev. From the energy ratios it has been concluded that the latter states are the 4+ and 6+ members of the ground state rotational band. States have also been observed at 700 kev and above(C57a,B56) but no information is available concerning their spins and parities. For this reason only reactions which occur with bombarding energies between 0 and 0.5 Mev will be considered.

2. A number of further assumptions have been made which limit the number of unknown quantities involved in the analysis. These are:

(i) Γ_γ is taken constant in energy, and independent of $J\pi$. It has been chosen equal to 24 mv. At the time these calculations were carried out this value was believed to be best; it agrees quite

well with the value of 25 mv used in Chapter 9, the difference being well within experimental error.

(ii) $D_{J\pi}$ is taken proportional to $(2J + 1)^{-1}$ with an energy dependence given by Lang and LeCouteur (L56). With this assumption $D \equiv \frac{(2J + 1)D_{J\pi}}{2(2I + 1)}$ is the level spacing observed with $\ell = 0$ neutrons. It is taken as 18 ev at zero bombarding energy.

(iii) The ratio $S_\ell = \left\langle \gamma^2_{J\pi s\ell} \right\rangle / D_{J\pi}$, the strength function, is taken independent of $J\pi$ and s. We have chosen $S_o = 0.036$ which is consistent with choosing $\Gamma^o_n = 2.5$ mv, D = 18 ev, and a nuclear radius of about 9f. The assumption of $J\pi$ and s independence deserves some further comment. A model for calculating the dependence of S on $J\pi s$ and has been suggested by Wigner, Lane, and Thomas (L55). On their view, the interaction of the neutron with the nucleus can be described in terms of an average potential, a point of view adopted by other workers (F54) on less fundamental grounds than those of (L55). The single particle levels of the average potential then "share" their reduced neutron width with nearby levels of the actual compound nucleus. The energy interval over which this sharing is considered appreciable is taken to be somewhat less than the separation of the single particle levels, giving rise to the now well known "giant resonance" phenomena. If the average potential is a spherically symmetric one with no spin dependent terms then S_ℓ is independent of $J\pi$ and s, and depends only on ℓ. [It is worth noting at this point that then the $B_L(\alpha,\alpha')$ take exactly the same form in either the Ij or $s\ell$

representations (see Chapter 12). In this chapter we shall use the more familiar channel spin ($s\ell$) representation.] It has been suggested, however, that the average potential does contain a spin-orbit coupling term, and the effect this will have on the following analysis is discussed in Chapter 12.

(iv) The fourth and last assumption is that $S_0 = S_2$, and that both these quantities are constant in the energy range 0 to 0.5 Mev.

This assumption is based on the following qualitative considerations: If one examines a plot of S_o (at zero bombarding energy) vs A (see, for example reference Z56) one notices that mass number 238 is situated at a minimum. Now, if the range and depth (only the product VR^2 is important here) of the average potential are taken to be smoothly varying functions of mass number, then the single particle levels will move smoothly past zero bombarding energy, E, into the well as VR^2 increases. Minimum S_o in this simple picture corresponds to s-wave single particle levels roughly symmetrically placed around E = 0, so as to insure that dS_o/dE vanishes at E = 0. For, if the range and depth of the well parameters are smooth functions of mass number $\frac{dS_o}{dE} \propto \frac{dS_o}{dA} = 0$. In such a case, if the width of the single particle levels is much larger than 0.5 Mev, S_o will not vary much in the first 0.5 Mev. The absorption width of the single particle levels is of the order of twice the imaginary part of the potential in the complex potential model (which is formally identical with that of L55); for the potential suggested by Weisskopf (W56b) this is about 7.0 Mev.

Near each s-wave level lies a d-wave level with a very similar wave function. Let us first consider a square well, and let us define the position

of a level by the vanishing of the logarithmic derivative of the radial wave function. [The radial wave function, u is defined by $\psi = \frac{u_\ell(r)}{r} Y_{\ell m}(\theta,\phi)$. This boundary condition corresponds to a level shift upwards of ℓ, the orbital momentum quantum number, times the single particle reduced width of the level, at zero bombarding energy.] As is shown in Appendix (1-11), the s-d splitting is then given by

$$\frac{1}{2}\frac{\Delta E}{E} = \frac{\Delta x}{x} = \frac{3}{x^2} \qquad (1\text{-}11)$$

where E is approximately the energy of either level measured from the bottom of the well, and $x = R/\lambda\!\!\!^-$, the ratio of the well radius to the inside reduced neutron width. Equation (1-11) is based on the assumption that $x >> \ell$, which is true for the virtual levels we are considering. For a well about 40 Mev deep, and 9 f in radius, Eq. (1-11) gives a splitting of about 1.5 Mev, at zero bombarding energy. This difference corresponds to about a 2% difference in wave length.

One can argue that if the edge of the well is tapered the splitting calculated with Eq. (1-11) will not change much, i.e., the s- and d-levels will travel together. This is because after several oscillations the wave functions have roughly the same shape, they have the same phase at the nuclear surface, and very nearly the same wave length. Only when the perturbation extends into the region where the action of the centrifugal potential is important will the splitting be altered. By an extension of the foregoing argument it may be expected that the contribution of these levels to their respective strength functions will be nearly the same, since the latter quantity depends only on the value of the wave function on the nuclear

surface. Hence we expect that $S_2 = S_o$ and that both quantities are fairly constant in the first 0.5 Mev of neutron energy.

It is possible to verify these conjectures by exact calculation in the case of a complex square well. Results of such a calculation are given in Table (1-11). X_o is the ratio of the nuclear radius to the inside wave

Table (1-11). s- and d-Strength Functions for a Complex Square Well

		E = 10 kev		E = 500 kev	
X_o	γ	S_o	S_2	S_o	S_2
11.65	0.03	0.01237	0.01017	0.009338	0.007733
11.95	0.03	0.007167	0.006320	0.006070	0.005434
12.25	0.03	0.005287	0.004902	0.004794	0.004609
12.55	0.03	0.004695	0.004563	0.004470	0.004642
12.85	0.03	0.004965	0.005093	0.004927	0.005608

length at zero bombarding energy, and γ is the ratio of the imaginary and real parts of the potential. When $X_o = 12.55$, which roughly corresponds to a minimum in S_o as a function of X_o, S_o and S_2 appear constant and equal within some 5% or less. Changing X_o from this value by ± 0.30, which corresponds to about a ± 2 Mev change in the well depth and level positions for uranium, keeps the constancy of S_o and S_2 within about 13% or less.

3. A considerable amount of data has been reported for inelastic scattering and radiative capture in U^{238} below 0.5 Mev (H55a, H57a, A57, C57b, B55, B56, N56b). Enough data is available on inelastic scattering to draw a continuous curve from 150 kev to about 2 Mev. Unfortunately, most of these data suffer from a systematic defect, viz.: only partial resolution of elastic neutrons and

neutrons scattered from the 44 kev state. Perhaps the easiest way to see this is to compare the time-of-flight measurements (C57b) at 550 kev with measurements made by other techniques at the same energy. The time-of-flight measurements clearly resolve the 44 kev level, as can be seen by inspection of the reported time spectra, and give a total non-elastic cross section of 1800 mb. On the other hand, the work of Allen (A57) and Batchelor (B56), both of which were done by sphere transmission and proportional counting, fail to resolve the 44-kev level as can be seen from an inspection of the reported pulse-height spectra. Both these experiments give a non-elastic cross section of about 800 mb, which is significantly lower than the time-of-flight value. Allen discusses the effects of this imperfect resolution on his experiments and concludes that his values for the excitation cross section of the 44-kev state, $\sigma(2+)$, by 150 kev neutrons and for the excitation cross section of the 146 kev state, $\sigma(4+)$, by 250 kev and 500 kev neutrons are probably correct. However, comparison of his value for $\sigma(4+)$ at 500 kev, viz., 490 $\pm$ 250 mb, and at 250 kev, viz., 290 $\pm$ 159 mb, with the time-of-flight value at 550 kev, viz., 290 $\pm$ 60 mb, indicates that Allen's values of $\sigma(4+)$ are probably too high. Since these values were obtained by a rather uncertain "unpeeling" technique we are inclined to the opinion that a systematic error is present in the analysis favoring too high values for $\sigma(4+)$. No such possibility of error arises in the case of the 150 kev data, where only the 44-kev state is excited; according to Allen inelastic neutrons ought to be separable from elastic neutrons at this bombarding energy.

4. Let us consider the available data at 550 kev, summarized in Table (2-11). In this table B(2+) is the coefficient of the $\cos^2\theta$ term

Table (2-11). Experimental Values of Cross Sections for E = 550 kev

Quantity	Measurement	Reference
σ (2+)	1430 $\pm$ 200 mb	C57b
σ (4+)	290 $\pm$ 60 mb	C57b
B (2+)	-0.45 $\pm$ 0.10	C57b
$\sigma(n,\gamma)$	135 $\pm$ 15 mb	B56, H55a

in the angular distribution, $1 + B\cos^2\theta$, of the neutrons inelastically scattered from the 2+ state. It has been determined experimentally that the coefficients of higher powers of $\cos\theta$ and zero. Only one value of $\sigma(n,\gamma)$ is given, and it represents an average of several excellently agreeing data reported in the corresponding reference.

According to Eq. (9-2), (10-2), (6-2) and (8-2), if we only consider s-, p-, d-, and f-waves, we can write

$$\frac{\sigma(2+)}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T_o(2T_2')}{T_o + 2T_2' + T_\gamma} \right\rangle_{\frac{1}{2}+} + \left\langle \frac{T_1(T_1' + T_3')}{T_1 + T_1' + T_3' + T_3'' + T_\gamma} \right\rangle_{\frac{1}{2}-}$$

$$+ 2\left\langle \frac{T^2(T_o' + 2T_2')}{T_2 + T_o' + 2T_2' + T_2'' + 2T_\gamma} \right\rangle_{\frac{3}{2}+} + 2\left\langle \frac{T_1(2T_.' + 2T_3')}{T_1 + 2T_1' + 2T_3' + 2T_3'' + 2T_\gamma} \right\rangle_{\frac{3}{2}-}$$

$$+ 3\left\langle \frac{T_2(T_o' + 2T_2')}{T_2 + T_o' + 2T_2' + 2T_2'' + 3T_\gamma} \right\rangle_{\frac{5}{2}+} + 3\left\langle \frac{T_3(2T_1' + 2T_3')}{T_3 + 2T_1' + 2T_3' + T_1'' + 2T_3'' + 3T_\gamma} \right\rangle_{\frac{5}{2}-}$$

$$+ 4\left\langle \frac{T_3(T_1' + 2T_3')}{T_3 + T_1' + 2T_3' + 2T_1'' + 2T_3'' + 4T_\gamma} \right\rangle_{\frac{7}{2}-} \qquad \text{(2a-11)}$$

$$\frac{\sigma(4+)}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T_1 T_3''}{T_1 + T_1' + T_3' + T_3'' + T_\gamma} \right\rangle_{\frac{1}{2}-} + 2\left\langle \frac{T_2 T_2''}{T_2 + T_o' + 2T_2' + T_2'' + 2T_\gamma} \right\rangle_{\frac{3}{2}+}$$

$$+ 2\left\langle \frac{T_1(2T_3'')}{T_1 + 2T_1' + 2T_3' + 2T_3'' + 2T_\gamma} \right\rangle_{\frac{3}{2}-} + 3\left\langle \frac{T_2(2T_2'')}{T_2 + T_o' + 2T_2' + 2T_2'' + 3T_\gamma} \right\rangle_{\frac{5}{2}+}$$

$$+ 3\left\langle \frac{T_3(T_1'' + 2T_3'')}{T_3 + 2T_1' + 2T_3' + T_1'' + 2T_3'' + 3T_\gamma} \right\rangle_{\frac{5}{2}-} + 4\left\langle \frac{T_3(2T_1'' + 2T_3'')}{T_3 + T_1' + 2T_3' + 2T_1'' + 2T_3'' + 4T_\gamma} \right\rangle_{\frac{7}{2}-} \tag{2b-11}$$

$$\frac{\sigma(n\gamma)}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T_o T_\gamma}{T_o + 2T_2' + T_\gamma} \right\rangle_{\frac{1}{2}+} + \left\langle \frac{T_1 T_\gamma}{T_1 + T_1' + T_3' + T_3'' + T_\gamma} \right\rangle_{\frac{1}{2}-}$$

$$+ 2\left\langle \frac{T_2(2T_\gamma)}{T_2 + T_o' + 2T_2' + T_2'' + 2T_\gamma} \right\rangle_{\frac{3}{2}+} + 2\left\langle \frac{T_1(2T_\gamma)}{T_1 + 2T_1' + 2T_3' + 2T_3'' + 2T_\gamma} \right\rangle_{\frac{3}{2}-}$$

$$+ 3\left\langle \frac{T_2(3T_\gamma)}{T_2 + T_o' + 2T_2' + 2T_2'' + 3T_\gamma} \right\rangle_{\frac{5}{2}+} + 3\left\langle \frac{T_3(3T_\gamma)}{T_3 + 2T_1' + 2T_3' + T_1'' + 2T_3'' + 3T_\gamma} \right\rangle_{\frac{5}{2}-}$$

$$+ 4\left\langle \frac{T_3(4T_\gamma)}{T_3 + T_1' + 2T_3' + 2T_1'' + 2T_3'' + 4T_\gamma} \right\rangle_{\frac{7}{2}-} \tag{2c-11}$$

The notation is as follows:

$$T_\ell = 4\pi \cdot s_\ell \cdot \frac{\langle \gamma^2_{J\pi\ell} \rangle}{D_{J\pi}} = 4\pi \cdot s_\ell \cdot S_\ell \tag{3-11}$$

We have omitted the subscript s on the reduced width, since we are specifically assuming it independent of the channel spin. T_ℓ of course is independent of $J\pi$, and is the penetrability factor of Hauser and Feshbach (H52). An unprimed T refers to the entrance channel ($I\pi = 0+$), a singly primed T refers to the exit channel in which the 44-kev state is excited ($I\pi = 2+$), and a doubly primed T refers to an exit channel in which the 146-kev state is excited ($I\pi = 4+$). Excitation of higher states in the ground state rotational band has been ignored because of the high angular momentum changes involved. Finally

$$T_\gamma = \frac{2\pi\Gamma_\gamma}{D} \text{ where } D = \frac{(2J + 1)D_{J\pi}}{2(2I + 1)} \qquad (4\text{-}11)$$

In accordance with the level density law of Lang and LeCouteur (L54) D has been taken to be 7.2 ev at 550 kev. The subscripts at the lower right of each term give the spin and parity of the associated compound state. The brackets denote averages with respect to the distribution of widths. For the purposes of this averaging each T has as many degrees of freedom as the coefficient which multiplies it ($\epsilon = 0,1,2$), except T_γ which always has $\nu = \infty$.

Equations (2a, b, c-11) possess a very useful property which arises from the fact that all the states excited in the reactions we are considering have the same parity. The orbital angular momenta involved in the formation and decay of a given compound state must always have the same parity. Hence some terms in Eqs. (2-11) only involve s- and d-waves, while others only involve p- and f-waves. Thus if a fixed ratio is assumed between the p- and f-wave strength functions, and if the radiative width is a small part of the total

width, Eqs. (2a-11) and (2b-11) can be written as linear functions of the p-wave strength function,* viz.:

$$\sigma = \sigma_{even} + \sigma^*_{odd}\left(\frac{S_1}{S_1^*}\right) \tag{5-11}$$

Here σ_{even} is the contribution to the cross section from the even parity terms calculated for $S_o = S_2 = 0.0358$, and σ^*_{odd} is the contribution from the odd parity terms for a value of the p-wave strength function equal to S_1^*. This linear relation allows rapid solution for the values of S_1 required to fit the experimental values of $\sigma(2+)$ and $\sigma(4+)$. If the ratio of p- to f-wave strength function has been chosen properly the two values of S_1 determined from $\sigma(2+)$ and $\sigma(4+)$ will be identical. Furthermore, by similar reasoning, $\sigma(n,\gamma)$ should be nearly independent of the p-wave strength function, except for very small values which make T_γ an appreciable part of the total width in the odd parity terms.

If we choose the ratio $\frac{S_3}{S_1} = 3$ and $S_1^* = S_o$, we obtain from Eqs. (2-11) the results

$$\sigma(2+) = 570 + 760\ (S_1/S_o)\ \text{mb} \tag{6a-11}$$

$$\sigma(4+) = 88 + 180\ (S_1/S_o)\ \text{mb} \tag{6b-11}$$

$$\sigma(n\gamma) = 140\ \text{mb} \tag{6c-11}$$

The linear law for $\sigma(2+)$ and $\sigma(4+)$, and the constancy of $\sigma(n\gamma)$ ought to hold quite accurately since T_γ is never more than about 5% of the total denominator in any of the terms in Eqs. (2-11). Choosing $\frac{S_1}{S_o} = 1.13$, gives $\sigma(2+) = 1430$ mb,

*This linear relation has been checked by direct calculation; these results are reported below.

$\sigma(4+) = 291$ mb in excellent agreement with experiment. Hence, the initial choice $\frac{S_3}{S_1} = 3$ was correct. Finally, the value of $\sigma(n\gamma)$ is in excellent agreement with experiment.

It may be asked with what precision the values of $\frac{S_1}{S_1^*}$ and $\frac{S_3}{3S_1}$ are determined by the above procedure? This question can be answered roughly as follows: As it happens the f-wave contribution to the total width in the odd parity terms of Eq. (2-11) is about 5 to 8% of the total. Hence, Eqs. (6a-11) and (6b-11) can be written

$$\sigma(2+) = 570 + \frac{S_1}{S_0}\left[520 + 210\left(\frac{S_3}{3S_1}\right) + 26\left(\frac{S_3}{3S_1}\right)^2\right] \qquad (7a\text{-}11)$$

$$\sigma(4+) = 88 + \frac{S_1}{S_0}\left[170\left(\frac{S_3}{3S_1}\right) + 13\left(\frac{S_3}{3S_1}\right)^2\right] \qquad (7b\text{-}11)$$

The first term in the bracket in Eq. (7a-11) represents events in which a p-wave neutron is incident and excident; the terms linear in $\left(\frac{S_3}{3S_1}\right)$ represent events in which a p- (f-) wave neutron is incident and f- (p-) wave neutron is excident; the terms quadratic in $\left(\frac{S_3}{3S_1}\right)$ represent events in which an f-wave neutron is incident and excident. Plotted in Fig. (1-11) are four curves defined by Eqs. (7-11) and obtained by setting $\sigma(2+)$ and $\sigma(4+)$ equal to the reported value $\pm$ the reported experimental error. Any point inside the area defined by these curves will give value of $\sigma(2+)$ and $\sigma(4+)$ within the reported errors. The cross marks the most probable values of $\frac{S_1}{S_0}$ and $\frac{S_3}{3S_1}$. Since the reported errors are stated to be 50% larger than the standard deviation of the measurements (C57b), the probability of any point lying inside the area is about 75%. The vertices are rather improbable; indeed, the probability

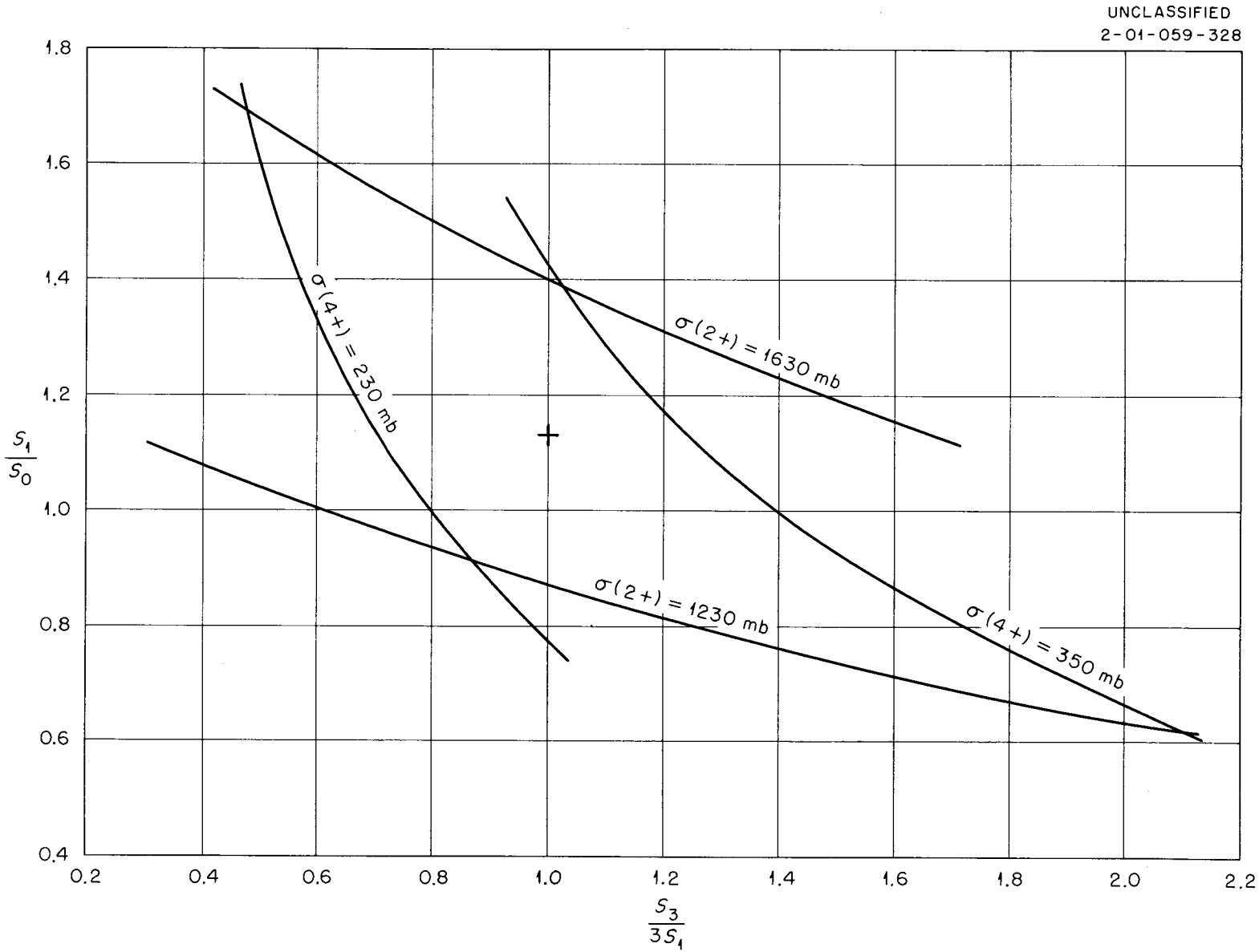
UNCLASSIFIED
2-01-059-328
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
$\frac{S_1}{S_0}$
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
$\frac{S_3}{3S_1}$
σ(4+) = 230 mb
σ(2+) = 1630 mb
σ(2+) = 1230 mb
σ(4+) = 350 mb

Fig. 1-11.

of lying outside both sets of lines is only about 2%. A rough estimate of the precision in the determination of $\frac{S_1}{S_0}$ and $\frac{S_3}{3S_1}$ is $\sim$ 30%.

5. The importance of correctly taking the fluctuations in the widths into account can be seen by analyzing the results analogous to Eqs. (7-11) in the case of no fluctuations, viz:

$$\sigma(2+) = 850 + \frac{S_1}{S_0}\left[900 + 245\left(\frac{S_3}{3S_1}\right) + 20\left(\frac{S_3}{3S_1}\right)^2\right] \tag{8a-11}$$

$$\sigma(4+) = 87 + \frac{S_1}{S_0}\left[190\left(\frac{S_3}{3S_1}\right) + 10\left(\frac{S_3}{3S_1}\right)^2\right] \tag{8b-11}$$

$\frac{S_3}{3S_1} = 2.70$, $\frac{S_1}{S_0} = 0.34$ is a solution to these equations; as one can readily see it is much different from the correct solution. For $\frac{S_3}{3S_1} = \frac{S_1}{S_0} = 1$ for which Eqs. (6-11), (7-11), and (8-11) are exact, $\sigma(2+)$ and $\sigma(4+)$ equal 1330 mb and 270 mb, respectively, with fluctuations and 2020 mb and 290 mb, respectively, without fluctuations. $\sigma(n\gamma)$ in these two cases is 140 mb with fluctuations and 130 mb without.

$\sigma(4+)$ and $\sigma(n,\gamma)$ are not strongly affected by the fluctuations in the neutron widths, although the individual terms in Eqs. (2-11) are. In $\sigma(4+)$ and $\sigma(n\gamma)$ a substantial portion of the cross section comes from terms in which a competing width greatly exceeds the sum of the entrance and exit widths. As pointed out in paragraph (5-11) such terms may be enhanced by the effect of fluctuations. The remaining terms are decreased by the fluctuations, and quite fortiutously, a near cancellation occurs. The case is otherwise with $\sigma(2+)$ where the net effect of fluctuations is to decrease the cross section by about 40%.

6. According to Eqs. (9-2) (10-2), (6-2), and (8-2), if we only consider s-, p-, d-, and f-waves, we can write

$$4B_2(2+) = -2.857 \left\langle \frac{T_2 T_2'}{T_2 + 2T_2' + T_2'' + 2T_\gamma} \right\rangle_{\frac{3}{2}} + -2.400 \left\langle \frac{T_1(T_1' - T_3')}{T_1 + 2T_1' + 2T_3' + 2T_3'' + 2T_\gamma} \right\rangle_{\frac{3}{2}} -$$

$$-0.6857 \left\langle \frac{T_3 T_1'}{T_3 = 2T_1' + 2T_3' + T_1'' + 2T_3'' + 3T_\gamma} \right\rangle_{\frac{5}{2}} -$$

$$+3.543 \left\langle \frac{T_3 T_3'}{T_3 + 2T_1' + 2T_3' + T_1'' + 2T_3'' + 3T_\gamma} \right\rangle_{\frac{5}{2}} -$$

$$+5.714 \left\langle \frac{T_3 T_1'}{T_3 + T_1' + 2T_3' + 2T_1'' + 2T_3'' + 4T_\gamma} \right\rangle_{\frac{7}{2}} -$$

$$+8.254 \left\langle \frac{T_3 T_3'}{T_3 + T_1' + 2T_3' + 2T_1'' + 2T_3'' + 4T_\gamma} \right\rangle_{\frac{7}{2}} - \qquad (9\text{-}11)$$

The notation is the same as before. The Z-coefficients were obtained from the tables of L. C. Biedenharn (B53a). Again choosing $\frac{S_3}{S_1} = 3$ and $S_1^* = S_0$ we have

$$2\pi\lambda\!\!\!^{-2} B_2(2+) = -40 - \frac{S_1}{S_0}\left[120 - 57\left(\frac{S_3}{3S_1}\right) - 10\left(\frac{S_3}{3S_1}\right)^2\right] \text{mb} \qquad (10\text{-}11)$$

It follows from Eqs. (10-11) and (9-2) that

$$B(2+) = \frac{3R}{2 - R} \; ; \quad R = \frac{B_2(2+)}{B_0(2+)} = \frac{2\pi\lambda\!\!\!^{-2} B_2(2+)}{\sigma(2+)} \tag{11-11}$$

Choosing $\frac{S_1}{S_0} = 1.13$ and $\frac{S_3}{3S_1} = 1$, $B(2+) = -0.10$ which is too low by a factor of about 4.5, and differs from the experimental value by more than 3 times the quoted error (4.5 standard deviations). Reasonable changes in $\frac{S_1}{S_0}$ and $\frac{S_3}{3S_1}$ cause very little change in the calculated value of B(2+). This discrepancy will be discussed in some detail later.

7. Table (3-11) summarizes the available data at 150 kev. If we again

Table (3-11). Experimental Values of Cross Sections at 150 kev

Cross Section	Measurement	Reference
$\sigma(n\gamma)$	160 ± 8 mb	B56
	200* mb	H55a
	240* mb	N56b
$\sigma(2+)$	440 ± 200 mb	A57

*Graphical interpolation.

choose $\frac{S_3}{3S_1} = 1$ and $S_1^* = S_0$ and choose D = 13.9 ev in accordance with reference L54 we obtain

$$\sigma(2+) = 190 + 490\left(\frac{S_1}{S_0}\right) \tag{12a-11}$$

$$\sigma(n\gamma) = 180 \text{ mb} \tag{12b-11}$$

For this case the linear dependence of $\sigma(2+)$ on $\frac{S_1}{S_0}$ has been checked by direct calculation. For $\frac{S_3}{3S_1} = 1$ and $S_1^* = 3S_0$ we obtain $\sigma(2+) = 1760$ mb directly, and 1660 from Eq. (12a-11), a difference of only 6%. For $\sigma(n\gamma)$ we obtain

205 mb directly, verifying the rough constancy of the radiative cross section. Since the linear law holds fairly accurately over such a large range of $\frac{S_1}{S_0}$ (a factor of 3) it should be much more accurate for smaller changes in $\frac{S_1}{S_0}$. Moreover, it should hold more accurately at higher energies, where the radiative width is a smaller fraction of the total width. For $\frac{S_1}{S_0} = 1.13$, $\sigma(2+)$ is given by Eq. (12a-11) as 740 mb, which is somewhat larger than the datum in Table (3-11). In view of the strong possibility that the datum in Table (3-11) is an underestimate we are not inclined to look upon this discrepancy as serious.

8. The insensitivity of the radiative capture cross section above the inelastic threshold to the value of $\frac{S_1}{S_0}$ makes it useless for a determination of this ratio. However, it can be used to check some of the assumptions used in the calculations. For example, if $D_{J\pi}$ is chosen to be independent of J rather than proportional to $(2J + 1)^{-1}$, the inelastic cross sections remain the same, but the radiative cross section will fall. At 150 kev (with $\frac{S_3}{3S_1} = \frac{S_1}{S_0} = 1$) this fall is about 45% from 180 mb to 125 mb, substantially worsening agreement. Again if the decrease of about 30% in the level spacing predicted by Lang and LeCouteur (L54) in going from zero bombarding energy to 150 kev is not permitted, the inelastic cross section remains unchanged, but the radiative cross section falls by about 30% to 140 mb. At 550 kev the decrease is by more than a factor of 2. This necessity for using the level density law of Lang and LeCouteur to calculate the radiative cross section correctly has been carefully pointed out by Lane and Lynn (L57).

Below the inelastic threshold, the radiative width becomes a substantial portion of the total width in the odd parity terms, and the radiative capture cross section is no longer independent of the ratio $\frac{S_1}{S_0}$. Hence, the radiative capture cross section can be used to determine S_1. Plotted in Fig. (2-11) are some experimental points of Newson (N56b) together with the 95% confidence limits of error (see Appendix 2-11). Also included in the figure are several curves calculated with Eq. (2c-11). Below 44 kev, of course, all singly and doubly primed T's vanish. In addition, f-wave contributions are to the total widths are extremely small, and have been neglected. The points above 10 kev agree quite well with the curve for $\frac{S_1}{S_0} = 1.35$, although any curve for which $\frac{S_1}{S_0}$ is between 1 and 2 is probably consistent with the data. The radiative capture cross section at 25 kev has been measured independently by Macklin, Lazar, and Lyon (M57) who obtain a value of 610 ± 61 mb, in good agreement with Newson. Their single determination gives $\frac{S_1}{S_0} = 1.6 \pm 0.5$. Agreement of the calculated curves for which $S_1 \gtrsim S_0$ with the data points below 10 kev is not too bad except at 6 kev. Whether the apparent point of inflection in the range 6-9 kev is real or not has already been the subject of considerable discussion. Newson has suggested that the inflection is due to the appearance of a rapidly rising p-wave contribution, but the smooth behavior of the calculated curves seem to contradict this hypothesis.

Cameron (C57b) has suggested a way of fitting the radiative cross section below 200 kev by allowing a dependence of the radiative width on the neutron orbital angular momentum. In particular, for p-waves he recommends $\Gamma_\gamma = 80$ mv. Plotted in Fig. (3-11) are several curves calculated with this

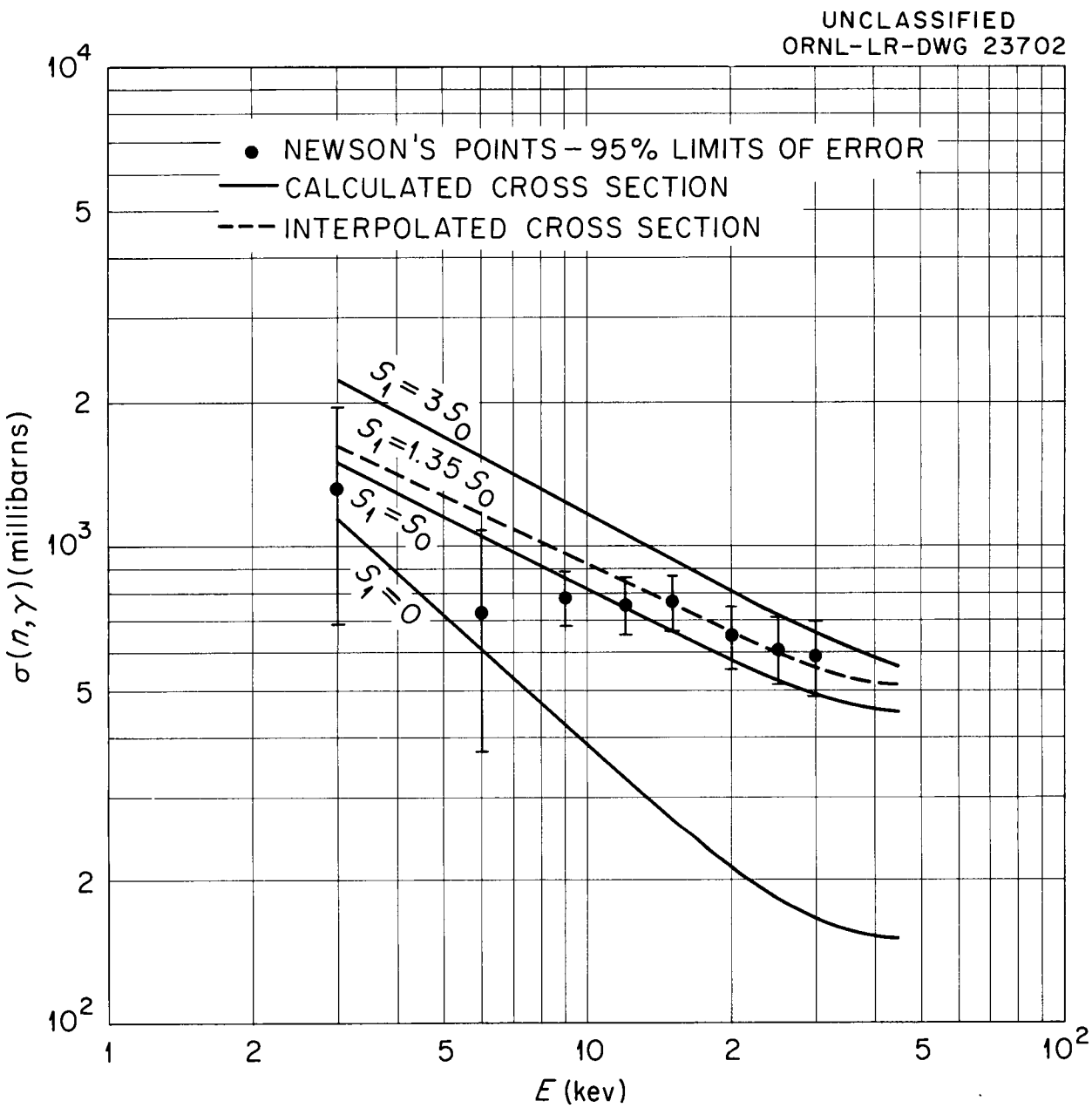

Fig. 2-11. Radiative Capture Cross Section as a Function of Energy.

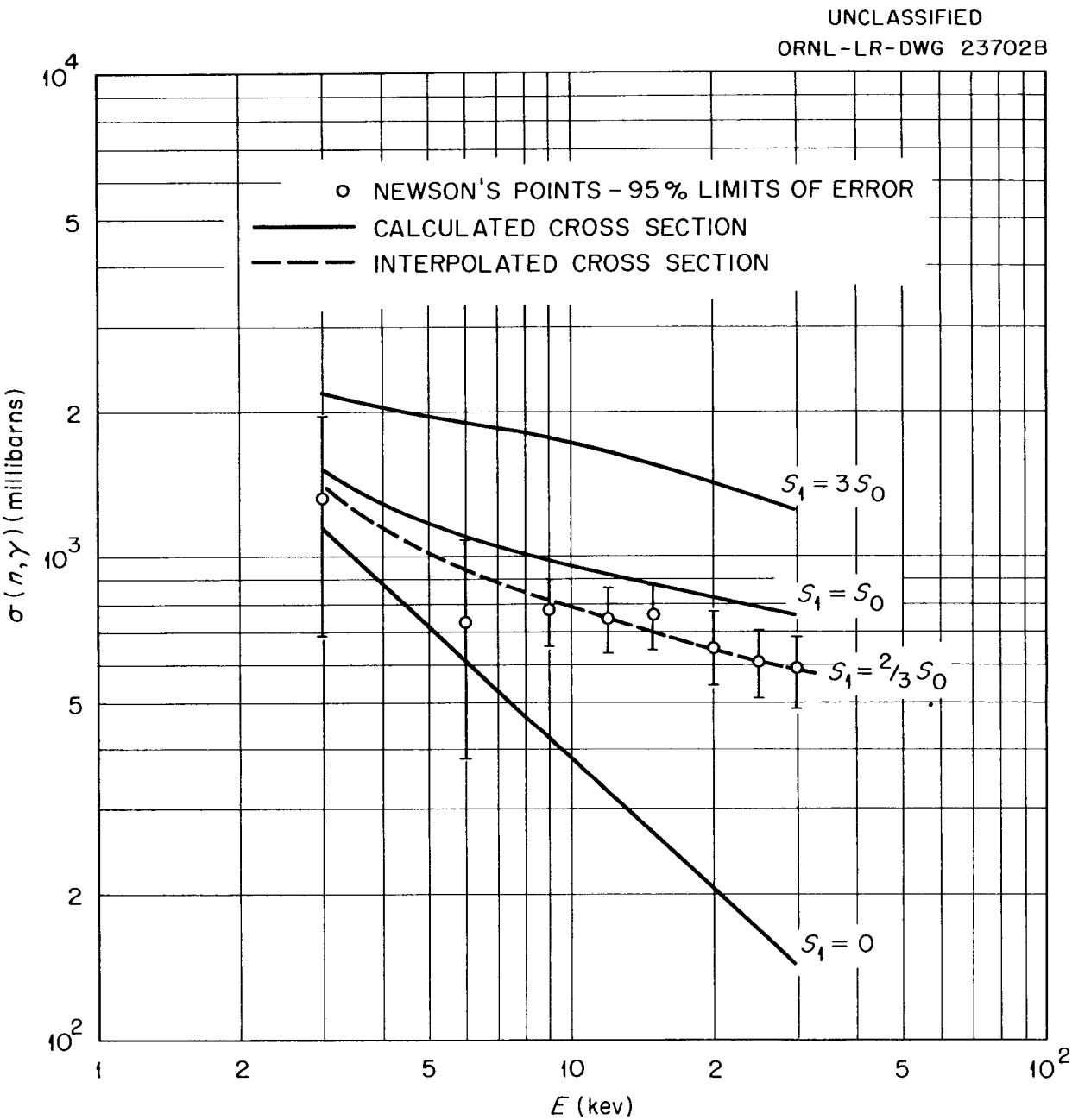

Fig. 3-11. Radiative Capture Cross Section as a Function of Energy.

assumption (and $\Gamma_{\gamma s} = \Gamma_{\gamma d} = 24$ mv). The curve for $S_1 = \frac{2}{3} S_0$ fits the data very well, except perhaps at 6 kev. Cameron's assumptions unfortunately have another important and disadvantageous consequence. To illustrate, let us consider radiative capture at 150 kev, where the f-wave contribution to $\sigma(n\gamma)$ will be small. With Cameron's assumption the s- and p-wave contributions to $\sigma(n\gamma)$ are already about 270 mb which is comparable with the experimental value. The additional d-wave contribution, calculated assuming Γ_γ for d-waves is 24 mv, is about 50 mb, making the total about 320 mv. This is considerably larger than the experimental value. At 550 kev, a similar situation occurs, where the sum of the s- and p-wave contributions is 150 mb, which is again comparable with experiment. The estimated d- and f-wave contributions (assuming $\Gamma_{\gamma d} = \Gamma_{\gamma f} = 24$ mv) raise this about 230 mb, which is much larger than the experimental value. Only if radiative capture of d- and f-wave neutrons nearly vanishes are Cameron's assumptions tenable.

9. By way of summary, then, it appears that the ratio $\frac{S_1}{S_0} \sim 1.1$ at 550 kev, and perhaps slightly higher (~ 1.4) at ~ 10 kev. The ratio $\frac{S_3}{3S_1} \sim 1$ at 550 kev. These choices appear to satisfactorily explain all of the total reaction cross section data within the limits of experimental uncertainty. With regard to the single datum concerning the angular distribution of neutrons inelastically scattered from the 44-kev state, the agreement of theory and experiment is poor. It has been suggested by Chase and Wilets (C57c) that an improvement might be expected if a significant portion of the excitation of the 44-kev state occurred by direct interaction with the non-spherical surface of the uranium nucleus. Calculations by these authors using a spheroidal variant of a typical optical model potential indicated about a 100 mb direct

excitation cross section for 550 kev neutrons. As a further check on this point a rough calculation was performed by the present author with the perturbation theory of Brink (B55a). The nucleus was assumed black with a radius of 9 b and a depth normalized to the measured s-wave strength function. This choice at least insures that the s-, p-, and d-wave strength functions are roughly the same as we have previously found, and that the s-wave potential scattering length is nearly equal to the experimental value found by Seth (S56c). With these parameters Brink's theory gives a cross section for direct excitation of the 44-kev state for 550 kev neutrons of 100 mb. If this direct cross section is assumed to have a B_2-coefficient of -1, which is the maximum possible if no higher Legendre components are present (as appears experimentally to be the case), then B(2+) is increased in magnitude to about -0.20 which is still much too low. Indeed, the direct excitation cross section would have to be nearly 400 mb and as anisotropic as allowable to account for the observed anisotropy in the total 44-kev excitation cross section. Finally, Cranberg (C57a)has stated that the results of successive runs on the accelerator used in the time-of-flight work did not repeat within the statistical uncertainties, and further that the conditions which gave the best data were only achieved once. In light of these remarks we are inclined not to attach too much significance to the discrepancy in predicted and measured B(2+) at 550 kev.

Appendix (1-11). Virtual Levels of a Square Well

The virtual levels of a square well are defined by the condition $f_\ell = 0$, where

$$f_\ell = 1 + \frac{xj_\ell'}{j_\ell} \tag{1-11.1}$$

and where j_ℓ are the spherical Bessel functions and the primes denote differentiation with respect to x, the channel radius in units of the inside reduced wave length. Now it has been shown by Feshbach, Porter, and Weisskopf (F54) to follow easily from the recurrence relations for the j_ℓ that

$$f_\ell = \frac{x^2}{\ell - f_{\ell-1}} - \ell \tag{2-11.1}$$

Furthermore, if we differentiate Eq. (1-11.1) with respect to x and then use Eq. (1-11.1) and the second order differential equation for the j_ℓ to eliminate the second derivatives we can write

$$\frac{df_\ell}{dx} = \frac{(\ell + 1 - f_\ell)(\ell + f_\ell) - x^2}{x} \tag{3-11.1}$$

Now by two applications of Eq. (2-11.1) we can write

$$f_{\ell+1} = \frac{x^2}{2\ell + 1 - \dfrac{x^2}{\ell - f_{\ell-1}}} - (\ell + 1) \tag{4-11.1}$$

Thus if $f_{\ell-1}(x_-) = 0$,

$$f_{\ell+1}(x_-) = \frac{x_-^2}{2\ell + 1 - \dfrac{x_-^2}{\ell}} - (\ell + 1) \tag{5-11.1}$$

Suppose $f_{\ell+1}(x_+) = 0$. If $x_- - x_+$ is small we can write

$$f_{\ell+1}(x_-) = (x_- - x_+) \frac{df_{\ell+1}}{dx_+} \tag{6-11.1}$$

It then follows from Eqs. (6-11.1), (5-11.1), and (3-11.1), after rearrangement, that

$$\frac{x_- - x_+}{x_+} = (2\ell + 1) \frac{x_-^2 - \ell(\ell + 1)}{\left[x_+^2 - (\ell + 1)(\ell + 2)\right]\left[x_-^2 - \ell(2\ell + 1)\right]} \tag{7-11.1}$$

When $x \gg \ell$, Eq. (7-11.1) reduces to

$$\frac{\Delta x}{x} = \frac{2\ell + 1}{x^2} \tag{8-11.1}$$

Clearly Eq. (7-11.1) is only valid when the left hand side is $\ll 1$, for which the condition is $x \gg \ell$.

The reduced neutron widths, γ^2, of these levels can now easily be found. According to the method of "perturbation of boundary conditions" described in the book of Blatt and Weisskopf (B52a)

$$\gamma_\ell^2 = -\left(\frac{\partial f_\ell}{\partial E}\right)^{-1} \tag{9-11.1}$$

evaluated at the point at which $f_\ell = 0$. But from Eq. (3-11.1) it follows that

$$\left(\frac{\partial f_\ell}{\partial E}\right)_{f_\ell=0} = \left(\frac{\partial f_\ell}{\partial x}\right)_{f_\ell=0}\left(\frac{dx}{dE}\right)_{f_\ell=0} = \frac{\ell(\ell + 1) - x^2}{2(E + V)} \tag{10-11.1}$$

where V is the depth of the well. Then

$$\gamma_\ell^2 = \frac{2(E + V)}{x^2 - \ell(\ell + 1)} \tag{11-11.1}$$

If the potential well has a small imaginary part, the virtual levels also have an absorption width given by

$$W_\ell = -2\,(\mathrm{Im} f_\ell)_{f_\ell=0}\,\gamma_\ell^2 \qquad (12\text{-}11.1)$$

where γ_ℓ^2 is the reduced neutron width (which is still calculated for the real well as described above), and $\mathrm{Im} f_\ell$ is the imaginary part of f_ℓ evaluated at the point where $f_\ell = 0$ for the real part of the potential. If $x = x_R + ix_I$, and if $x_I << x_R$

$$f_\ell(x_R + ix_I) = f_\ell(x_R) + ix_I f_\ell'(x_R) \qquad (13a\text{-}11.1)$$

$$= ix_I \cdot \frac{\ell(\ell+1) - x_R^2}{x_R} \qquad (13b\text{-}11.1)$$

since $f_\ell(x_R) = 0$. If ζ is the ratio of the real to imaginary part of the square well, $x_I/x_R = 1/2\,\zeta$ if $\zeta << 1$ and $V >> E$. In such a case

$$W = 2\zeta(E + V) \approx 2\zeta V \qquad (14\text{-}11.1)$$

Appendix (2-11). Estimation of Statistical Errors for Newson's Data

Newson's reported data does not include any error estimate, but it is possible to obtain one since at some energies the results of two independent determinations are given. If we assume that individual cross section determinations are normally distributed with mean m, and variance σ, then we may ask the following question: If we choose n independent determinations with mean M and variance S, what is the probability that $|m - M| \geq kS$? This question is answered by a theorem of statistics (C56a) which states that M is normally distributed with mean m and variance $\sigma/\sqrt{n}$, and that the random variable nS^2/σ^2 is distributed in a chi-squared distribution of n - 1 degrees of freedom. For n = 2, the variable $\zeta = \sqrt{2}\,\frac{m - M}{\sigma}$ is normally distributed with zero mean and unit variance. The probability that $|m - M| \geq kS$ is the probability that $|\zeta| \geq k\sqrt{2}\,\frac{S}{\sigma}$ $\left(\text{which equals Erfc}\left[k\sqrt{2}\,\frac{S}{\sigma}\right]\right)$ averaged over the σ-distribution. Since the square of the variable $\frac{S\sqrt{2}}{\sigma} = \tau$ is distributed in a chi-squared distribution of one degree of freedom, we can write

$$P(|m - M| \geq kS) = \int_0^\infty \mathrm{Erfc}(k\tau)(2\pi\tau^2)^{-\frac{1}{2}}\, e^{-\frac{1}{2}\tau^2}\, d(\tau^2) \qquad (1\text{-}11.2)$$

Now

$$\frac{dP}{dk} = -\frac{\sqrt{2}}{\pi}\int_0^\infty e^{-(k^2+\frac{1}{2})\tau^2}\, d(\tau^2) = -\frac{\sqrt{2}}{\pi}\,\frac{1}{k^2+\frac{1}{2}} \qquad (2\text{-}11.2)$$

and

$$P(0) = 1 \qquad (3\text{-}11.2)$$

Thus

$$P = \text{constant} \times \int_{k\sqrt{2}}^{\infty} \frac{dy}{y^2 + 1} \qquad (4\text{-}11.2)$$

The integral is elementary; combining Eqs. (4-11.2) and (3-11.2) we obtain

$$P(|m - M| \geq kS) = \frac{2}{\pi}\left[\frac{\pi}{2} - \arctan(k\sqrt{2})\right] \qquad (5a\text{-}11.2)$$

$$= \frac{2}{\pi} \operatorname{arccot}(k\sqrt{2}) \qquad (5b\text{-}11.2)$$

Some numerical values are given in Table (1-11.2) below. The distribution has a very slowly vanishing tail, very unlike the normal distribution in which nearly all the area is concentrated with three variances of the mean.

Table (1-11.2)

k	0	1/2	1	3/2	2	5/2	3	5	10
$P(\lvert m - M\rvert \geq kS)$	1	0.61	0.40	0.28	0.22	0.18	0.15	0.09	0.04_5

CHAPTER 12. ANALYSIS OF NEUTRON REACTIONS IN U^{238} (continued)

1. It is the purpose of this chapter to analyze the effect of spin-orbit forces in the optical potential on the conclusions of the last chapter. We shall carry this program out in the following steps:

(i) First, we shall derive the connection between the strength functions of the actual nucleus and the parameters of the levels of the optical potential.

(ii) Using the strength functions deduced from experiment in the last chapter we shall then determine the positions of the single particle levels using the results of (i).

(iii) Thirdly, we shall estimate the level splitting induced by the spin-orbit part of the optical potential.

(iv) Then we shall use these split levels to obtain the strength functions in the presence of spin-orbit coupling.

(v) Finally, we shall examine the changes which result in the calculated cross sections.

2. According to Feshbach, Porter, and Weisskopf the optical potential is so chosen that the diagonal elements of its scattering matrix, $\eta_{\alpha j\ell,\alpha j\ell}$, are equal to the averages over many resonances of the diagonal elements of the actual scattering matrix, $\left\langle S^{J\pi}_{\alpha j\ell,\alpha j\ell}\right\rangle$. This stipulation implies as it is intended to that the total cross sections in the various channels of the actual nucleus averaged over many resonances are correctly given by the optical model. This can easily be seen by slightly generalizing the procedure outlined by Feshbach, Porter, and Weisskopf in connection with Eq. (2.7) of their paper (F54) to Eq. (4.7) of reference (B52) in the Ij representation [see Eq. (11-2)]. Let us first consider the case of target spin zero ($I = 0$, $J = j$).

The average of $S^{J\pi}_{\alpha j\ell,\alpha j\ell}$ can be obtained from Eq. (7-2) using the relation

$$\int_{-\infty}^{+\infty} \frac{dx}{x - i\epsilon} = i\pi; \quad \epsilon > 0 \tag{1-12}$$

It is

$$\left\langle S^{J\pi}_{\alpha j\ell,\alpha j\ell} \right\rangle = e^{2i\xi\alpha\ell}\left(1 - \frac{\pi\left\langle \Gamma_{\alpha j\ell}\right\rangle}{D_{J\pi}}\right) \tag{2-12}$$

It then follows from Eq. (2-12) that

$$1 - \left|\eta_{\alpha j\ell,\alpha j\ell}\right|^2 = \frac{2\pi\left\langle \Gamma_{\alpha j\ell}\right\rangle}{D_{J\pi}}\left(1 - \frac{\pi}{2}\,\frac{\left\langle \Gamma_{\alpha j\ell}\right\rangle}{D_{J\pi}}\right) \tag{3-12}$$

At fairly low energies, where the resonances are well separated, the second quantity in the parenthesis is usually quite small compared to unity. Even at 0.5 Mev, in the calculations described in the last chapter, $\frac{\pi}{2}\,\frac{\left\langle \Gamma_{\alpha j\ell}\right\rangle}{D_{J\pi}}$ never exceed about 0.15. In view of the comparatively large uncertainties in the strength functions calculated in the last chapter, we feel nothing is lost by setting the parenthesis equal to unity in Eq. (4-12). Finally, the scattering matrix for the optical model is also given, in the vicinity of a single particle level, by Eq. (7-2).* If we identify the parameters of the single particle levels by dots above them, then it follows that

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*Since the optical scattering matrix is not unitary, the usual derivation of Eq. (7-2) is not applicable. The result can be obtained using the channel elimination procedure of Teichmann and Wigner [cf. R. G. Thomas, Phys. Rev. 97 224 (1955)], or more simply, by the method of "perturbation of boundary conditions" of Blatt and Weisskopf (B52a).

$$\frac{2\pi \left\langle \Gamma_{\alpha j \ell} \right\rangle}{D_{J\pi}} = \frac{\dot{\Gamma}_{\alpha j \ell}(\dot{\Gamma} - \dot{\Gamma}_{\alpha j \ell})}{(E - \dot{E}_o)^2 + \left(\frac{\dot{\Gamma}}{2}\right)^2} \tag{4-12}$$

The resonance energy $\dot{E}_o$ contains the so-called level shift, and can be written

$$\dot{E}_o = \dot{E}_{\ell j} - \Delta_\ell \, \dot{\gamma}^2_{\alpha j \ell} \tag{5-12}$$

where Δ_ℓ is defined in Eq. (18-2), and $\dot{E}_{\ell j}$ is the formal resonance energy, defined by the vanishing of the logarithmic derivative of the radial wave function on the nuclear surface. Combining Eq. (4-12) and (3-12) we can write

$$\frac{\left\langle \dot{\gamma}^2_{\alpha j \ell} \right\rangle}{D_{J\pi}} \equiv S_{\alpha j \ell} = \frac{\dot{\gamma}^2_{\alpha j \ell}}{2\pi} \; \frac{(\dot{\Gamma} - \dot{\Gamma}_{\alpha j \ell})}{(E - \dot{E}_{\ell j} + \Delta_\ell \, \dot{\gamma}^2_{\alpha j \ell})^2 + \left(\frac{\dot{\Gamma}}{2}\right)^2} \tag{6-12}$$

where $S_{\alpha j \ell}$ is the strength function in the channel $\alpha j \ell$, assumed independent of J and π. Equation (6-12) has been arrived at assuming the target spin, I, is zero. If this is not so and the equality of $\eta_{\alpha j \ell, \alpha j \ell}$ and $\left\langle S^{J\pi}_{\alpha j \ell, \alpha j \ell} \right\rangle$ must be replaced by

$$\eta_{\alpha j \ell, \alpha j \ell} = \sum_{J=|j-I|}^{j+I} \frac{2J + 1}{(2j + 1)(2I + 1)} \left\langle S^{J\pi}_{\alpha j \ell, \alpha j \ell} \right\rangle \tag{7-12}$$

If we assume that $S_{\alpha j \ell}$ is independent of $J\pi$, then so is $\left\langle S^{J\pi}_{\alpha j \ell, \alpha j \ell} \right\rangle$. The summation then gives unity, and the final result is again Eq. (6-12). [The correct many level generalization of Eq. (6-12) is

$$S_{\alpha \ell j} = -\frac{1}{\pi} \; \frac{\mathrm{Im}\, f_{\alpha \ell j}}{(\mathrm{Re}\, f_{\alpha \ell j} - \Delta_\ell)^2 + (\mathrm{Im}\, f_{\alpha \ell j} - s_\ell)^2} \tag{8-12}$$

where $f_{\alpha \ell j}$ is the logarithmic derivative of the radial wave function corresponding to a scattering function $\eta_{\alpha \ell j, \alpha \ell j}$].

3. As we have seen in the last chapter from a study of the uranium s-wave and strength function, near zero bombarding energy a condition of s- (and d-) wave anti-resonance exists. We expect, therefore, that there are odd parity single particle states near zero bombarding energy. We shall, therefore, try to explain the p- and f-strength functions deduced in the last chapter on the basis of one single particle level approximation using Eq. (6-12). According to the arguments presented in paragraph (2-11) the reduced widths for the odd-parity levels ought to be nearly equal, since near the nuclear surface the wave functions are very similar. Furthermore, as previously pointed out, the p-f level splitting for the actual optical potential ought to be the same as for a square well of comparable depth and radius. Finally, the single particle reaction width, $W = \Gamma - \Gamma_{\alpha j \ell}$, of the actual optical potential should be very nearly equal to that of the comparable square well if the only difference between them is a rounded edge.

According to Weisskopf's latest calculations (W56b) the best optical potential is

$$V(r) = \frac{V_o(1 + i\zeta)}{1 + \exp\left[2(r - R)/d\right]} \tag{9-12}$$

with $V_o = 42$ Mev, $\zeta = 0.08$, $d = 1.15$ f, and $R = 1.35\ A^{\frac{1}{3}}$f. For this potential

$$W \approx 2\zeta V_o = 6.7 \text{ Mev} \tag{10a-12}$$

$$E_p - E_f \approx 2.9 \text{ Mev} \tag{10b-12}$$

It is possible to obtain easy confirmation of Eq. (10-12) by inspecting the published calculation of S_o vs A. The widths of the S-wave peaks at A = 55 and A = 160 are related to W; this relation can be approximately derived by assuming that for particular s-wave single particle levels KR is a slowly varying function of radius. Here K is appropriate to the related square well ($d \rightarrow 0$) for which KR is exactly constant. Then

$$\frac{d\mathring{E}_o}{dA} = \frac{2}{3}\,\frac{V_o}{A} \tag{11-12}$$

when $\mathring{E}_o$ corresponds to zero bombarding energy. From Eq. (7-12) for $E = \ell = 0$ we then obtain

$$W = \left(\frac{2}{3}\,V_o\right)\,\frac{\Delta A}{A_o} \tag{12-12}$$

where A_o corresponds to a maximum in S_o, and ΔA is its full width at half maximum. According to Eq. (12-12) both the peak at A = 55 and the peak at A = 160 give W = 7 Mev, confirming Eq. (10a-12). The maximum value of S_o permitted by Eq. (6-12) for $E = \ell = 0$ is $\frac{2}{\pi}\,\frac{\xi^2}{W}$. With W = 7 Mev the peaks at A = 55 and 160 give $\mathring{\gamma}^2_{\ell=o}$ = 1.7 and 2.2 Mev, respectively.

Using the value W = 7 Mev, and assuming $\mathring{\gamma}^2_{\ell=1} = \mathring{\gamma}^2_{\ell=3}$ in Eq. (6-12), one can obtain the p- and f-wave strength functions at E = 0.5 Mev as functions of $\mathring{\gamma}^2_{\ell=1}$. For $\mathring{\gamma}_{\ell=1}$ = 2.5 Mev the values deduced in Chapter 11 are reproduced and the single particle p-wave level is found to be at -6.3 Mev and the f-wave level at -9.1 Mev. Finally, the p- and f-level splitting is 2.8 Mev, making the choice $\mathring{\gamma}^2_{\ell=1}$ unique.

4. To estimate the level splitting caused by the introduction of a spin orbit force in the optical potential we must solve Shrodinger's equation. This can be done easily in two cases: (i) a square well central potential plus a square well spin-orbit potential of the same radius, and (ii) a square well potential plus a surface spin-orbit potential.

Case (i)

Schrödinger's equation can be written

$$-\frac{\hbar^2}{2m}\nabla^2\psi - V_c\psi - V_{so}\frac{\vec{L}\cdot\vec{S}}{\hbar^2}\psi = E\psi \quad r < R \tag{13a-12}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \quad r > R \tag{13b-12}$$

We can choose our eigenfunctions as simultaneous eigenfunctions of $j^2(\vec{j} = \vec{\ell} + \vec{s})$, ℓ^2, and s^2 since all of these operators commute with the Hamiltonian, i.e.,

$$\psi^m_{j\ell s} = \frac{1}{r}\, u^m_{j\ell s}(r) \sum_{m_\ell m_s} (jm\ell s|\ell s m_\ell m_s)\, Y^m_\ell(\theta\phi)\, \chi^{m_s}_s \tag{14-12}$$

Since $\vec{\ell}\cdot\vec{s} = \frac{1}{2}(j^2 - \ell^2 - s^2)$ Schrödinger's equation becomes

$$u''(r) + \left[\frac{2m}{h^2}\left\{E + V_{so}\frac{j(j+1) - \ell(\ell+1) - s(s+1)}{2}\right\} + \frac{2m}{\hbar^2}V_c - \frac{\ell(\ell+1)}{r^2}\right] u(r) = 0$$

$$r < R \tag{15a-12}$$

$$u''(r) + \left[\frac{2m}{\hbar^2}E - \frac{\ell(\ell+1)}{r^2}\right] u(r) = 0 \quad r > R \tag{15b-12}$$

Equation (15-12) has the same structure as the Schrödinger equation for an ordinary central square well except for an energy shift from E to $E + \frac{1}{2}V_{so}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]$. This immediately gives the desired level splitting, viz.: $E_+ - E_o = -\frac{\ell}{2}V_{so}$, $E_- - E_o = \frac{\ell+1}{2}V_{so}$, where E_+ denotes the energy of the virtual state for which $j = \ell + s$, etc. Note that the space part of the spin-orbit potential is taken as attractive.

Case (ii)

Before we can treat case (ii) we must first obtain appropriate boundary conditions to use at a surface on which a delta function potential exists. We can do this as follows: Consider a one-dimensional region in which the potential looks like it does in Fig. (1-12). Let the dotted line denote the total energy. The wave function appropriate to this problem is

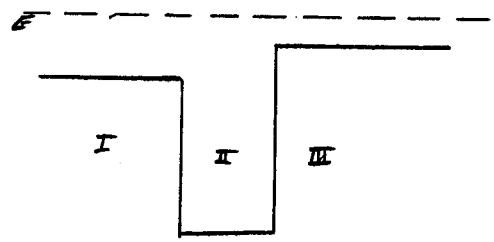

Fig. (1-12)

$$\left.\begin{array}{ll} \psi = A \cos kx + B \sin kx & \text{Region I} \\ \psi = A' \cos k'x + B' \sin k'x & \text{Region II} \\ \psi = A'' \cos k''x + B'' \sin k''x & \text{Region III} \end{array}\right\} \quad (16\text{-}12)$$

The conditions of continuity of the wave function and its derivative at $x = 0$ and $x = a$ can be written, after some rearrangement as

$$A \cos k'a + \frac{kB}{k'} \sin k'a = A'' \cos k''a + B'' \sin k''a \qquad (17a\text{-}12)$$

$$- k'A \sin k'a + kB \cos k'a = - k''A'' \sin k''a + k''B'' \cos k''a \qquad (17b\text{-}12)$$

Now let the potential hole in Fig. (1-12) become infinitely deep and infinitesimally narrow, i.e., let $k' \longrightarrow \infty$ and $a \longrightarrow 0$, but let $k'^2 a$, which is proportional to the integrated potential in region II, remain finite. Then Eqs. (17-12) can be rewritten as

$$\frac{k''B''}{A''} = \frac{kB}{A} - k'^2 a \qquad (18\text{-}12)$$

An equivalent form for Eq. (18-12) is

$$\left(\frac{1}{\psi}\frac{d\psi}{dx}\right)_{x=o+} - \left(\frac{1}{\psi}\frac{d\psi}{dx}\right)_{x=o-} = \frac{2m}{\hbar^2}\int V(r)dr \qquad (19\text{-}12)$$

where V(r) is taken as negative in the case of a potential hole. Hence, the logarithmic derivative of the wave function has a discontinuity of magnitude $-\frac{2m}{\hbar^2}$ times the integrated delta function potential. If the delta function potential in region II is a spike rather than a hole, the trigonometric functions in the region II wave functions are replaced by hyperbolic functions, and the derivation then proceeds as before. The result is again Eq. (19-12), but with the sign of the potential reversed, as it should be.

With this boundary condition we can now study the Shrodinger's equation for the nuclear problem. The counterpart of Eq. (15-12) in the case of a delta function spin-orbit potential on the nuclear surface is

$$u''(r) + \left[\frac{2m}{\hbar^2}(E + V_c) - \frac{\ell(\ell+1)}{r^2}\right]u(r) = 0 \qquad r < R \qquad (20a\text{-}12)$$

$$u''(r) + \left[\frac{2m}{\hbar^2}E - \frac{\ell(\ell+1)}{r^2}\right]u(r) = 0 \qquad r > R \qquad (20b\text{-}12)$$

$$\left(\frac{R}{u}\frac{du}{dr}\right)_{r=R+} - \left(\frac{R}{u}\frac{du}{dr}\right)_{r=R-} = -\frac{2m}{\hbar^2}\cdot V_{so}R\cdot\frac{j(j+1) - \ell(\ell+1) - s(s+1)}{2} \qquad (20c\text{-}12)$$

where V_{so} is the integrated value of the space part of the spin-orbit potential (taken positive for an <u>attractive</u> force).

Now $\left(\frac{R}{u}\frac{du}{dr}\right)_{r=R+}$ is, by definition, just $f_{\ell j}$, whereas $\left(\frac{R}{u}\frac{du}{dr}\right)_{r=R-}$ is f_ℓ of the same problem without spin orbit coupling. Hence,

$$f_{\ell j} = f_\ell - \frac{2m}{\hbar^2}V_{so}R\cdot\frac{1}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right] \qquad (21\text{-}12)$$

Now suppose $f_{\ell j}(E_{\ell j}) = f_\ell(E_\ell) = 0$. Then

$$0 = f_{\ell j}(E_{\ell j}) = (E_{\ell j} - E_\ell) f'_\ell(E_\ell) - \frac{2m}{\hbar^2} V_{so} R \frac{1}{2} \left[j(j+1) - \ell(\ell+1) - s(s+1) \right] \tag{22-12}$$

Since $f'_\ell(E_\ell) = -\frac{1}{\mathring{\gamma}_\ell^2}$, we have finally,

$$E_{\ell j} = E_\ell - \mathring{\gamma}_\ell^2 \cdot \frac{2m}{\hbar^2} V_{so} R \cdot \frac{1}{2} \left[j(j+1) - \ell(\ell+1) - s(s+1) \right] \tag{23a-12}$$

or

$$E_{\ell\pm} = E_\ell - \mathring{\gamma}_\ell^2 \cdot \frac{2m}{\hbar^2} V_{so} R \cdot \left(\begin{matrix} \ell/2 \\ -\frac{\ell+1}{2} \end{matrix} \right) \tag{23b-12}$$

5. It is rather conventional in analysis of spin orbit coupling to choose the spin orbit potential as some multiple, γ_{so}, of the Thomas potential, which is given as

$$V_{Thomas} = \frac{1}{2} \left(\frac{\hbar}{mc^2} \right) \frac{1}{r} \frac{dV_c}{dr} \left(\frac{\vec{L} \cdot \vec{S}}{h^2} \right) \tag{24-12}$$

where V_c is the central potential. For an attractive square well of depth of V_o, Eq. (24-12) gives for the quantity $\frac{2m}{\hbar^2} V_{so} R$ the value $-\frac{V_o}{mc^2}$.

A number of workers have analyzed various nuclear data using Eq. (24-12) for the form of the spin-orbit potential (L56a, F58, R56b, G56a) and various central potentials. All these analyses have given values of $\gamma_{so} \sim -30$ to -50. For the remainder of this work we shall take $\gamma_{so} = -40$. With this value, $\mathring{\gamma}^2_{\ell=1} = 2.5$ Mev, and $V_o = 42$ Mev, $E_{p1/2} - E_{p3/2} = 6.8$ Mev. Adair (A54) has analyzed some reaction data using a potential of type (i) and finds V_{so} about 2 Mev, giving $E_{p1/2} - E_{p3/2} = 3.0$ Mev. In the remainder of this work we shall use the larger value. In this case the level positions are:

E(p1/2) = - 1.8 Mev, E(p3/2) = - 8.6 Mev, E(f5/2) = - 0.08 Mev, E(f7/2) =-15.9 Mev. Because these levels are not shifted by a very large fraction of their energy relative to the bottom of the potential well, we shall assume for them also W = 7.0 Mev, $\overset{\circ}{\gamma}{}^2_{\ell j}$ = 2.5 Mev. With these assumptions we then have S(p1/2) = 0.077, S(p3/2) = 0.027, S(f5/2) = 0.060, S(f7/2) = 0.025 at E = 0.5 Mev.

5. Let us now complete the final step of the program outlined in (1-12), i.e., consider the effect of these new ℓj strength functions on the reaction cross sections. Let us begin by considering radiative capture below the inelastic threshold. The odd-parity contribution to this cross section is, with extremely small error, due only to p-waves, and is given by Eq. (9-2), (14-2) and Eq. (8-2) modified in accordance with the discussion after Eq. (14-2) as:

$$\frac{\sigma(n\gamma)\Big]_{\text{p-wave}}}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T(p\,\frac{1}{2})\;T_\gamma}{T(p\,\frac{1}{2}) + T_\gamma} \right\rangle_{\frac{1}{2}-} + 2\left\langle \frac{T(p\,\frac{3}{2})(2T_\gamma)}{T(p\,\frac{3}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}-} \qquad (25\text{-}12)$$

Where $T(p\,\frac{1}{2}) \sim T(p\,\frac{3}{2}) \sim T_1 >> T_\gamma$, the right hand side of Eq. (25-12) approaches $5T_\gamma$ independent of $T(p\,\frac{1}{2})$, $T(p\,\frac{3}{2})$, or T_1. (T_1 is the value to which $T(p\,\frac{1}{2})$ and $T(p\,\frac{3}{2})$ tend when $V_{so} \rightarrow 0$.) Thus in this limit the odd wave contribution to $\sigma(n\gamma)$ is independent of the extent of the spin-orbit coupling. If, on the other hand, $T(p\,\frac{1}{2}) \sim T(p\,\frac{3}{2}) \sim T_1 << T_\gamma$, the right hand side of Eq. (25-12) approaches $T(p\,\frac{1}{2}) + 2T(p\,\frac{3}{2})$. Now we shall show below that under the circumstances pertaining to our calculation this last sum is very nearly equal to $3T_1$, and is consequently also independent of

the extent of the spin-orbit coupling. In view of the behavior of the p-wave contribution to $\sigma(n\gamma)$ in these extreme limits we expect it to be very nearly independent of the extent of the spin-orbit coupling. This point is tested by direct calculation below.

To prove $T(p\,\frac{1}{2}) + 2T(p\,\frac{3}{2}) = 3T_1$ we proceed as follows: If $\left|E_{\ell j} - E_\ell\right|$ is not too large compared to Γ we can write

$$S_{\ell j} = S_\ell + (E_{\ell j} - E_\ell)\left(\frac{dS_\ell}{dE_\ell}\right) \tag{26-12}$$

Furthermore, if the level splitting $\left|E_{\ell j} - E_\ell\right|$ is small compared to E_ℓ (measured from the well bottom) it also follows that

$$\sum_{j=\left|\ell-\frac{1}{2}\right|}^{\ell+\frac{1}{2}} (2j+1)E_{\ell j} = 2(2\ell+1)E_\ell \tag{27-12}$$

This result can be derived from first order perturbation theory, or in case (ii) from Eq. (23b-12), or from the energy shift derived in case (i). It follows from Eqs. (26-12) and (27-12) that

$$\sum_{j=\left|\ell-\frac{1}{2}\right|}^{\ell+\frac{1}{2}} (2j+1)S_{\ell j} = 2(2\ell+1)S_\ell \tag{28-12}$$

from which the desired result follows when ℓ is set equal to 1.

These results are true for any angular momentum ℓ, but depend on taking <u>zero target spin</u>. In such a case

$$\sigma(n\gamma) = \frac{\pi\lambda\!\!\!^{-2}}{2} \sum_{\ell=0}^{\infty} \sum_{j=\left|\ell-\frac{1}{2}\right|}^{\left|\ell+\frac{1}{2}\right|} (2j+1)\,\frac{2\pi}{D_{j\pi}} \left\langle \frac{\Gamma_{j\ell}\Gamma_\gamma}{\Gamma_{j\ell}+\Gamma_\gamma} \right\rangle \tag{29-12}$$

since $j = J$ and $\pi = (-)^{\ell}$. No other neutron width but $\Gamma_{j\ell}$ can appear in the total width since $I = 0$ and parity is conserved. Proceeding as before we can show that for orbital angular momenta for which $\Gamma_{j\ell} >> \Gamma_{\gamma}$,

$$\sigma^{(\ell)}(n\gamma) = \sum_{j=\left|\ell - \frac{1}{2}\right|}^{\ell + \frac{1}{2}} (2j + 1) \frac{2\pi\Gamma_{\gamma}}{D_{j\pi}} \tag{30-12}$$

while for orbital angular momenta for which $\Gamma_{j\ell} << \Gamma_{\gamma}$, we can use Eq. (28-12) to show:

$$\sigma^{(\ell)}(n\gamma) = (2\ell + 1)\, 4\pi s_{\ell} S_{\ell} \tag{31-12}$$

Both of these results are independent of V_{so}.

Thus as long as Eq. (28-12) holds, $\sigma(n\gamma)$ should be independent of V_{so}. For p-waves the level shift $\left|E_{\ell j} - E_{\ell}\right|$ is of the order of 2.5-4.5 Mev, compared to a total width, Γ, of 7 or more Mev and an energy of $\sim$ 40 Mev above the well bottom. Hence, we expect Eq. (28-12) to hold. Indeed, for the strength functions given at the end of paragraph (4-11), $\frac{1}{3}\, T(p\, \frac{1}{2}) + \frac{2}{3}\, T(p\, \frac{3}{2})$ is only 9% larger than T_1.

Presented in Table (1-12) are calculated values of the p-wave contribution to $\sigma(n\gamma)$ at several energies spanning the range $T_1 >> T_{\gamma}$ to $T_1 << T_{\gamma}$. Values have been calculated for $T_1 = 0.040$, and $T(p\, \frac{1}{2}) = 0.077$, $T(p\, \frac{3}{2}) = 0.027$. From the tabular entries the anticipated independence of the strength of the spin-orbit coupling is verified. At the lower energies the relative contribution of the p-waves is rather small compared to the s-waves, and the change in the total radiative capture cross section caused by the introduction of the spin-orbit coupling is never more than 3%.

Table (1-12). P-Wave Contribution to $\sigma(n\gamma)$

Energy (kev)	With Spin-Orbit Force (mb)	Without Spin-Orbit Force (mb)
3	289	245
9	302	292
15	276	271
21	249	247
27	224	224

For nuclei with a non-zero target spin and spin-orbit independence of $\sigma(n\gamma)$ cannot be demonstrated even if Eq. (28-12) holds, since then other orbital angular momenta besides that of the entrance width can enter the total width. There is one exception, however, and that is in the range in which only s- and p-waves need be considered. Since these partial waves cannot appear in the same term, by parity conservation, Eq. (29-12) again holds, but with the ℓ-sum restricted to 0 and 1. The circumstance is of the greatest importance because it allows unambiguous analysis of data like that of Macklin, Lazar, and Lyon (M57) $\left[\sigma(n\gamma) \text{ for Sb-Be neutrons}\right]$ for the quantity $\frac{2}{3} S(p\,\frac{3}{2}) + \frac{1}{3} S(p\,\frac{1}{2}) = S_1$. These results have several important consequences: In the first place, the analysis of Newson's data carried out in Chapter 11 gives physically meaningful results in the sense that independently the precise extent of the spin-orbit coupling the parameter $\frac{2}{3} S(p\,\frac{3}{2}) + \frac{1}{3} S(p\,\frac{1}{2}) = S_1$ is well determined by the experimental data. In the second place, the procedure can be inverted, for if $S_\ell = \frac{2j+1}{2(2\ell+1)} \times$

$\sum_{j=|\ell-\frac{1}{2}|}^{\ell+\frac{1}{2}} S_{\ell j}$ only is known, and if the spin-orbit coupling is not too large, $\sigma(n\gamma)$ may be reliably calculated below the inelastic threshold for the spin zero nuclei, or for any nucleus if only s- and p-waves are important.

This last point has an important practical significance because an independence theorem similar to that for the radiative capture cross section below inelastic threshold also holds for the cross section for compound nucleus formation, and the total cross section <u>for any target spin</u>. This can easily be shown as follows: From the results of Chapter 2 we can write

$$\sigma(\alpha,\alpha') = \frac{\pi\lambda\!\!\!^{-2}}{2(2I+1)} \sum_{j=0}^{\infty} \sum_{j=|J-I|}^{J+I} \sum_{j'=|J-I'|}^{J+I'} \sum_{\ell=|j-\sigma|}^{j+\sigma} \sum_{\ell'=j'-\sigma'}^{j'+\sigma'} (2J+1) \times$$

$$\left| \delta_{\alpha\alpha'}\delta_{\ell\ell'}\delta_{jj'} - S^{J\pi}_{\alpha j\ell,\alpha' j'\ell'} \right|^2 \qquad (32\text{-}12)$$

If we sum this equation over all $\alpha' \neq \alpha$ and carry out the indicated sums over ℓ' and j', we obtain

$$\sigma_c(\alpha) = \frac{\pi\lambda\!\!\!^{-2}}{2(2I+1)} \sum_{j=0}^{\infty} \sum_{j=|J-I|}^{J+I} \sum_{\ell=|j-\sigma|}^{j+\sigma} (2J+1) \frac{2\pi}{D_{J\pi}} \left\langle \Gamma_{\alpha\ell j} \right\rangle \qquad (33\text{-}12)$$

where σ_c is the cross section for compound nucleus formation. Here we have made use of the equation obtainable from Eq. (7-2)

$$\left\langle \left| S^{J\pi}_{\alpha j\ell,\alpha j\ell} \right|^2 \right\rangle = 1 + \frac{2\pi}{D_{J\pi}} \left\langle \frac{\Gamma^2_{\alpha j\ell}}{\Gamma} \right\rangle - \frac{2\pi}{D_{J\pi}} \left\langle \Gamma_{\alpha j\ell} \right\rangle$$

If we assume the strength functions to be independent of J, then we can carry out the J-sum obtaining

$$\sigma_c(\alpha) = \frac{\pi\lambda\!\!\!^{-2}}{2} \sum_{\ell=0}^{\infty} \sum_{j=|\ell-\sigma|}^{\ell=\sigma} (2j+1)\cdot 4\pi s_\ell \cdot S_{\ell j} = \pi\lambda\!\!\!^{-2} \sum_{\ell=0}^{\infty} (2\ell+1) 4\pi s_\ell S_\ell \qquad (34\text{-}12)$$

from Eq. (28-12). This last result is clearly independent of V_{so}.

If we carry out the sum over all α including α', and over ℓ' and j', we obtain

$$\sigma_t(\alpha) = \frac{\pi\lambda\!\!\!^{-2}}{2(2I+1)} \sum_{J=0}^{\infty} \sum_{j=|J-I|}^{J+I} \sum_{\ell=|j-\sigma|}^{j+\sigma} (2J+1)2\mathrm{Re}\left(1 - \left\langle S^{J\pi}_{\alpha\ell j\ \alpha\ell j}\right\rangle\right) \qquad (35\text{-}12)$$

Using Eq. (3-12) for the averaged diagonal S-matrix element one obtains

$$\sigma_t(\alpha) = \frac{\pi\lambda\!\!\!^{-2}}{2(2I+1)} \sum_{J=0}^{\infty} \sum_{j=|J-I|}^{J+I} \sum_{\ell=|j-\sigma|}^{j+\sigma} 2(2J+1)$$

$$\left[1 - \cos(2\xi_{\alpha\ell})(1 - 2\pi s_\ell S_{\alpha\ell j})\right] \qquad (36\text{-}12)$$

If we take $S_{\alpha\ell j}$ independent of J the J-sum can be carried out, and the j sum as well, giving:

$$\sigma_t(\alpha) = \pi\lambda\!\!\!^{-2} \sum_{\ell=0}^{\infty} (2\ell+1)2\left[1 - \cos(2\xi_{\alpha\ell})(1 - 2\pi s_\ell S_\ell)\right] \qquad (37\text{a-}12)$$

$$= \pi\lambda\!\!\!^{-2} \sum_{\ell=0}^{\infty} (2\ell+1)\left[4\sin^2\xi_{\alpha\ell} + \cos(2\xi_{\alpha\ell}) \cdot 4\pi s_\ell S_\ell\right] \qquad (37\text{b-}12)$$

which is again independent of V_{so}.

The optical model of Feshbach, Porter, and Weisskopf is based on fitting σ_t and σ_c as functions of neutron energy. From Eqs. (37-12) and (34-12) it follows that it is not necessary to consider a spin-orbit part in the optical potential. Since the radiative capture cross section below inelastic threshold also depends only on the central potentials it follows that calculations of the latter quantity based on such an optical model should

be quite reliable for spin zero nuclei or when only s- and p-waves are important.

Another example of a cross section which is independent of V_{so} is the inelastic scattering cross section near its threshold. The inelastic scattering cross section can be written

$$\sigma(\alpha,\alpha') = \frac{\pi\lambda\!\!\!^{-2}}{2(2I+1)} \sum_{J=0}^{\infty} \sum_{j=|J-I|}^{J+I} \sum_{j'=|J-I'|}^{J+I'} \sum_{\ell=|j-\sigma|}^{j+\sigma} \sum_{\ell'=|j'-\sigma'|}^{j'+\sigma'}$$

$$\cdot\ (2J+1)\ \frac{2\pi}{D_{J\pi}} \left\langle \frac{\Gamma_{\alpha j \ell}\Gamma_{\alpha' j' \ell'}}{\Gamma} \right\rangle \qquad (38\text{-}12)$$

Now if we are very close to threshold (of the <u>first</u> inelastic level), and if radiative capture is small, $\Gamma = \sum_{j\ell} \Gamma_{\alpha j \ell}$. We can then write

$$\sigma(\alpha,\alpha') = \frac{\pi\lambda\!\!\!^{-2}}{2(2I+1)} \sum_{J=0}^{\infty} \sum_{j'=|J-I'|}^{J+I'} \sum_{\ell=|j'-\sigma'|}^{j'+\sigma'} (2J+1)\ \frac{2\pi \left\langle \Gamma_{\alpha' j' \ell'} \right\rangle}{D_{J\pi}}$$

$$\cdot \sum_{j=|J-I|}^{J+I} \sum_{\ell=|j-\sigma|}^{j+\sigma} \left\langle \frac{\Gamma_{\alpha j \ell}}{\Gamma} \right\rangle \qquad (39\text{-}12)$$

Carrying out the last two sums gives unity. Since $\frac{2\pi \left\langle \Gamma_{\alpha' j' \ell'} \right\rangle}{D_{J\pi}}$ is assumed to be independent of $J\pi$ we can carry out the J sum first and then the j' sum, using Eq. (28-12) giving finally:

$$\sigma(\alpha,\alpha') = \pi\lambda\!\!\!^{-2}\ \frac{2I'+1}{2I+1} \sum_{\ell'=0}^{\infty} (2\ell'+1)\ 4\pi s_{\ell'} s_{\ell} \qquad (40\text{-}12)$$

This is just the reciprocity relation

$$\frac{(2I+1)\sigma(\alpha,\alpha')}{\lambda\!\!\!^{-2}_{\alpha}} = \frac{(2I'+1)\sigma_c(\alpha')}{\lambda\!\!\!^{-2}_{\alpha'}} \qquad (41\text{-}12)$$

which under the stated circumstances must hold. Since the right hand side of Eqs. (40-12) and (41-12) are independent of V_{so}, so is $\sigma(\alpha,\alpha')$.

6. In general, however, the partial reaction cross sections are not independent of V_{so}. In the Ij representation the equations analogous to Eqs. (2-11) and (9-11) are:

$$\frac{\sigma(2+)}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T(S\,\tfrac{1}{2})\left[T'(d\,\tfrac{5}{2}) + T'(d\,\tfrac{3}{2})\right]}{T(S\,\tfrac{1}{2}) + T'(d\,\tfrac{5}{2}) + T'(d\,\tfrac{3}{2}) + T_\gamma} \right\rangle_{\frac{1}{2}+}$$

$$+ \left\langle \frac{T(p\,\tfrac{1}{2})\left[T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2})\right]}{T(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + T_\gamma} \right\rangle_{\frac{1}{2}-}$$

$$+ 2\left\langle \frac{T(d\,\tfrac{3}{2})\left[T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2})\right]}{T(d\,\tfrac{3}{2}) + T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{5}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}+}$$

$$+ 2\left\langle \frac{T(p\,\tfrac{3}{2})\left[T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2})\right]}{T(p\,\tfrac{3}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}-}$$

$$+ 3\left\langle \frac{T(d\,\tfrac{5}{2})\left[T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2})\right]}{T(d\,\tfrac{5}{2}) + T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{3}{2}) + T''(d\,\tfrac{5}{2}) + 3T_\gamma} \right\rangle_{\frac{5}{2}+}$$

$$+ 3\left\langle \frac{T(f\,\tfrac{5}{2})\left[T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2})\right]}{T(f\,\tfrac{5}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 3T_\gamma} \right\rangle_{\frac{5}{2}-}$$

$$+ 4\left\langle \frac{T(f\,\tfrac{7}{2})\left[T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2})\right]}{T(f\,\tfrac{7}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{1}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 4T_\gamma} \right\rangle_{\frac{7}{2}-}$$

(42a-12)

$$\frac{\sigma(4+)}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T(p\,\tfrac{1}{2})T''(f\,\tfrac{7}{2})}{T(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2})\;T_\gamma} \right\rangle_{\frac{1}{2}} -$$

$$+\,2\left\langle \frac{T(d\,\tfrac{3}{2})\cdot T''(d\,\tfrac{5}{2})}{T(d\,\tfrac{3}{2}) + T'(s\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{5}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}} +$$

$$+\,2\left\langle \frac{T(p\,\tfrac{3}{2})\left[T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2})\right]}{T(p\,\tfrac{3}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}} -$$

$$3\left\langle \frac{T(d\,\tfrac{5}{2})\left[T''(d\,\tfrac{3}{2}) + T''(d\,\tfrac{5}{2})\right]}{T(d\,\tfrac{5}{2}) + T'(s\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{3}{2}) + T''(d\,\tfrac{5}{2}) + 3T_\gamma} \right\rangle_{\frac{5}{2}} +$$

$$3\left\langle \frac{T(f\,\tfrac{5}{2})\left[T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2})\right]}{T(f\,\tfrac{5}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 3T_\gamma} \right\rangle_{\frac{5}{2}} -$$

$$+\,4\left\langle \frac{T(f\,\tfrac{7}{2})\left[T''(p\,\tfrac{1}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2})\right]}{T(f\,\tfrac{7}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{1}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 4T_\gamma} \right\rangle_{\frac{7}{2}} -$$

(42b-12)

$$\frac{\sigma(n\gamma)}{\pi\lambda\!\!\!^{-2}} = \left\langle \frac{T(s\,\tfrac{1}{2})\;T_\gamma}{T(s\,\tfrac{1}{2}) + T'(d\,\tfrac{5}{2}) + T'(d\,\tfrac{3}{2}) + T_\gamma} \right\rangle_{\frac{1}{2}} +$$

$$+\left\langle \frac{T(p\,\tfrac{1}{2})\;T_\gamma}{T(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + T_\gamma} \right\rangle_{\frac{1}{2}} -$$

$$+ 2\left\langle \frac{T(d\,\tfrac{3}{2})(2T_\gamma)}{T(d\,\tfrac{3}{2}) + T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{5}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}+}$$

$$= 2\left\langle \frac{T(p\,\tfrac{3}{2})(2T_\gamma)}{T(p\,\tfrac{3}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}-}$$

$$+ 3\left\langle \frac{T(d\,\tfrac{5}{2})(3T_\gamma)}{T(d\,\tfrac{5}{2}) + T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{3}{2}) + T''(d\,\tfrac{5}{2})\ 3T_\gamma} \right\rangle_{\frac{5}{2}+}$$

$$+ 3\left\langle \frac{T(f\,\tfrac{5}{2})(3T_\gamma)}{T(f\,\tfrac{5}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 3T_\gamma} \right\rangle_{\frac{5}{2}-}$$

$$+ 4\left\langle \frac{T(f\,\tfrac{7}{2})(4T_\gamma)}{T(f\,\tfrac{7}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 4T_\gamma} \right\rangle_{\frac{7}{2}-} \cdots$$

(42c-12)

$$4B_2(2+) = -\left\langle \frac{T(d\,\tfrac{3}{2})\left[2.400T'(d\,\tfrac{3}{2}) + 0.4572T'(d\,\tfrac{5}{2})\right]}{T(d\,\tfrac{3}{2}) + T'(S\,\tfrac{1}{2}) + T'(d\,\tfrac{3}{2}) + T'(d\,\tfrac{5}{2}) + T''(d\,\tfrac{5}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}+}$$

$$+\left\langle \frac{T(p\,\tfrac{3}{2})\left[-\,2.400T'(p\,\tfrac{3}{2}) - 0.472T'(f\,\tfrac{5}{2}) + 2.856T'(f\,\tfrac{7}{2})\right]}{T(p\,\tfrac{3}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 2T_\gamma} \right\rangle_{\frac{3}{2}}$$

$$+\left\langle \frac{T(f\,\tfrac{5}{2})\left[-\,0.6858T'(p\,\tfrac{3}{2}) + 0.6858T'(f\,\tfrac{5}{2}) + 2.858T'(f\,\tfrac{7}{2})\right]}{T(f\,\tfrac{5}{2}) + T'(p\,\tfrac{1}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 3T_\gamma} \right\rangle_{\frac{5}{2}-}$$

$$+\left\langle \frac{T(f\,\tfrac{7}{2})\left[5.713T'(p\,\tfrac{3}{2}) + 3.810T'(f\,\tfrac{5}{2}) + 4.444T'(f\,\tfrac{7}{2})\right]}{T(f\,\tfrac{7}{2}) + T'(p\,\tfrac{3}{2}) + T'(f\,\tfrac{5}{2}) + T'(f\,\tfrac{7}{2}) + T''(p\,\tfrac{1}{2}) + T''(p\,\tfrac{3}{2}) + T''(f\,\tfrac{5}{2}) + T''(f\,\tfrac{7}{2}) + 4T_\gamma} \right\rangle_{\frac{7}{2}-}$$

(42d-12)

Let us first consider $\sigma(2+)$ at 550 kev. If we assume no change in the d-wave strength function (which is reasonable in view of the discussion of paragraph 11-2), then only the odd-wave contributions to the cross sections show dependence on the spin-orbit coupling. For $\sigma(2+)$, the main odd wave contribution ($\sim$ 70%) comes from pure p-wave interactions [cf. Eq. (7a-11), for example]. The corresponding terms in Eq. (42a-12) are those labelled $\frac{1}{2}$ - and $\frac{3}{2}$ - . The sum of these two terms is coincidentally not very sensitive to the extent of the spin-orbit coupling, which we can show roughly as follows:

Let us ignore in these terms the effects of the statistical distribution of the reaction widths, the f-wave and radiative widths, and let us further assume that $T_{\ell j} = T'_{\ell j}$ at 550 kev (in truth the ratio $T'_{\ell j}/T_{\ell j} = 0.94$ at this energy). In such case the p-wave term has the form

$$P = \frac{T(p\,\frac{3}{2})T(p\,\frac{1}{2})}{T(p\,\frac{3}{2}) + T(p\,\frac{1}{2})} + 2\,\frac{T(p\,\frac{3}{2})\left[T(p\,\frac{3}{2}) + T(p\,\frac{1}{2})\right]}{2T(p\,\frac{3}{2}) + T(p\,\frac{1}{2})} \tag{43a-12}$$

with the constraint

$$2T(p\,\tfrac{3}{2}) + T(p\,\tfrac{1}{2}) = 3T_1 \tag{43b-12}$$

It can easily be shown that

$$\left[\frac{T(p\,\frac{3}{2})}{P}\;\frac{dP}{dT(p\,\frac{3}{2})}\right]_{T(p\,\frac{3}{2})=T_1} = -\frac{7}{22} \qquad (44\text{-}12)$$

Thus a change of $S(p\frac{3}{2})$ from 0.040 to 0.027 (about 33%) will cause roughly a 10% reduction in P. Exact calculation including the effects neglected above, and using the strength functions of obtained at the end of paragraph (4-12) gives about a 7% reduction in the contribution to $\sigma(2+)$ from the $\frac{1}{2}$ - and $\frac{3}{2}$ - compound states. For, according to Eq. (7a-11) this contribution is about 590 mb when $S_1 = 0.040$, while in the presence of the spin-orbit coupling assumed in this chapter it is about 550 mb.

The total calculated $\sigma(2+)$ cross sections with spin-orbit coupling is 1220 mb, which is just barely outside the quoted experimental error. Because the s; p; and d-wave parts of this result are essentially independent of V_{so}, and because the f-wave part is both a small contribution ($\sim$ 15%) and comparable with the experimental uncertainty ($\pm$14%), $\sigma(2+)$ tells us nothing about S_3 or V_{so}. It does, however, give information on S_1 (since the p-wave contribution is nearly independent of V_{so}) and indeed indicates that $S_1 \sim S_o$, in accordance with our findings from the analysis of Newson's data on $\sigma(n\gamma)$. This agreement between two separate determinations of S_1 increases our confidence in this result.

$\sigma(4+)$, on the other hand, depends quite strongly on the f-wave strength functions. Of the 180 mb contributed to $\sigma(4+)$ by odd-waves in Eq. (7b-11), 145 mb come from the $\frac{5}{2}$ - and $\frac{7}{2}$ - compound states, 40 mb from the $\frac{5}{2}$ - state, and 105 mb from the $\frac{7}{2}$ - state. The corresponding contributions using this chapter's strength functions are 17 and 29 mb, respectively. These contributions

are roughly in the ratios of $S(f\,\frac{5}{2}):S_3$ and $S(f\,\frac{7}{2}):S_3$, indicating that the dependence of these terms on V_{so} through the p-wave penetrabilities is rather slight (as one might expect from the form of these terms given in Eq. 42b-12). The total 4+ cross section is 145 mb using the spin-orbit strength functions, which is much too low.

In order to increase this value we must increase $S(f\,\frac{5}{2})$, $S(f\,\frac{7}{2})$, or both. Because of the large splitting of the $f\,\frac{5}{2}$ and $f\,\frac{7}{2}$ levels is not possible to increase them both. Furthermore, increasing $S(f\,\frac{5}{2})$ to its maximum allowable value $\frac{2\mathcal{J}^2}{\pi W} \sim 0.18$ and setting $S(f\,\frac{7}{2}) \sim 0$ will give a total contribution from the $\frac{5}{2}$ - and $\frac{7}{2}$ - states of the order of 60 mb, which is still much too small. Increasing $S(f\,\frac{7}{2})$, however, to the maximum value, and decreasing $S(f\,\frac{5}{2})$ to zero gives a contribution from the $\frac{5}{2}$ - and $\frac{7}{2}$ - states of the order of 160 mb which is nearly right. Hence, we are inclined to think that the level structure proposed so far is incorrect, and that the correct one is characterized by the following requirements:

(1) When $V_{so} = 0$, $S_1 \doteqdot 0.040$; and moreover the extent of the spin-orbit coupling is such that Eq. (28-12) holds for p-waves.

(2) After the spin-orbit coupling has been introduced, the $f\,\frac{7}{2}$ partial wave is in nearly perfect resonance at E = 0.5 Mev, i.e., $S(f\,\frac{7}{2}) \sim 0.15 - 0.20$ when E = 0.5 Mev.

(3) In all likelihood the unsplit p-level lies at positive rather than negative energies. If it lies at negative energies, then as the bombarding energy decreases the total width decreases while the level shift increases pushing the effective level position closer to the bombarding energy, both of which phenomena cause a

rapid rise in S_1. On the other hand, if the level is at positive energy, these effects work in contrary directions. In any case the resulting level scheme must maintain S_1 reasonably constant over the range 0 - 0.5 Mev, as required by our analysis of Newson's data and the $\sigma(2+)$ data at 550 kev. Finally, since the f $\frac{7}{2}$ level is the lowest of the four we are concerned with, if it is to resonate at 0.5 Mev, the other levels must be at positive energies.

If we again assume W = 7.0 Mev, $\overset{\circ}{\gamma}{}_1^2$ = 2.5 Mev, γ_{so} = - 40 we find that E_1 = 5.6 Mev will give S_1 = 0.040 when E = 0.5 Mev. We can determine the position of the f $\frac{5}{2}$ and f $\frac{7}{2}$ levels from the requirement $E_1 - E_3$ = 2.8 Mev, and from Eqs. (23-12). The results are $E\left(f\,\frac{5}{2}\right)$= 11.8 Mev, $E\left(f\,\frac{7}{2}\right)$= - 4.0 Mev. $E(p\frac{1}{2})$= 10.1 Mev and $E(p\frac{3}{2})$= 3.3 Mev. The corresponding strength functions

are $S(p\,\frac{1}{2})$ = 0.020, $S(p\,\frac{3}{2})$ = 0.060, $S(f\,\frac{5}{2})$ = 0.0086, $S(f\,\frac{7}{2})$ = 0.170. The p-wave strength functions again approximately obey Eq. (28-12). Finally, S_1 at E = 0 is 0.036 which is near S_1 at E = 0.5 Mev as required. For the previous choice (E_1 = - 6.3 Mev) S_1 at E = 0 was about 0.10 which was too large.

7. With the above choice of strength functions exact calculations at 550 kev give $\sigma(2+)$ = 1420 mb, $\sigma(4+)$ = 270 mb, and $\sigma(n\gamma)$ = 140 mb in excellent agreement with experiment. A similar calculation gives B(2+) = - 0.25 in better agreement with experiment than before, but still far outside the quoted experimental error. The increase is primarily due to the increase in the p $\frac{3}{2}$ - p $\frac{3}{2}$ term in Eq. (42d-12). It is probably possible to make slight adjustments in the level scheme so as to increase $S(p\,\frac{3}{2})$ somewhat and improve the

agreement of B(2+) with experiment, without disturbing the other quantities too much. Furthermore, a small amount of highly anisotropic direct excitation may affect B(2+) considerably. 200 mb of direct, excitation with a P_2-component of - 0.8 (the value obtained by Chase and Wilets) of its isotropic component brings B(2+) to - 0.35 which is just barely within experimental error.

8. In concluding this chapter let us recapitulate our findings: As we have seen $\sigma(n\gamma)$ at low energies and $\sigma(2+)$ at 550 kev seem rather independent of V_{so} and hence can be used to analyze the central part of the optical potential. Assuming $S_o = S_2$ as usual these data overdetermine the p-wave strength function and indicate that it is slightly larger than the s-wave strength function, and fairly constant in the first 0.5 Mev of neutron bombarding energy. This constraint, plus the measured s-wave strength function and potential scattering radius, together with the general properties of reasonable optical potentials known from survey works of the type of reference (F54) should determine the central optical potential. This central potential can then be tested by calculating the total cross section. To this a spin-orbit potential should be added whose strength is of the order of - 40 times the Thomas term, and which brings the f $\frac{7}{2}$ strength function near its maximum at a bombarding energy of 0.5 Mev.

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