Conf-751227--1

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By

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Prepared For Presentation at

IAEA Consultants Meeting

on the Use of Nuclear Theory in

Neutron Nuclear Data Evaluation Trieste

December 8-12, 1975

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ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

operated under contract W-31-109-Eng-38 for the

U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

Review paper RP2 prepared for presentation at the IAEA Consultants Meeting on the Use of Nuclear Theory in Neutron Nuclear Data Evaluation Trieste, December 8-12, 1975.

Statistical Theory of Neutron Nuclear Reactions*

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ABSTRACT

The statistical theory of average neutron nucleus reaction cross sections is reviewed with emphasis on the justification of the Hauser Feshbach formula and its modifications for situations including isolated compound nucleus resonances, overlapping and interfering resonances, the competition of compound and direct reactions, and continuous treatment of residual nuclear states.

1. STATISTICAL THEORY AND THE OPTICAL MODEL

The fundamental description of a quantum mechanical system, such as the atomic nucleus is provided by the wave function ψ which is obtained from the solution of the Schrödinger equation $(H-E)\psi=0$, where H is the Hamiltonian energy operator, which includes all kinetic and interaction energies of the system, and E is the energy of the system. Even in a relatively light nucleus, the many interaction terms between the nuclear constituents give rise to strong and rapid variations of ψ when the energy is varied at excitations of several MeV or higher, where neutron induced reactions can take place. The details of these variations are often difficult to ascertain theoretically and they are often irrelevant to nuclear power applications because they are washed out by Doppler broadening and by effective flux averaging. It is therefore useful to treat these variations statistically, that is to say, by discussing energy averages of relevant quantities, such as cross sections.

For the discussion of scattering and reactions we are interested only in the asymptotic wave function which is specified by the S-matrix whose typical component S_{cd} is the coefficient of the outgoing wave in channel d when a unit flux plane wave is incident only in channel c. The S-matrix is required to be symmetric and unitary because of time-reversal invarience and flux conservation, and its elements completely determine all observable cross-sections. For example the differential cross section for scattering from a neutron channel c to the same or any other channel d has the form

$$\frac{d\sigma_{cd}(\Theta)}{d\Omega} = \sum_{L} P_L(\cos\Theta) \sum_{c',d'} f_{Lcc'dd'} \, \mathrm{Re}\left[(\delta_{cc'} - S_{cc'})(\delta_{dd'} - S^*_{dd'})\right]$$

$$f_{Lcc'dd'} = (-1)^{s_c - s_d} \frac{\lambda_c^2}{4(2s_c+1)} \sum_{\ell_{c'}\ell_{d'}J_1J_2} i^{\ell_c - \ell_{c'} + \ell_d - \ell_{d'} - 2L}$$

$$\times Z(\ell_c J_1 \ell_{c'} J_2; s_c L) Z(\ell_d J_1 \ell_{d'} J_2; s_d L)$$

$$Z(\ell_1 J_1 \ell_2 J_2; sL) = \sqrt{(2\ell_1+1)(2\ell_2+1)(2J_1+1)(2J_2+1)}$$
$$\times (\ell_1 \ell_2 00 | L0) \times W(\ell_1 J_1 \ell_2 J_2, sL)$$

and where ℓ_c and s_c are the orbital angular momentum and channel spin in channel c and the Z-coefficients are products of one Clebsch-Gordon coefficient and one Racah coefficient W. The angle integrated cross section is

$$\sigma_{cd} = \pi\lambda^2 |\delta_{cd} - S_{cd}|^2 \tag{2}$$

and the total cross section is

$$\sigma_c^{tot} = 2\pi\lambda^2 (1 - \mathrm{Re}S_{cc}) \tag{3}$$

In order to treat the energy variations of these cross sections statistically, we must give a statistical description of the energy variations of the S-matrix elements S_{cd}. The simplest and most important statistical property of S is its energy average $\bar{S}$. Energy averaging does not affect the symmetry property, but it does destroy unitarity, and thereby flux conservation. Averaging cannot create new flux, it can only "absorb" flux into the "compound nucleus" so that the re-emission of this absorbed flux is not described by $\bar{S}$. Therefore $\bar{S}$ must be "less than unitary", which means that the transmission coefficients

$$T_c = 1 - \sum_d |\bar{S}_{cd}|^2 \tag{4}$$

must satisfy

$$0 \leq T_c \leq 1 \tag{5}$$

where the lower limit implies unitarity of $\bar{S}$, and therefore an energy independent S, and the upper limit implies complete absorption of all incoming flux into the compound system. The transmission coefficient T_c represents the compound nucleus "absorption" cross section in units of $\pi\lambda^2$.

The cross sections obtained by substituting $\bar{S}$ in place of S in Eqs. (1)-(3) are referred to as "direct" cross sections and the direct elastic scattering cross section is called the "shape elastic" cross section. To obtain the complete average cross section $\bar{\sigma}_{cd}$, the direct cross section must be complemented with the average compound nucleus cross section $\sigma_{cd}^{f\ell}$ (also called the fluctuation cross section) which arises from the re-emission into channel d of the absorbed flux T_c.

The calculation of this average compound nucleus cross section is the principal object of the statistical theory that is of interest to nuclear power applications.

The average S-matrix $\bar{S}$ is obtained from the optical model by solving the Schrödinger equation with a complex potential interaction between the neutron or other scattered particle and the residual nucleus [1. The real part of this potential produces shape elastic scattering and the imaginary part is responsible for the compound nucleus absorption. If the optical model Hamiltonian contains also interaction potentials between particles in different reaction channels, then we have a coupled channels optical model with non-vanishing off-diagonal elements of $\bar{S}$ and with nonvanishing direct reaction cross sections between these channels [2]. Optical and coupled channels models are discussed in greater detail in paper RP5. Among recent developments in the statistical theory is the discussion of the effects of such direct reaction cross sections upon competing compound nucleus cross sections [3,4,5].

The compound nucleus or fluctuation cross section arises from the fluctuating part of the S-matrix

$$S^{f\ell} = S - \bar{S} \tag{6}$$

in the following way

$$\sigma_{cd}^{f\ell} = \bar{\sigma}_{cd} - \sigma_{cd}^{direct} = \pi\bar{\lambda}^2 \overline{|S_{cd}^{f\ell}|^2} \tag{7}$$

where the superposed bar denotes an energy average. The differential fluctuation cross section is

$$\frac{d\sigma_{cd}^{f\ell}(\Theta)}{d\Omega} = \sum_L P_L(\cos\Theta) \sum_{c'd'} f_{Lcc'dd'} \overline{\mathrm{Re}S_{cc'}^{f\ell} S_{dd'}^{f\ell *}} \tag{8}$$

The simplest assumption leading to expressions for the fluctuation cross section considers that "the average compound nucleus" behaves like a single state of the nuclear system which emits particles into the various reaction channels in the same proportions as it absorbs them. This assumption immediately leads to the well-known Hauser-Feshbach formula for the compound nucleus cross section [6,7].

$$\sigma_{cd}^{H.F.} = \pi\bar{\lambda}^2 \, T_c T_d / \sum_e T_e \tag{9}$$

where the sum in the denominator is taken over all open channels. Adding the assumption that the average of products of different S-matrix elements vanishes, we obtain the differential Hauser-Feshbach formula for the compound nucleus cross section from Eq. (8) and

$$\mathrm{Re}\,\overline{S^{f\ell}_{cc'}S^{f\ell*}_{dd'}} = \left[\delta_{cd}\delta_{c'd'} + (1-\delta_{cc'})\,\delta_{cd'}\delta_{c'd}\right] T_c T_{c'} / \sum_e T_e \qquad (10)$$

In the usual Optical Model with spin-orbit coupling the channel transmission coefficients T_c depend upon the channel orbital angular momentum ℓ_c and the total projectile angular momentum $\vec{j}_c = \vec{\ell}_c + \vec{s}_c$ (vector addition), where s_c is the projectile spin (½ in the case of nucleons). With this dependence, Goldman and Lubitz have derived the following formula for the differential compound nucleus cross section for spin ½ particles [8].

$$\frac{d\sigma^{H.F.}_{cd}(\Theta)}{d\Omega} = \frac{\lambda\!\!\!^{-2}_c(-1)^{I_c - I_d}}{8(2I_c+1)} \sum \frac{T_c T_d}{T_e} P_L(\cos\Theta) \qquad (10a)$$

$$(2J+1)^2(2j_c+1)(2j_d+1)(j_c\tfrac{1}{2}j_c-\tfrac{1}{2}|L0)(j_d\tfrac{1}{2}j_d-\tfrac{1}{2}|L0)$$

$$W(Jj_cJj_c;\,I_cL)W(Jj_dJj_d;I_dL)$$

where the summation is over all $J, j_c, j_d, \ell_c, \ell_d$, and all even L, and where I_c and I_d are the target and residual nucleus spins in channels c and d.

The angle integrated cross section averaged over all initial angular quantum numbers and summed over all final angular quantum numbers is then

$$\sigma^{H.F.}_{[cd]} = \pi\lambda\!\!\!^{-2} \sum_J \frac{2J+1}{2(2I_c+1)} \frac{T_c T_d}{\sum_e T_e} \qquad (9a)$$

where the summation extends also over all j_c, ℓ_c, j_d, ℓ_d, consistent with total angular momentum J. In both Eqs. (9a) and (10a) the channels e must have total angular momentum J and the same parity as channels c and d. We will henceforth omit the averaging and summation over angular momenta and discuss the individual channel cross sections as in Eq. (9).

The following three sections review the main features of statistical theories and how their predictions of the fluctuation cross section agree or differ from the Hauser-Feshbach formula. The final section deals with situations in which the residual nuclear states have a continuous spectrum or are treated as such.

2. ISOLATED RESONANCES

At low neutron energies, the energy dependences of neutron cross sections are well known to arise from sequences of well isolated Breit-Wigner resonances [9]. This behavior is described by an S-matrix which has the form [10].

$$S_{cd} = e^{-i(\phi_c + \phi_d)} \left(\delta_{cd} - i \sum_{\mu} \frac{f_{\mu c} f_{\mu d}}{E - E_{\mu} + \frac{1}{2} i \Gamma_{\mu}} \right) \tag{11}$$

where the total widths Γ_{μ} are related to the partial widths $\Gamma_{\mu c}$ and the real width amplitudes $f_{\mu c}$ by

$$\Gamma_{\mu c} = f^2_{\mu c} , \; \Gamma_{\mu} = \sum_{c} \Gamma_{\mu c} \tag{12}$$

and where all widths Γ_{μ} are small compared to the spacings between resonance energies E_{μ}.

Averaging Eq. (11) over energy, we obtain the optical model S-matrix elements

$$\bar{S}_{cd} = e^{-i(\phi_c + \phi_d)} \left(\delta_{cd} - \pi \langle f_{\mu c} f_{\mu d} \rangle_{\mu} / D \right) \tag{13}$$

where D is the mean spacing of the E_{μ} and the bracket $\langle \; \rangle_{\mu}$ refers to an average with respect to the resonance index μ, taken over all resonances within the averaging interval. We see immediately that in the absence of direct reactions when $\bar{S}_{cd}$ vanishes for $c \neq d$, $\langle f_{\mu c} f_{\mu d} \rangle_{\mu}$ must also vanish, and vice versa. We shall assume here that $\bar{S}$ is diagonal and return to the case of direct reactions in Section 4. Then we have

$$\bar{S}_{cd} = \delta_{cd} e^{2i\phi_c} \left(1 - i\pi \langle \Gamma_{\mu c} \rangle_{\mu} / D \right) \tag{14}$$

which leads to

$$T_c = 1 - |\bar{S}_{cc}|^2 = \frac{2\pi \langle \Gamma_{\mu c} \rangle_{\mu}}{D} - \frac{\pi^2 \langle \Gamma_{\mu c} \rangle^2}{D^2} \tag{15}$$

where we will ignore the second term in the limit of small $\langle\Gamma_{\mu c}\rangle/D$, that is in the limit of small transmission coefficients.

In this same limit the fluctuation cross section is easily calculated from the S-matrix (11) with the assumption that $\bar{S}$ is diagonal, and one obtains

$$\sigma_{cd}^{f\ell} = \frac{2\pi^2\lambda\!\!\!^{-2}}{D} \left\langle \frac{\Gamma_{\mu c}\Gamma_{\mu d}}{\Gamma_\mu} \right\rangle_\mu \tag{16}$$

which, on omitting the second term in Eq. (15) becomes [11-14]

$$\sigma_{cd}^{f\ell} = \pi\lambda\!\!\!^{-2}_c \, \sigma_{cd}^{H.F.} F_{cd} \tag{17a}$$

where

$$F_{cd} \equiv \left\langle \frac{\Gamma_{\mu c}\Gamma_{\mu d}}{\Gamma_\mu} \right\rangle_\mu \Big/ \frac{\langle\Gamma_{\mu c}\rangle_\mu \langle\Gamma_{\mu d}\rangle_\mu}{\langle\Gamma_\mu\rangle_\mu}$$

$$= \left(1+2\,\frac{\delta_{cd}}{\nu_d}\right) \int_0^\infty dt \prod_f \left(1 + \frac{2tT_f}{\nu_f \sum_g T_g}\right)^{-(\frac{1}{2}+\delta_{fc}+\delta_{fd})} \tag{17b}$$

In this integral evaluation of the width fluctuation correction F_{cd} to the Hauser Feshbach formula, it is assumed that the distribution of values of the partial widths $\Gamma_{\mu c}$ for each channel c are given by the chi-squared distribution law with ν_c degrees of freedom, which is defined for any positive real ν by the frequency function

$$F_\nu(x) = x^{(\frac{\nu}{2}-1)} e^{-\frac{x}{2}} \Big/ \left(2^{\frac{\nu}{2}}\Gamma(\tfrac{\nu}{2})\right) \tag{18}$$

Tepel et al. [15] found a formula which yields a very good approximation to the width fluctuation c..rected Hauser Feshbach formula of Eqs. (17) in most instances, but does not require the integration of Eq. (17b). According to these authors

$$\sigma_{cd}^{f\ell} \approx \pi\lambda\!\!\!^{-2}_c \left(Y_c Y_d + 2\delta_{cd} Y_d^2/\nu_d\right) \Big/ \sum_e Y_e \tag{19a}$$

where

$$Y_c = \frac{T_c}{1+\frac{2}{\nu_c}\frac{T_c}{\sum_e T_e}} \tag{19b}$$

Clearly, in the case of isolated resonances with no direct reactions, the only information which we need in order to evaluate the fluctuation cross sections is the optical model transmission coefficients and the partial width distribution laws for all open channels. There is considerable theoretical as well as experimental evidence that in this isolated resonance limit the $f_{\mu c}$ of Eq. (11) are normally distributed with zero means. It follows from this that the $\Gamma_{\mu c}$ are distributed according to the chi-squared distribution with one degree of freedom (the Porter-Thomas distribution) for any "channel" c which is specified by a single complete set of quantum numbers describing the channel angular momenta and the state of the residual nucleus [16-17]. This is the case for neutron and proton partial widths in channels having a specified orbital and total angular momentum and a specified residual nuclear level. Any "channel" that is specified by n independent quantum channels all having the same average partial width, is distributed according to a chi-squared distribution with n degrees of freedom. Thus "capture" generally encompasses a large number of independent gamma ray transitions to various low lying levels of the compound nucleus, and therefore the capture width has a very narrow distribution corresponding to a large degree of freedom (see paper RP3). Fission, which often proceeds by one of several independent processes, gives rise to fission widths which have generally between two and three degrees of freedom, depending on isotope and energy. Fission will be discussed in paper RP7.

The effect of the width fluctuation correction is to increase the compound elastic fluctuation cross section and to decrease non-elastic cross sections correspondingly. The effect of this correction is particularly pronounced for the inelastic scattering to the first excited state of an even A nucleus, which can be reduced by almost a factor of ½ compared to Hauser-Feshbach. Correspondingly the compound elastic cross-section is enhanced by almost 50% compared to Hauser-Feshbach. When many channels are open, the effect on each inelastic cross section becomes less pronounced, but the compound elastic effect increases to a possible maximum enhancement by a factor of 3. Some typical magnitudes of the width fluctuation correction are shown in the graphs of Fig. 1 and a typical example of the effect upon inelastic scattering to the first excited state in even A nuclei is shown in Fig. 2.

There are, of course, other interesting statistical properties that affect the details of the energy variations of the cross sections, such as the behavior of the level densities and the distribution of level spacings. The level densities will be reviewed in paper RP4. Level spacing distribution laws have been very intensively studied by a number of authors [14,17]. But this subject is of very limited interest to nuclear power applications.

In computing elastic and non-elastic neutron scattering cross sections, it is important, particularly at low energies, to include the contribution $T_\gamma = 2\pi\Gamma_\gamma/D$ of the capture channels to the transmission factor sum in the Hauser-Feshbach cross section in Eq. (17), as is done in the computer program NEARREX [18]. The effect of the capture channels on the width fluctuation correction (17) can be taken into account by an additional factor of $\exp[-tT_\gamma/\sum_g T_g]$ in the integral [13]. This treatment assumes that the capture widths do not fluctuate. Computer programs for the calculation of average cross sections by the width-fluctuation corrected Hauser-Feshbach formula include NEARREX [18], ALTE [19], and STAX 2 [20].

3. INTERFERING RESONANCES

As we have seen in Eq.(15), the results of the previous section break down as soon as T_c for some channel is no longer very small, as will happen for low angular momentum neutron channels at quite moderate energies of typically some tens of kilovolts. Then $\langle\Gamma_\mu\rangle_\mu/D$ is no longer very small and consequently at some energies more than one term in the resonance sum of Eq.(11) will contribute significantly to S. At such energies the expression (11) is not unitary and it can be shown that it is in fact impossible to make Eq.(11) unitary at all such energies with real parameters $f_{\mu c}$.

In order to retain unitarity, Eq.(11) must be modified to read [10,21,22]

$$S_{cd} = S^b_{cd} - i\sum_\mu \frac{g_{\mu c}g_{\mu d}}{E-E_\mu+\frac{1}{2}i\Gamma_\mu} \tag{20}$$

where the S^b_{cd} and the $g_{\mu c}$ are complex parameters that are only slowly energy dependent, and that satisfy complicated and not yet fully understood relations in place of Eq. (12).

Two known relations that the parameters of Eq. (20) must satisfy in the case of diagonal $\bar{S}$ are, first of all [23]

$$2\pi \langle g_{\mu c}{}^2 \rangle_\mu/D = \bar{S}^{*-1} - \bar{S} \tag{21a}$$

or

$$|2\pi \langle g_{\mu c}{}^2\rangle_\mu/D|^2 = T_c{}^2/(1 - T_c) \tag{21b}$$

where D is the mean spacing of the E_μ in (20). Secondly we have the requirement that [24,25]

$$\bar{S}_{cc} = e^{-\pi\langle\Gamma_{\mu c}\rangle_\mu/D}\ , \quad \langle\Gamma_\mu\rangle_\mu = \sum_c \langle\Gamma_{\mu c}\rangle_\mu \tag{22a}$$

or

$$T_c = 1 - e^{-2\pi\langle\Gamma_{\mu c}\rangle_\mu/D} \tag{22b}$$

and it follows from (21) and (22) that

$$\pi|\langle g_{\mu c}^2 \rangle_\mu|/D = \sinh(\pi\langle\Gamma_{\mu c}\rangle_\mu/D) \tag{23}$$

which shows that the mean partial width becomes logarithmically infinite as T_c approaches unity, and that the absolute mean square amplitudes $g_{\mu c}$ grow exponentially compared to the mean partial widths.

We can again calculate the optical model S-matrix and the fluctuation cross section and obtain [21]

$$\bar{S}_{cd} = S^b_{cd} - \pi\langle g_{\mu c}g_{\mu d}\rangle_\mu/D \tag{24}$$

which implies quite generally, that in order for $\bar{S}$ to have off-diagonal elements, either S^b or $\langle g_\mu \times g_\mu\rangle_\mu$ or both must have off-diagonal elements. The possibility that the two terms cancel is effectively excluded. The fluctuation cross section for diagonal $\bar{S}$ is [21,25]

$$\sigma_{cd}^{f\ell} = \pi ƛ^2 \; (2\pi/D)\langle |g_{\mu c}|^2 |g_{\mu d}|^2/\Gamma_\mu \rangle - M_{cd} \tag{25}$$

where

$$M_{cd} = \tfrac{1}{2}\, \delta_{cd} T_c{}^2/(1-T_c) - (2\pi i/D)\Big\langle \sum_{\nu\neq\mu} \frac{g_{\nu c} g_{\nu d} g^*_{\mu c} g^*_{\mu d}}{(E_\mu - E_\nu)+\frac{1}{2} i(\Gamma_\mu+\Gamma_\nu)} \Big\rangle_\mu \tag{26}$$

The first term in Eq. (25) looks like Hauser-Feshbach but is difficult to evaluate because we know nothing about the $|g_{\mu c}|^2$ except that they are proportional to the $\Gamma_{\mu c}$ independent of channel index [10,21].

$$|g_{\mu c}|^2/\Gamma_{\mu c} = N_\mu \geq 1 \tag{27}$$

This fact permits us to define the quantities [21]

$$\Theta_{\mu c} = (2\pi/D) N_\mu{}^2 \Gamma_{\mu c} \;, \; \Theta_\mu = \sum_c \Theta_{\mu c} \tag{28}$$

from which

$$\sigma_{cd}^{f\ell} = \pi ƛ^2 \; (\langle \Theta_{\mu c} \Theta_{\mu d}/\Theta_\mu \rangle - M_{cd}) \tag{29}$$

and

$$T_c = \langle \Theta_{\mu c} \rangle_\mu - \sum_d M_{cd} \tag{30}$$

The evaluation of the first term of Eq. (29) is complicated by the fact that it can be shown that there exist correlations between the $\Theta_{\mu c}$ for different channels [26] even in the absence of direct reactions, and these correlations make the evaluation much more difficult than in the case of Eq. (16) where the $\Gamma_{\mu c}$ were not correlated for different channels. Also the evaluation of the second term in Eq. (26) depends on a knowledge of possible resonance-resonance correlations of the $g_{\mu c}$ [27].

It has been shown that in a certain class of cases, the effect of the channel-channel correlations of the $\Theta_{\mu c}$ just cancels the contribution of M [26]. Assuming this M-cancellation to be generally valid one arrives at a formula for the fluctuation cross section that is identical to the width fluctuation corrected Hauser-Feshbach formula (17). The only difference is that now we do not know the values of the fluctuation indices ν_c for the various channels as we did in the case of isolated resonances. From general theoretical considerations one deduces that for each independent channel the value of ν_c rises from 1 towards a limiting value of 2 as $\langle\Gamma\rangle/D$ increases. From certain numerical studies Tepel et al. [15] have deduced an empirical expression for ν_c as a function of T_c

$$\nu_c = 1 + T_c^{1/2} \tag{31}$$

Other more complicated functional relationships have been proposed elsewhere [4]. However almost certainly the value of ν_c does not only depend on T_c but also on the transmission coefficients of all competing channels. If channels with large transmission coefficients compete with a channel c having a small T_c, the value of ν_c will be larger than indicated by Eq. (31) [26]. More work is required in this area.

It is important to note that the M-cancellation principle replaces an earlier attempt to take into account the second term in Eq. (30) by modifying the definition of T_c, using parameter Q_c [18,21, 25].

There exist two other methods for treating the fluctuation cross section which are so far applicable only to the limit of very large $\langle\Gamma\rangle/D$. They may therefore not be usable in many situations of interest to nuclear power applications. The first of these is the treatment of Kawai, Kerman and McVoy which is based upon a representation of the S-matrix that looks very much like Eq. (20), but whose parameters are chosen in such a way that S is not unitary at all energies [3]. The resulting fluctuation cross section formula, which does not involve the difficult expression M in Eq. (24) yields virtually identical results to those obtained from the M-cancellation procedure in the limit of large Γ/D if all channel fluctuation indices are chosen to have the value $\nu_c = 2$. We shall return to this formula in the next section.

There is also a new and entirely different method due to Agassi and Weidenmüller which is based upon the doorway state description of the nuclear reaction mechanism (see paper RP6), and which yields correction terms to the Hauser-Feshbach formula in the limit of large $\langle\Gamma\rangle/D$ [28].

4. DIRECT REACTION EFFECTS

As we saw in Eq. (13), one obvious effect of direct reactions is that they can produce correlations between the partial widths of different channels. (Actually, Eq. (11) must be modified to permit also nonresonant off-diagonal terms if direct reactions are present.) Correlations in partial widths of different channels must be expected to produce enhanced fluctuation cross sections between these channels. The reason for this is the same as the reason for the width-fluctuation enhancement of the elastic fluctuation cross section, Eq.(17), which arises from the complete correlation of entrance and exit channel widths in the elastic case, where the two are identical. Thus the effect of direct reactions upon average compound nucleus cross sections is basically an aspect of the width fluctuation correction. In the case of isolated resonances the direct effect can be calculated in this way [29,30]. However the most general and useful method is the use of the Engelbrecht-Weidenmüller transformation [31] which is a linear transformation of the reaction channels that results in a transformed unitary S-matrix with a diagonal average.

This transformation is specified by the unitary matrix U that diagonalizes the Hermitean penetration matrix P of Satchler [32]

$$P = 1 - \overline{S}\,\overline{S}^* \tag{32}$$

$$P' = UPU^{-1} \text{ is diagonal,} \tag{33}$$

where $U^{-1} = U^{\dagger}$.

It follows then that

$$S' = US\tilde{U} \tag{34}$$

is unitary, where $\tilde{U}$ is the transpose of U, and

$$\overline{S}' = U\overline{S}\tilde{U} \text{ is diagonal} \tag{35}$$

Arguments have also been given that S' has the same statistical properties as a physical S-matrix with diagonal average [4]. For the case of only two directly coupled channels, the transformation U is easily written down explicitly [5]. Writing

$$\overline{S} = \begin{pmatrix} f_1 e^{i\Theta_1} & f_3 e^{i\Theta_3} \\ f_3 e^{i\Theta_3} & f_2 e^{i\Theta_2} \end{pmatrix} \tag{36}$$

and $$U = \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \tag{37}$$

we find that

$$\tan 2\alpha = \frac{f_2 \sin\Theta_{23} - f_1 \sin\Theta_{13}}{f_2 \cos\Theta_{23} + f_1 \cos\Theta_{13}}$$

$$\tan 2\beta = \frac{2f_3}{f_2 \cos(\Theta_{23}-\alpha) - f_1 \cos(\Theta_{23}-\alpha)} \qquad (38)$$

where $\Theta_{13} = \Theta_1 - \Theta_3$, $\Theta_{23} = \Theta_2 - \Theta_3$.

For three or more coupled channels the direct effect will in general not be very significant as we shall see. In such cases numerical diagonalization of P is required.

With the help of the Engelbrecht-Weidenmüller transformation the fluctuation cross section can be expressed entirely in terms of the elements of the transformation matrix U, and certain averages of the transformed S-matrix S'. Two types of such averages occur. The first is of the form $\overline{|S'^{f\ell}_{cd}|^2}$, which is just the fluctuation cross section (7) in the transformed channel space and can be evaluated by the width fluctuation corrected Hauser-Feshbach formula as described in Sections II or III. For this one requires the transmission coefficients in the transformed channel space, which are just the diagonal values of the transformed penetration matrix P'. One also requires the fluctuation parameters ν'_c (Eq. 31) for each of the transformed channels in order to compute the width fluctuation correction factors F'_{cd}. Then

$$\begin{aligned} \sigma'^{f\ell}_{cd} &= \pi\lambda^2_c \, \overline{|S'^{f\ell}_{cd}|^2} \\ &= \pi\lambda^2_c \, (P'_{cc}P'_{dd}/\mathrm{tr}P') \, F'_{cd}. \end{aligned} \qquad (39)$$

In addition there also occur averages of another type, which can be estimated by means of the M-cancellation procedure as follows

$$\pi\lambda^2_c \, \overline{S'^{f\ell}_{cc} S'^{f\ell *}_{dd}} = \sqrt{\frac{2-\nu'_c}{\nu'_c} \cdot \frac{2-\nu'_d}{\nu'_d}} \, \sigma'^{f\ell}_{cd} \qquad (40)$$

Using Eqs. (35), (39), (40) one obtains for the fluctuation cross section in the presence of direct reactions [5]

$$\sigma_{cd}^{f\ell} = \sum_{e} |U_{ec}|^2 |U_{ed}|^2 \sigma'^{f\ell}_{ee}$$
$$+ \sum_{f \neq e} \Big[U^{*}_{ec} U^{*}_{fd} (U_{ec} U_{fd} + U_{fc} U_{ed}) \tag{41}$$
$$+ \sqrt{\frac{2-\nu'_e}{\nu'_c} \frac{2-\nu'_f}{\nu'_f}} \; U^{*}_{ec} U^{*}_{ed} U_{fc} U_{fd} \Big] \sigma'^{f\ell}_{ef}$$

A very similar formula that yields almost entirely equivalent results, but is a little more complicated to evaluate, has been given by Hofmann et al. [4]. The formula of Kawai, Kerman and McVoy [3] yields results equivalent to Eq. (41) only in the limit of large $\langle\Gamma\rangle/D$ when all ν'_c are equal to 2. Then this formula reads

$$\sigma_{cd}^{f\ell} = X_{cc} X_{dd} + X_{cd} X_{dc}, \quad \langle\Gamma\rangle >> D \tag{42}$$

$$P_{cd} = \sum_{e} (X_{cd} X_{ee} + X_{ce} X_{ed}) \tag{43}$$

Here Eq. (43) must first be solved for X by numerical iteration and then substituted into Eq. (42).

Qualitatively we see from Eq. (41) that the enhancement of the fluctuation cross section due to direct reactions is at most equal to the width-fluctuation enhancement of the transformed elastic fluctuation cross section $\sigma'^{f\ell}_{ee}$. This enhancement amounts at most to a factor of $1 + 2/\nu'_e$ and will in practice almost always be less than a factor of 2. The maximum enhancement is achieved when only two channels are directly coupled to one another and det P = 0. In that case the transmission coefficients for one of the two transformed channels vanishes, and therefore there is only one independently fluctuating transformed channel. As a result, the fluctuations in the two coupled physical channels are completely correlated, just as in the case of compound elastic scattering. The case det P = 0 is called the causality limit because causality considerations are violated when det P is negative [5]. Eq. (41) predicts that enhancements due to direct reactions are appreciable only quite close to the causality limit when that limit is not identical to the unitarity limit trP=0. Ordinarily large enhancements will occur only when the rank of P is no greater than 2. Fig. 3 shows the enhancement due to direct reactions as computed by means of Eq. (40) for two types of $\overline{S}$ matrices. In one of these (upper right) the causality limit coincides with the unitarity limit, and there is no appreciable enhancement. In the other case the causality limit is not equal to the unitarity limit and enhancements close to a factor of 2 occur.

The validity of the results of Eq. (41) have been confirmed by computer averaging of computer generated statistical model cross sections [5]. Such calculations have also been used to confirm the M-cancellation principle for a wide variety of $\overline{S}$ matrices [26].

5. CONTINUOUS CHANNELS

With increasing neutron energy the number of open exit channels increases rapidly until it is either impossible or undesirable to enumerate all such channels and discuss their cross sections in detail. It then becomes necessary to discuss the differential cross section for transitions to channels of a given type (e.g., neutron or protons, etc.) leaving the residual nucleus with an excitation energy within a differential interval at E_d.

$$\frac{d\sigma_{cd}^{f\ell}(\text{cont.})}{dE_d} = \sigma_{cd}^{f\ell}(\text{discr.})\ \rho_d(E_d) \tag{44}$$

where $\sigma_{cd}^{f\ell}(\text{discr.})$ is the cross section for excitation of a discrete channel with residual nuclear excitation E_d, and $\rho_d(E_d)$ is the level density at excitation E_d of the residual nucleus in channel d for states having spin and parity specified by the channel index d. We refer again to paper RP4 for a detailed discussion of level densities.

If the dependence of ρ_d upon the relevant residual spins I_d is given by the factor $(2I_d+1)$, then it can be shown that the fluctuation cross section (44) summed over I_d is isotropic. Though this spin dependence of ρ_d is not correct, the anisotropies of fluctuation cross sections at such high energies are expected to be small and can often be ignored.

Also, in the presence of large numbers of competing channels, the width fluctuation correction and direct effect upon non-elastic fluctuation cross sections becomes negligible. On the other hand for $\langle\Gamma\rangle >> D$ we expect an elastic width fluctuation correction factor of 2, so that in the present domain we expect that

$$\sigma_{cd}(\text{discr.}) \cong (1 + \delta_{cd})\sigma_{cd}^{H.F.} , \qquad (45)$$

where again, the channel indices c and d carry all relevant energy and angular momentum quantum numbers.

The transmission factor sum $\sum_e T_e$ which occurs in the denominator of $\sigma_{cd}^{H.F.}$, Eq. (9), must also be evaluated statistically

$$\sum_e T_e = \sum_e \int_0^{E_e(\max)} T_e(E_e)\rho_e(E_e)dE_e \qquad (46)$$

which involves the level densities for the residual nuclei in all competing channels. Again, if ρ_e depends on the residual nucleus spin through a factor $(2I_e+1)$, then the transmission sum (46) is given by [33]

$$\sum_e T_e = (2J+1)G/\pi \qquad (46a)$$

where J is the total angular momentum and G depends only upon excitation energy of the compound nucleus.

Another empirical method for determining the transmission factor sum makes use of the relation [34]

$$\sum_e T_e \cong 2\pi\Gamma^{corr}/\rho \qquad (47)$$

where Γ^{corr} is the correlation width and ρ is the compound nucleus level density for states of the same total angular momentum and parity as the channels e that are summed over. The correlation width can under some circumstances be estimated from fluctuation experiments [35]. The validity of the relation (47) was recently confirmed by numerical studies [26]. Comparison of Eqs. (22b) and (47) shows that the correlation width of Eq. (47) is not the same as the average of the widths $\langle\Gamma_\mu\rangle_\mu$ of Eq. (20).

Difficulties remain in the reliable treatment of compound nucleus cross sections at high energies. These are caused by a number of different circumstances. First, there is the uncertainty regarding the effects of gamma ray transitions between highly excited compound nuclear states in softening the spectrum of emitted neutrons and protons. Secondly, there are empirical results which disagree with the shapes of the particle spectra predicted by the above statistical picture. This effect has been treated with considerable success by means of the pre-equilibrium models which will be discussed in paper RP6 [36].

Finally, at neutron energies exceeding 10 to 20 MeV, residual nuclear levels become unstable and emit secondary particles which further add to the particle flux generated by the reaction. From a theoretical viewpoint, such physically continuous channels pose a three- or more body problem in the channel portion of configuration space, not just in the compound nucleus. While theoretical methods exist now for treating three-body problems [37], they are complicated and time-consuming and have not yet been applied to neutron induced reactions in heavy nuclei. It is therefore generally assumed that above the threshold for three body breakup, the breakup proceeds sequentially. That is, in addition to the particle spectrum produced according to Eq. (44), there are additional particles produced by the breakup of the residual nuclei in each channel d which is given by

$$\int_0^{E_d(\max)} dE_d \sigma_{cd}^{f\ell}(\text{discr.}) \rho_d(E_d)\ T_{d'} \rho_{d'}(E_{d'}) / \sum_{e'} T_{e'} \tag{48}$$

where the channels d' are decay channels of the residual nucleus of channel d, considered as a new compound system, etc.

When level densities are computed from the model of the nucleus which pictures it as a gas of fermions, characterized by a temperature parameter, the particle spectra produced according to Eqs. (44), (48), etc., are called evaporation spectra. Probably in most instances, the doorway state models involving precompound or pre-equilibrium decay (see paper RP6) give a better account of these spectra.

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*Work performed under the auspices of the U.S. Energy Research and Development Administration.

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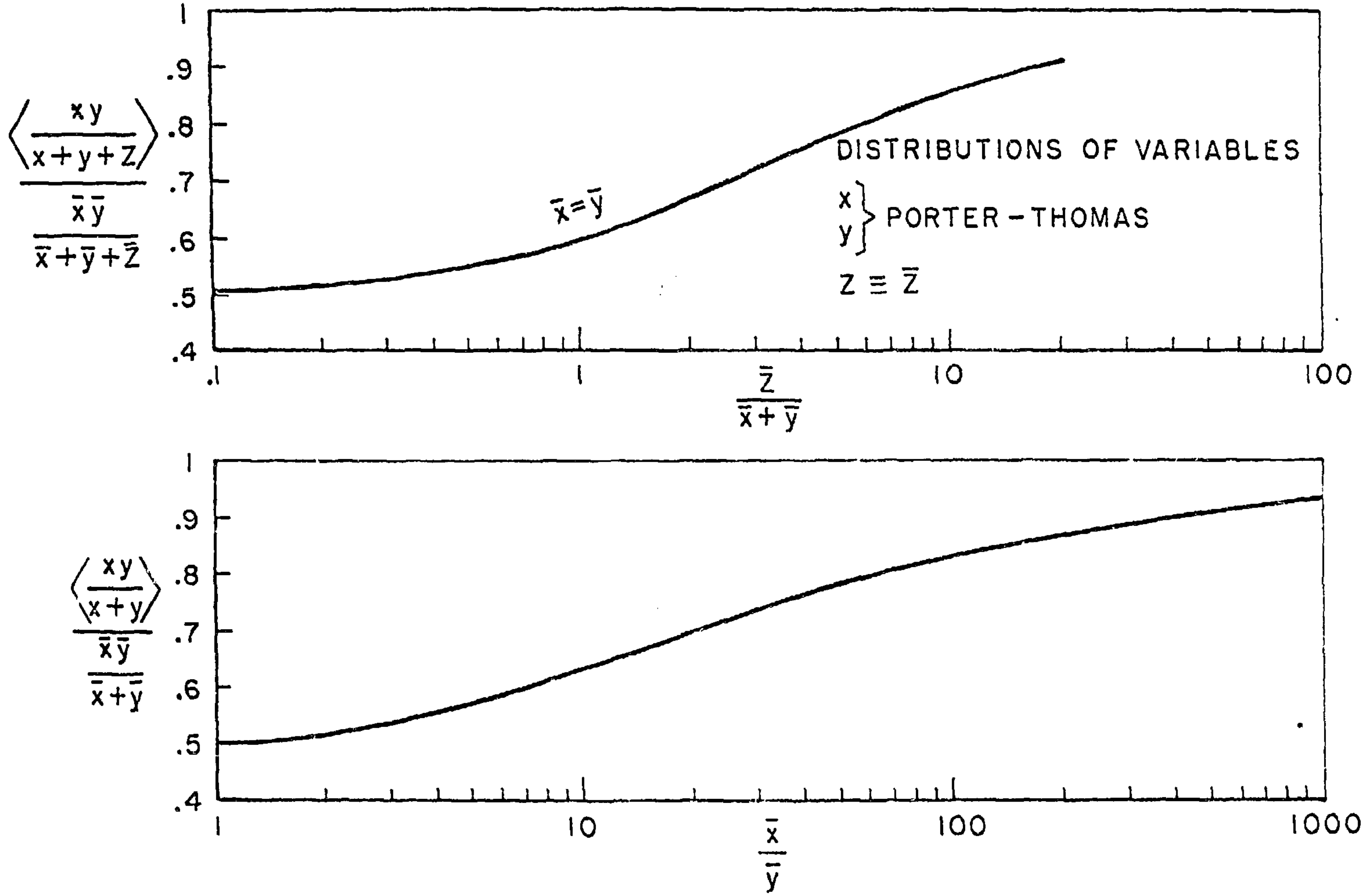
FIGURE CAPTIONS

Fig. 1. Some non-elastic width fluctuation correction factors for two channels (x and y) having $\nu=1$ (Porter-Thomas) and one channel (Z) having $\nu=\infty$ (exponential, equivalent to large numbers of competing channels).

Fig. 2. A typical example of the effect of the width fluctuation correction on the excitation cross section of the first 2^+ state in an even target nucleus. Shown are the Hauser-Feshbach prediction and the width fluctuation corrected predictions for $\nu=1$ and $\nu=2$ for the 845 keV level in iron. Optical potential and data points are from Ref. [38]. (Neutron time-of-flight spectroscopy.) The data curve is from Ref. [39] (gamma ray spectroscopy.)

Fig. 3. Predicted enhancements of compound non-elastic cross sections due to competition with direct reactions for two classes of coupled channel $\overline{S}$-matrices (From Ref. [5])



DISTRIBUTIONS OF VARIABLES
x
y
PORTER-THOMAS
Z ≡ Z̄
x̄=ȳ
.4
.5
.6
.7
.8
.9
1
.1
1
10
100
1000

Fig. 1.

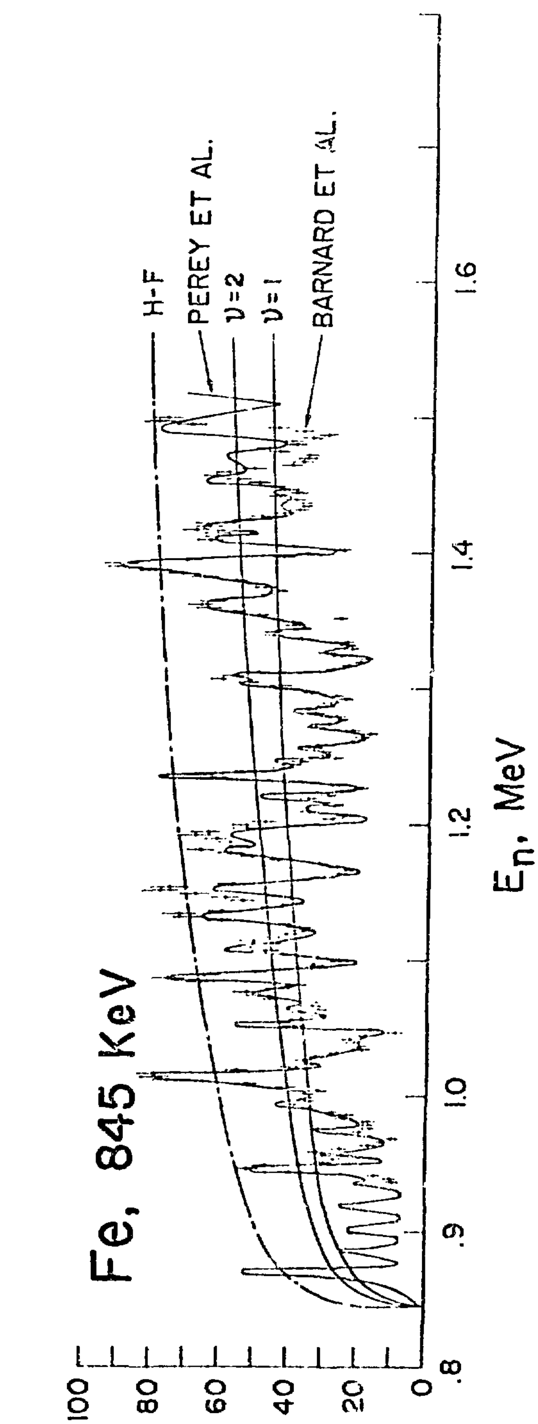
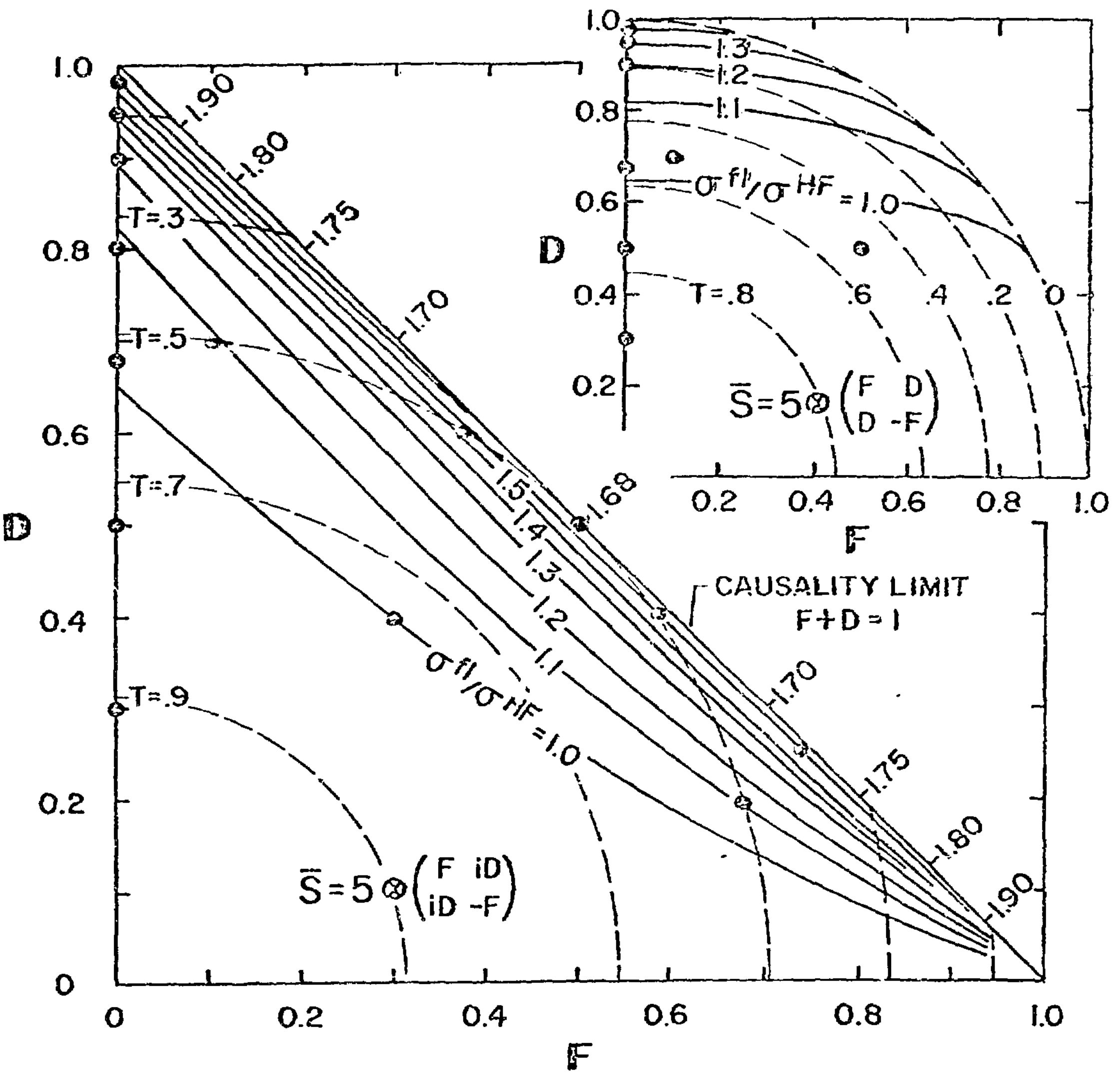

Fe, 845 KeV
H-F
PEREY ET AL.
ν=2
ν=1
BARNARD ET AL.
100
80
60
40
20
0
.8
.9
1.0
1.2
1.4
1.6
En, MeV
dσ/dΩ (90°), mb/sr

Fig. 2.



1.0
0.8
0.6
0.4
0.2
0
D
F
1.90
1.80
1.75
1.70
1.68
1.5
1.4
1.3
1.2
1.1
T=.3
T=.5
T=.7
T=.9
σfl/σHF=1.0
CAUSALITY LIMIT
F+D=1
S̄=5⊗(F iD / iD -F)
S̄=5⊗(F D / D -F)
T=.8
.6
.4
.2
0

Fig. 3.