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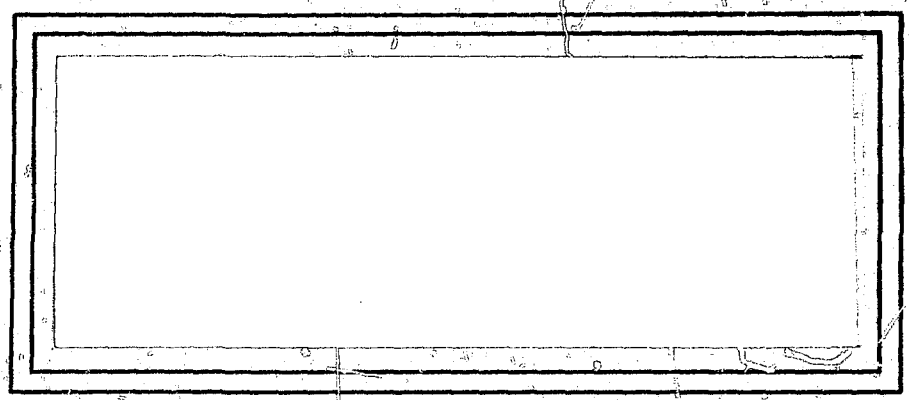

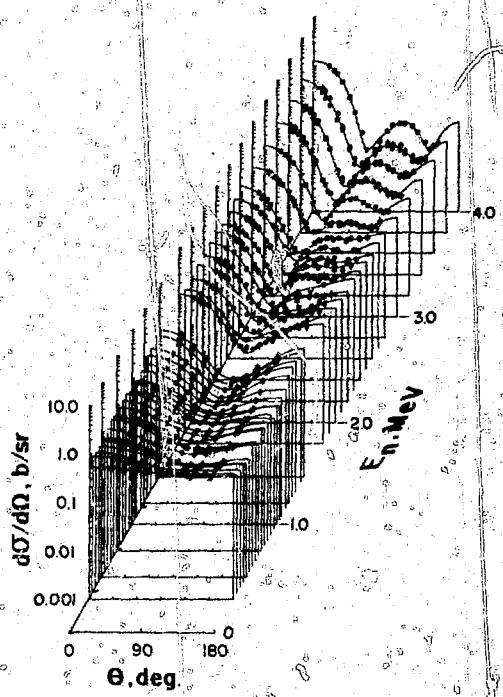

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STATISTICAL THEORY OF NEUTRON NUCLEAR REACTIONS

by

P. A. Moldauer

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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.

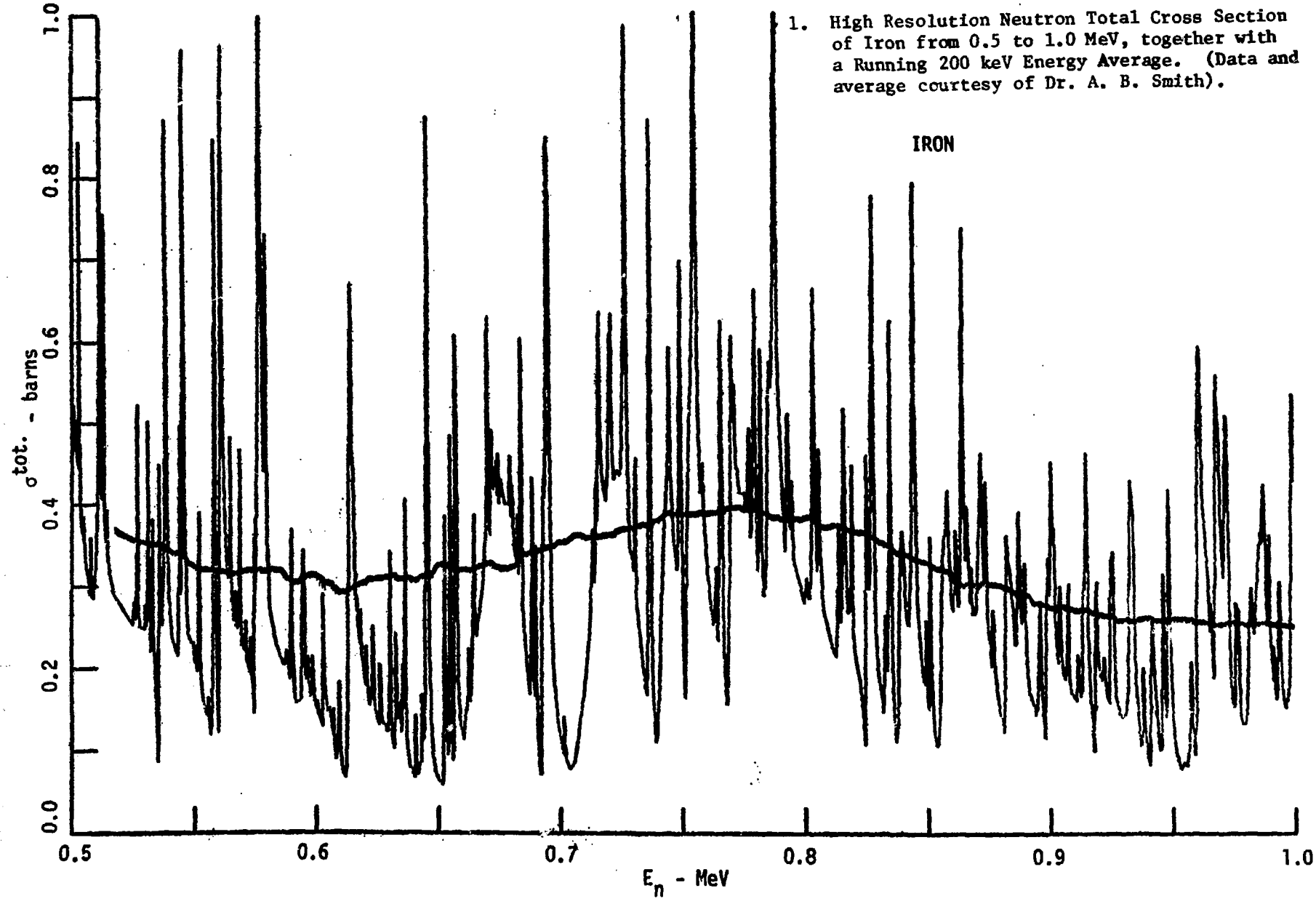
*This work supported by the U. S. Department of Energy.

I. STATISTICS

We shall review theories of certain statistical properties of neutron reaction cross section data. Statistics is a method for the partial description of sets of data. Specifically it relies on averages of the data and of functions of the data. If $\{\sigma_i\}$, 1, 2, ... N is a set of cross section data, then one familiar set of statistics is the average $\langle\sigma\rangle = \Sigma_i\sigma_i/N$ and the central moments $m_\nu(\sigma) = \Sigma_i(\sigma_i - \langle\sigma\rangle)^\nu/N$ where $m_2(\sigma)$ is the square of variance s of $\{\sigma_i\}$. For two sets of data $\{\sigma_i\}$, $\{\tau_i\}$ one has a matrix of central moments $m_{\mu\nu}(\sigma,\tau) = \Sigma_i(\sigma_i - \langle\sigma\rangle)^\mu(\tau_i - \langle\tau\rangle)^\nu/N$ where m_{11} is the covariance of σ and τ and the correlation of σ and τ is $\rho = m_{11}(\sigma,\tau)/(s(\sigma)s(\tau))$. One obtains the autocovariance and the autocorrelation ρ_n for a single set of data $\{\sigma\}$ by stubstituting in the above expression σ_{i+n} for τ_i. These statistics are, of course, also applied to continuous variables by substituting integrals for the summations.

The basic statistics that we will be interested in will be the energy averages of fluctuating neutron cross sections. Fig. 1 shows an example of such a cross section and its energy average. Clearly, the value of an energy averaged cross section depends upon the averaging interval, both its size and its location. Each point in the average cross section curve in Fig. 1 represents the average obtained over an interval of 200 keV which is centered on the point in question. This is how we interpret an energy dependent average cross section. Clearly one can discuss also the variance of such a cross section curve, its autocorrelation, or other statistics which describe the fluctuations about the average. In addition one can discuss the correlation between different cross sections, such as the elastic and inelastic cross section, or the cross sections for scattering at different angles, etc. These fluctuation statistics are, however, of minor interest in applications.

Reaction theory describes the complicated energy fluctuations of cross sections in terms of discrete sets of parameters, the "resonance" or "pole" parameters. The aims of statistical theory are to relate the average cross sections and their fluctuations to the statistics of resonance or pole parameters, and to further relate the latter to physical models and to basic principles. Some of these basic principles on the distributions and correlations of resonance spacing and the distributions



1. High Resolution Neutron Total Cross Section of Iron from 0.5 to 1.0 MeV, together with a Running 200 keV Energy Average. (Data and average courtesy of Dr. A. B. Smith).

Fig. 1

of partial resonance widths were already discussed in the lectures of Sec. II.6. And the relations of resonance statistics to physical models were discussed in Sec. III on the optical model. We will briefly review these matters as we need to.

II. NOTATION

A neutron nuclear reaction proceeds by the interaction of an incident neutron of a certain energy with a target nucleus (Z,A) which together comprise a compound system (Z,A+1). Following the interaction the system breaks up into one of several possible reaction channels consisting of one, two, or more nuclei or nuclides having various internal and relative states. A Roman lower case subscript a,b,c, etc. will be used to label a specific such channel, that is the fragments present, their internal states, and their relative states. In the case of a two product channel, e.g., neutron scattering, the channel index incorporates the relative orbital angular momentum ℓ of the fragments, the total angular momentum $j = \ell + s$ of one (usually the lighter) fragment, where s is that fragment's spin angular momentum and the sum is, of course, the quantitized vector sum, and the total angular momentum $J = j + I$ where I is the spin angular momentum of the heavier fragment. The relative energy of fragments is not included in the channel index as it will usually be the parameter to be averaged over. The Greek subscript γ will be reserved for gamma ray channels in which all possible gamma rays are lumped together. The Greek subscripts α,β will be reserved to indicate the alternatives specifying only the fragments and their internal states.

States of the compound system (Z,A+1) will be labeled by lower case Greek subscripts μ,ν, etc. These incorporate all internal quantum numbers including the total angular momentum J and parity π.

III. ISOLATED RESONANCES [1]

When a low energy neutron interacts with a nucleus, one of two types of things can happen. Either the neutron is scattered elastically without involving the internal degrees of freedom of the target nucleus. This is potential scattering. Or the neutron is absorbed by the target, forming a compound system in one of a number of metastable resonance states. These are states consisting primarily of bound single particle

configurations whose total energy is above the neutron threshold at the energy of the scattering system. However, because of its coupling to the neutron scattering channel and possible other open channels, having positive channel energies, these resonance states do decay with a mean lifetime which is τ_μ for the μth such state. The inverse of this lifetime $1/\tau_\mu \equiv 2\pi\Gamma_\mu/h$ is the probability of decay of the state per unit time. Here h is Planck's constant. The width Γ_μ is the energy uncertainty of the μth state in accordance with Heisenberg's uncertainty principle and it is proportional to the decay probability per unit time of the μth state. If this state can decay into any one of several channels a,b,c, etc., then there will be decay probabilities proportional to partial widths $\Gamma_{\mu a}$, $\Gamma_{\mu b}$, $\Gamma_{\mu c}$, etc. for each of these channels so that $\Gamma_\mu = \Gamma_{\mu a} + \Gamma_{\mu b} + \Gamma_{\mu c} + \ldots$

By reciprocity, the probability of formation of the compound state μ by absorption of an incident neutron in, say, channel a is also proportional to $\Gamma_{\mu a}$, and the relative probability for decay of into channel b is clearly $\Gamma_{\mu b}/\Gamma_\mu$. The cross section for the reaction proceeding from incident channel a to exit channel b through the compound state μ is then proportional to the product of Γ_μ and $\Gamma_{\mu b}/\Gamma$ and is in units of π/k_a^2

$$\sigma_{ab}^{(\mu)} = 2\pi\Gamma_{\mu a}\Gamma_{\mu b}/\Gamma_\mu. \tag{3.1}$$

From this it is clear that the average compound nuclear cross section for the reaction a,b within the energy interval Δ is

$$\bar{\sigma}_{ab}^{c.n.} = \frac{2\pi}{D}\left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle_{\mu\in\Delta}. \tag{3.2}$$

Where D is the mean energy spacing of compound states with correct J and π in Δ and the bracket signifies the average over compound states within Δ. The average absorption cross section into the compound system from channel a is called the transmission coefficient T_a.

$$\bar{\sigma}_a^{c.n.} = \Sigma_b \bar{\sigma}_{ab}^{c.n.} = \frac{2\pi}{D}\left\langle \Gamma_{\mu a} \right\rangle_\mu \equiv T_a. \tag{3.3}$$

These transmission coefficients are specified by various physical models for different types of channels, the optical model for neutron,

proton and other nuclear channels, and corresponding models for fission and capture channels. These models are discussed elsewhere in these lectures. We shall return to the optical model later.

With the definition (3.3), Eq. (3.2) can be rewritten as

$$\bar{\sigma}_{ab}^{c.n.} = \sigma_{ab}^{H.F.} W_{ab} \tag{3.4}$$

where the well-known Hauser-Feshbach formula

$$\sigma_{ab}^{H.F.} = T_a T_b / \Sigma_c T_c \tag{3.5}$$

is completely specified by the transmission coefficients of all open channels, and hence by the physical models for these channels. The second factor in (3.4) is the width fluctuation correction

$$W_{ab} = \left\langle \frac{\Gamma_{\mu a}\Gamma_{\mu b}}{\Gamma_\mu} \right\rangle \Big/ \frac{\langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle}{\langle \Gamma_\mu \rangle} \tag{3.6}$$

This factor depends upon the distributions and correlations of the partial widths and we shall discuss it further in the next section.

The total average reaction cross section consists of the sum of the potential or direct scattering cross section and the average compound cross section. In the absence of direct reactions, which will be treated later, the only potential cross section is the shape elastic contribution

$$\bar{\sigma}_{ab} = \delta_{ab}\sigma_a^{s.e.} + \bar{\sigma}_{ab}^{c.n.}. \tag{3.6}$$

Here $\sigma_a^{s.e.} = \sigma_{aa}^{dir.}$ is also determined by the optical model, as will be seen below.

IV. WIDTH FLUCTUATION CORRECTION

It has become well established that the distribution of partial widths for a channel as defined in Sec. 2 is given by the Porter-Thomas distribution law. According to it the probability that for some state μ the quantity $\Gamma_{\mu a}/\langle \Gamma_{\mu a} \rangle_\mu$ has a value between x and x + dx is

$$F_{P.T.}(x)\,dx = (2\pi x)^{-\frac{1}{2}} e^{-\frac{1}{2}x} dx. \tag{4.1}$$

This Porter-Thomas distribution belongs to the class of chi-squared distributions with ν degrees of freedom

$$F_\nu(x) = \frac{(\frac{1}{2}\nu)^{\frac{1}{2}\nu}}{\Gamma(\frac{1}{2}\nu)}\, x^{\frac{1}{2}\nu - 1}\, e^{-\frac{1}{2}\nu x} \tag{4.2}$$

where $F_{P.T.}(x) = F_1(x)$ is the chi-squared distribution with one degree of freedom. In Eq. (4.2) ν can have any real positive value. If the states of a given J, π can decay into n channels, all having the same $\langle \Gamma_{\mu a_i} \rangle$, then we can consider the partial widths for decay into the alternative α consisting of any one of these n channels. Clearly $\langle \Gamma_{\mu\alpha} \rangle = n \langle \Gamma_{\mu\alpha_i} \rangle$ and the $\Gamma_{\mu\alpha}$ are distributed according to the chi-squared distribution with n degrees of freedom F_n. For example, if neutrons are scattered by a $\frac{1}{2}^+$ target nucleus, then compound states of total angular momentum and parity 1^- can be formed by the absorption of either a $p_{\frac{1}{2}}$ or a $p_{3/2}$ neutron. If the average partial widths for these two channels were the same, then the total neutron widths for these 1^- states would be distributed according to the chi-squared distribution with two degrees of freedom $F_2(x) = \frac{1}{2}e^{-\frac{1}{2}x}$. If the transmission coefficients for $p_{\frac{1}{2}}$ and $p_{3/2}$ neutrons were not equal, the neutron widths of 1^- states would not have exactly any chi-squared distribution but could still be well approximated by $F_\nu(x)$ with ν somewhere between 1 and 2.

Analyses of fission widths have shown that their distributions can be approximated by chi-squared distributions with between one and four degrees of freedom, depending on isotope and J. The gamma ray radiation alternative consists generally of a large number of possible gamma ray transition channels and is therefore best represented by a chi-squared distribution of perhaps 10 or 20 or more. Since such distributions involve only very small fluctuations about the average value, the total radiation width is often assumed not to be fluctuating at all.

From Eq. (4.2) it follows that if x is distributed according to $F_\nu(x)$ then

$$\langle x^k \rangle = \frac{\Gamma(k + \frac{1}{2}\nu)}{(\frac{1}{2}\nu)^k \Gamma(\frac{1}{2}\nu)} \tag{4.3}$$

and the variance of x is $(2/\nu)^{\frac{1}{2}}$.

It is useful to factor the width fluctuation correction into

$$W_{ab} = G_{ab} C_{ab}, \tag{4.4}$$

where

$$G_{ab} = \frac{\langle \Gamma_{\mu a} \Gamma_{\mu b} / \Gamma_\mu \rangle}{\langle \Gamma_{\mu a} \Gamma_{\mu b} \rangle / \langle \Gamma_\mu \rangle} \tag{4.5}$$

and

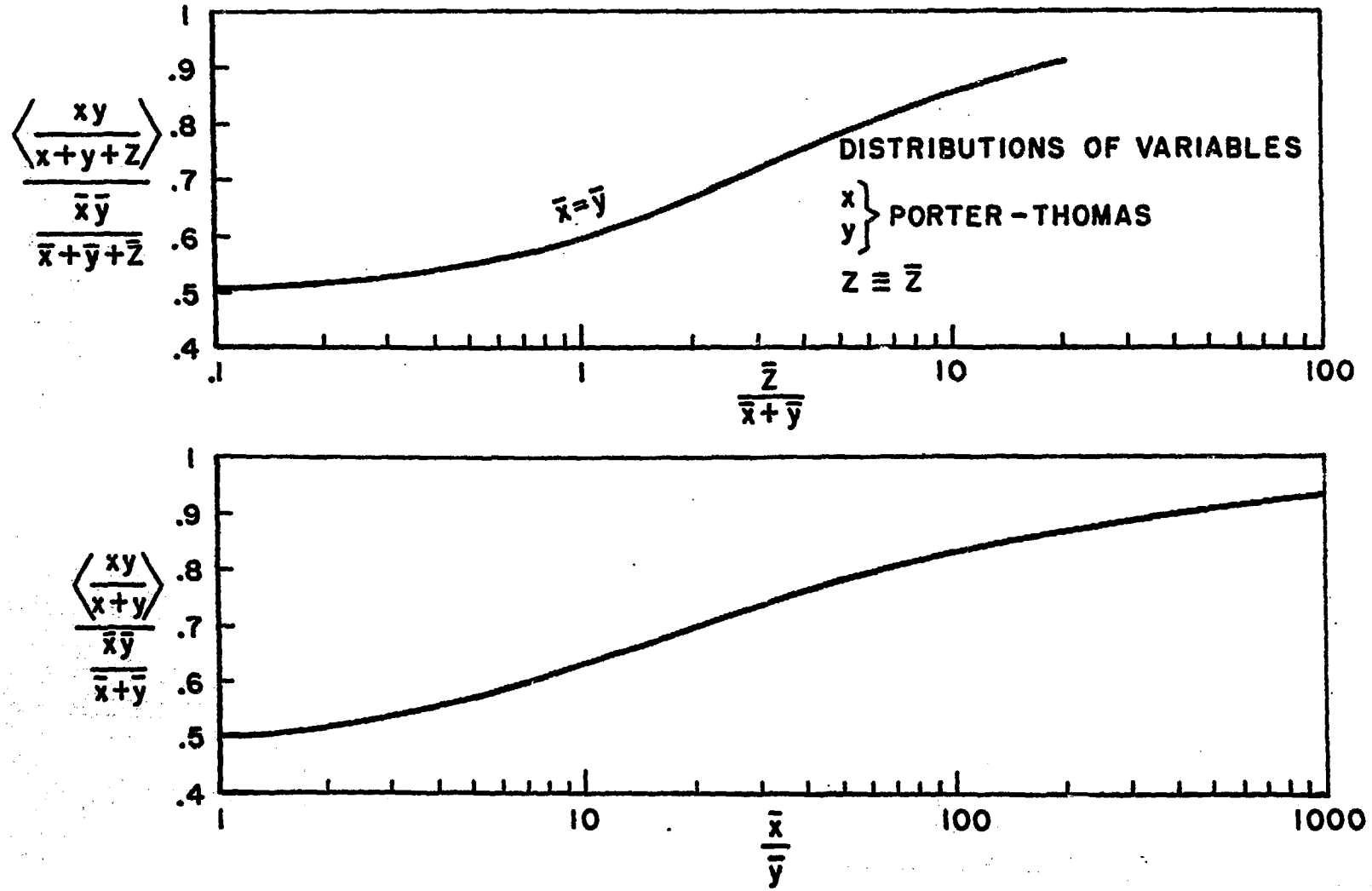
$$C_{ab} = \frac{\langle \Gamma_{\mu a} \Gamma_{\mu b} \rangle}{\langle \Gamma_{\mu a} \rangle \langle \Gamma_{\mu b} \rangle}. \tag{4.6}$$

Here G_{ab} arises from the correlation between $\Gamma_{\mu a}\Gamma_{\mu b}$ and Γ_μ^{-1} which is due to the fact that both contain $\Gamma_{\mu a}$ and $\Gamma_{\mu b}$. It is easily shown that if the $\Gamma_{\mu c}$ are distributed according to the chi-squared distribution with ν_c degrees of freedom, then G_{ab} can be expressed as the following single integral

$$G_{ab} = \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{\langle \Gamma_{\mu c} \rangle}{\langle \Gamma_\mu \rangle} t\right)^{-(\frac{1}{2}\nu_c + \delta_{ac} + \delta_{bc})}. \tag{4.7}$$

A capture channel which is assumed to have a non-fluctuating partial width Γ_γ will contribute a factor $\exp(-t\Gamma_\gamma/\langle \Gamma_\mu \rangle)$ to the integral of Eq. (4.7). Some examples of numerical values are shown in Fig. 2. The factor C_{ab} arises from correlations between the partial widths of channels a and b for chi-squared distributions can be expressed in terms of the partial widths correlation coefficient ρ_{ab}

$$C_{ab} = 1 + \frac{2\rho_{ab}}{(\nu_a \nu_b)^{\frac{1}{2}}}. \tag{4.8}$$



2. Width Fluctuation Correction for Two Channels Having Porter-Thomas Distributed Partial Widths when These are the only Channels (bottom), and when They Compete with a Large Number of Channels Having a Lumped Non-fluctuating Partial Width (top).

In the absence of a direct reaction between channels a and b, ρ_{ab} is expected to vanish for $a \neq b$ and of course $\rho_{aa} = 1$. Therefore

$$C_{ab} = 1 + 2\delta_{ab}/\nu_a \qquad \text{(no direct reactions.)} \tag{4.9}$$

The case of direct reactions will be discussed in greater detail later.

The factor C_{ab} is seen to enhance the average elastic compound cross section by a factor of 3 for the case of the Porter-Thomas distribution and by a factor of 2 for the case of the $\nu = 2$ exponential distribution. This enhancement is compensated by a reduction of all cross sections due to the factor G_{ab} of Eq. (4.7) so that the sum (3.3) is preserved.

It is, however, also possible for G_{ab} to be greater than unity [2]. This will occur where the transmission factors for channels a and b are both very small (weak cross section) and when the total width is dominated by one of a very few competing channels. In that case it is useful to factor G_{ab} once more into

$$G_{ab} = \frac{\left\langle \Gamma_{\mu a}\Gamma_{\mu b}\Gamma_{\mu}^{-1} \right\rangle}{\left\langle \Gamma_{\mu a}\Gamma_{\mu b} \right\rangle \left\langle \Gamma_{\mu}^{-1} \right\rangle} \times \left\langle \Gamma_{\mu}^{-1} \right\rangle \left\langle \Gamma_{\mu} \right\rangle . \tag{4.10}$$

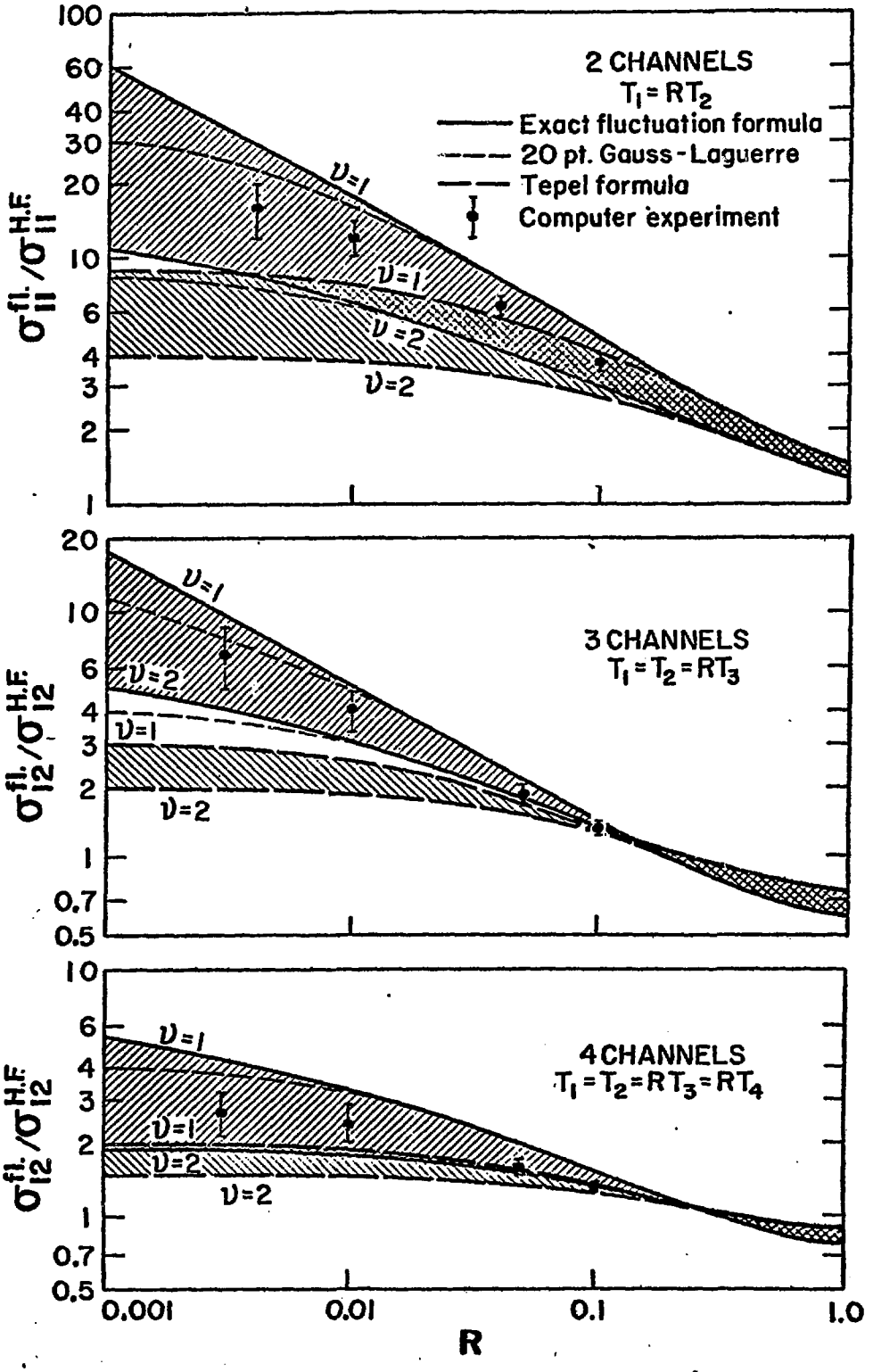
Here the first factor is close to unity because $\Gamma_{\mu a}$ and $\Gamma_{\mu b}$ do not contribute appreciably to the magnitude to Γ_{μ}^{-1}. The second factor can be evaluated

$$\left\langle \Gamma_{\mu}^{-1} \right\rangle \left\langle \Gamma_{\mu} \right\rangle = \frac{1}{1 - 2/\nu_t} \quad \text{for } \nu_t > 2 \tag{4.11}$$

where Γ_{μ} is distributed according to F_{ν_t}. When $\nu_t \leq 2$ this factor acdiverges, though of course G_{ab} will always be finite. It can be seen that large enhancements of small cross sections are possible in this way. Examples of calculations of this effect are shown in Fig. 3.

V. S-MATRIX THEORY

The discussion of Sec. 3 is reliable only in the case of very low neutron energies, typically up to several tens of keV. With increasing energy, neutron partial widths increase and the number of open channels also increases, while the level spacing decreases. As a result at higher energies the total widths become comparable to the spacings and the



3. Enhancement of Weak Average Cross Sections for Values of ν Ranging from 1 to 2 and Various Combinations of Channels. The Tepel curves refer to the results obtained from Ref. 11; the points are the results of STASIG calculations.

different resonances begin to interfere with one another. A neutron can then be absorbed coherently by two or more resonance states and this situation must be discussed quantum mechanically.

In quantum mechanics, the scattering system is described by the Schrödinger equation

$$(H - E)\Psi = 0 \tag{5.1}$$

where H is the hermitean hamiltonian describing the interactions of the system, E is the energy, and the wave function Ψ describes all properties. We are interested in scattering solutions of the Schrödinger equation with boundary conditions at infinity which specify an incoming spherical wave of unit flux I_a in channel a only and outgoing waves of unit flux O_c in all open channels c. The asymptotic wave function for this boundary condition has the form

$$\Psi_a^{as.} = I_a - \Sigma_c S_{ac} O_c \tag{5.2}$$

where the S-matrix components S_{ac} give the amplitude for transitions from channel a to channel c. From time reversal invariance of H it follows that S is symmetric

$$S_{ab} = S_{ba}, \quad S = \tilde{S} \tag{5.3}$$

where $\tilde{S}$ is the transpose of S.

For a general asymptotic wave $\Psi^{as.} = \Sigma_a x_a \Psi_a^{as.}$ the incident flux is $\Sigma_a |x_a|^2$. The total outgoing flux is $\Sigma_{ab} x_a^* S_{ca}^* S_{cb} x_b$ which must equal the incident flux if no flux is absorbed or created. This leads to the unitarity property of S

$$S_{ca}^* S_{cb} = \delta_{ab}, \quad S^\dagger S = 1 \tag{5.4}$$

A third property of the S-matrix follows from the causality principle. According to it the S-matrix considered as a function of energy has an analytic continuation without singularities in the upper half plane. This requirement can be understood by remembering that the time dependence of the wave function has the form $\exp(-iEt/\hbar)$ where E is the energy of the system. A complex energy state at a singularity of the S-matrix will have

an exponentially growing time dependence for a singularity in the upper half plane and an exponentially decaying behavior in the lower half plane. The causality principle requires us to exclude exponentially growing states.

In the absence of any scattering $S_{ac} = \delta_{ac}$ and $\psi_a^{as.} = I_a - O_a$. Then we can write (5.2) in the general case as

$$\psi_a^{as.} = (I_a - O_a) - \Sigma_c (S_{ac} - \delta_{ac}) O_c$$

where the first parentheses represent the unscattered wave and the sum represents the scattered wave. The cross section for the process $a \to b$ is now just the scattered flux in channel b for incident unit flux in channel a which in our units is

$$\sigma_{ab} = |\delta_{ab} - S_{ab}|^2. \tag{5.5}$$

I will generally discuss this cross section (5.5) because it is the simplest example of the kind of bilinear expression in the S-matrix elements that occurs in all observable cross sections. On the other hand, it is important to remember that the expression (5.5) which represents a reaction proceeding from one particular partial wave to another is seldom of practical interest. The quantities that are of practical interest are the following.

The differential cross section for the process originating with an incident wave in the alternative α and a scattered wave in the differential solid angle $d\Omega$ at scattering angle θ in the alternative β is given by

$$\frac{d\sigma_{\alpha\beta}(\theta)}{d\Omega} = \frac{1}{4\pi} \Sigma_L B_L P_L(\cos\theta) \tag{5.6a}$$

where the P_L are the Legendre polynomials of integer order L. For the case where the projectile in both alternatives α or β has either spin 0 or spin $\frac{1}{2}$, B_L can be written

$$B_L = \left(\frac{\hat{L}}{\hat{I}_\alpha \hat{s}_\alpha}\right)^2 \sum \hat{J}^2 \hat{J}'^2 A(\alpha,L) A(\beta,L) \left(\delta_{\ell_\alpha \ell_\beta} \delta_{j_\alpha j_\beta} - S^{J\Pi}_{\ell_\alpha j_\alpha, \ell_\beta j_\beta}\right)$$

$$\times \left(\delta_{\ell'_\alpha \ell'_\beta} \delta_{j'_\alpha j'_\beta} - S^{J'\Pi'*}_{\ell'_\alpha j'_\alpha, \ell'_\beta j'_\beta}\right) \tag{5.6b}$$

and

$$A(\alpha,L) = (-1)^{s_\alpha+I_\alpha+j_\alpha+j'_\alpha}\hat{j}_\alpha\hat{j}'_\alpha\begin{pmatrix} j'_\alpha & j_\alpha & L \\ s_\alpha & -s_\alpha & 0\end{pmatrix}\begin{Bmatrix} j'_\alpha & j_\alpha & L \\ J & J' & I_\alpha\end{Bmatrix} \tag{5.6c}$$

and the karet means $\hat{k} = (2k+1)^{\frac{1}{2}}$. The round bracket in (5.6c) is a Wigner 3j coefficient, the curly bracket is a 6j coefficient, and the sum in (5.6b) is over total angular momenta J,J' and parities π,π' as well as over all four orbital angular momenta ℓ and all four projectile angular momenta j, primed, unprimed, α, and β. s_α and I_α are the projectile and target spins in α.

Integrating Eq. (5.6) over all solid angles, we obtain the integrated cross section

$$\sigma_{\alpha\beta} = \Sigma_{J,\pi,\ell_\alpha,j_\alpha,\ell_\beta,j_\beta} g_J |\delta_{\ell_\alpha\ell_\beta}\delta_{j_\alpha j_\beta} - S^{J,\pi}_{\ell_\alpha j_\alpha,\ell_\beta j_\beta}|^2 \tag{5.7}$$

which is a sum over terms (5.5) with coefficients

$$g_J = (\hat{J}/\hat{I}_\alpha\hat{s}_\alpha)^2. \tag{5.7}$$

Summing (5.7) over all β yields to total cross section

$$\sigma_\alpha^{tot.} = \Sigma_{J,\pi,\ell_\alpha,j_\alpha} 2g_J\,(1 - \mathrm{Re}S^{J\pi}_{\ell_\alpha j_\alpha,\ell_\alpha,j_\alpha}) \tag{5.9}$$

which depends linearly on the real part of the diagonal S-matrix elements.

VI. S-MATRIX PARAMETERS AND THE OPTICAL MODEL

The energy variations of the S-matrix elements arise from two types of singularities in the finite energy plane. Branch points at the thresholds of channels and poles or other singularities in the lower half plane. The threshold branch points won't concern us here. We can always arrange all branch cuts so that they do not fall along our averaging interval. Also the energy dependences produced by these branch points are generally very weak. Only in the immediate vicinity of an s or p-wave neutron threshold is it generally necessary to be cautious. Similar statements apply to the contribution of entire functions to the S-matrix elements. Among singularities in the lower half plane, single poles are of greatest interest to us because, as we shall see, they correspond to the compound

state resonances of Sec. 3. Accordingly we write the S-matrix for a given J, π in the form of the pole expansion

$$S_{ab} = S^B_{ab} + S^P_{ab}$$

$$S^P_{ab} = -i \sum_\mu \frac{g_{\mu a} g_{\mu b}}{E - E_\mu + \frac{1}{2} i \Gamma_\mu} . \qquad (6.1)$$

This formula requires some discussion. The justification for the factorized form of the pole residues will emerge later. The backbackground term S^B_{ab} is smoothly varying in the energy interval of interest and arises from distant singularities as well as the contribution of entire functions. Generally we shall assume that S^B can be approximated by an energy independent constant matrix in our energy interval. For purposes of statistical analysis it will be useful to be able to consider the poles of S^P to consist of an infinite ergodic sequence extending from $\mathrm{Re}E = -\infty$ to $+\infty$ with constant statistical properties, i.e. constant averages, distributions and correlations of the pole parameters E_μ, Γ_μ and $g_{\mu c}$. This can be done by defining a region in the energy plane such that poles within that region (near poles) contribute to the energy variation in our interval, but singularities outside that region (distant poles) do not contribute significantly to that energy variation. Then we define a statistical S-matrix which has the form (6.1), where the pole parameters form an infinite ergodic extension of the actual parameters of the near poles. Then S^B contains the contribution within the energy interval of interest of the difference between the actual distant poles and the distant poles belonging to the ergodic sequence. In what follows I shall always assume such a statistical S-matrix [3].

We first confirm that the S-matrix (6.1) yields isolated resonances as in Sec. 3. Considering only the simplest situation where $S^B_{ab} = \delta_{ab}$, we obtain from Eqs. (5.5) and (6.1) for the μth isolated resonance

$$\sigma^{(\mu)}_{ab}(E) = \frac{|g_{\mu a}|^2 |g_{\mu b}|^2}{(E - E_\mu)^2 + \frac{1}{4}\Gamma^2_\mu} , \qquad a \neq b$$

and integrating this over energy the total contribution of the μth resonance to the cross section is

$$\sigma_{ab}^{(\mu)} = 2\pi|g_{\mu a}|^2|g_{\mu b}|^2/\Gamma_\mu$$

which by comparison with Eq. (3.1) yields

$$\Gamma_{\mu a} = |g_{\mu a}|^2, \quad \Gamma_{\mu b} = |g_{\mu b}|^2.$$

It is also easily verified that this identification with $\Gamma_\mu = \Gamma_{\mu a} + \Gamma_{\mu b} + \ldots$ guarantees the unitarity of the S-matrix when only a single resonance term is included.

When more than one resonance term is included in the sum of Eq. (6.1), and in particular when the widths of such resonances are comparable or greater than their spacing, the conditions which unitarity of S imposes on all the resonance parameters become exceedingly complex. We return to that problem later. Of course the S-matrix of Eq 6.1 is symmetric provided S^B is symmetric and it is causal if all Γ_μ are non-negative.

In order to calculate the average cross sections from the S-matrix (6.1) we write

$$S = \overline{S} + S^{f\ell} \tag{6.2}$$

where $\overline{S}$ is the energy averaged S-matrix and since we regard S^B as constant we have

$$\begin{aligned} \overline{S} &= S^B + \overline{S}^P \\ S^{f\ell} &= S^P - \overline{S}^P \end{aligned} \tag{6.3}$$

and averaging Eq. (5.5) we have

$$\overline{\sigma}_{ab} = \sigma_{ab}^{dir.} + \sigma_{ab}^{f\ell} \tag{6.4}$$

where

$$\sigma_{ab}^{dir.} = |\delta_{ab} - \overline{S}_{ab}|^2 \tag{6.5}$$

$$\sigma_{ab}^{f\ell} = \overline{|S_{ab}^{f\ell}|^2}. \tag{6.6}$$

The problem has evidently been split into two parts, finding the average S-matrix for Eq. (6.5) and finding the average absolute square of $S^{f\ell}$ for Eq. (6.6).

Considering first the problem of the average S-matrix we have from Eqs. (6.3) and (6.1)

$$\bar{S}^P_{ab} = -\frac{\pi}{D}\langle g_{\mu a} g_{\mu b}\rangle_\mu \tag{6.7}$$

where now D is the mean spacing of the E_μ and the bracket $\langle\ \rangle_\mu$ indicates an average with respect to μ. We now demonstrate a result [4] about $\bar{S}^P$ by means of integration around the two contours in Fig. 4. The contour in Fig. 4a encloses no singularities and therefore the integral of S(E) around this contour vanishes. If we assume that on the average the contributions from the two vertical members of the contour cancel and that S(E + iW) on the upper horizontal member is sufficiently constant for sufficiently large W, then we have

$$\bar{S} = S(E + iW) \tag{6.8}$$

where in fact W is of order of the averaging interval for $\bar{S}$. The contour of Fig. 4b encloses the poles in the interval ΔE. Assuming again that the contributions from the vertical members cancel, we have

$$2\pi\Sigma_\mu g_{\mu a} g_{\mu b} = \Delta E[S_{ab}(E - iW) - S_{ab}(E + iW)],$$

which together with the analytic continuation of the unitarity relation

$$S(E^*) = S^{*-1}(E),$$

gives using Eq. (6.7)

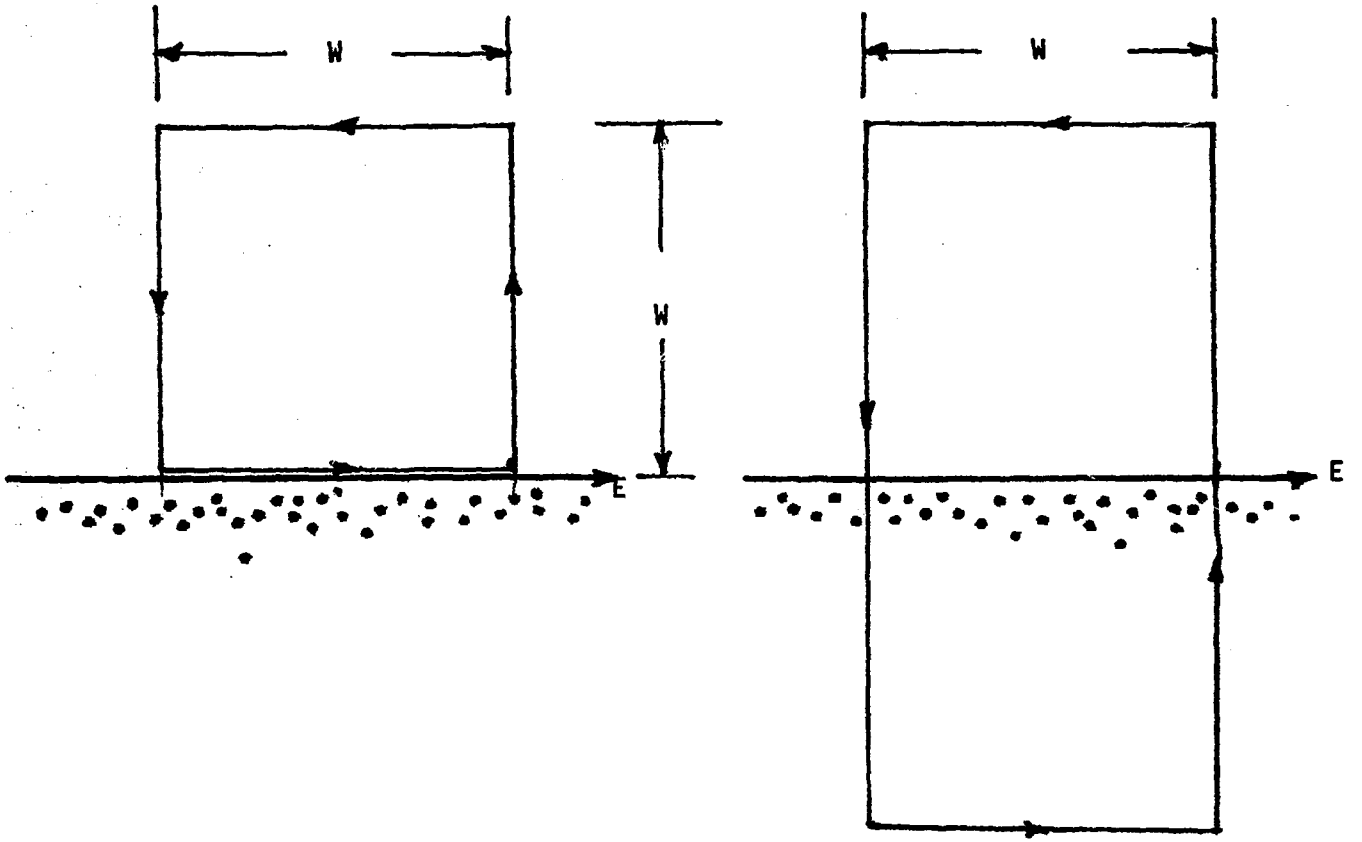
$$\bar{S}^P = \tfrac{1}{2}(\bar{S} - \bar{S}^{*-1}), \tag{6.9a}$$

from which

$$S^B = \tfrac{1}{2}(\bar{S} + \bar{S}^{*-1}). \tag{6.9b}$$

This allows us to express each part of $\bar{S}$ in Eq. (6.7) in terms of $\bar{S}$ itself.

Next we note that Eq. (6.5) looks just like the cross section formula (5.5). We may suppose therefore that there exists an interaction hamiltonian $H^{O.M.}$ that gives rise to $\bar{S}$ in the same way that H of Eq. (5.1) gives rise to S. This optical model hamiltonian $H^{O.M.}$ produces then the direct cross section $\sigma^{dir.}$ in the same way that H produces σ. Provided the fluctuation cross section $\sigma^{f\ell}$ does not vanish, $\bar{S}$ cannot exhaust the incident



4. Integration Contours Used in Deriving Eqs. (6.8) and (6.9).

flux and is therefore non-unitary and hence $H^{O.M.}$ must be non-hermitean, causing absorption of flux. Subtracting

$$\bar{\sigma}_a^{tot} = 2(1 - Re\bar{S}_{aa}) \tag{6.10}$$

from the sum over b of Eq. (6.6) we find that the unitarity defect of $\bar{S}$ gives

$$1 - \Sigma_b|\bar{S}_{ab}|^2 = \Sigma_b\sigma_{ab}^{f\ell} \equiv T_a. \tag{6.11}$$

By the unitarity of S, the optical model transmission coefficients T_a cannot exceed unity

$$T_a \leq 1 \qquad \text{(unitarity)}. \tag{6.12a}$$

Similarly causality, which limits absorption into decaying states only, requires that $\bar{S}$ be absorptive rather than emissive, thus limiting T_a to be positive

$$T_a \geq 0 \qquad \text{(causality)}. \tag{6.12b}$$

For the present we will restrict ourselves to the case where $\bar{S}$ is diagonal. Then the optical model is a separate scattering model in each channel $\underline{a}$ with an absorptive complex potential. Then there are also no direct reactions $\sigma_{ab}^{dir.}$ only an elastic potential scattering cross section $\sigma_{aa}^{dir.} = \sigma_a^{s.e.}$ and

$$T_a = 1 - |\bar{S}_{aa}|^2, \qquad (\bar{S} \text{ diagonal}). \tag{6.13}$$

From this and Eqs. (6.7) and (6.8) we have [4]

$$2|\bar{S}_{aa}^{P}| = \frac{2\pi}{D}|\langle g_{\mu a}^2\rangle| = T_a/\sqrt{1 - T_a}. \tag{6.14}$$

Another relationship valid for diagonal $\bar{S}$ is

$$\frac{2\pi}{D}\langle\Gamma_{\mu a}\rangle = -\ln(1 - T_a). \tag{6.15}$$

For the isolated resonance limit Eqs. (6.14) and (6.15) reduce to

$$\frac{2\pi|\langle g_{\mu a}^2\rangle|}{D} = \frac{2\pi\langle\Gamma_{\mu a}\rangle}{D} = T_a, \qquad (T << 1) \tag{6.16}$$

which verifies Eq. (3.3).

We give the proof of Eq. (6.15) in the form given by Simonius [5]. Since S is unitary, det S is unimodular and since it is assumed to have only simple poles and the pole residues factor, forming a rank 1 matrix, we can write it in the form

$$\det S = e^{2i\phi} \prod_\mu \frac{E - E_\mu - \frac{1}{2}i\Gamma_\mu}{E - E_\mu + \frac{1}{2}i\Gamma_\mu}$$

then to first order in the inverse averaging interval W^{-1}

$$\ln \det \langle S \rangle = \ln \det S(E + iW) = \Sigma_\mu \frac{-i\Gamma_\mu}{E - E_\mu + iW} + 2i\phi$$

$$= \frac{\pi}{D} \langle \Gamma_\mu \rangle - i \left(\Sigma_\mu \frac{\Gamma_\mu (E - E_\mu)}{(E - E_\mu)^2 + W^2} - 2\phi \right).$$

The last sum vanishes for the case of the statistical S-matrix because the terms are odd in $(E - E_\mu)$ and from the real part of this equation the channel sum of Eq. (6.15) follows.

Eqs. (6.11), (6.14) and (6.15) relate averages of S-matrix parameters to the optical model. To evaluate the fluctuation cross section requires also knowledge about the distributions of these parameters. We now turn to this question.

VII. R-MATRIX THEORY

The unitarity condition imposes severe restrictions on the S-matrix parameters. This can be seen from the fact that a unitary symmetric matrix has only half as many independent components as a general complex symmetric matrix. Since S(E) must be unitary for each value of the energy E and since some Γ/D resonance terms contribute to S at each energy, it is clear that unitarity must impose complicated correlations upon the resonance parameters. One way of avoiding this difficulty is by defining the S-matrix in terms of R-matrix states. The R-matrix states are solutions of the Schrödinger equation (5.1), subject to a boundary condition at the nuclear surface so that the solutions are stationary, real states ϕ_μ with real energies E_μ. The real symmetric R-matrix formed with these states is

$$R_{ab} = R^B_{ab} + \Sigma_\mu \frac{\gamma_{\mu a}\gamma_{\mu b}}{E - E_\mu} \qquad (7.1)$$

where

$$\gamma_{\mu a} = \int_S ds \psi_a^* \phi_\mu$$

is the real overlap on the nuclear surface of the solution ϕ_μ with the channel wave function ψ_a. The background R-matrix R^B is assumed to be constant in a statistical R-matrix in the same way that S^B was constant in the statistical S-matrix.

It is generally expected that the statistical distributions of the E_μ and the $\gamma_{\mu a}$ are represented by the distributions of the eigenvalues and the eigenvectors of the orthogonal matrix ensemble as discussed in Sec. II.6. Therefore the spacings of the E_μ follow the Wigner distribution and the $\gamma_{\mu a}$ are normally distributed with zero mean for varying state index μ and given channel a. The $\gamma_{\mu a}$ for different channels are expected to be statistically independent.

A relation between the R and the S-matrices is obtained by expanding the solution of the Schrödinger equation with scattering boundary conditions (5.2) in terms of the R-matrix states with boundary conditions at the nuclear surface. This expansion inside the nuclear surface is then fitted to the known channel wave functions in the exterior. In this procedure the channel wave functions are described by channel phase shift χ_c and by channel shift and penetration factors S_c^0 and P_c. These make up the two complex diagonal channel matrices

$$\Omega = e^{-i\chi}, \qquad L^0 = S^0 + iP. \tag{7.2}$$

With the help of these the relationship between R and S is expressed by the following channel matrix equation

$$S = \Omega P^{\frac{1}{2}}(1 - RL^0)^{-1}(1 - RL^{0*})P^{-\frac{1}{2}}\Omega \tag{7.3}$$

we can establish the connection between the R-matrix parameter statistics and the optical model by evaluating Eq. (7.3) at the energy E + iW and assuming Ω and L^0 to be constant within the averaging interval W. Then we get for diagonal $\bar{S}$

$$\bar{S}_{cc} = e^{-2i\chi_c} \frac{1 - L_c^0 \tilde{R}_{cc}}{1 - L_c^0 \tilde{R}_{cc}} \tag{7.4}$$

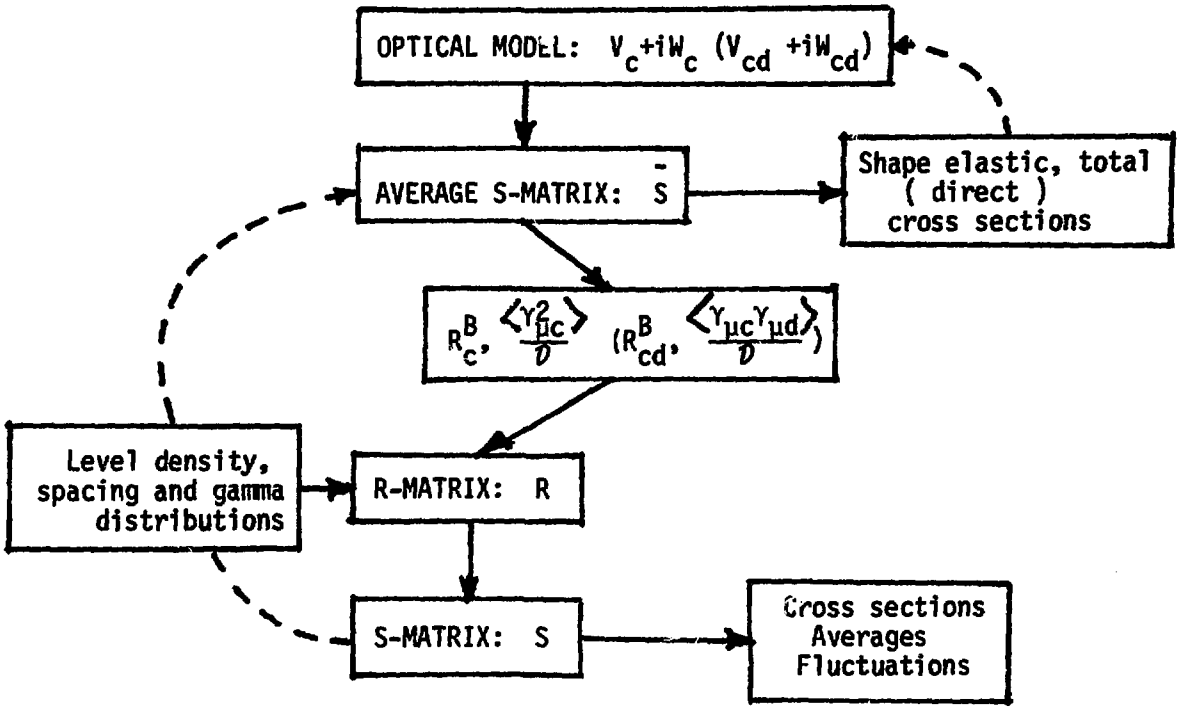
where

$$\tilde{R}_{cc} \equiv R_{cc}(E + iW) = R^B_{cc} + i\pi \frac{\langle \gamma^2_{\mu c} \rangle_\mu}{D} \tag{7.5}$$

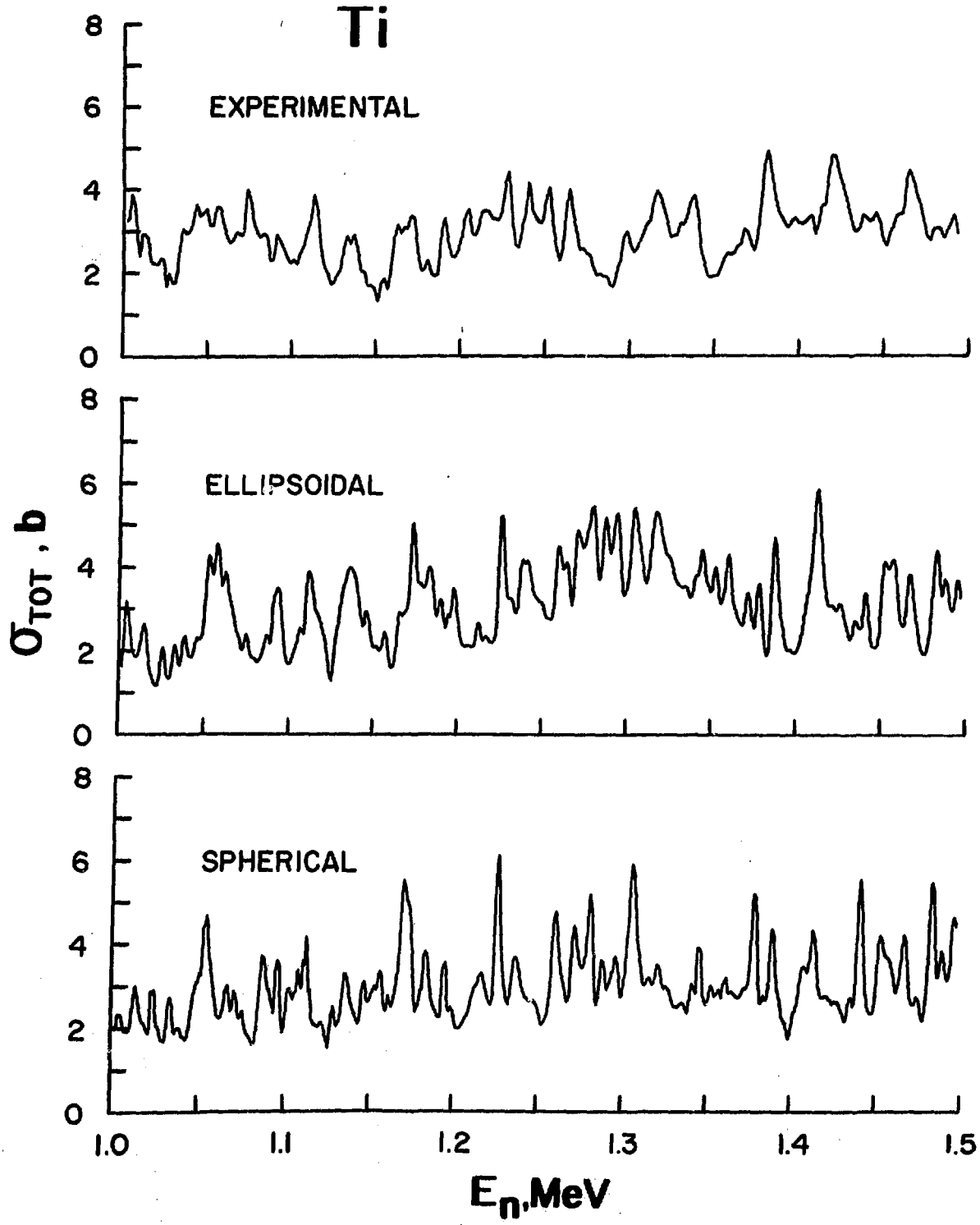
and where D is the mean spacing of R-matrix states E_μ. Since χ_c and L_c^0 are known functions of the energy in channel c, Eqs. (7.4) and (7.5) uniquely determine the two statistical R-matrix parameters R^B_{cc} and $\langle \gamma_{\mu c}^2 \rangle / D$ in terms of the real and imaginary parts of the optical model S-matrix $\bar{S}_{cc}$. This, together with the statistical assumptions discussed above, and an appropriate choice of the level density D makes it possible to construct a unitary statistical S-matrix and cross sections from the optical models for any number of competing channels with arbitrarily large values of Γ/D.

The steps in such a procedure are outlined in Fig. 5. First the Schrödinger equations with the optical model potentials are integrated to give the optical model S-matrices, $\bar{S}_{cc}$ in all channels. Then Eqs. (7.4) and (7.5) are solved for R^B_{cc} and $\langle \gamma_{\mu c}^2 \rangle / D$ for all channels. Then R-matrix parameters E_μ and $\gamma_{\mu c}$ are selected by a random number generator, so as to agree with the above value of $\langle \gamma_{\mu c}^2 \rangle / D$ and to yield the appropriate level density and distribution laws. From this parameters and energy dependent R-matrix is constructed, using Eq. (7.1) from which our energy dependent S-matrix is calculated using Eq. (7.3). Energy dependent cross sections are then calculated using Eqs. (5.5) to (5.9). These energy dependent cross sections can then be compared with experimental high energy resolution measurements, or they can be averaged and statistically analyzed to compare with theoretical predictions. A computer program STASIG has been written to perform such calculations [6]. Fig. 6 shows an example of differing cross section fluctuations obtained with two optical models which yield equivalent average total cross sections.

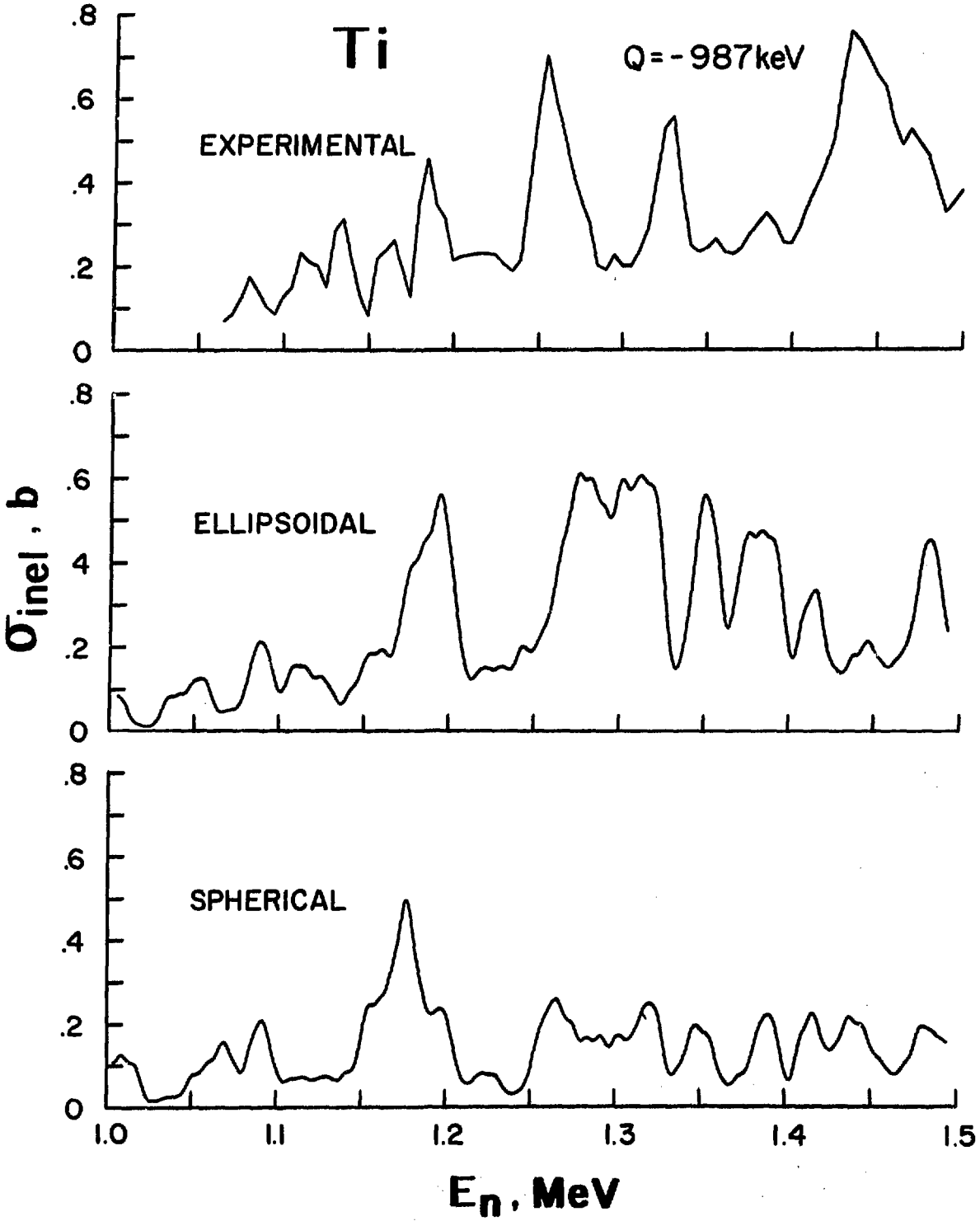
With the help of the R-matrix formalism it is also possible to determine numerically the pole parameters E_μ and $g_{\mu a}$ of a unitary S-matrix. This is done with the aid of the level matrix L with components



5. Method Used in STASIG to Generate Statistical Cross Sections.



6a. Example of STASIG Generated Cross Total Neutron Sections for Titanium. The top curve is the experimental result. The middle curve was generated from a coupled channels optical model, the bottom for a single channel optical model.



6b. STASIG Generated Inelastic Neutron Cross Sections for Titanium from the Same Models as in Fig. 6a.

$$L_{\mu\nu} = E_\mu \delta_{\mu\nu} - \Sigma_{ab} \gamma_{\mu a} \left[L^0 (1 - R^B L^0)^{-1} \right]_{ab} \gamma_{\nu b} \tag{7.6}$$

whose eigenvalues are the S-matrix poles $E_\mu - \frac{1}{2} i \Gamma_\mu$ and whose eigenvectors $T_\nu^{(\mu)}$ specify the S-matrix pole amplitudes by

$$g_{\mu a} = e^{-i x_a} \; 2 P_a \; \Sigma_{\nu, b} T_\nu^{(\mu)} \left[(1 - R^B L^0)^{-1} \right]_{ab} \gamma_{\nu b} \; . \tag{7.7}$$

One important parameter that arises in the level matrix formalism is the level normalization

$$N_\mu = \Sigma_\nu |T_\nu^{(\mu)}|^2 \geq 1 \tag{7.8}$$

which enters into a relationship between the pole width Γ_μ and the pole amplitudes $g_{\mu a}$

$$\Gamma_\mu = \Sigma_a |g_{\mu a}|^2 / N_\mu \tag{7.9}$$

for every pole μ. This formula permits a definition of partial widths

$$\Gamma_{\mu a} = |g_{\mu a}|^2 / N_\mu \tag{7.10}$$

which add up to the total width.

The difficulty encountered in using this level matrix formalism numerically arises from the fact that it cannot be applied to a statistical S-matrix, but only to one with a finite set of poles. Here one encounters systematic end effects and large level matrices must be constructed in order to yield a satisfactory sample of poles in the middle of the energy interval where they are not disturbed by end effects [7]. However the method has been successfully applied in the computer program MATDIAG to confirm the relations (6.14) and (6.15) over a wide range of parameters [8]. It has also been learned from such studies that for large Γ/D, the level correlations of the Wigner distribution tend to disappear and the E_μ tend to be distributed only with an exponential spacing distribution

(see Fig. 7). On the other hand the widths in such cases tend to have a broader distribution than would be expected from sums of partial widths, each having the Porter-Thomas distribution law (see Fig. 8). It was also found that the average of N_μ increases with increasing Γ/D. We shall return to further applications of this method in the next section.

VIII. THE FLUCTUATION CROSS SECTION

Our aim here is to evaluate the average reaction cross section in terms of optical model transmission coefficients and general statistical laws. Since the direct cross section (6.5) is, for diagonal $\bar{S}$, already given by the optical model, we turn to the fluctuation cross section (6.6). By Eqs. (6.1), (6.3) and (6.7) we find that [3]

$$\sigma_{ab}^{f\ell} = \frac{2\pi}{D}\left\langle \frac{|g_{\mu a}|^2 |g_{\mu b}|^2}{\Gamma_\mu} \right\rangle - M_{ab}$$

$$M_{ab} = 2|\bar{S}_{ab}^{P}|^2 - \frac{2\pi i}{D}\left\langle \frac{g_{\nu a} g_{\nu b} g_{\mu a}^* g_{\mu b}^*}{(E_\mu - E_\nu) + \frac{1}{2}i(\Gamma_\mu + \Gamma_\nu)} \right\rangle_{\mu \neq \nu} \tag{8.1}$$

with the definition

$$\Theta_{\mu a} = \frac{2\pi}{D} N_\mu |g_{\mu a}|^2, \tag{8.2}$$

where N_μ is the normalization parameter of Eq. (7.8), we can rewrite (8.1)

$$\sigma_{ab}^{f\ell} = \left\langle \frac{\Theta_{\mu a}\Theta_{\mu b}}{\Theta_\mu} \right\rangle - M_{ab} \tag{8.3}$$

where

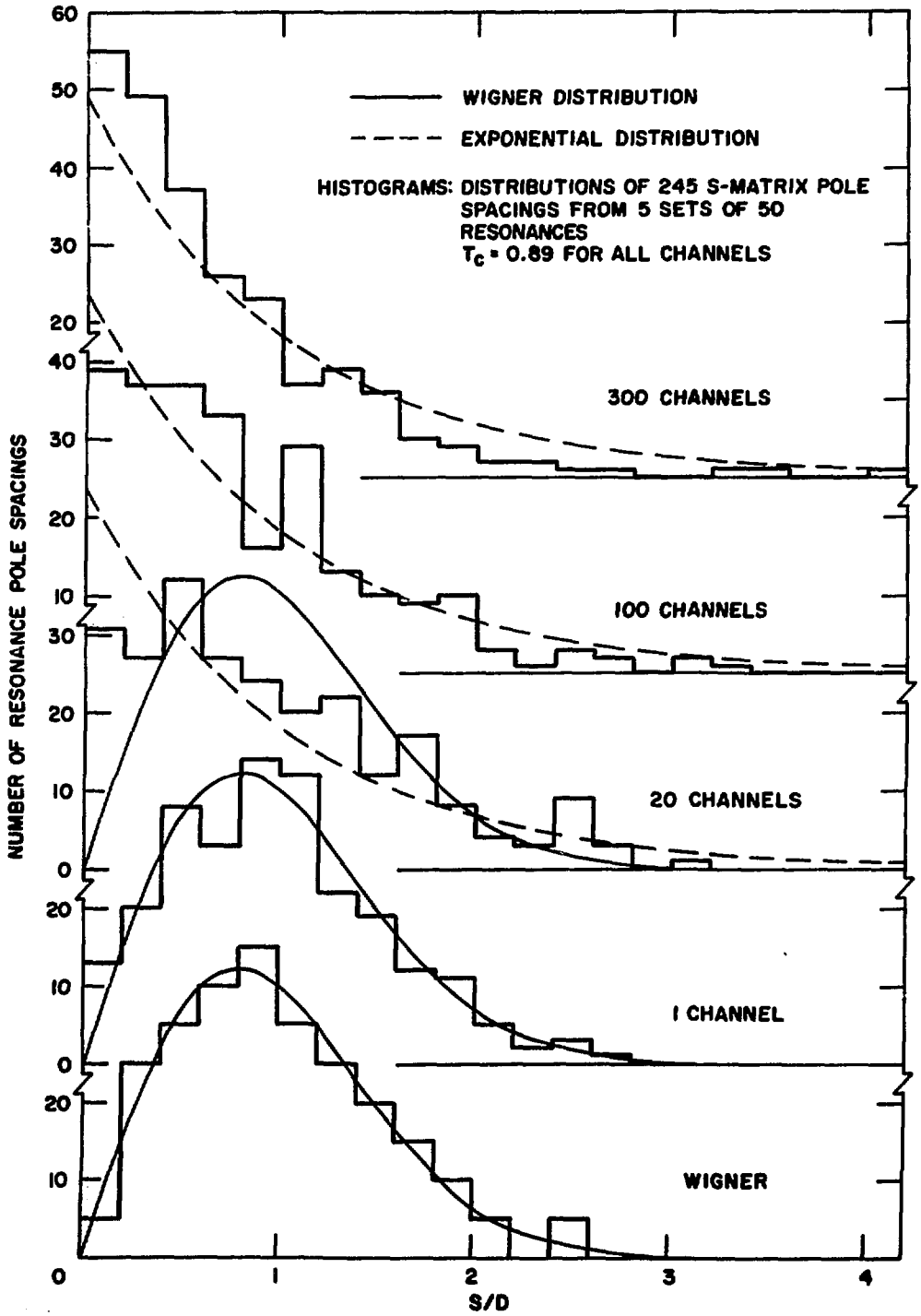
$$\langle \Theta_{\mu a} \rangle = T_a + \Sigma_b M_{ab} \tag{8.4}$$

and

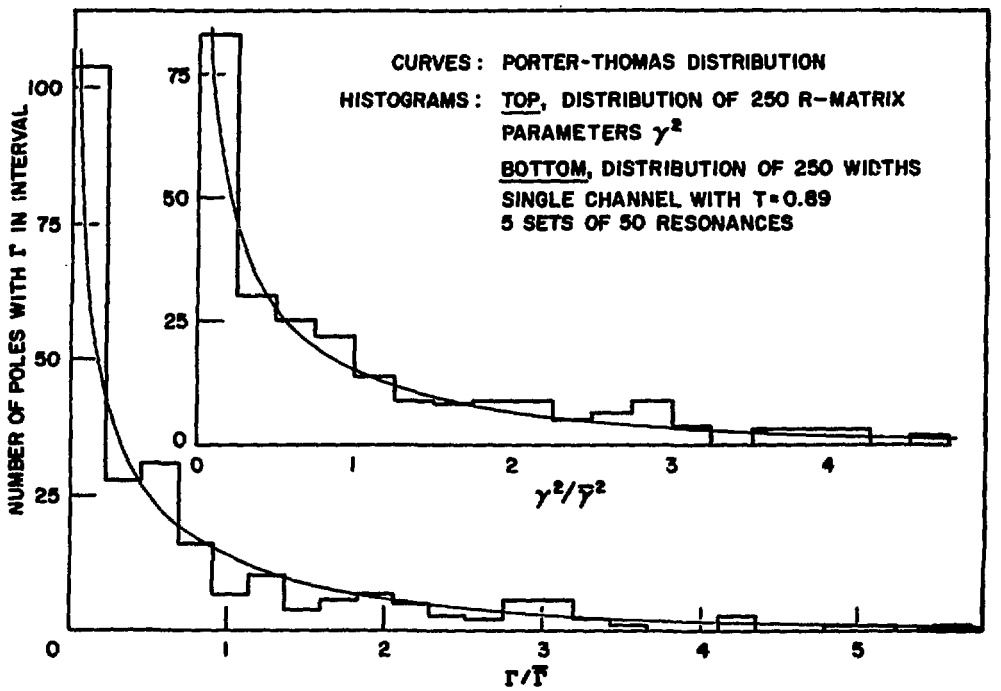
$$\langle \Theta_\mu \rangle = \Sigma_c \langle \Theta_{\mu c} \rangle. \tag{8.5}$$

The similarity of the first term in Eq. (8.3) with Eq. (3.2) suggests that we use the notation of Sec. 4 to write

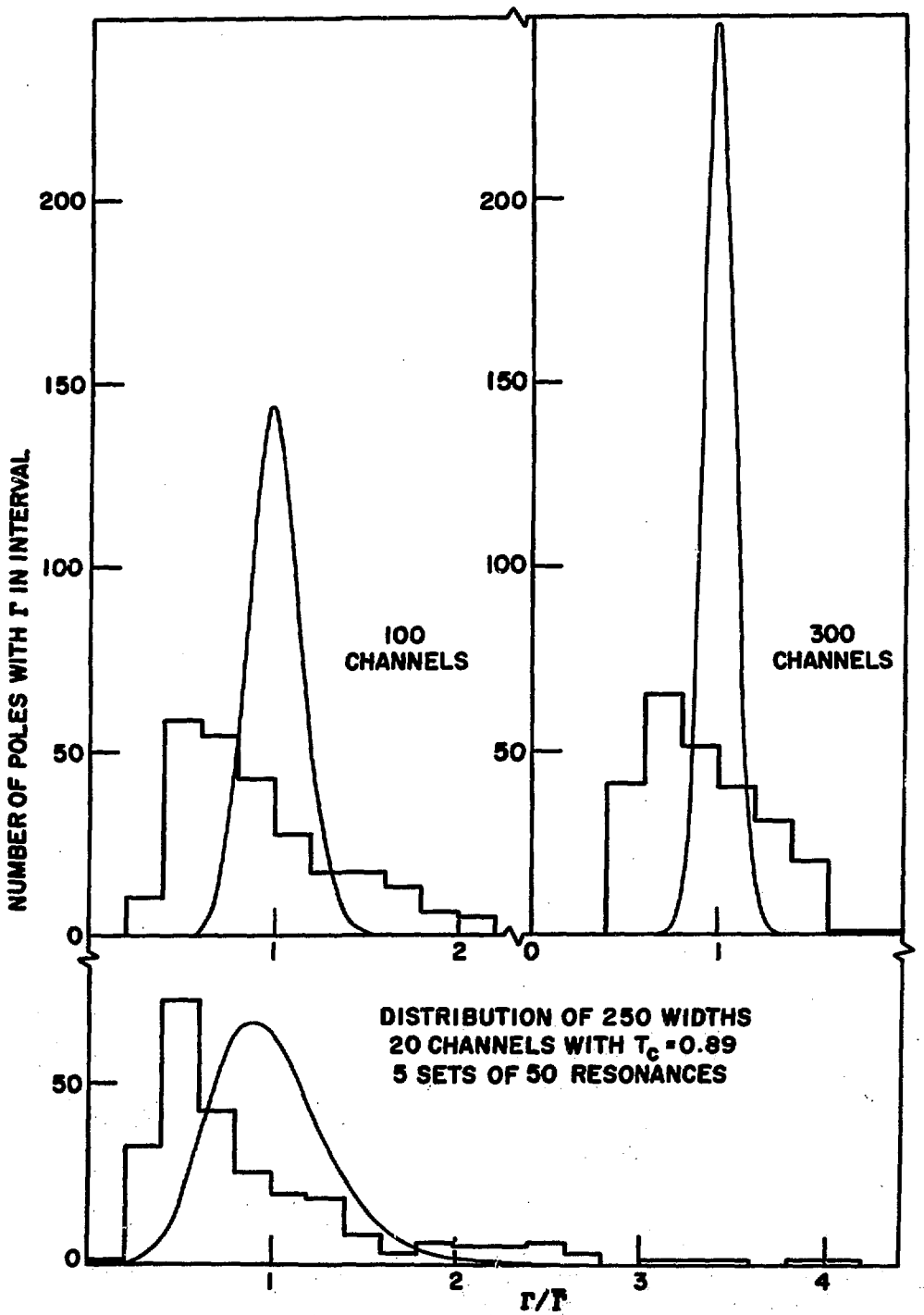
$$\sigma_{ab}^{f\ell} = \frac{\langle \Theta_{\mu a} \rangle \langle \Theta_{\mu b} \rangle}{\langle \Theta_\mu \rangle} G_{ab} C_{ab} - M_{ab} \tag{8.6}$$



7. MATDIAG Generated Changes in the Level Spacing Distribution with Increasing Numbers of Competing Strongly Absorbed Channels (histograms).



8a. MATDIAG Generated Changes in the Total Width Distribution with Increasing Numbers of Competing Strongly Absorbed Channels. (histograms). The curves are the distributions that would be expected from independently Porter-Thomas distributed partial widths.



8b. MATDIAG Generated Changes in the Total Width Distribution with Increasing Numbers of Competing Strongly Absorbed Channels. (histograms). The curves are the distributions that would be expected from independently Porter-Thomas distributed partial widths.

with

$$G_{ab} = \left\langle \frac{\Theta_{\mu a}\Theta_{\mu b}}{\Theta_\mu} \right\rangle \Big/ \frac{\langle \Theta_{\mu a}\Theta_{\mu b}\rangle}{\langle \Theta_\mu \rangle} \tag{8.7}$$

$$C_{ab} = \frac{\langle \Theta_{\mu a}\Theta_{\mu b}\rangle}{\langle \Theta_{\mu a}\rangle\langle \Theta_{\mu b}\rangle} = 1 + 2\frac{\rho_{ab}}{\sqrt{\nu_a \nu_b}} \tag{8.8}$$

where we have assumed that the distribution of $\Theta_{\mu a}$ can be described by the chi-squared distribution with ν_a degrees of freedom and where the channel correlation coefficient ρ_{ab} is given by

$$\rho_{ab} = \frac{C_{ab} - 1}{(C_{aa} - 1)(C_{bb} - 1)} \tag{8.9}$$

At this point one might hope that the term M_{ab} might vanish at least in the limit of large Γ/D, leaving again a simple Hauser-Feshbach formula. Unfortunately, as was pointed out by Weidenmüller [9], this is not possible. For, comparing the average of (8.2) with Eq. (6.14) and substituting this with Eq. (8.4), we find that

$$\Sigma_b M_{ab} \geq T_a \left(\frac{1}{\sqrt{1 - T_a}} - 1 \right) \tag{8.10}$$

which diverges as T_a approaches unity.

To make further progress it is useful to analyze a simple case which is described by a limited number of parameters and yet has arbitrarily large Γ/D. This is the case of n statistically equivalent channels [10]. By this we mean that

$$\begin{aligned} &T_c \equiv T, \qquad \nu_c \equiv \nu \quad \text{for all} \quad c = 1,2,3, \ldots n \\ &\rho_{cd} \equiv \rho \quad \text{for all} \quad c \neq d. \end{aligned} \tag{8.11}$$

Then also for all distinct c and d from 1 to n

$$\begin{aligned} C_{cc} &= 1 + 2/\nu \equiv C \\ C_{cd} &= 1 + 2\rho/\nu \equiv D \\ M_{cc} &\equiv M \\ M_{cd} &\equiv P \\ G_{cc} &= G_{cd} = \frac{n}{C + (n-1)D} \end{aligned} \tag{8.12}$$

Upon substitution into Eqs. (8.7) and (8.8) we find that

$$\sigma_{cc}^{f\ell} = \frac{\frac{C}{D}T}{\frac{C}{D} + n - 1} - \frac{n - 1}{\frac{C}{D} + n - 1}\left(M - \frac{C}{D}P\right) \tag{8.13a}$$

$$\sigma_{cd}^{f\ell} = \frac{T}{\frac{C}{D} + n - 1} + \frac{1}{\frac{C}{D} + n - 1}\left(M - \frac{C}{D}P\right). \tag{8.13b}$$

The actual behavior of these parameters was studied by means of MATDIAG calculations using channel numbers which varied from 5 up to 15 and using various values of channel transmission coefficients T distributed between 0 and 1. In all cases the results indicated the relationship [10]

$$C' \equiv \frac{C}{D} = \frac{M}{P} \tag{8.14}$$

which makes the second terms in Eqs. (8.13) vanish and leaves

$$\sigma_{cd}^{f\ell} = \frac{1 + \delta_{cd}(C' - 1)}{C' + n - 1}\ T \tag{8.15}$$

which is precisely the width fluctuation corrected Hauser-Feshbach formula for n equivalent channels each having transmission coefficient T and partial widths that are uncorrelated between different channels and are distributed according to a chi-squared distribution with ν' degrees of freedom where

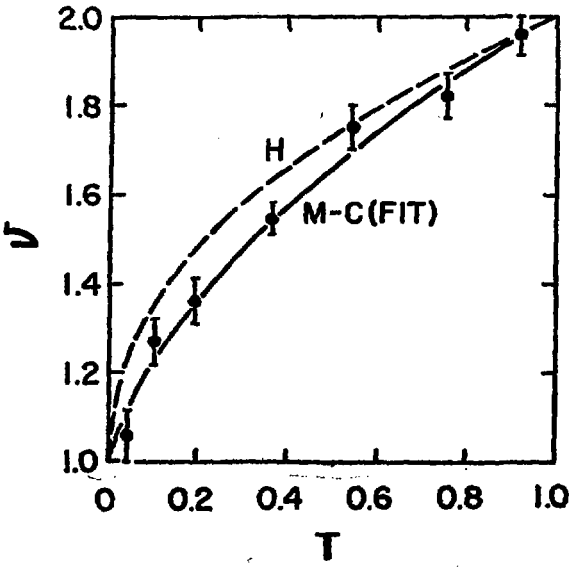
$$C' = 1 + 2/\nu'. \tag{8.16}$$

Furthermore, the values of ν' deduced from the MATDIAG calculations showed that ν' varied from a value of 1 for small values of T to a value of 2 for values of T near unity. Tepel, Hofmann and Weidenmüller [11] have given the following empirical formula for the dependence of ν'_c on T_c

$$\nu' = 1 + \sqrt{T}. \tag{8.17}$$

Another slightly different graphical relationship is shown in Fig. 9.

The Porter-Thomas distribution $\nu' = 1$ characterizes a random variable which is the square of a real normally distributed variable with zero mean. The exponential $\nu' = 2$ distribution characterizes a variable that is the sum of squares of two such real normally distributed variables with equal



9. Relation between ν and T Obtained from Numerical Calculations (Ref. 15) Compared to the Prediction of the Formula of Ref. 16 (H).

dispersions, or in other words the absolute square of a complex number with normal real and imaginary parts, isotropically distributed in the complex plane about the origin. This suggests that we consider a complex random variable $t_{\mu a}$ for every channel a, having normally distributed real and imaginary parts with zero means such that

$$T_a = \left\langle |t_{\mu a}|^2 \right\rangle_\mu \tag{8.18}$$

and

$$x_a = \left\langle (\mathrm{Im} t_{\mu a})^2 \right\rangle_\mu \Big/ \left\langle (\mathrm{Re} t_{\mu a})^2 \right\rangle_\mu . \tag{8.19}$$

If we now require

$$\frac{(1 + x_a)^2}{1 + x_a^2} = \nu_a' \tag{8.20}$$

then $|t_{\mu a}|^2$ has the same dispersion as the chi-squared distribution with ν_a' degrees of freedom, and is in fact quite close to it.

We can now summarize the development which started with the consideration of n competing equivalent channels in Eq. (3.11) by saying that

$$\sigma_{ab}^{f\ell} = \left\langle |S_{ab}^{f\ell}|^2 \right\rangle = \left\langle \frac{|t_{\mu a}|^2 |t_{\mu b}|^2}{\Sigma_c |t_{\mu c}|^2} \right\rangle_\mu \tag{8.21}$$

with the specifications (8.18) through (8.20) and with ν_a' given by (8.17). The final calculation of Eq. (8.21) proceeds then exactly in the way discussed in Sec. 4 for the Hauser-Feshbach formula with width fluctuation correction. Analogously we can evaluate other averages, such as

$$\begin{aligned} S_{aa}^{f\ell} S_{bb}^{f\ell *} &= \frac{t_{\mu a}^2 t_{\mu b}^{*2}}{\Sigma_c |t_{\mu c}|^2} \\ &= \sqrt{\left(\frac{2}{\nu_a'} - 1\right)\left(\frac{2}{\nu_b'} - 1\right)}\ \sigma_{ab}^{f\ell}, \end{aligned} \tag{8.22}$$

while for the case where $\bar{S}$ is diagonal, all averages such as $\left\langle S_{ab}^{f\ell} S_{ac}^{f\ell *} \right\rangle$ which involve indices that are not repeated vanish.

These results have been found consistent with MATDIAG calculated samples also in cases of inequivalent competing channels. They will be referred to as the M-cancellation formulas because they depend crucially on the cancellation of the M term in Eq. (8.6) by the channel-channel correlation effect as expressed in Eq. (8.14).

In evaluating average differential cross sections, we average Eqs. (5.6) which requires the evaluation of averages of the type

$$\left\langle S_{ab}^{J\pi f\ell} S_{a'b'}^{J'\pi' f\ell *} \right\rangle . \tag{8.23}$$

According to the above we have three types of nonvanishing contributions from (8.23). The first comes from terms of the type of Eq. (8.21).

$$\delta_{JJ'}\delta_{\pi\pi'}\delta_{aa'}\delta_{bb'} \frac{T_a T_b}{\Sigma_{c\epsilon J,\pi} T_c} G_{ab} C_{ab} . \tag{8.24}$$

The second contribution comes from terms of the type of Eq. (8.22)

$$\delta_{JJ'}\delta_{\pi\pi'}\delta_{ab}\delta_{a'b'} \sqrt{\left(\frac{2}{\nu_a} - 1\right)\left(\frac{2}{\nu_{a'}} - 1\right)} \frac{T_a T_{a'}}{\Sigma_c T_c} G_{aa'} C_{aa'} \tag{8.25}$$

The third contribution occurs for compound elastic scattering of neutrons from odd-A targets and arises from spin-flip elastic scattering

$$\delta_{JJ'}\delta_{\pi\pi'}\delta_{ab'}\delta_{ba'} \frac{T_a T_b}{\Sigma_c T_c} G_{ab} C_{ab} . \tag{8.26}$$

Besides the M-cancellation formula of Hauser-Feshbach times width fluctuation correction, there exists an empirically derived formula based on calculation of the STASIG type which in many instances gives results very similar to the M-cancellation formula. According to Tepel, Hofmann and Weidenmüller [11]

$$\begin{aligned} \sigma_{ab}^{f\ell} &= X_a X_b + 2\delta_{ab} X_b^2/\nu_b \\ T_a &= X_a \Sigma_c X_c + 2X_a^2/\nu_a \end{aligned} \tag{8.27}$$

This formula also depends only on the channel transmission coefficients and the channel parameters ν_c which have essentially the same numerical values as in the width fluctuation correction. Instead of evaluating the integrals (4.7) of the width fluctuation correction, Eq. (8.27) requires the solutions of the coupled equations for X_a in terms of the transmission coefficients which are then used to evaluate the fluctuation cross section. Numerically there appears to be little advantage of either procedure. The major difference arises in cases such as discussed in Eqs. (4.10) and (4.11) which give rise to enhanced nonelastic cross sections. This effect is not predicted by Eqs. (8.27). In the limit of large Γ/D when $\nu_a = 2$ for all channels, Eq. (8.27) becomes identical to a formula proposed by Kawai, Kerman, and McVoy [12].

IX. DIRECT REACTION EFFECTS

We now give up the assumption that $\bar{S}$ is diagonal. Then the optical model becomes a coupled channels model in which, in addition to the complex potential for each channel there are coupling potentials between channels. Such a generalization is particularly important in the excitation by neutron inelastic scattering of vibrational or rotational collective states of the target nucleus.

One immediate effect of a nonvanishing $\bar{S}_{ab}$ is suggested by Eq. (6.7). Unless only S^B_{ab} contributes to $\bar{S}_{ab}$, there will also be contributions from $\bar{S}^P_{ab} = -\pi \langle g_{\mu a} g_{\mu b} \rangle / D$ and hence the pole amplitudes $g_{\mu a}$ and $g_{\mu b}$ for the two channels a and b will be correlated. In the isolated resonance limit this produces a nonvanishing correlation ρ_{ab} between the partial widths $\Gamma_{\mu a} = |g_{\mu a}|^2$ and $\Gamma_{\mu b} = |g_{\mu b}|^2$, which, by the width fluctuation correction factor C_{ab} of Eq. (4.8) causes an enhancement of the average compound cross section between channels a and b. In the isolated resonance limit this enhancement can be calculated from the coupled channels optical model value of $\bar{S}$. But for appreciable Γ/D we must again turn to S-matrix theory.

The crucial technique for treating such cases is the Engelbrecht-Weidenmüller transformation [13] which permits one to transform to the case of a diagonal $\bar{S}$, calculate $\sigma^{f\ell}$ for that diagonalized $\bar{S}$ in the manner of Sec. 8, and then transform the result back to the non-diagonal case. This transformation is best described in terms of Satchler's hermitean

penetration matrix P which is a generalization of the optical model transmission coefficient for non-diagonal $\bar{S}$ [14]

$$P_{ab} = \delta_{ab} - \Sigma_c \bar{S}_{ac} \bar{S}^*_{bc}, \qquad P = 1 - \bar{S}\bar{S}^\dagger. \tag{9.1}$$

The transmission coefficients (6.11) are then just the diagonal elements of the P-matrix. Unitarity still requires these transmission coefficients to be no greater than unity

$$T_a = P_{aa} \leq 1 \quad \text{(unitarity)} \tag{9.2}$$

It can also be shown that causality now requires that

$$P \text{ is positive semidefinite} \quad \text{(causality)} \tag{9.3}$$

which means that all eigenvalues of P are non-negative. I shall refer to the case where P is a singular matrix, i.e., has a vanishing eigenvalue as the causality limit.

The Engelbrecht-Weidenmüller transformation is the unitary transformation U that diagonalizes P

$$UPU^{-1} = P' \text{ is diagonal.} \tag{9.4}$$

It follows that

$$U\tilde{S}\tilde{U} = S' \text{ is unitary if S is} \tag{9.5}$$

and that

$$U\bar{S}U = \bar{S}' \text{ is diagonal.} \tag{9.6}$$

In the case of two coupled channels we can write

$$\bar{S} = \begin{pmatrix} f_1 e^{i\Theta_1} & f_3 e^{i\Theta_3} \\ f_3 e^{i\Theta_3} & f_2 e^{i\Theta_2} \end{pmatrix} \tag{9.7}$$

and

$$U = \begin{pmatrix} \cos\beta & -\sin\beta \\ \sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \tag{9.8}$$

and find that

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

$$\tan 2\beta = \frac{2f_3}{f_2 \cos(\Theta_{23} - \alpha) - f_1 \cos(\Theta_{23} - \alpha)} \,. \tag{9.9}$$

where

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

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.

Using Eq. (9.5) the fluctuation cross section $\sigma_{ab}^{f\ell}$ can be written in terms of the elements of S'. In this expression averages of the form $\left\langle S'^{f\ell}_{ab} S'^{f\ell *}_{cd} \right\rangle$ occur. From the discussion in Sec. 8 we know that the only non-vanishing such averages are of this form

$$\sigma'^{f\ell}_{ab} = \left\langle |S'^{f\ell}_{ab}|^2 \right\rangle \tag{9.10}$$

which is evaluated in terms of the elements T' of P' by means of the width fluctuation corrected Hauser-Feshbach formula as in Eq. (8.21), or they are of the form

$$\left\langle S'^{f\ell}_{aa} S'^{f\ell}_{bb} \right\rangle = \left(\frac{2}{\nu'_a} - 1\right)^{\frac{1}{2}} \left(\frac{2}{\nu'_b} - 1\right)^{\frac{1}{2}} \sigma'^{f\ell}_{ab} \tag{9.11}$$

by Eq. (8.22). With these results we get [15]

$$\begin{aligned} \sigma^{f\ell}_{ab} = {} & \Sigma_c |U_{ca}|^2 |U_{cb}|^2 \sigma'^{f\ell}_{cc} \\ & + \Sigma_{d \neq c} \Big[U^*_{ca} U^*_{db} (U_{ca} U_{db} + U_{da} U_{cb}) \\ & + \left(\frac{2}{\nu'_c} - 1\right)^{\frac{1}{2}} \left(\frac{2}{\nu'_d} - 1\right)^{\frac{1}{2}} U^*_{ca} U^*_{cb} U_{da} U_{db} \Big] \sigma'^{f\ell}_{cd}. \end{aligned} \tag{9.12}$$

Hofmann et al. [16] have evaluated a very similar formula differing only in the evaluation of the matrix elements (9.11) and employing the

Tepel formula (8.27) for the evaluation of $\sigma'^{f\ell}_{cd}$ instead of the width fluctuation corrected Hauser-Feshbach formula. Kawai et al. [12] have given the following formula which gives equivalent results only in the limit when all $\nu' = 2$

$$\sigma^{f\ell}_{ab} = X_{aa}X_{bb} + X_{ab}X_{ba}$$
$$P_{ab} = \Sigma_c(X_{ab}X_{cc} + X_{ac}X_{cb}. \qquad (9.13)$$

In addition to the fluctuation cross section (9.12) we will in general also have a direct contribution to the average reaction cross section due to Eq. (6.5).

For $a \neq b$ the cross section (9.12) can be enhanced over the value one would obtain with the ordinary width fluctuation corrected Hauser-Feshbach formula. This is because of the occurrence of the correlation enhanced elastic fluctuation cross section $\sigma'^{f\ell}_{cc}$ in the primed channels in the first sum of Eq. (9.12). The enhancement of $\sigma'^{f\ell}_{cc}$ will be greatest when the relative contribution of this first term is greatest. The maximum effect will occur when P has only one non-vanishing eigenvalue, for then only one diagonal primed cross section $\sigma'^{f\ell}_{cc}$ can contribute, all others vanishing. In this case, clearly, the direct enhancement is of the order of the elastic enhancement, namely $1 + 2/\nu$. The above situation where eigenvalues of P vanish is what we have called the causality limit. It is likely to be achieved only in the case of two strongly coupled channels.

We have investigated the behavior of the direct enhancement for two classes of average S-matrices involving only pairs of coupled channels

$$\bar{S}_A = 5 \otimes A, \qquad A = \begin{pmatrix} F & iD \\ iD & -F \end{pmatrix}$$
$$\bar{S}_B = 5 \otimes B, \qquad B = \begin{pmatrix} F & D \\ D & -F \end{pmatrix} \qquad (9.14)$$

Here $5 \otimes A$ means that $\bar{S}_A$ is a 10×10 matrix consisting of five identical 2×2 blocks A along the diagonal. Both $\bar{S}_A$ and $\bar{S}_B$ represent two parameter families of average S-matrices depending on F and D. The non-trivial submatrices of the P matrix in the two cases are

$$P_A = \begin{pmatrix} T & 2iFD \\ -2iFD & T \end{pmatrix}$$
$$P_B = \begin{pmatrix} T & 0 \\ 0 & T \end{pmatrix} \qquad (9.15)$$

with $T = 1 - F^2 - D^2$ in both cases. In case B the causality limit $\det P_B = 0$ coincides with the usual limit $T = 0$ and imposes no separate restriction beyond $F^2 + D^2 \leq 1$. However in case A, the causality condition requires

$$F + D \leq 1 \qquad \text{(case A)} \qquad (9.16)$$

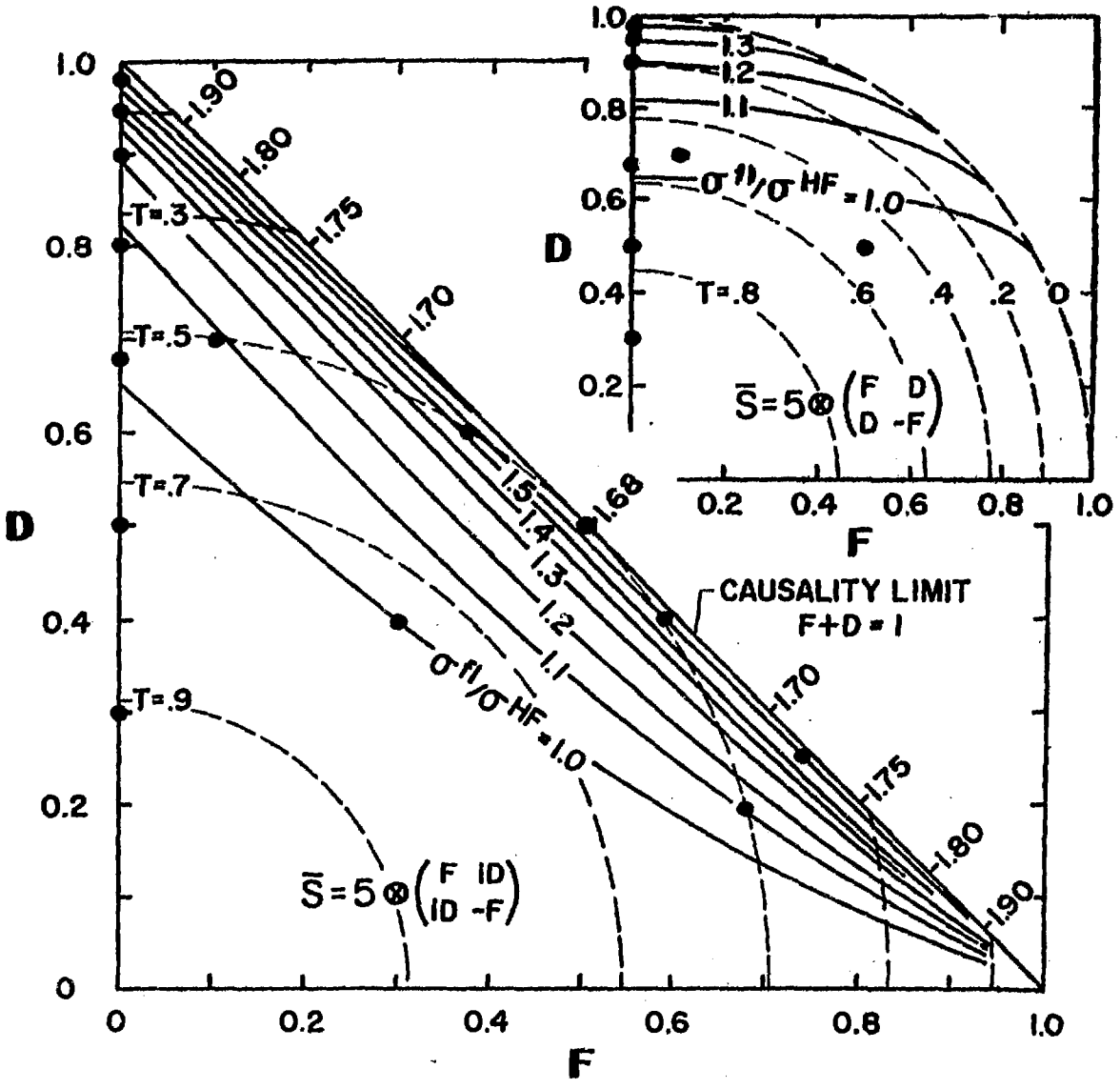
and we expect a maximum enhancement of the non-elastic cross sections between any two directly coupled channels. Fig. 10 shows the parameter space of the two average S-matrices of Eq. (9.14) and the calculated compound enhancements over the Hauser-Feshbach formula according to Eq. (9.12). As expected the enhancements are largest and comparable to elastic enhancements along the causality limit (9.16) and the enhancements quickly drop off as one moves away from this limit. In the case of $\bar{S}_B$ where the causality limit imposes no restriction on the available parameter space, there are no appreciable enhancements except along the line $F = 0$ which case B shares with case A.

The predictions of the direct enhancement in these and other cases have been confirmed by computer studies with randomly generated unitary S-matrices. In Fig. 10 the parameters of such computer studies are indicated by black dots.

X. 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 leaving the residual nucleus with an excitation energy within a differential interval at E_d.

$$\frac{d\sigma_{cd}^{f\ell}(\text{cont.})}{dE_d} = \sigma_{cd}^{f\ell}(\text{discr.})\rho_d(E_d) \qquad (10.1)$$



10. Distribution of Enhancements of Average Compound Cross Sections Due To Competing Direct Reactions for Two Classes of Average S-matrices.

where $\sigma_{cd}^{f\ell}$(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.

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 (10.1) 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 $\Gamma \gg D$ we expect an elastic width fluctuation correction factor of 2, so that in the present domain we expect that

$$\sigma_{cd}(\text{discr.}) \cong (1 + \delta_{cd})\sigma_{cd}^{H.F.}. \tag{10.2}$$

The transmission factor sum $\Sigma_e T_e$ which occurs in the denominator of $\sigma_{cd}^{H.F.}$, Eq. (3.5), must also be evaluated statistically

$$\Sigma_e T_e = \Sigma_e \int_0^{E_e(\max)} dE T_e(E_e)/D_e(E_e) \tag{10.3}$$

which involves the level spacings D_e for the residual nuclei in all competing channels. Again, if D_e depends on the residual nucleus spin through a factor $(2I_e + 1)^{-1}$, then the transmission sum (10.3) is given by

$$\Sigma_e T_e = (2J + 1)G/\pi$$

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

$$\Sigma_e T_e \cong 2\pi\Gamma^{corr}/D \tag{10.4}$$

where Γ^{corr} is the correlation width and ρ is the compound nucleus level spacing 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 [17]. The validity of the relation (10.4) was recently confirmed by numerical studies [10]. Comparison of Eqs. (6.15) and (10.4) shows that the correlation width is not the same as the average of the widths $\Gamma_{\mu\ \mu}$.

Difficulties remain 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 indicates a breakdown of our basic statistical assumptions which is dealt with in the lectures on preequilibrium decay.

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 [18], 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. (10.1), there are additional particles produced by the breakup of the residual nuclei in each channel d which is given by

$$\int_0^{E_d(\max)} dE_d \sigma_{cd}^{f\ell}(\text{discr.}) \rho_{d'}(E_d) T_{d'} \rho_{d'}(E_{d'}) / \Sigma_{e'} T_{e'} \qquad (10.5)$$

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

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