Strength Distributions and Statistical Spectroscopy.

1. General Theory

J. P. Draayer

Department of Physics and Astronomy, Louisiana State University,
Baton Rouge, Louisiana 70803

J. B. French

Department of Physics and Astronomy, University of Rochester,
Rochester, New York 14627

AND

S. S. M. Wong

Department of Physics, University of Toronto, Toronto, Ontario, Canada

Received December 1, 1976

The strength distribution for an arbitrary excitation is given in terms of a double expansion, and its sum rule by single expansion, in polynomials defined by the initial and final energy spectra. In model spaces which are not too large, a rapid convergence, to within fluctuations, is assured by the action of a central limit theorem, as is shown in particular by considering the response of the system under infinitesimal deformations of the Hamiltonian. When larger spaces are decomposed into subspaces defined by partitioning of the single-particle space a similar convergence results. At the same time, close contact is made with, and important corrections are found in, intuitive procedures which are often used for approximating strength distributions. The general features of the distribution are often easily understood in terms of a simple geometry made effective by the model space by the central limit theorem, and further features by exploiting the connection of this geometry to the unitary group of transformations in the single-particle space. Extensions are given for multipole strengths and sum rules, appropriate when the angular momenta (and isospins) are specified for the states involved in the transitions. Measures for the RMS fluctuations in the same-coupling quantities, and correlations between them, are given by combining the low-order-polynomial (statistically smoothed) strengths with an assumed Porter-Thomas distribution for the (high-order) strength fluctuations.

* Supported in part by the U.S. Energy Research and Development Administration, the U.S. National Science Foundation, and the National Research Council of Canada.

Copyright © 1977 by Academic Press, Inc.
All rights of reproduction in any form reserved.

ISSN 003-8110
STRENGTH DISTRIBUTIONS: GENERAL THEORY

1. INTRODUCTION

We give in this paper a theory of strength distributions for a wide class of nuclear excitations, applicable for example to $\beta$- and $\gamma$-transitions and to excitation via particle transfer. As always there is an excitation operator $O$ which induces transitions, $\left| W' \right> \rightarrow O \left| W \right>$, between the starting states $\left| W \right>$ and final states $\left| W' \right>$. In the usual way we define the microscopic strength as

$$ R(W', W) = \left< W' \left| O \right| W \right>^2 \tag{1} $$

the square of the expansion coefficient of the state $O \left| W \right>$ in terms of the final Hamiltonian eigenstates $\left| W' \right>$, which may (as in $\beta^{-}, \beta^{+}, \gamma$) or may not (as in particle transfer) belong to the same model subspace. The $p$th-order energy-weighted sum rule is

$$ \mathcal{M}_p(W) = \sum_{W'} R(W', W)(W')^p = \int \left< W' \left| (\mathcal{H} - E) \right| W \right> \left< W' \left| O \right| W \right> dW' = \left< W \left| O^p \mathcal{H} \left| W \right> \right. \tag{2} $$

where $P(z)$ is the eigenstate density in the final-state space whose dimensionality is then $\int P(z) dz = d$. We see that $\mathcal{M}_p(W)$ is, on the one hand, a starting-state expectation value and, on the other, the $p$th moment of the strength distribution which originates with $\left| W \right>$. Other types of strength moments, closely related to the $\mathcal{M}_p$, are the polynomial moments which we encounter ahead (13), and moments in which the strength weighting is $(W' - W)^p$ which give rise to expectation values involving multiple commutators. For finite-dimensional spaces, the only ones we encounter, the strength is determined by the set $\mathcal{M}_p(W)$ for all $p \geq 0$ or by the corresponding sets of the other moments.

The fact that sum rules determine everything is, however, not of direct practical consequence because of a number of interchanging difficulties. The first difficulty is that, because of the undue weighting which they give to small unobservable strengths at high excitations, high-order $\mathcal{M}_p(W)$, say $p \geq 2$, and consequently the strength distributions themselves, are not measurable. This is not to say, however, that these quantities are devoid of interest for there are many cases in which measurable quantities depend on the strengths; an example would be the radiation emitted during a cascade reaction. It will often happen moreover, that even for low-order moments one can experimentally determine only the endothermic $(W' > W)$ or exothermic $(W < W)$ strengths, and these are adequate only to give lower limits to the low-order $\mathcal{M}_p$; in order to decompose the starting-state expectation values into exothermic and endothermic parts we also need the strength $R(W', W)$ itself.

In some cases when the sums are measurable the analysis will yield quantities which are of immediate significance (as is often the case with occupations), but, particularly with complicated sum rules, the significance may not be clear at all. In this second case, and very often in the first as well, one will wish to proceed further with the
analysis and ask, for example, what the measurements imply about the nature of the interaction which is effective in the target state. In the conventional procedure one would construct the starting state, for example by a shell-model diagonalization, evaluate the required expectation values, and perhaps attempt thereafter to determine the sensitivity of the expectation values to the input parameters. In that procedure the starting state is treated differently from the final states for which no explicit construction is needed. But beyond that the construction of a state will often be hopelessly complicated; and if to achieve it we make radical simplifications in the Hamiltonian and the model space considered, we must compound that error by using the simplified $\mathcal{H}$ in the operators $\mathcal{O}^* \mathcal{H} \mathcal{O}$ which come into the energy-weighted sum rules (3) if we want self-consistency, or else give up self-consistency which in itself involves errors beyond our control. Very often then the further analysis is not carried out at all and the significance of the measurements is not explored. And of course the same argument applies if one wishes to make sum-rule predictions, and a fortiori if one’s interest is with the strength itself rather than in its low-order moments (the sum-rule quantities).

The purpose of the present paper is to demonstrate that there are major simplications associated with strength distributions and sum rules in many-particle spaces, and to exploit them in such a manner as to dispose of these difficulties. The theory which we propose now, which has been briefly discussed in earlier papers [1–3], makes use of spectral distribution methods. These in turn derive from a recognition of the role of the central limit theorem (CLT) in the small many-particle model spaces constructed by distributing nucleons over some finite set of single-particle states. In an asymptotic limit, that of large particle number, the smoothed eigenvalue density for “almost all” Hamiltonians which could act in the model space will, by the action of the CLT, be close to Gaussian [4, 5]. Since the state density determines the partition function it is then not surprising that the strength distribution will, to within fluctuations which we shall have to consider separately, also have a characteristic simple asymptotic form. In favorable cases it is in fact linear in the energies (linear in both $W$ and $\mathcal{O}^* \mathcal{H} \mathcal{O}$), the sum rules for the strength originating at $W$ will then determine starting-state expectation values $\langle W | \mathcal{O}^* \mathcal{H} \mathcal{O} | W \rangle$, which are similarity (again to within fluctuations) linear in $\mathcal{O}^* \mathcal{H} \mathcal{O}$. The sum rules and strengths are thus determined by a small number of quantities, which in fact are traces over the model space, and some of its subspaces, of operators $\mathcal{O}^* \mathcal{H} \mathcal{O} | \mathcal{O}^* \mathcal{H} \mathcal{O}$ with small $p,q$, being calculable therefore by methods which do not involve the construction of any Hamiltonian (or other) eigenfunctions. Because of this feature the methods can be applied in model spaces of arbitrarily large dimensionality. They have a further advantage that they give the results as more or less explicit functions (involving low-order powers) of the Hamiltonian matrix elements so that one can see what features of the Hamiltonian are implied by particular properties of the strength distribution; with standard methods in which explicit starting-state wavefunctions are required this is feasible only in most exceptional circumstances. The problem discussed above of the endothermic-exothermic separation is solved by the construction of the strength itself, which of course solves also the problem of the high-order moments of the smoothed distribution. The implication of the latter remark is that moments, of order high enough to fix the secular variations of the strength (not its
fluctuations), are in fact calculable because of the simplicities generated by the central limit theorem.

These preliminary remarks raise a number of questions. The first is about the way in which the CLT originates and acts in the many-particle model space; the important thing to keep in mind here is that the CLT is a very "strong" principle whose operation dominates much of the behavior and gives rise to quite different approximations than would come to if its operation were ignored. We shall briefly review these matters ahead.

As a second general problem we must face the fact that only a small fraction of the model-space states can have any physical significance; this arises from the fact that the many-particle spectrum spans are far greater than the corresponding single-particle span (100 MeV compared with 5 MeV, for example, in $\alpha$-decay) so that all but the lowest states have an inadequate single-particle basis. This feature is of course shared by shell-model and other calculations which make use of microscopic model spaces (those with a finite single-particle basis) but they are put more deeply into view in the spectral methods in which many things are "tied to" the spectrum centroid which lies far above the states which are adequately treated. The questions here are whether the CLT is adequate to extend things into the physical domain and whether we can deal with model spaces large enough to treat things adequately when our interest is in physical domains which themselves span a considerable energy range (say $>10$ MeV); these matters also are by now well understood, and the answers are positive.

A third general question concerns the nature and magnitude of the fluctuations which are ignored and the consequences of ignoring them. Ignoring the fluctuations will, of course, induce an error in the predictions for the strength and so forth involving individual levels, and for that reason, if no other, we should understand their general magnitude. Concerning the nature of the fluctuations we remark first that the eigenvalue density rapidly smooths out and converges to Gaussian as the particle number increases, so that the second deviations (measured over a fixed energy interval) from the asymptotic Gaussian rapidly disappear. The natural unit for the spectrum fluctuations is, however, the local level spacing which itself would rapidly decrease as we increase the particle number in order to take advantage of the CLT smoothing. The consequence (not yet completely understood) is that the CLT smoothing has essentially no effect on the spectrum fluctuations which may be regarded as having an existence of their own, undisturbed by the changes in the eigenvalue density generated by changing the particle number. To the extent that the Porter-Thomas distribution [6] describes the strength fluctuations they also may be regarded as having an independent existence; we shall see, moreover, how the secular variation is the strength will combine with the Porter-Thomas fluctuations to give measures for the fluctuations in, and correlations between, the sum-rule quantities.

There is still the general question whether level-to-level fluctuations carry information, or equivalently, whether the errors involved in ignoring them are of physical consequence. It is known [7] that energy-level fluctuations at high excitation are determined by parameter-free statistical laws and therefore carry little or no information; the same seems to be true for the strengths. It would not be safe to assume that
this behavior holds at all excitations, and indeed it seems quite clear, and is understoed, that fluctuations in the ground-state domain are considerably modified by collective effects. On the other hand, it is also known that when collectivity is not dominant, these aspects of the fluctuations which are measurable both at high and low excitations do indeed exist in the ground state domain [5]. This is incompatible with the point of view, encountered for example in discussions of effective interaction theory [9], that the major physical interest involves only the first few levels and that high accuracy is essential, implying that fluctuation-free results are without interest. These arguments do not seem to be valid even for phenomena involving ground states and, of course, high accuracy is pointless for almost all phenomena occurring at high excitations.

In summary then, while questions may be raised concerning statistical methods for strength distributions, it appears that their simplicity does not involve a high-handed neglect of much of the physics involved but rather derives from the recognition that the phenomena involved are fairly simple. We shall demonstrate this in the examples of the following paper.

In Section 3 of this paper we derive orthogonal-polynomial expansions for the smoothed strength function $R(W, W)$ and the associated sum-rule quantiles. The polynomials are those defined by taking the eigenvalues densities in the $R$ and $W$ subspaces as weight functions. The whole success of our procedure derives from the rapid convergence of the expansions (Eq. 11) which is guaranteed by the C.L.T. whose origin and method of operation we describe in Section 3. We show moreover, that there is, for our operators of the system, a geometry which determines much of the behavior. In Section 4 we show the connection of the strength and sum-rule results with a theory of the linear response of the system under a perturbation of the Hamiltonian. For details of this see not as important as the general connections which are established between Hamiltonian "deformations" and the associated strength distributions and expectation values.

The basic energy dependences which are generated by the C.L.T. bilinear in the energy for the strengths and linear for the sum rules, give at least a semi-quantitative description for an extremely wide range of cases. They derive from the first two terms in the polynomial expansions, the only terms which are unimpaired by the action of the C.L.T. We can omit a few further terms in the expansions to generate the corrections to the linear forms; alternatively we can partition the single-particle space into "orbits" and the model space thereby by configurations, in order to produce a simpler theory which should be accurate in arbitrarily large spaces. The results of this are given in Section 5, which sketches a detailed derivation of the simplest of all theories for the strength distribution; it then goes on to demonstrate the remarkable way in which the polynomial expansions take account of the correlations between Hamiltonian and excitation operator in order to confront the simple schematic theory into an exact one.

Section 6 gives, for future reference, the basic equations required to deal with the angular-momentum decomposition of the strengths and sum rules.

In Section 7 we give an introduction to the relationships between the geometry of the model-space operators and the symmetries generated by unitary transformations.
in the single-particle space. As an example we use these results to show, in a particular case, how information is "propagated" over a wide energy domain in the spectrum.

In Section 8 we combine the Porter-Thomas distribution in the elementary transition strengths with the polynomial theory for the secular energy variation in order to calculate the mean-squared fluctuations in the sum-rule quantities and the correlations between them.

The purpose of this paper then is to give the general theory. In the following paper we assess its accuracy via a comparison with detailed shell-model results for a variety of electromagnetic transitions. In later papers we shall give further methods for evaluating the necessary input terms and shall apply the theory to particle transfer, to beta decay, and to other excitations. We should stress that "excitations" which are not physically realizable, and expectation values which do not derive from sum rules, are often of great interest also, in some cases for example because of their connection with symmetries. We shall discuss these also.

2. POLYNOMIAL EXPANSIONS

As in (1), (2) the Hamiltonian is $H$ and the excitation operator $O$. We are interested in transitions $| W' \rangle \rightarrow | W \rangle$, where we label the states by their energies and where the $| W \rangle$ states span one model subspace (an eigenspace for $H$) and the $| W' \rangle$ another (the two subspaces may coincide, and then we do not corresponding states); in case of degeneracies a more complete labeling will be adopted as needed. Besides the state density $\rho(z)$ it is convenient to introduce the corresponding probability density

$$\rho(x) = \text{d}^2(x) = 1.$$ (3)

In the case where the subspaces are distinct we can, of course, consider the inverse transitions by a simple relabeling ($W \rightarrow W'$, $O \rightarrow O'$) but that will not be convenient if we are interested in the relationships between the two distributions $| W \rangle \rightarrow | W' \rangle$ and $| W' \rangle \rightarrow | W \rangle$.

The total strength originating with $| W \rangle$, its centroid, and its variance (of the width), are given respectively in terms of the moments $M_n(W)$ (3) by

$$M_n(W) = \langle W | O^n O | W \rangle - \langle W | O^n | W \rangle \langle O | W \rangle$$ (4)

and similarly for higher-order quantities. Since finite-space distributions are determined by their moments the set of $M_n(W)$ for all $n$ determines the distribution of the strength which originates in $| W \rangle$; its Fourier transform (characteristic function) is

$$R(x, W) = e^{-ixW} \left( \frac{\pi}{2} \right)$$ (5)

where the prime on $\Gamma(x)$ indicates that we are dealing with the state density for the $W'$ space, and inversion gives

$$\Gamma(W') R(W, W') = \langle W | O | W' \rangle$$ (6)
a result which we can verify by making an intermediate eigenstate expansion of the expectation value and using \(\sum_{n} \langle n | \mathbf{f}(\mathbf{W}) | n \rangle \mathbf{W}^n \). We could of course have started with (6) but we have derived it instead in order to stress the relationship between zero roots and these \(n\) moments.

As they stand these moment expansions are not directly applicable. For one thing, there is no convergence in the moment order and, for another, as described in Section 1, it is impossible to measure high moments; and to calculate any moments at all we need the model states \(\{\mathbf{W}\}\), which, in complicated nuclei, we are unable to construct. Even in "simple" cases most measured wavefunctions promise more than they can really deliver, and give many-particle correlations which are inadequate for dealing with operations of high "particle rank" (a \(k\)-body operator has particle rank \(k\)).

To circumvent the last difficulty we sum \(\langle z \rangle\) over the starting states as well; setting \(\{z\}\) run over the \(\{\mathbf{W}\}\) states we have

\[
\mathbf{f}(\mathbf{W}) \mathbf{R}(\mathbf{W}, \mathbf{W}) \mathbf{R}(\mathbf{W}) = \langle \mathbf{W} | \mathbf{O}^z \mathbf{R}(\mathbf{W}, \mathbf{W}) \mathbf{O}^z | \mathbf{W} \rangle \mathbf{R}(\mathbf{W})
\]

\[
= \sum_{z} \langle z | \mathbf{O}^z \mathbf{R}(\mathbf{W}, \mathbf{W}) \mathbf{O}^z | z \rangle \mathbf{R}(z) \mathbf{R}(z - \mathbf{W}) dz
\]

\[
= \sum_{z} \langle z | \mathbf{O}^z \mathbf{R}(\mathbf{W}, \mathbf{W}) \mathbf{O}^z | z \rangle \mathbf{R}(z) \mathbf{R}(z - \mathbf{W}) dz
\]

\[
= \sum_{z} \langle z | \mathbf{O}^z \mathbf{R}(\mathbf{W}, \mathbf{W}) \mathbf{O}^z | z \rangle \mathbf{R}(z) \mathbf{R}(z - \mathbf{W}) dz
\]

where we have introduced the notation that \(\langle z \rangle^m = d \times \langle z \rangle^m\) is the trace of \(\mathbf{O}\) over the \(\{\mathbf{W}\}\) mode space so that \(\langle z \rangle^m\) is the average expectation value.

To deal with the convergence problem we replace the moment (Taylor series) expansion by a polynomial (normal mode) expansion. The appropriate polynomials are \(P_{\lambda}(x)\), the orthonormal polynomials defined by the (nonnegative-definite) \(\mathbf{W}\) density, \(\rho(\mathbf{x})\), as weight function (there are of course a corresponding set \(\mathbf{P}_{\lambda}\) for the final state space). Then

\[
\int P_{\lambda}(x) P_{\lambda}(y) \rho(x) dx = \delta_{\lambda, \lambda},
\]

\[
\delta_{\lambda, \lambda} = \langle \mathbf{w} | P_{\lambda}(x) P_{\lambda}(y) | \mathbf{w} \rangle.
\]

The polynomials can be constructed directly from (8) and appear as functions of the density moments

\[
\mathbf{m}_{\alpha} = \int \rho(x) z^\alpha dx = \langle \mathbf{w} | z^\alpha | \mathbf{w} \rangle.
\]

For the first two we have \(P_{0}(x) = 1, P_{1}(x) = (x - \delta)\varphi\) where \(\delta = \mathbf{m}_{0}\) and \(\varphi = \mathbf{m}_{1} - (\mathbf{m}_{0})^2\) are the density centroid and variance. The unnormalized polynomial
which the strengths are weighted, as in the second form, by polynomials in the energy rather than by simple powers. Observe that the \( A_i \) for \( \alpha \leq \beta \) are linear combinations of the \( \mathcal{M}_p \) for \( p \leq \beta \), and inversely, so that the sets carry the same information; specifically if \( x^p = \sum_i \xi_i f_i(x) \) then \( \mathcal{M}_p(W) = \sum_i \xi_i A_i(W) \). From (11), (13) we have

\[
d' \times \mathcal{G}(m', m) = \int \mathcal{A}(x) \mathcal{P}(x) \phi(x) \, dx
\]

\[
d' \times \mathcal{R}(W', W) = \sum_{x} P_x(W') P_x(W) \int \mathcal{A}(x) \mathcal{P}(x) \phi(x) \, dx 
\]

\[
= \sum_{x} A_x(W') P_x(W) - \sum_{x} A_x(W) P_x(W'),
\]

which gives alternative expressions for the strength in terms of the (polynomial) moments.

We observe also that for the expectation value of an arbitrary operator \( K \), not necessarily one which derives from a sum rule, we have

\[
\langle W' | \mathcal{K} | W \rangle = \mathcal{K}(W) - \mathcal{K}(W)(\mathcal{H} - W)^{\mu} = \sum_{x} \mathcal{K}(x) (\mathcal{H} - W)^{\mu} P_x(W)
\]

With \( \mathcal{K} = \mathcal{O}^{\mathcal{H}O} \) this becomes a polynomial expansion for the strength moments \( \mathcal{M}_p(W) \). Finally the density itself is expressible as a t-nice,

\[
\rho(W) = \langle \mathcal{K}(\mathcal{H} - W)^{\mu}\rangle.
\]

3. CONVERGENCE AND THE CENTRAL LIMIT THEOREM; CORRELATION COEFFICIENTS AND SIMPLE GEOMETRY

Simply writing the strength and its sum rules in the forms (11), (13) does not of course solve the problems which we have described above (following (6)); the new feature which does solve them derives from the many-particle nature of the model spaces of interest, more specifically from the direct product structure of these spaces, which ensures a rapid convergence (to within fluctuations) in the polynomial expansions (11), (13). Everything indeed will derive from the fact, which has been known for some years and is by now well understood, that as we increase the number of particles the model-space eigenvalue density goes rapidly to Gaussian, this feature deriving from the central limit theorem. We shall briefly describe the origin and function of the CLT and show how it leads to convergence of our expansions.

For the simplest possible case, that of noninteracting particles, the density convolutes as we add particles; thus

\[
\rho_n(x) = \int \rho_{n-1}(x - y) \rho_1(y) \, dy = \rho_{n-1} \otimes \rho_1(x) = \rho_1 \otimes \rho_1 \otimes \rho_1 \cdots \otimes \rho_1[x]
\]

in which \( m \) now stands for the particle number. Now, by the simplest version of the
CLT, $\mu_0(x) \to$ Gaussian for large enough particle number (for characteristic single-particle spectra a half-dozen particles is enough for a good Gaussian). It must not be
genominal however that, as described in Section 1, convergence of the density to
gaussian does not imply convergence of the spectrum to a characteristic form. We
shall therefore always have in mind convergence of “smoothed” functions or “con-
vergence to within fluctuations.”

Equation (18) represents an approximation, even for noninteracting particles, since
in deriving it we have ignored a Pauli “blocking effect” (which would be of no conse-
quence however for a “dilute” system, one with $m \ll N$ where $N$ is the number of
single-particle states). If we construct the $m$-particle status by adding one particle at a
time we may think of the energy of the single-particle state into which a particle is
placed as a random variable, and the convolution defines the density of a sum of
random variables. The CLT requirements are that the variables be additive (which is
satisfied for noninteracting particles) and that they be independent (which is disturbed
by the blocking effect since a state filled by one particle is not accessible to another).
An extremely nonuniform single-particle spectrum might in fact require such a high
order of convolution (large number of particles) that a Gaussian spectrum is not
achievable. In practical cases, however, this does not occur and one can very simply that
noninteracting-particle systems generate Gaussian spectra.

For interacting particles or the other hand the energies are not additive, and there is
no necessary convergence to Gaussian even if the usually strong blocking effects are
ignored (suppose for example that $H$ is a type of separable interaction, represented by
the square of a one-body operator whose centroid is zero and whose spectrum is
Gaussian; then $H$ has a $\chi^2$ distribution, $\rho(x) \sim x^{-1/2} \exp(-x/2)$, which is highly
non-Gaussian). Despite this, it is found that all nuclear Hamiltonians which give
reasonable agreement with experimental data have model-space spectra which are
quite close to Gaussian. To understand this one introduces an ensemble of Hamiltoni-
ans, for example a Gaussian Orthogonal Ensemble (GOE) of $k$-body interactions
(in which the two-body matrix elements are chosen independently according to similar
zero-centroid Gaussian laws) which contains members giving rise to every possible
spectra of the specified dimensionality. One can now show [5] that the ensemble-
averaged density becomes Gaussian for large enough particle number, and that more-
over, the relative weight of those $H$’s in the ensemble which give deviant densities
become negligible for large systems (an aspect of ergodicity). For “most” Hamiltoni-
ans then the measure being defined by the GOE we have effectively a CLT for
interacting particles as well as for noninteracting. Drawing now on our experience
we assert that successful model-space Hamiltonians are characteristic members of the
ensemble and follows then that, as we increase the particle number, the eigenvalue
density converge to Gaussian even when the particles are interacting.

In case the sudden appearance of an ensemble is mysterious we remark that its real
function is to reproduce, for interacting particles, the dominance [5, 11] of the binary
correlations between matrix elements which is found automatically for noninteracting
particles when $1 \ll m \ll N$ (the corresponding physical assumption). In accord with
experience, is that such dominance is indeed found with reasonable model Hamilton-
ions). To show this consider a one-body Hamiltonian, $H = \sum i \epsilon_i$, with $\epsilon_i$, the number operator and $\sum \epsilon_i = 0$ (so that $\langle H \rangle^\dagger$ is the central moment). Thus $\langle H^2 \rangle^\dagger$ decomposes into a number of parts according to the partitions of $p$ (for $p \leq 4$) characteristic [3, 21] for example being $\epsilon_1 \epsilon_2 + \epsilon_3 \epsilon_4$, with $\epsilon_i \neq \epsilon_j$ since $\epsilon_i \neq \epsilon_j$ and $(\Delta \epsilon_i - \epsilon_i)^2 < (4)$ where $\Delta$ is the number of different operators in the product. It is almost obvious, and easy to verify, that the partition with the largest number of parts will be dominant, with the proviso however that partitions containing $1^4$ [3]; [21] for example) will contain a power of $\langle \epsilon^2 \rangle^\dagger = 0$ as a factor and are therefore ruled out. Thus binary correlations are dominant, corresponding totensoring of particle pairs. Doing the same calculations in a general (non-ideal) basis, $H = \sum \epsilon_i^2 \epsilon_i^\dagger \epsilon_i$, we find correlations between the Hamiltonian matrix elements $\epsilon_i \epsilon_j$. The argument leading to this simple result is obviously invalid for interacting particles, but on the other hand, the binary correlations are precisely those which are dominant for the GOE in our $(N \gg m \gg 1)$ limit. Their dominance arises in this case because the "one-particle" do not contribute (nor do others involving an odd factor) because of the vanishing of the ensemble-averaged matrix element $W_{ij}$, while, compared with the number of binary-correlation terms, the number involving quaternary and higher-order correlations goes to zero in our limit.2

The ensemble methods used in exploring these questions are closely analogous to the methods of statistical mechanics involving ensembles of Hamiltonians rather than states however. They are useful for many general purposes, for example to verify the role of convergence and other properties of the transition to Gaussian, and they give the only available method for studying the fluctuations. It must be emphasized however, that ensemble are used in this paper only for general arguments. When dealing with a specific system, as we shall be from now on, we work with the given Hamiltonian; we shall make no use of ensembles nor shall we ignore blocking effects not the nonadditivity of the energy.

Returning now to the strength distributions, we consider first thebart rules, or more generally the expectation value of an operator $K$. The polynomial expansion of $\langle K(W) \rangle$ is given by (19). The convergence of the densities to Gaussian implies an asymptotic similarity to $\langle K(W) \rangle$. This is demonstrated in Fig. 4, the corresponding argument being that if $H$ has eigenvalues $\lambda_i$ then $H_i = \lambda_i H_i$ with small $i$ has eigenvalues $\lambda_i H_i$, both spectra being Gaussian, being identical therefore to within a scale change, it follows that $\langle K(W) \rangle$ is linear in $W_i$, and is given therefore by the first two terms of (19).

$$\langle K(W) \rangle = \sum_i \langle K(\lambda_i) \rangle \lambda_i^2 = \langle KH \rangle + \langle \epsilon_i \rangle^2 \langle W \rangle - \langle \epsilon_i \rangle^2 \langle \epsilon_i \rangle^2.$$ (19)

This result is, of course, valid to within level-level fluctuations. It relies on the fact that, starting in the spinor space at the point $H$ we may, when there are enough particles, move an infinitesimal distance in "almost" any direction without modifying the smoothed spectrum shape, at least to first order in $\epsilon_i$. With $K = H(1)$ is an identity but, on the other hand, $K = H^2$ whose expectation value is quadratic in $W$ and

---

1 These may prove their relative contribution vanish, for that depends on the matrix-elements distribution and with a "singular" distribution they could dominate.
Fig. 1. The expectation value $\langle W | \hat{H} | W \rangle = \langle W | \hat{H} | W \rangle = \langle W | \mathcal{O}(\delta \hat{H}) | W \rangle$, as determined by the response of the system under $H \rightarrow H + \delta \hat{H}$, is the only quantity (to within fluctuations) in the linear scale variation, $\delta = \langle (H - \hat{H})^2 \rangle \rightarrow \langle (H - \hat{H})^2 \rangle \cdot \delta \hat{H}$, and then the levels shift are linear in the energy as shown. Allowing for a nonzero value of $\langle \mathcal{O} \rangle$ gives a (constant) centroid shift as well.

which by itself would generate a non-Gaussian spectrum defines an exceptional or singular direction in the operator space, as would other operators closely correlated with a power of $H$, which would similarly require further terms in (19).

If linearity obtains for the moments of the strength generated by the excitation operator $\mathcal{O}$ and its adjoint $\mathcal{O}^\dagger$ we see from (12), (13) that the polynomial strength moments $\delta^m \langle W | \hat{H} | W \rangle$ vanish when $\mathcal{O} = 1$; thus in the CLT limit the strength itself (always to within fluctuations) is bilinear in the energies

$$
d' \times \langle W | \mathcal{O}(H - \delta^2) \mathcal{O}^\dagger | W \rangle = \langle \mathcal{O}^\dagger \mathcal{O} \rangle (W' - \delta^2) \langle \mathcal{O}^\dagger \mathcal{O} \rangle (W - \delta^2) \langle \mathcal{O}^\dagger \mathcal{O} \rangle (W - \delta^2) \langle \mathcal{O}^\dagger \mathcal{O} \rangle (W - \delta^2)$$

a special case of (11), important in giving for many cases the general trend of the energy variation of the strength.

Although the low-order shape corrections, giving nonlinearities in $\mathcal{O}(H)$ and $\mathcal{O}(\hat{H})$, are not necessarily small, it is worthwhile paying special attention to the asymptotic case because there we can see very easily an important geometrical structure which is essentially maintained when we proceed to higher order. In particular,
the linear form (19) for $K(W)$ has a simple geometrical interpretation. For an operator $F$ the bilinear trace $(F^*F)$ (we shall often drop the $m$-superscript which labels the model space; note too that $(F^*F)$ is the trace of $A^*(F^*F)$) defines a proper norm and then, for Hermitian operators, $(FG)$ defines an inner product in terms of which magnitudes of operators, $\|F\| = (FG_0^2)^{\frac{1}{2}}$, and angles between operators, can be defined, the operators then residing in a (normal) Euclidean space. Subtracting out the centroid for an operator $K = K - <K> = \langle K \rangle$; $H \rightarrow H - \langle e \rangle = \langle \langle e \rangle \rangle$ has the geometrical significance of projecting in a plane perpendicular to the "one" operator 1. For these centered operators we write the unit operators or unit vectors as

$$k = \langle e \rangle$$

and then (19) takes on the forms

$$F(W) = \langle e \rangle \langle F \rangle (W - \langle e \rangle)^{1/2},$$

$$H(W) = (k - h)(W - \langle e \rangle)^{1/2} \rightarrow \langle e \rangle (W - \langle e \rangle)^{1/2},$$

in which $\nabla_{\langle e \rangle} = (k - h)$, whose value lies in the interval $(-1, 1)$ may be regarded, in geometrical terms, as the cosine of the angle between the two centered operators or, in statistical terms, as the correlation coefficient between them.

A strong correlation between $X$ and $\langle e \rangle$ (i.e., alignment, either parallel or anti-parallel) implies a strong energy dependence of $K(W)$, the states of maximum expectation value lying low if the operators are antiparallel and high if parallel. A good example occurs with the isocorollar-quadrapole transition strength, for which $K = G \cdot Q$ while $(H - \langle e \rangle)$ "contains" a large part of $Q$ - $Q$ with negative coefficient, the "strong" states are then low-lying. On the other hand, if $(H - \langle e \rangle)$ should contain only a small part of $K$ (i.e., if the operators are essentially orthogonal) then the smoothed expectation value $\langle K \rangle(W)$ will be essentially constant over the entire spectrum. Of course the notion that one operator contains a multiple of another is given a precise formulation by the geometry which we have introduced, the appropriate operation being that of projecting one operator along the other, or, more completely, of decomposing one of the operators into a part directed along the other and a part orthogonal. Thus the projection of $(H - \langle e \rangle)$ along $(G - \langle G \rangle)$ is the operator $\langle [G - \langle G \rangle]^2 [H - \langle H \rangle] (G - \langle G \rangle)\rangle$, in which for the inner product we could just as well have written $\langle (G - \langle G \rangle) (H - \langle H \rangle) \rangle$ or $\langle (G - \langle G \rangle) \rangle$, since $\langle (H - \langle H \rangle) \rangle = \langle (G - \langle G \rangle) \rangle = 0$; more generally still we could write as an operator equivalent of (16)

$$K = \sum_k \langle (K) \rangle (H) \cdot P_k (H)$$

valid of course only for linear expectation values of $K$.

As a minor illustration we have that the correlation coefficient in $(dh)^2$ between the isocorollar $Q \cdot Q$ operator and any reasonable interaction is negative and large in magnitude; for the Kuo interaction [12] $\zeta = -0.56$ and comparable values are found for other "realistic" interactions. With a normalization such that $Q \cdot Q = \langle A \rangle = 2\langle A \rangle$, where $\langle A \rangle$, the SU(3) bilinear Casimir operator, has eigenvalues $\lambda^2 + \mu^2 + \nu^2 + 3(\lambda + \mu)$
is the \((\lambda, \mu)\) representation, we have in linear approximation then that \(Q \cdot Q(\hat{W}) \rightarrow 156.5 - 22.3x\) where \(x = (W - \hat{W})/\mu\) has the value \(-5.1\) at the ground state (for a nondegenerate ground state and a Gaussian density \(x\) is given in terms of an error function by \(x = \text{erfc}^{-1}(1/\mu)\) which is very roughly \((2\pi \mu)^{1/2}\); excellent approximations are available [13]). This would give a \(Q \cdot Q\) ground-state expectation value \(\approx 20\) quite compatible with the fact that the largest \(Q \cdot Q\) eigenvalue in \((\hat{W})\) is 720 deriving from the representations \((12, 0)\) or \((0, 12)\).

This example, in fact, is quite instructive, for at the upper end of the energy spectrum (where we would find the small-eigenvalue \(S(1)\) representations) the linear form for \(Q \cdot Q(\hat{W})\) goes negative even though \(Q \cdot \hat{Q}\) is a positive definite operator. This comes about because the circumstances in this example are [14] unfavorable for a Gaussian density and a corresponding linear \(K(W)\). The space is too large \((d = 2.7 \times 10^6)\) for these approximations to extend over the entire spectrum span (the shape deformations of course show up first near the extremes); \(Q \cdot \hat{Q}\) is strongly correlated with \(H\) so that \(Q \cdot Q(W)\) has a large slope, and, \(Q \cdot \hat{Q}\) being the sum of five squares, is somewhat related to the square of a one-body operator which we have mentioned above as a prototype of an operator with a non-Gaussian spectrum. In fact the necessary cut-off in the \(Q \cdot \hat{Q}\) spectrum at small eigenvalues generates quite a strong deviation from Gaussian at the large-eigenvalue end, which would correspond to low-lying states in the energy spectrum; the deviations in density are also large but the expectation value (which has a polynomial rather than an exponential form) is given reasonably. Even so for good accuracy we should take into account the shape deformations either by including some more terms in the expansions given above or by using the partitioning procedure (to be discussed in the next section) which is more efficient and more instructive. It will be seen, however, from the examples in the next paper that the geometry will survive, giving quantitative results in favorable circumstances and at least a qualitative description in unfavorable ones.

A Euclidean (or Unitary) geometry can be introduced into any model space. However, the physical significance of the geometry as we have introduced it above derives from the CLT which for centered operators, and always within fluctuations, assures us that the norms of operators and the scalar products which derive from the norms, determine everything about the asymptotic behavior. In other words the significance of the geometry derives from the direct-product nature of the model spaces. But this same structure determines also symmetries, defined by the group \(U(\Lambda)\) of unitary transformations among the \(N\) single-particle states with which we build the model spaces, and its various subgroups. Quite new consequences follow from this as we shall discuss briefly in Section 7.

4. LINEAR RESPONSE THEORY

The asymptotic results (19), (20) may be thought of as deriving from the linear response of the system under the deformation \(H \rightarrow H_\lambda = H + \lambda K\). In the general (nonasymptotic) case there will be a deformation of the spectrum shape, as well as the
variations in the centroid and with which lead to (19), (20). We might expect then to relate the higher terms in the polynomial expansions to the shape deformation, and thereby the rate of convergence of the expansions to the rate determined by the CLT for the density, which is well understood.

Let us first derive a compact form for $\mathcal{K}(W)$ in terms of the density deformation. Under $H \rightarrow H_0 + H + \alpha K$, with small $\alpha$, we have $W_1 \rightarrow W_1 + \alpha K(W_1)$, as in Fig. 1. Let $W < W_0 < W_{\max}$ and agree that $K(W), K(W_{\max}) > 0$ (the other cases lead to the same result). Since $d \times F(W)$ counts the number of levels below $W$, the deformation will either produce no change in $F(W)$, or a change in $F(W)$ of value $(-d)^3$, the probability of the latter being the ratio of the shift $\alpha K(W)$ to the local level spacing $(W_{\max} - W)$. For smoothed distributions, adequate for our purpose, this ratio is $ad \times \rho(W)K(W)$ and then, taking the small-$a$ limit, we have the result [2]

$$
\frac{\partial F(W)}{\partial a} = \left( \frac{\partial F(W)}{\partial a} \right)_{a=0} = \left( \frac{\partial}{\partial a} \right)_{a=0} \rho(z) \delta z.
$$

Recognizing that $F(W)$ is a staircase function and that the change in $F(W)$ takes place only for $W$ in the neighborhood of an eigenvalue $W_1$, we see that (26) is valid in general.

A density $\rho(z)$ may be defined in terms of its location, extent, and shape, respectively by its centroid $z_0 = \mathcal{S}_0(z) = \langle H \rangle^m$, its variance $\sigma^2 = \mathcal{S}_2(z) = \langle (H - \langle H \rangle)^2 \rangle^m$, and a set of shape parameters $\mathcal{S}_m(\sigma)$ which must then be translated and scaled invariants. It follows by linear independence of the moments that we can take the $\mathcal{S}_m$ to be 8th order polynomial moments of the form

$$
\mathcal{S}_m(s) = \frac{1}{2^m} \left[ \mathcal{S}_m(s) - \mathcal{S}_m(s) \right] dz = \langle s(H + \alpha K) - s(H)^m \rangle^m = s(H)^m \langle s(H)^m \rangle^m + \ldots
$$

where $s_8(z)$ is the 8th order polynomial. In the case of the centroid and its dependence on the density, the $\mathcal{S}_m(z)$ must be functions only of $(z - \langle \rangle)$. Under the Hamiltonian deformation the density $\rho(z)$ becomes $\rho_1(z)$ and the variation of each parameter $\delta$, gives a contribution to $K(W)$, specifically, from (24)

$$
\frac{\partial P(W)}{\partial \mathcal{S}_m} = - \sum_m \left( \frac{\partial \mathcal{S}_m(z)}{\partial a} \right)_{a=0} \frac{\partial F(W)}{\partial \mathcal{S}_m}.
$$

The $(n - 1, 2)$ terms, exactly as we would expect, give back the CLT result (19); formally $\mathcal{S}_m$ has the functional form $\sigma^2 f(n - \langle \rangle)$ and then (19) follows from the results that [2]

$$
\frac{\partial F(W)}{\partial \mathcal{S}_1} = -\rho(W), \quad \frac{\partial F(W)}{\partial \mathcal{S}_2} = -\frac{(W - \langle W \rangle)^2}{2\sigma^2} \rho(W).
$$
We now have for the deformed density and distribution function

\[ \rho(x) = \rho_0 \left\{ 1 + \sum_{\alpha} S_\alpha(x) T_\alpha(x) \right\}, \]

\[ F(x) = \int_0^x \rho(x) \, dx. \]  

(28)

The centroid and variance deformations are included in \( \rho(x) \) but since their contributions to \( K(W) \) are already known (26), (7) we may as well ignore them here. In (28) the \( S_\alpha(x) \) are given by (25) and the functions \( T_\alpha(x) \) will follow from the fact that the \( S_\alpha \) are polynomial monotonic. Since from (25), (26)

\[ \langle S_\alpha(x) \rho(x) \rangle = \langle K(\rho(x)) \rangle S_\alpha, \]

\[ \langle (K(x))^{\alpha} \rangle = \int_0^x \rho(x) T_\alpha(x) \, dx, \]

we have, on writing \( K(W) = K_{exx}(W) + d K(W) \), that \( d K(W) \), the shape-deformation correction to \( K(W) \), is given (26), (29) by

\[ K(W) \Delta K(W) = \sum_{\alpha} \langle S_\alpha(x) \rangle \langle (K(x))^{\alpha} \rangle \int_0^x \rho(x) T_\alpha(x) \, dx. \]  

(30)

We fix the \( x \) polynomials and the \( T_\alpha \) functions in terms of the orthogonal polynomials \( P_n \) by

\[ x(x) = P_{-\alpha}(x), \]

\[ \rho(x) T_\alpha(x) = \int_0^x (dx) \rho(x) P_{\alpha}(x). \]  

(31)

(the integration constant being of no consequence in the first of these may be taken zero) and then (30) reproduces the \( K(W) \) expansion (16).

We have now a term-by-term association between the polynomial expansions of the strength and that of the expectation values (and therefore of the mean-squared quantities and the strengths themselves) which assures that the CLT convergence of the density implies a similar convergence of these quantities as well. In particular as we add partials the shorter-wavelength (higher polynomial order) deviations from linearity are attenuated more rapidly so that the most significant corrections to the CLT terms \( \Delta K(W) \) and \( R(W, W) \) will be those of low order.

For completeness we mention two technical points. (1) There is a derivative relationship (as in (31)) between the density and strength deformations which, for a given order, are not strictly related to each other on a point-by-point basis. However for Gaussian \( \rho(x) \) we have \( \alpha^2 \delta(x)b(x) \rho_0(x) P_{\alpha}(x) \sim b(x) \) so that in this case the correspondence is precise; a slightly more complicated correspondence exists for a small class of other density forms, namely those for which there is a generalized Rodriguez formula (13). (2) Even for Gaussian the convergence is not best exhibited
by an orthogonal polynomial expansion. In the standard Gram-Charlier expansion about a Gaussian density the $r \gg 6$ coefficients are not strictly Hermite-polynomial moments, and the differences are more pronounced with the Edgeworth-series which exhibit the CLT convergence in a more uniform fashion [16]. Neither of these points, however, will have any real effect on our arguments and results.

The results above have followed from the linear response of the system under the $(\mathcal{H} \to \mathcal{H} + \mathcal{O})$ "deformation" of the Hamiltonian. The quadratic response, in which we take account of the $(\partial^2 \mathcal{H}/\partial \phi^2)_{\phi=0}$ terms, and the response of higher order, can be used to give a theory for the inverse-energy-weighted sum rules, a subject which will be discussed and applied in a later paper.

5. Partitioning for Strengths, Sum Rules, and Expectation Values

Simple notions about the distribution of shell-model configurations throughout the spectrum lead naturally to procedures for calculating strength distributions which have been often used though they are approximate and in many cases quite inaccurate. We start with a sequence of such procedures and then give an exact polynomial expansion which in form is closely related to the simple ones but which, unlike them, takes full account of the interactions and in particular of the correlations between the Hamiltonian and the excitation operator.

We consider the single-particle space as composed of orbits (perhaps spherical) as in the $d_2$ shell with $d_{1p}, d_{1f}, d_{2p}$, and the $m$-particle space as decomposed thereby into configurations (3 for $m = 1, 4$ for $m = 2$ in our $d_2$ example), schematically

$$N = \sum N_i,$$

$$n = \sum m_i = \sum m_i$$

where $l$ is the number of orbit; for simplicity we ignore the angular-momentum and isospin labels so that we consider together the transitions involving the various $(J, T)$ values.

We can now give an approximate strength in the $m$-particle space in terms of the dimensionsality of the configurations $d(m)$, the centroids, $\delta(m) = (\mathcal{H} \rightarrow \sum c_m)$, for noninteracting particles and the mean-squared excitation matrix element $\mathcal{H}^2$, $\delta(m)$which connects two configurations. For the (average) strength connecting two states we have, with $\delta(m), \delta(m')$ the configuration centroids, that

$$R(W', W) \rightarrow \sum M'(m', m) \delta(W' - \delta(m')) \delta(W' - \delta(m))$$

so that the strength appears as a series of "spikes"; for the total strength in a spike we must of course include the configuration-dimensionality factors.
To give a form for $M'$ we observe that, for $F$, $G$ defined in $m$,

$$
\langle FG \rangle^m = \sum_m \langle FG(m' - m) \rangle^m = \sum_m \langle G(m' - m)F \rangle^m. \tag{34}
$$

Here we have written $G = \sum G(q)$ where $G(q)$ acting on any vector in $m$ gives a vector in $m + q$ (i.e., with partition numbers $(m_i + q_i)$). This decomposition is quite immediate; for example with a one-body operator, $G = \sum_{A' A} A' A$, a restriction of $F$ to the orbit $N_i$ and of $\rho$ to orbit $N_i$, gives an operator which generates only transformations $[m_i, m_{i-1}, ..., m_1 - l_{i-1}, m_1 + 1, ..., m_0]$. $F$ could similarly be decomposed but the simultaneous decomposition of $F$ and $G$ is obviously unnecessary for quadratic traces. As a point of notation we shall write $F(q) = (F(q))^{1 \rho}$ and is therefore an operator of type $(-q)$. Observe that $(F(q)G(q))^{1 \rho}$ is a partial variance of $I$, the contribution to the variance of the term $m - m + q - q$.

Using (34) we have that $d(m')d(F(m' - m)) = \langle O(m' - m)O \rangle^m$ so that (33) gives for the simplest version of the strength,

$$
R(W', W) = \sum_{m'} d(m')^{-1} \langle O(m' - m)O \rangle^m \delta(W' - \mathcal{E}(m')) \delta(W - \mathcal{E}(m)). \tag{35}
$$

This very crude "schematic" theory already accomplishes something. In the $d\alpha$ shell for example, there are considerable energy differences between the three $j$-orbits (the relative primary single-particle energies are $6\alpha = 0.98$, and 5.08 MeV for $d_{5/2}$, $d_{3/2}$, $d_{9/2}$, respectively) and as a consequence the centroids of the $45 (d\alpha)^N$ configurations themselves span a measurable part of the entire spectrum (with the primary energies the centroid span is $(6\alpha + 4\alpha) \approx 44$ MeV and renormalization of the single-particle energies (which takes some account of the interaction) will increase this somewhat. Thus (35) spreads the strength over a considerable energy domain, not adequate however, because the spectrum span will be 100-125 MeV depending on the interaction and we would expect the strength to spread over the entire spectrum.

We can improve things by taking account of the spread of the configurations and making the simple assumption that the strength "follows" the densities. Then, since the $m$-states form, at $W$, a fraction $I_m(W) = \rho(W)$ of the total states, we have, as the extension of the simplest model, the approximation

$$
R(W', W) = \sum_{m'} \frac{I_m(W')}{I_m(W)} \frac{I_m(W)}{I_m(W)} \frac{d(m')}{d(m)}^{-1} \langle O(m' - m)O \rangle^m \tag{36}
$$

which now does spread the strength over the entire spectrum. We have introduced here the decomposition of the density into partial (configuration) densities,

$$
I_m(W) = \sum_n I_n(W) = \sum_n d(n) \rho_n(W) = \sum \langle H_n - z \rangle^m, \quad d(m) M_{ij}(m) = \sum_n \langle H_n \rangle^m. \tag{37}
$$
In contrast to the total density, the partial densities are not densities of eigenvalues except in the special case where the configuration subspaces are Hamiltonian eigenspaces; instead \( \mu(\mathbf{x}) \) measures the total \( m \)-intensity in the eigenstates located in the energy interval \( dx \) at \( x \).

Observe very carefully that this linear decomposition involving, as it does, quantities nonlinear in the energy, does not imply that the configuration distributions are non-interesting; in evaluations \( \langle HQ \rangle_m \) for \( p = 1 \) we would logically take account of intermediate excitations to other configurations so that, taking \( p = 2 \) for example, (which along with the centroids would often suffice) the variance for one configuration has both an "internal" part (\( m \rightarrow m \rightarrow m \)) and a set of "external" parts (\( m \rightarrow m \rightarrow m \)). Then (36) does take account of some of the correlations induced by the interaction.

With the strength as given by (36) we find, for the energy-weighted sum rules, the expected result that

\[
\mathcal{M}_4(W) \rightarrow \sum_m \frac{I_m(W)}{I_m(W)} M_4(m) \langle O^+(m^+ + m)O^m \rangle
\]  

(38)

with \( M_4(m) \) a final-state density moment. The expectation value result follows from

\[
\mathcal{K}(W) \rightarrow \sum_m \frac{I_m(W)}{I_m(W)} \langle K \rangle_m
\]

(39)

But this intuitively simplest form, which has been used, for example [15], in evaluating spin cutoff factors (with \( K = J^Z \)), does not even take account of the first-order \( K-H \) correlation which, depending on its sign, raises or lowers the states with larger-than-average \( K \) expectation values, and which is taken account of in the CLT limit. We see then that the approximate results (38), (39), and a fortiori (36) have no proper basis at all except for operators very weakly correlated with \( H \) (as \( J^Z \) usually is, so that the earlier spin-off evaluations are still more or less satisfactory). The major difficulty with these approximations is with the assumption that the strength follows the density, which ignores the correlation between the Hamiltonian and the excitation and which is in general not at all correct. A related difficulty is the partial neglect of interference between configurations, which there is no natural way to take account of in the schematic theory. To give an exact theory which will include the schematic theory as a very poor approximation, and the CLT-limit theory as a much better one, it is simplest to start all over again.

For very large spaces the CLT approximations (19), (20), will not be sufficiently accurate in the ground-state domain and consequently correction terms are required. It is quite satisfactory in some cases to include a few higher terms in the general expansions (11), (16). The traces required for these corrections, however, become rapidly harder and harder to evaluate as the order increases. Just as in the schematic models just described, it pays us to purify by orbits and configurations, which we do exactly as above. Let us now rewrite the polynomial expansions (11), (16) in accord with the new forms (37) for the density.
For the expectation values and hence the sum-rule quantities we define

$$K(W: m) = \sum_{\nu} \langle H\nu | \hat{K}(H-H')^{\nu} | \hat{K}(H-W)\rangle$$

(40)

and then from (16)

$$K(W) = \sum_{\nu} \langle H\nu | \hat{K}(H-W)\rangle^{\nu} = \sum_{\nu} \langle H\nu \hat{K}(H-W)\rangle^{\nu}$$

(41)

$$- \sum_{\nu} \langle H\nu \hat{K}(W) \rangle^{\nu} \sum_{\nu} \langle H\nu \hat{K}(H-W)\rangle^{\nu}$$

$$\sum_{\nu} \langle H\nu \hat{K}(W) \rangle^{\nu} K(W: m)$$

which is quite different from (30). We have here first decomposed the trace according to \( m = \sum_{\nu} m \) and have then taken the physically motivated step of introducing separate polynomial sets for the separate subspaces, namely for a given \( m \) the polynomials defined by the partial density \( \mu_m(W) \). Since a configuration density is to some extent localized in the spectrum a given term is not now required to give results over the entire spectrum and much lower polynomial orders are appropriate. It should be remarked also that, while there will be more of them, configuration traces are no harder to evaluate than the \( m \)-space ones (whereas the complexity increases extremely rapidly with polynomial order). The net result is that our partitioning gives a major simplification.

If, as we usually do, we take the partial densities \( \mu_m(W) \) to be Gaustavian the \( \mu_m^{(n)}(W) \) are of course Hermite polynomials, \( \mu^{(n)}(W) = \mu^{(n)}(H) \), where \( \mu^{(n)}(x) = H_{n}(x) \). In some cases, particularly for low-lying configurations, it would be worthwhile to include skewness and excess corrections.

In (41), just as in (30), \( I_m(W) = I_m(W, m) \) is a natural intensity ratio while \( K(W: m) \), as defined in (40) is given by the standard \( K(W) \) form (16) but restricted to the \( m \) subspace. Superficially then (41) has exactly the form to be expected. \( K(W) \) appearing as a properly weighted fixed-energy average of its subspace values. This expectation is quite logical if the subspaces are Hamiltonian eigenspaces (which in practice does not really happen with configurations) for then \( K(W: m) \) is indeed a \( \mu \) expectation value.

But in the general case it is not a priori so because of the \( m \rightarrow m \) excitations induced by \( H \). It is a remarkable property of (41), that, without changing its form, it properly takes account of correlations and interferences of all orders, and gives then a formally exact expansion for \( K(W) \). Note incidentally that, in the CLT limit in which we take only polynomials of order \( 0 \), (41), \( K(W: m) \) is a true expectation value as long as \( m \) is an eigenspace for either \( H \) or \( K \), so that with configurations the CLT limit of (41) does give for occupations an uncoupled superposition. The \( \mu = 0 \) terms of (41) give back the schematic theory result (39) but, as indicated above, there is in general no logic in ignoring the \( \mu = 1 \) terms which are similarly uninfluenced by the CLT.
For the strength we proceed similarly

\[
\mathcal{L}_a(W^o) R(W^o, m'; W, m) \mathcal{L}_a(W) = \sum_{\mu, m} \langle O^\dagger(\mathbf{H} - W) O(\mathbf{H} - W) \rangle_{a, \mu, m} \mathcal{L}_a(W^o) \mathcal{L}_a(W) \delta^a(\mu, m') \times \sum_{\nu, m} \langle O^\dagger(\mathbf{H} - m') O^{\dagger}(\mathbf{H}) \rangle_{a, \nu, m} \delta^a(\mu, m') \mathcal{L}_a(W^o) \mathcal{L}_a(W^o, m'; W, m) \]

(42)

and thus

\[
R(W^o, m'; W, m) = \sum_{a, \mu, \nu, m} \mathcal{L}_a(W^o) \mathcal{L}_a(W) \mathcal{L}_a(W^o, m'; W, m) \]

(43)

with \( R(W^o, m'; W, m) \) defined by the fourth form occurring in (42). We have introduced here, for each initial and each final subspace \((m, m')\), a set of polynomials generated by the subspace densities, the argument for doing this being identical with that given for expectation value (41). In (43) we find the intuitively obvious form for the strength decomposition as a superposition, with the natural initial- and final-state branching ratios, of the strengths connecting the subspaces, but once again all correlations and interferences are properly included and the result is formally exact. The CLT limit takes account of all polynomials of order \(<1\), thus \((\mu, \nu) = (0, 0), (0, 1), (1, 0)\), and \((1, 1)\), just as in (20) for the spaces not partitioned. The \((0, 0)\) terms gives for \( R \) the mean-squared matrix elements connecting two configurations which leads to the schematic theory derived above. It is easily verified that an integration over the strength (43) reproduces the sum rules (41), just as in the nonpartitioned case, an integration over (11) gives back (16). The same is true for the schematic version of (43) and the corresponding sum rules (39). We stress also that, in all three cases, integration over a restricted energy domain will produce the exothermic or endothermic sums disposed then of a difficulty discussed in the Introduction.

6. MULTIPLE STRENGTHS AND SUM RULES

If we consider \( J = 0^- \rightarrow 2^+ \) quadrupole excitations we may start with \( J = 0 \) model space and then the selection rule automatically yields \( J = 2 \). For a case such as this no formal expansion of the procedures described above is needed (though of course the technical problem of evaluating the traces for fixed particle number and angular momentum will be harder than for fixed number only). By symmetry (42) the same is true for the inverse transitions \( J = 2^+ \rightarrow 0^- \) even though final states \( J = 0^- \).
are accessible, but things are quite different for example for $J = 2 \rightarrow 1$ and more generally for nonscalar excitations connecting nonscalar states. We need that to decompose the strength according to angular momentum.

In principle this can be done by introducing a projection operator for the final states (infinite intermediate ones in the sum-rule expectation values). Such an operator is easily written as a polynomial in $J^2$, but, in general calculations, as opposed, for example, to matrix ones in which they are automatically taken care of, it is hardly feasible to deal directly with operators of such high particle rank. (The fact though that there is an alternative procedure for solving the problem implies that there is an indirect way of dealing with them but we shall not explore that.)

We follow instead the methods [9] used in generalizing the multipole sum rules from the conventional "scalar" ones. We assume that the model spaces "accommodate" the angular momentum in the sense that if a state with given $J$ is found in it, so will the complete level (i.e., all $2J + 1$ $I_J$ values); this simply implies that the model spaces supply representations (in general reducibles of the rotation group. The basic rules are now very simple; every quantity should be displayed as a spherical tensor (or a linear combination of such); ordinary multipole is replaced by tensor (Clebsch-Gordan) coupling, ordinary matrix elements by zero-coupled ones (zero because only scalars can survive integration over the coordinates of the system; the zero-coupled matrix elements may also be written as vacuum-expectation values or as Racah's double-barred matrix elements (ghost). Then elementary recoupling algebra will solve for us all the problems connected with tensorial behavior. The same operations work also for isospin and in fact we shall use a direct-product notation which will work for angular-momentum or isospin or both together (e.g., $I = J$ or $I$ or $J, T$). In this connection we remark parenthetically that, although the $J$ and $T$ coupling operations are identical, things are very different for the trace evaluation. This comes about because all the states of given $J$ belong to an irreducible representation of a (direct-product) group, but this is not true at all for $T$. Specifically we use the notation of Ref. [16]. We also need a definition of "double-barred" traces. Let us lab the states by $(m, \Gamma, M, s)$ where $M$ is the component of $I$ so that the $(|I|)$-dimensional set with fixed $(m, \Gamma, s)$ constitutes a level and the non-angular-momentum label $s$ counts the levels. Let $d(m, \Gamma)$ be the state dimensionality for fixed $(m, \Gamma)$, and $d(m, \Gamma, I)$ the level dimensionality, and similarly for $l(m, \Gamma, W)$ and $l(m, \Gamma, W)$. Then

$$d(m, \Gamma, I) = \sum_{m} d(m, \Gamma)$$

$$l(m, \Gamma, W) = (|I|) l(m, \Gamma, W) = d(m, \Gamma) l(m, \Gamma, W)$$

$$\sum_{m} [I] d(m, \Gamma, W) |2W| = d(m, \Gamma, W) \sum_{m} l(m, \Gamma, W) |2W| dW.$$  \hspace{1cm} (44)

We define

$$\langle O(r)|n^r = d(m, \Gamma) \langle O(r)|n^r = \sum_{m} \langle m| \Gamma, r \rangle \langle m\Gamma r \rangle$$

$$= \int d(m, \Gamma, W) d(m\Gamma W, r \rangle \langle m\Gamma W, r \rangle dW.$$  \hspace{1cm} (45)
in the last form of which we have used the Hamiltonian basis, taking for granted that we have a scalar Hamiltonian.

Consider first the (tensorial) expectation values of $K'$ in the $(m', \Gamma)$ eigenfunctions:

$$
\langle K'(H - W)|\langle m', \Gamma W \rangle = \sum_n \langle \bar{p}^m_n | \bar{p}^{m'}_n (H - W) | \bar{p}^m_n \rangle
$$

$$
= \int \rho(\epsilon, W) (\epsilon - m\Gamma W - \tilde{W} m\Gamma W) \langle \bar{p}^m_n | \bar{p}^{m'}_n \rangle d\tilde{W}
$$

and hence

$$
\langle \bar{p}^m_n | \bar{p}^{m'}_n \rangle = \chi(W, \frac{\epsilon}{m\Gamma W}) = \sum_n \langle \bar{p}^m_n | \bar{p}^{m'}_n (H - W) | \bar{p}^m_n \rangle
$$

(46)

which gives the tensorial extension of (16); taking $\beta = 0$, only we have the CLT limit, the corresponding extension of (19). The polynomials introduced here are of course, those defined by the $(m, \Gamma)$ partial density.

We may derive the van t's rule from the strength itself, which we consider next. We have then for a pure multipole transition, $(m'\Gamma' M' W')$, in which only the $(M' - M)$ component of $\Omega'$ contributes to the transition,

$$
\rho(m'\Gamma' M' W'; m\Gamma W) = \langle \bar{p}^m_n | \bar{p}^{m'}_n (H - W) | \bar{p}^m_n \rangle
$$

$$
= \langle \Gamma' (\rho_{\Gamma' M' W' - \rho_{\Gamma M W}}^{\text{tensor}}) | \langle \tilde{W} | \Omega | \tilde{W} \rangle \rangle
$$

$$
= \langle \Omega | (\rho_{\Gamma' M' W' - \rho_{\Gamma M W}}^{\text{tensor}}) | \tilde{W} \rangle
$$

(48)

$$
R(\Gamma' M' W' - \Gamma M W) = \langle \Omega | \tilde{W} \rangle
$$

(49)

where we have used the Wigner-Eckart theorem and, for convenience, have suppressed the $(m, m')$ labels. The polarized strength has been defined precisely as in Section 2 while the unpolarized strength $R(\Gamma' W' - \Gamma W)$ ($= R(\Gamma W' - \Gamma W)$) for a self-adjoint excitation is, for electromagnetic and other hole-particle transitions, essentially the $BD$ or $BMD$ value, differing by a statistical factor since we have summed over initial states instead of averaging. For angular momentum $(\Gamma = J)$, our interest is usually in the unpolarized strength, for isotropic $(\Gamma = -J$) usually in the polarized strength. Then for $(\Gamma = J, \Gamma)$ we are left with a Cebuhov-Greinse isotopic factor.

In the polarized cases there is, of course, interference between multipoles. We therefore need the more general quantity

$$
R(m'\Gamma' M' W'; m\Gamma M W) = \langle \bar{p}^m_n | \bar{p}^{m'}_n (H - W) | \bar{p}^m_n \rangle
$$

$$
= \langle \bar{p}^m_n | \bar{p}^{m'}_n (H - W) | \bar{p}^m_n \rangle
$$

(50)

$$
R(\Gamma' M' W' - \Gamma M W) = \langle \tilde{W} | \tilde{W} \rangle
$$

(51)
We have dropped a complex conjugate since all dimes can be taken real. Observe that $H = 0$, so that a polynomial expansion for $F^w$ will be adequate for all cases, rational or unipolarized, pure monople or mixed.

We have now, using (3.17) of Ref. [16] which we label as (V 3.17)

\[
\rho(g^w; W') R^w(gW; P'W)\rho(gW)
\]

\[
- (-1)^{\nu-\nu'} \int \rho(g^w; x') dx' \int \rho(gW; x) dx
\]

\[
\times \times (T_2 \parallel O(H - W)) (\Gamma' \times (\Gamma' \parallel O(H - W)) \Gamma_2)
\]

(52)

and then from (44), (45), (V 3.25)

\[
I(m^\nu\Gamma' W; W') R^w(m^\nu\Gamma' W; m\Gamma W) I(m^\nu\Gamma' W)
\]

(53)

\[
= (-1)^{\nu-\nu'} \sum_{\nu} (-1)^{\nu} \int (T_2 \parallel \Gamma_2) (\Gamma_2 \omega) (O(h - h - W)) \times O(H - W - W') (T_1)^{\nu-\nu'}
\]

It is seen from the LHS that the intermediate states in the RHS trace must all be $\nu$ states and thus our expansion is completed by expanding $B(H - W')$ and $B(H - W)$ in $\rho^{\nu^2}$ and $\rho^{\nu^3}$ polynomials respectively, hence

\[
d_\nu(m^\nu\Gamma') R^\nu(m^\nu\Gamma' W; m\Gamma W) d(m\Gamma)
\]

\[
= (-1)^{\nu-\nu'} \sum_{\nu} (-1)^{\nu} \int (T_2 \parallel \Gamma_2) (G_2)
\]

\[
\times \times (O^{\nu} p^{\nu}(H) \times O^{\nu} p^{\nu}(H) \times O^{\nu} p^{\nu}(W) \times p^{\nu}(W))
\]

(54)

which extends (11). It should be clear of course that the sum in (53), (54) is responsible for the $\nu$ projection. In fact, for the diagonal case ($\nu = 0$), $U(T^\nu\Gamma' \parallel \Gamma' \omega) \sim p_{\nu}(\cos \theta)$ where $\theta$ is the $(\nu + 1 - \nu)$ coupling angle and the symbol $(\sim)$ denotes the Rash–Legendre correspondence (V 3.29); thus, $\sum_{\nu}$ generates the usual spherical harmonic transform. We have, with the subscript zero defining a vacuum expectation value, that

\[
\sum_{\nu} (-1)^{\nu} \int (T_2 \parallel \Gamma_2) (\Gamma_2 \omega) (\Gamma_2 \parallel \Gamma_2) = \langle \phi(\omega) \times \phi(\omega) \rangle_{\nu=0}
\]

(55)

and then (35), (54) become

\[
I(m^\nu\Gamma' W; W') R^w(m^\nu\Gamma' W; m\Gamma W) I(m^\nu\Gamma' W)
\]

\[
= (-1)^{\nu-\nu'} \sum_{\nu} (-1)^{\nu} \int (\phi(\omega) \times O(h - h - W)) (\times O(H - W - W') (T_1)^{\nu-\nu'}
\]

(56)

\[
d_\nu(m^\nu\Gamma' W; W') d(m\Gamma)
\]

\[
= (-1)^{\nu-\nu'} \sum_{\nu} (-1)^{\nu} \int (\phi(\omega) \times O^{\nu} p^{\nu}(H) \times O^{\nu} p^{\nu}(H) \times O^{\nu} p^{\nu}(W) \times p^{\nu}(W))
\]

\[
\times p^{\nu}(W) p^{\nu}(W)
\]

(57)
in which the \( z \) sums define a new variety of coupled trace (a graphical transform of the original given by (45)). The technical problem of trace evaluation is of course essentially the same for the two variables. The multiple sum rules follow immediately from these basic equations, as does also the decomposition by configurations (which is somewhat complicated, however, by the interorbit couplings). We leave these matters until we come to applications in later papers.

7. UNITARY GEOMETRY

In Section 3 we have introduced a geometry for the (unselected) operators which operate in a model space by taking the square of the norm of an operator to be defined by its variance. It has been stressed that the effectiveness of this geometry (the fact that we can understand phenomena and even calculate parameters by making use of it) derives from the CLT which, in the many-particle limit, assigns great significance to the widths (norms). The CLT is turn derived from the direct-product nature of the model spaces, which is best described in group theoretical terms; specifically the \( (2) \) states formed by distributing \( n \) fermions over \( N \) single-particle states form an irreducible representation of the group \( U(N) \) of unitary transformations in the single-particle space. It is not surprising that these symmetry considerations \( (2) \) will give a deeper understanding of the results derived above; \( (2) \) will make explicit the particle number dependence (see for example (59) ahead) so that we can explore how a given phenomenon changes as we consider a set of neighboring models; \( (3) \) will give group theoretical methods for evaluating the necessary traces; \( (4) \) will lead to major extensions of the geometry when we consider subgroups of \( U(N) \).

In this section we give an introduction to these states, considering \( U(N) \) only and not its subgroups. We leave the extensions and applications for later papers. We shall, however, answer, in a particular case, a general question discussed in the introduction, namely: How is information propagated over a very wide energy range in the model spectrum so that, although most of the model states are highly "unphysical," the space nevertheless does supply real information about the low-lying states? Remember that the Hamiltonian norm is determined by the sum of square of all its model-space eigenvalues, only a negligible fraction of which will be "physical" so that this question is very important for us.

The \( n \)-particle states generate the \( U(N) \) irreps defined by a one-columned Young shape with \( n \) boxes. Since all the representations we encounter will be predominantly antisymmetric (many times, few columns) we shall label them by their columnar structure rather than by rows, thus \( \hat{a}^\dagger \) for the \( n \)-particle antisymmetric states. A general \( k \)-body operator does not transform irreducibly but instead [15]

\[
F(k) = \sum_\alpha F(\alpha) - \sum_{\alpha \neq \beta} \left( \frac{N - \alpha}{k} \right) \delta(\alpha)
\]

where \( \epsilon \), which describes the unitary symmetry, and which we shall define as the unitary
rank, indicates that \( F(k) \) transforms as one- or two-columned representations \( [N-\nu, \nu] \), \( n \) is the number operator and the last equality expresses the fact that any \( k \)-body operator of definite unitary rank contains (if \( s < k \)) an \( n \)-polynomial factor which is the result of a \( (k - \nu) \)-fold contraction of \( F(k) \). We may describe the \( D(\nu) \) for more simply \( \pi(\nu) \) as fully reduced or contracted tensors. They vanish in \( (s < \nu) \) hole or particle spaces and behave simply under the hole \( \leftrightarrow \) particle transformation \( (\pi(\nu) \leftrightarrow (-1)^{n-\nu} \pi(\nu)) \). Their unitary and particle ranks are equal.

We have thus that the space of the \( k \)-body operators (whose dimensionality is \( 2\nu \)), that being the number of independent matrix elements decomposes into a set of \( (k - 1) \) subspaces each defining an irreducible tensor; the subspaces dimensionalities are \( D(\nu) = \binom{N}{\nu} \), \( \text{link} \). \((N - 1)\binom{N - 2\nu + 1}{\nu} \) (in spaces generated by distributing \( \nu \)-tensors over \( N \) single-particle states, every contracted tensor of rank \( n \) expands itself in terms of \( D(\nu) \) tensors). A general \( k \)-body operator has a component in each subspace. In particular a two-body interaction has a \( (n - 1) \) part which behaves like a number-dependent (because of the \( (n - 1) \) factor) irreducible (traceless) one-body operator and which renormalizes the single-particle energies; it contains also a “number-dependent zero-body operator,” a multiple of \( \Omega \), which for \( m = N \) gives the closed-shell energy and for arbitrary \( m \) the average energy, or eigenvalue centroid; this is subtracted out of course, when the operator is centered.

The square of the norm of \( F(k) \) now decomposes as a sum of squares, no cross-terms occurring because only the scalar \((\nu = 0)\) part of the product contributes to the trace

\[
\langle \pi(\nu) | F(k) | \pi(\nu) \rangle = \sum_{m=0}^{N} \left( \begin{array}{c} N - m \\ \nu \end{array} \right)^2 \langle \pi(\nu) | \pi(\nu) \rangle^m \]

\[
= \sum_{m=0}^{N} \left( \begin{array}{c} m - \nu \\ \nu \end{array} \right)^2 \left( \begin{array}{c} N - m \\ \nu \end{array} \right)^2 \langle \pi(\nu) | \pi(\nu) \rangle^m (59)
\]

where \( \langle \pi(\nu) | \pi(\nu) \rangle \) is the matrix element of \( \pi(\nu) \) between states \( \alpha, \beta \) which belong to an orthonormal basis for the \( \nu \)-particle space. The first equality here derives from (58) and the second from the fact that, since \( \langle \pi(\nu) | \pi(\nu) \rangle \) is an operator of various particle ranks \( \langle 2\nu | \pi(\nu) | \pi(\nu) \rangle \) is a polynomial in \( m \) of order \( 2\nu \), which must be invariant under \( m \rightarrow (N - m) \), must vanish for \( m < \nu \), and must reduce to unity for \( m = \nu \), these conditions then defining the polynomial to have the form indicated. \( \langle \pi(\nu) | \pi(\nu) \rangle^m \), defining the bare norm of \( F(k) \), is simply the mean square defining matrix element of \( \pi(\nu) \). Observe that the different tensorial parts of \( F(k) \) grow in magnitude (norm) at different rates as the particle number increases; the simplest tensors (smaller \( \nu \) ) grow more rapidly than the more complex ones. A completely similar decomposition follows immediately for the scalar product \( \langle \pi(\nu) | \pi(\nu) \rangle^m \langle \pi(\nu) | \pi(\nu) \rangle \). Note that if \( k = k' \) (say \( k < k' \)) then the \((r > k)\) parts of \( G(k') \) contribute nothing to the scalar product, an obvious
result but, as we shall see, an important one. (This property can indeed be used to
define the irreducible tensors and to carry out the explicit reduction of $F(k)$; the
key statement here is that any $k$-body operator with highest unitary rank ($t = k$) is
orthogonal in all $m$-particle space to every operator of lower particle rank.)

In the Introduction we commented on the fact that, with the methods we are using,
everything is "tied to" the spectrum centroid which may lie very high (this will change
somewhat when we partition the space but the essential truth will remain). The natural
question is how is the significant information transmitted over the wide energy span
extending from the centroid to the ground state. We are now in a position to deal with
a much more specific version of the same question, namely, how is "single-particle
information" transmitted, and above all how does it "survive" in the presence of
strong two-body interactions. From the fact that level densities can be adequately
calculated in terms of single-particle energies, and from the success of the Strutinsky
method for shell corrections, we know that single-particle information does survive;
we shall deal here with a different aspect of the problem, involving ground-state
occupancies which can be deduced from single-nucleon-transfer experiments. The
result which we draw on is the fact that the number operator for the single-particle
states, having $s = (0, 1)$, are not correlated with the unitary-rank-two part of $H$, so
that the scalar product $\langle \phi|H|\phi\rangle^{(2)}$ which enters into the CLT result (19) for
$n_s(W)$ (where $n_s$ is the operator for the single-particle state numbered $s$) depends only
on the (traceless) one-body interaction including the interaction operator $(s - 1)|H(1)|$
which renormalizes it. Since $\langle \phi|H|\phi\rangle^{(2)} = mN$ and $\alpha^2$ is the sum of two parts $(s = 1, 2)$
we have, with $H(1)$ the unrenormalized one-body $H$ and $\delta(1) = \langle H(1)|\phi(1)\rangle^{(1)}$ its centroid operator

$$n_s(W) \propto \frac{m}{N} \frac{\langle \phi|H(1)|\phi\rangle^{(1)} - \delta(1)}{\delta(1) + (s - 1)|H(1)|} (W - \delta) \quad (60)$$

whose slope $n_s(W)$ is proportional then to the correlation coefficient with the (renor-
malized) one-body $H$. The only role played by the "intrinsic" ($s = 2$) interaction is
to damp the correlation coefficient and only its norm is of consequence for that. If
the two parts are comparable in magnitude so that the damping is not too large,
and provided that the CLT result is adequate (and both of these things are often true),
the one-body information $n_s(W)$ extends to the ground state. If, moreover, the renor-
malization of $H(1)$ is appreciable $n_s(W)$ carries with it information about the two-body
interaction (through its $(s = 1)$ part) and the experimental occupancy results can be
used to test the interaction. This has been recently done for de-shell nuclei [3], the
occupancies being considered throughout the entire shell. It is of course a major
advantage of the methods being used that the number dependences of the norms
and scalar products (as well as the dependence on the matrix elements) are explicitly
exhibited [15].

In the asymptotic limit for a dilute system ($N \to \infty, m \to \infty, m/N \ll 1$) the "induced"
one-body interaction $(s - 1)|H(1)|$, assumed not to vanish identically, will dominate
both the geometry $\delta(1)$ and the $(s = 2)$ interaction (in each case because of its explicit
number dependence $\sim (s - 1)$; from (25) we have $\langle \phi|H|\phi\rangle^{(2)} \sim m^2 \rho(\phi)^{1/2}$;
8. Fluctuations and Correlations

It will be useful in order to calculate a measure for the probable errors (deviations between statistically smoothed and exact values), and instructive for other reasons as well, to consider the level-to-level fluctuations in the moments \( \mathcal{M}_j(W) \) and the correlations between moments of different order. In principle of course the complete (exact) polynomial expansion (11) for \( R(W', W) \) determines everything but, as stressed in Section 1, we can deal explicitly with the polynomial terms of low order which determine the secular variations, and we need a different method for handling those of high order which determine the fluctuations.

Specifically we shall combine the Porter-Thomas distribution for the local behavior of the individual matrix elements \( \langle W' | O | W' \rangle \), with the secular variations of \( \langle W' | O | W' \rangle \) as given above, to derive the mean-squared deviations in \( \mathcal{M}_j(W) \) and, more generally, the covariance of \( \mathcal{M}_j \) and \( \mathcal{M}_k \). Leaving some general remarks about the procedure until the end of this section we take for granted that, for one energy fixed and the other varying locally (over a domain in which the secular energy variations can be ignored), the matrix elements \( \langle W' | O | W' \rangle \) have a zero-centered Gaussian distribution. We assume, moreover, that with respect to local energy averaging (defined then by low-order polynomials) different strengths are entirely uncorrelated. Thus

\[
\langle W' | O | W' \rangle \text{ distributes as Gaussian (0, } \sigma^2) \quad (61)
\]

\[
\mathcal{M}_j(W') = \mathbb{E} \left( \sum_{W} R(W', W) \langle W' | O | W \rangle \right)
\]

where, in (61) \( \sigma^2 \) is the variance and in (62) the strengths are distinct. We now have

\[
\mathcal{M}_j(W') = \sum_{W} R(W', W) \langle W' | O | W \rangle \quad (63)
\]

\[
\mathcal{M}_j(W') \mathcal{M}_j(W) = \sum_{W} (W')^p R(W', W) \langle W' | O | W \rangle \langle W' | O | W \rangle
\]

\[
- \left( \sum_{W} (W')^p R(W', W) \right) \mathbb{E} \left( \sum_{W} R(W', W) \langle W' | O | W \rangle \right)
\]

\[
= \sum_{W} (W')^p \mathbb{E} \left( R(W', W) \sum_{W} \langle W' | O | W \rangle \right)
\]

\[
+ \sum_{W} (W')^p \mathbb{E} \left( \langle W' | O | W \rangle - \mathbb{E} \langle W' | O | W \rangle \right) (64)
\]
so that

$$
\Sigma_{\mu}(W) = \mathbb{H}(\bar{W}, \tilde{\mu}(\bar{W}) - \mathbb{H}(\bar{W}) \cdot \tilde{\mu}(\bar{W})
$$

$$
- d' \times \int \rho(x) \frac{\partial^2 \rho(x, \mu)}{\partial \mu^2} \, dx
$$

(65)

$$
- 2d' \times \int \rho(x) \frac{\partial \rho(x, \mu)}{\partial \mu} \, dx
$$

does not exist. This is due to the fact that the function of the cumulative distribution function is not continuous. (Note that $\mathbb{H}(\bar{W})$ is by (61) distributed as $\chi^2(1)$ but we do not need the entire distribution, only the relationship between the central and variance.) In (65), $\mathbb{H}(\bar{W}, \tilde{\mu}(\bar{W}))$ is simply the low-order polynomial approximation to $\mathbb{H}(\bar{W})$ given therefore by a restricted summation in (11).

Consider first the total strength originating with $\| W \|$. Our interest in particular is in the relative mean-squared fluctuation of the non-energy-weighted sum. We write $\Sigma_{\mu} = \Sigma_{\mu \nu} = (\Sigma_{\mu})^\mu$. Then

$$
\Sigma_{\mu}(W) = \frac{1}{d'} \int \rho(x) \frac{\partial \rho(x, \mu)}{\partial \mu} \, dx
$$

$$
- \frac{1}{2} (\mathbb{H}(\bar{W}))^\mu \sum \rho(x) \frac{\partial \rho(x, \mu)}{\partial \mu} \, dx
$$

$$
= \frac{1}{2} \frac{\partial \rho(x, \mu)}{\partial \mu} \left[ \frac{\partial \rho(x, \mu)}{\partial \mu} \right] W
$$

The second form here follows immediately from (11), (65) and the third, in which the $\mu$-index is restricted to those values used in defining the smoothed strengths, by using the last form of (11). In the expression (66) we have incoherent contributions to the mean-squared deviation, one for each value of $\mu$, indicating a mode-mix decomposition. But, by (15), $\mathbb{H}(\bar{W})$ is the coefficient in the final-state-polynomial decomposition of $\mathbb{H}(\bar{W}, \tilde{\mu}(\bar{W}))$ for fixed $\bar{W}$, and this defines the normal modes involved. Observe that, for a repreparation of secular and fluctuations effect, the results of (66) should be independent of the value of $\mu$ as the only thing that is large enough so that $\mathbb{H}(\bar{W})$ gives the secular behavior properly but small enough so that it takes no account of the level-level fluctuations. In the corresponding case of the energy-level fluctuations (for particle number much larger than the particle rank of the interaction) this is in fact well understood, we have at first a very rapid convergence as $\mu$ increases and a result then essentially independent of $\mu$ until the fluctuations set in. From the results of Section 3 we can expect that the same will apply here.

If the smoothed strength for fixed $\bar{W}$ is constant over the final spectrum we can see, from either the second or third form in (66), that the mean-squared fluctuations $-2d'$, exactly as expected for then $\mathbb{H}(\bar{W})$ distributions as $\chi^2(1)$, being the sum of $d'$ squares of similar zero-centered Gaussian random variables (even more simply, the ratio would be 2 for a single random variable and therefore $-2d'$ for $d'$ of them). Conversely we can use (66), as indicated by its
last form, to define \( d' \), the effective number of final states which participate in the excitation (the analogy of the number of "open channels" in reaction theory).

For the CLT result we recall that \( F_1(x) = 1 \), \( F_2(x) = (1 - x)^{-1/2} \) and then, by (13), \( \lambda(W) = \mathcal{A}(W) \) and \( \lambda_2(W) = \mathcal{A}(W) - \mathcal{A}(W')d' \) where as always \( \lambda'(\sigma) \) is the centroid and width of the final state density (independent therefore of \( W' \)) while \( \lambda(
abla) \) is the centroid of the strength which originates with \( W \).

Thus, in the CLT limit, when \( \mathcal{A}(W) \) is such that the strength and final-state-density centroids coincide, we have \( \lambda = \lambda' \). the strength should divide evenly through the final states and the fluctuations are minimal. When the CLT is inadequate (as would happen in large vector spaces, or even in smaller ones if the excitation strength is localized in energy) we must of course use higher-order polynomials in (66) or have resort to configuration decomposition.

Analogous results of course follow from (65) for the mean-squared fluctuation \( \Sigma_2(W) \) in the power-weighted sums, and similarly for the covariances and the polynomial-weighted sums. For the correlation coefficients we have (with \( \Sigma_2 = \mathcal{A}(W)^2 \) as above)

\[
\lambda_2(W) = \mathcal{A}(W) \Sigma_2(W) \Sigma_2(W)
\]

which, as always, lies in the interval \((-1, 1)\). It should be clear from (65) that, if the strength spreads through many states (large \( d' \)), then the fluctuations in the various strength sums are always small. They are closely correlated if the strengths lie in a narrow energy band (\( \sigma \ll \sigma' \)) and essentially uncorrelated in the opposite case. On the other hand, if \( \sigma' \) is very small, the fluctuations are large and correlated.

Concerning the Porter-Thomas distribution we remark finally that it is very well supported by experimental evidence and follows easily from the CLT for sums of random variables if we are willing to assume them uncorrelated. More formally we can introduce a Hamiltonian ensemble, such as GOE, and make certain plausible assumptions about the excitation, both the ensemble, \( \mathcal{A}(W) \) of a scalar product of the "plants resonant state" and the states of a general basis. But both of these procedures are rather unsatisfactory, the first because it requires an assumption about matrix-element correlations and the second mainly because the ergodicity question, the equivalence of ensemble and spectral averaging, is ignored. No entirely satisfactory derivation of this general law appears to have been given. It might be possible to produce one by ensemble averaging the polynomial expansion for the strength; we shall look into that later.

9. CONCLUSION

We have outlined a theory of considerable generality and have indicated several directions in which it can be extended, to inverse energy weighting for example and to mixed use of geometries defined by \( U(N) \) subgroups. In order to assess the accuracy
which can be achieved, we give in the next paper a comparison of the predictions with shell-model results for several electromagnetic excitations. After that of course the important thing is to proceed to an analysis of the experimental data; a little of this has already been done for single-nucleon transfer but we have, in mind considerable more systematic and extensive studies and for a wide variety of excitations. At the same time we shall extend the theory and give methods for evaluating the traces which it makes use of.

References
