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Spectral Distributions in Nuclei*

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Given a finite many-particle vector space, which may be of large dimensionality, and a Hamiltonian which operates inside it, we may investigate the general properties of the system by a method of expanding preselected basis states in terms of the Hamiltonian eigenfunctions. The corresponding intensity, considered as a function of the Hamiltonian eigenvalues, is a spectral distribution which may be studied via its energy moments; we consider such distributions averaged over subsets of basis states. The properties of these averaged distributions are discussed, as well as methods for applying them in general studies of complicated systems; methods are given for evaluating the moments in some significant cases. Detailed formal results are given for configuration distributions in the spherical shell model.

1. INTRODUCTION

There has been steady progress in the attempt to give, in the domain of the conventional shell model, a microscopic description of nuclear structure. But there remain great difficulties. For one thing there are severe limitations on the dimensionalities of the vector spaces in which one can work, and it is clear that, in many or all nuclear problems, much of the interesting physics will "lie outside" the spaces which can be handled in the most conventional way. One attempts to get around this by introducing effective Hamiltonians (and effective transition operators for various processes), determining such operators either directly, from experimental data[1] or by theoretical considerations, usually grounded in perturbation theory, which begin with the free nucleon-nucleon interaction.[2] Besides this problem, and of course related to it, one often does not know how to choose the subspace, compatible with a given dimensionality limit, which is optimal for considering a problem at hand, and an *a posteriori* recourse to comparison with experiment is often not satisfactory. There has been much progress here too, especially via Hartree-Fock theory and its various extensions[3] which achieve a degree of self-consistency in the choice of single-particle states which underly the subspace in which one works.

The aim of the theoretical considerations mentioned above has been almost exclusively that of simplifying a nuclear many-body problem so that a detailed ("microscopic") solution becomes feasible in the domain of conventional spectroscopy. In this pair of papers, and in others to follow, we suggest methods in which conventional spectroscopy plays a much less prominent role, and in which some of the limitations and ambiguities of the standard methods are missing. These methods do not, for the most part, consider the detailed spectrum of the Hamiltonian operator or the detailed strengths for various processes. They deal instead with certain distributions associated with these quantities, examining these in terms of their low-order moments ("spectral" or "strength" moments) with respect to energy, isospin, angular momentum, and so on.[4] They are not limited by the dimensionalities of vector spaces, since they involve neither complete matrix-element calculations nor matrix diagonalization. They do not solve the problems associated with detailed spectroscopy, but deal instead with more general questions. An essential feature of these spectral-moment methods is that, at the beginning when we deal with very low-order moments, we throw away almost all the "information" implicit in a given problem; then as we proceed (taking higher and higher moments, or more or less equivalently, as we shall see, dealing with finer and finer group structures) we gradually regain the lost information. While it is *in principle* possible by proceeding in this way to reproduce exactly the results of a conventional microscopic calculation, that would in fact be feasible only in quite trivial cases and it does not at all represent our view as to a reasonable way of proceeding.

It is in fact our belief that, in many cases, low-order moments of various distributions are more

significant quantities than the individual energies and transition strengths which come from detailed calculations. The low-order moments depend essentially on interactions between small numbers of particles, interactions which we can indeed expect to be reasonably treated by our nuclear models; the moments, being defined as averages over sets of states, are properly insensitive to minor variations in the model or interaction parameters. On the other hand, the experimentalist usually deals with and measures detailed quantities, so that the use of spectral-moment methods would then, in many cases, inhibit a *direct* comparison of experiment and theory. We will see in fact that a low-moment spectral distribution can sometimes give a surprisingly good account of the detailed spectra; and when we deal later with excitation strengths rather than Hamiltonian spectra it will turn out that the moments of the appropriate distributions are much more closely connected to experimental measurement. Nonetheless, there will be a burden upon us to demonstrate how, direct comparisons with experiment being often ruled out, we can still make progress via spectral-moment methods.

From the mathematical standpoint, the calculation of spectra moments can make good use of a number of concepts and methods of linear algebra together with elementary notions borrowed from a less familiar domain, in particular the theory of partially-ordered finite sets. These are combined with the usual second-quantization procedures used in many-fermion problems. It will become clear that representations of groups or chains of groups are essential ingredients, and indeed the entire method has everywhere a group-theoretical foundation. Parenthetically then it will turn out, because of this, that spectral-moment methods are ideally suited to a study of the goodness of group symmetries in many-particle systems, an important subject in which progress has been very slow. Although group theory underlies the whole thing, we can consider several important distributions without explicit reference to groups, and in order to make things as clear and simple as possible, we shall, in the first two papers do exactly that. We shall, moreover, discuss the essential ideas in considerable detail even though they may already be familiar to many people.

All the present work concerns itself with the behavior of an m-particle system, described in terms of a finite vector space, a basis for which is given by the states of m fermions distributed over a finite number of single-particle states. We shall describe such a space as a *spectroscopic space*, a term which will remind us that the things we do are still related to the standard operations of spectroscopy. However, we shall ask questions of such a sort and answer them in such a way that the dimensionality of these spaces will not be limiting. And eventually we would in fact hope to deal with spaces which have a more complicated basis.

In Sec. 2 of this paper we introduce the idea of spectral distributions and the moments which characterize them, and give also a brief account of the way in which they may be used. Section 3 will deal, as an illustrative example, with the "scalar" distribution in which one averages over all the states for a fixed number of particles. The theory of spectral moments leads to the discussion of averaging over sets of states as given in Sec. 4. Section 5 contains derivations of certain trace operators and the law of propagation of averages of the configuration distribution. In Sec. 6 the centroid energies and dispersions of the complete scalar and configuration distributions are derived in terms of the one- and two-body matrix elements of the nuclear shell-model Hamiltonian. Various properties of the resulting moment formulas are then investigated in Sec. 7.

2. SPECTRAL DISTRIBUTIONS

Suppose that the problems in which we are interested are describable in terms of a finite set of N single-particle states: For the nuclear (ds) shell in an isospin formalism we have, for example, $N=24$. These N states form a basis for a vector space which we shall call the *orbital space* and denote by $\{N\}$. The states for m fermions distributed over these states[5] form an $\binom{N}{m}$-dimensional vector space [$\binom{N}{m}$ being a binomial coefficient] which we shall label as $\vec{m}$ or $(\vec{m})$ or $(N;\vec{m})$, the last of these when we need to indicate N explicitly. The vector space for any number of fermions ($m=0, 1 \ldots N$) distributed over $\{N\}$ we shall indicate as $\vec{\mathfrak{N}}$. We have then $\vec{\mathfrak{N}}=\sum\vec{m}$. The dimensionality of $\vec{\mathfrak{N}}$ is $\sum_{m=0}^{N}\binom{N}{m}=2^N$. More generally, we may decompose $\vec{\mathfrak{N}}$ in other ways, introducing subspaces $\vec{\alpha}$ or $(\vec{m},\vec{\alpha})$, the latter symbol indicating that $\vec{\alpha}$ is also a subspace of $\vec{m}$. We assume that the Hamiltonian H is a linear operator in $\vec{\mathfrak{N}}$, this implying that H operating on any vector in $\vec{\mathfrak{N}}$ yields another vector in $\vec{\mathfrak{N}}$. Then of course H^p is the pth power[6] of a transformation of $\vec{\mathfrak{N}}$ and is itself a transformation of $\vec{\mathfrak{N}}$.

Let $\{\phi_\alpha(m)\}$ denote an orthonormal basis set in $\vec{m}$. The standard spectroscopic problem is to compute and diagonalize the ϕ-matrix representation of H, thus producing the eigenvalues E_i and eigenvectors $\psi_i(m)$ as linear combinations of the basis functions $\phi_\alpha(m)$.

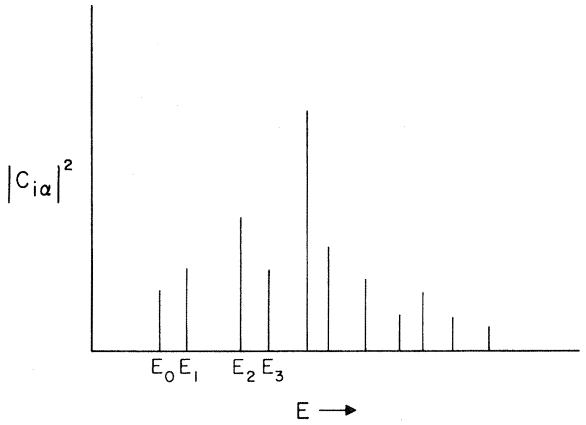

FIG. 1. Schematic representation of the spectral distribution of a vector ϕ_α over the eigenvectors of H.

$$H\psi_i(m) = E_i\psi_i(m)\,, \tag{1}$$

$$\psi_i(m) = \sum_\alpha C_{i\alpha}\phi_\alpha(m)\,. \tag{2}$$

Equally well, one may consider the basis vectors to be expanded in terms of the eigenvectors of H

$$\phi_\alpha(m) = \sum_i C_{i\alpha}{}^*\psi_i(m)\,. \tag{3}$$

Figure 1 gives a schematic picture of the distribution of the intensity of the vector $\phi_\alpha(m)$ over the eigenvectors of H. We refer to this as the "spectral distribution" of $\phi_\alpha(m)$. Such a distribution is completely characterized by its energy moments where the pth moment $M_p(m, \alpha)$ is defined by

$$M_p(m, \alpha) = \sum_i (E_i)^p |C_{i\alpha}|^2\,. \tag{4}$$

Using the definition of the expansion coefficients it is easily seen that $M_p(m, \alpha)$ may be rewritten as

$$M_p(m, \alpha) = \langle\phi_\alpha(m)H^p\phi_\alpha(m)\rangle\,, \tag{5}$$

where H^p denotes the pth power of the Hamiltonian. Equation (5) tells us that the distribution of ϕ_α over the eigenvectors of H is completely determined by expectation values of powers of H in the state ϕ_α, and that knowledge of the detailed eigenvalues and eigenvectors of H is unnecessary for this purpose.

The zeroth moment $M_0(m, \alpha)$ is unity, which merely expresses the normalization of the ϕ_α. The first moment $M_1(m, \alpha)$, which we shall also call $\mathcal{E}(m, \alpha)$ is the *centroid energy* of the distribution. Going beyond this it is more convenient to introduce either the pth *central moment* [defined for $p \geq 2$ as the pth moment of $H - \mathcal{E}(m, \alpha)$], or the pth cumulant, which we shall turn to later. The nonnegative-definite variance of the distribution is denoted by $\sigma^2(m, \alpha)$ and is defined as the second central moment, i.e.,

$$\sigma^2(m, \alpha) = \langle\phi_\alpha(m)[H - \mathcal{E}(m, \alpha)]^2\phi_\alpha(m)\rangle$$
$$= M_2(m, \alpha) - [M_1(m, \alpha)]^2\,. \tag{6}$$

The positive square root of the variance is the "width" $\sigma(m, \alpha)$ of the distribution. The skewness or asymmetry of the distribution about its centroid is measured by the third central moment $\langle\phi_\alpha(m) \times[H - \mathcal{E}(m, \alpha)]^3\phi_\alpha(m)\rangle$, and similarly for higher moments.

In the event that $\phi_\alpha(m)$ is an eigenvector of H then $\mathcal{E}(m, \alpha)$ is the corresponding eigenvalue, and all central moments of order two or more will vanish. A nonvanishing value for $\sigma(m, \alpha)$ may be called a pure "mixing" width, since it implies that $\phi_\alpha(m)$ is actually distributed over a number of eigenvectors of H. In general, the smaller the value of $\sigma(m, \alpha)$ the better is the approximation that $\phi_\alpha(m)$ is an eigenvector of H with $\mathcal{E}(m, \alpha)$ the approximate eigenvalue.

There are as many single-state distributions of the kind discussed above as there are vectors in the vector space, and thus, of course, no individual one is, on an *a priori* basis, of any particular interest. So we next proceed to the notion of distributions averaged over a set $(\vec{m}, \vec{\alpha}) \equiv \vec{\alpha}$ of the m-particle states. The moments of this distribution are then defined as

$$M_p(\vec{m}, \vec{\alpha}) = d^{-1}(\vec{m}, \vec{\alpha}) \sum_{\alpha\in\vec{\alpha}} M_p(m, \alpha)$$
$$= d^{-1}(\vec{m}, \vec{\alpha}) \sum_{\alpha\in\vec{\alpha}} \langle\phi_\alpha(m)H^p\phi_\alpha(m)\rangle\,, \tag{7}$$

where $d(\vec{m}, \vec{\alpha})$ is the dimensionality of the $\vec{\alpha}$ subspace of $(N; \vec{m})$.

From the purely formal standpoint now, the set $\vec{\alpha}$ must be chosen in such a way that its moments (at least as far as $p = 2$) can be evaluated. We rule out evaluation by means of an explicit construction of the individual matrix elements, since our major interest is in large spaces where such construction is not feasible; hence we require new techniques which are not to be found among those of conventional spectroscopy. Not surprisingly, it will turn out that to produce such techniques it will be advantageous for the subsets to define representations of groups or chains of groups.

From the standpoint of physics it should be clear that if the resultant averaged distributions are narrow then they are interesting, and, besides that, the groups which define $\vec{\alpha}$ then correspond to approximately good symmetries for the problem. But, as we shall see, there is much more to it than that, and, in particular, wide distributions are not necessarily uninteresting. Among the groups which we shall study in detail in early papers are the $U(N)$ group (which dominates almost everything), the direct-sum unitary group which

defines configurations, and the isospin, angular momentum, symplectic, and space-symmetry groups.

It follows immediately from Eq. (7) that the $\vec{\alpha}$ centroid energy is simply the average of the centroid energies for the individual states,

$$\mathcal{E}(\vec{m}, \vec{\alpha}) = d^{-1}(\vec{m}, \vec{\alpha}) \sum_{\alpha \in \vec{\alpha}} \mathcal{E}(m, \alpha) \ . \tag{8}$$

Things are different for higher-order quantities; in particular we have for the variance

$$\begin{aligned}\sigma^2(\vec{m}, \vec{\alpha}) &\equiv M_2(\vec{m}, \vec{\alpha}) - [M_1(\vec{m}, \vec{\alpha})]^2 \\ &= d^{-1}(\vec{m}, \vec{\alpha}) \sum_{\alpha \in \vec{\alpha}} \sigma^2(m, \alpha) \\ &\quad + \tfrac{1}{2} d^{-2}(\vec{m}, \vec{\alpha}) \sum_{\alpha, \alpha' \in \vec{\alpha}} [\mathcal{E}(m, \alpha) - \mathcal{E}(m, \alpha')]^2 \\ &= d^{-1}(\vec{m}, \vec{\alpha}) \sum_{\alpha \in \vec{\alpha}} \{\sigma^2(m, \alpha) \\ &\quad + [\mathcal{E}(m, \alpha) - \mathcal{E}(\vec{m}, \vec{\alpha})]^2\} \ . \end{aligned} \tag{9}$$

The energy term in Eq. (9) expresses a new contribution to the width which enters when averaged distributions are considered. Thus, even if every state of $\vec{\alpha}$ were an eigenstate of H, in which case there would be zero mixing widths for all the states, the width of the averaged distribution would still not vanish, since, in general, the eigenvectors would not be degenerate. We remark also that Eq. (9), applied to the Hamiltonian eigenstate representation [in which $\sigma^2(m, \alpha) = 0$], informs us that $\sigma^2(\vec{m}, \vec{\alpha})$ is a measure connected with the spacing distribution of the eigenvalues of H. Thus, though we make no statistical assumptions, we do have here a first contact with the statistical theory of spectra.[7]

The distribution moments $M_p(\vec{m}, \vec{\alpha})$, for a basis subset $(\vec{m}, \vec{\alpha})$, of the space $\vec{m}$ which we have introduced above are not really adequate for our purposes. In dealing with second moments, for example, it will be important to know what part of the width comes from intermediate states in $(\vec{m}, \vec{\alpha})$ and what part from states outside $(\vec{m}, \vec{\alpha})$. Therefore we should divide the width into an *internal*, or self-width, and an *external* width, according to

$$\begin{aligned} M_2(\vec{\alpha}) &= M_2^{\mathrm{i}}(\vec{\alpha}) + M_2^{\mathrm{e}}(\vec{\alpha}) \ , \\ M_2^{\mathrm{i}}(\vec{\alpha}) &= d^{-1}(\vec{\alpha}) \sum_{\alpha, \alpha' \in \alpha} \langle \alpha | H | \alpha' \rangle \langle \alpha' | H | \alpha \rangle \\ &= d^{-1}(\vec{\alpha}) \sum_{\alpha \in \vec{\alpha}} \langle \alpha | H P(\vec{\alpha}) H | \alpha \rangle \ , \\ M_2^{\mathrm{e}}(\vec{\alpha}) &= d^{-1}(\vec{\alpha}) \sum_{\substack{\alpha \in \vec{\alpha} \\ \beta \notin \vec{\alpha}}} \langle \alpha | H | \beta \rangle \langle \beta | H | \alpha \rangle \\ &= d^{-1}(\vec{\alpha}) \sum_{\alpha \in \vec{\alpha}} \langle \alpha | H [1 - P(\vec{\alpha})] H | \alpha \rangle \ , \end{aligned}$$

$$\begin{aligned} \sigma^2(\vec{\alpha}) &= \sigma^2{}_{\mathrm{i}}(\vec{\alpha}) + \sigma^2{}_{\mathrm{e}}(\vec{\alpha}) \ , \\ \sigma^2{}_{\mathrm{i}}(\vec{\alpha}) &= M_2^{\mathrm{i}}(\vec{\alpha}) - [M_1(\vec{\alpha})]^2 \ , \\ \sigma^2{}_{\mathrm{e}}(\vec{\alpha}) &= M_2^{\mathrm{e}}(\vec{\alpha}) \ . \end{aligned} \tag{10}$$

Here we have written $P(\vec{\alpha})$ for the projection operator onto the set $\vec{\alpha}$.

The separation above is that of $\vec{m}$ into two parts, $\vec{m} = \vec{\alpha} + (\vec{m} - \vec{\alpha})$. If we have a group in mind, for which $\vec{m}$ supplies a reducible representation, a more complete decomposition into irreducible representations may be relevant; thus $\vec{m} = \vec{\alpha} + \vec{\beta} + \vec{\gamma} + \ldots$. In terms of this, or any other decomposition into disjoint parts, we then define *partial widths* by

$$\begin{aligned} \sigma^2(\vec{\alpha}; \vec{\beta}) &= M_2(\vec{\alpha}; \vec{\beta}) - \delta_{\alpha\beta} [M_1(\vec{\alpha})]^2 \ , \\ M_2(\vec{\alpha}; \vec{\beta}) &= d^{-1}(\vec{\alpha}) \sum_{\substack{\alpha \in \vec{\alpha} \\ \beta \in \vec{\beta}}} \langle \alpha | H | \beta \rangle \langle \beta | H | \alpha \rangle \ . \end{aligned} \tag{11}$$

Then it follows easily that

$$\begin{aligned} \sigma^2(\vec{\alpha}) &= \sum_{\vec{\beta}} \sigma^2(\vec{\alpha}; \vec{\beta}) \ , \\ \sigma^2{}_{\mathrm{i}}(\vec{\alpha}) &= \sigma^2(\vec{\alpha}; \vec{\alpha}) \ , \\ d(\vec{\alpha}) \sigma^2(\vec{\alpha}; \vec{\beta}) &= d(\vec{\beta}) \sigma^2(\vec{\beta}; \vec{\alpha}) \ . \end{aligned} \tag{12}$$

We see that $\sigma^2(\vec{\alpha}; \vec{\beta})$ is the average over the states of $\vec{\alpha}$ of the squares of the matrix elements connecting the two subspaces. A corresponding (but more complicated) decomposition can be made also for higher moments.

What now can one learn from spectral distributions? The simplest thing is about the general eigenfunction structure, for example, about which representations contribute significantly in a particular range of energy. This would follow in an obvious way from the centroids and widths of the representations, which we could regard for this purpose as defining the distributions, assumed, for example, to be normal.

If the distribution for a particular representation is then found to span an energy region which contains the centroid of another representation, we would naturally suspect (unless that is forbidden by the exact symmetries) that the two representations would be strongly admixed. But we might be misled in assuming this; for it could happen that the width of the representation is predominantly a self-width, in which case the admixings would be small, we would have a peaceful coexistence of the states of the two representations, and separate transformations in the separate subspaces would produce good eigenfunctions; and of course similarly if many representations are involved. Thus we see the need for the partial-width decomposition of the total widths.

For more detailed results, if, for example, our interest is with the low-lying states, we may use the partial widths and centroids to supply a basis for a truncation of the original space to produce a resultant space small enough for detailed calculation. These quantities might, for example, indicate a small number of representations strongly coupled to a low-lying $\vec{\alpha}$ (or set of such $\vec{\alpha}$'s) in which case we might discard the other representations and make a more detailed calculation in the reduced space. The criterion for weak coupling of two representations is, of course, that the partial width[8] be small compared with the difference between their centroid energies.

We have, of course, been assuming here that the distributions are decently represented via moments of order $p \leq 2$. We shall, in fact, go beyond that and assume that they are close to "normal" or Gaussian, an assumption which has been found valid in the various examples, calculable in detail, which we have studied; we hope, in a later paper, to discuss the theoretical basis for it. It is, of course, possible to consider higher moments, which would measure departures from normality and would enable us to judge the validity of the entire moment procedure for studying the eigenfunction structures; at present, in the cases which we consider, it is feasible to go as far as the fourth moment. Besides the sequence of higher and higher moments for a given decomposition of $\vec{\mathfrak{N}}$, there is also the sequence in which we restrict the order (say to $p = 2$) but take a nested set of finer and finer subspace decompositions. This technique is successful if, as we proceed along the sequence, the widths, or better the partial-width matrix, indicate a structure of weakly interacting subspaces. When it works, the second technique is superior; on the one hand, the low moments of the finer distribution do carry information about the high moments of the coarser, while, on the other hand, since the finer decomposition will always correspond to some group structure, we learn at the same time about the group symmetries. It is important in both cases to study some examples which we can calculate in detail.

Going in the opposite direction we can study what happens when we enlarge a space by including more single-particle states both above and below the Fermi surface, i.e., proceeding to an enlarged orbital space $\{N'\} \supset \{N\}$. Not only do new distributions enter but the original distributions will spread. Thus, one can study the stability of the makeup of low-excitation spectra to changes in the size of the vector space. One may also introduce variational methods to study, for example, the way distributions involving deformed orbitals vary with the deformation parameters.

It is also clear that such distributions can provide information about the localization of interesting wave-function components at excitation energies appropriate to nuclear reactions exploring single-particle resonances and intermediate structure. They supply also, in an obvious way, a foundation for the microscopic theory of level densities, and in a less obvious way, perhaps also a basis for a statistical theory of reactions.[9] And as mentioned above it should be possible, by averaging over states corresponding to exactly good quantum numbers, to make contact with the statistical theory of spectra.

The considerations above give a method for studying group symmetries, involving as they do the question of the admixing of different representations. As an alternative method one may use mean-squared energies as an orthonormalization measure in terms of which one can decompose H^2 into orthogonal parts, some of which preserve the symmetry while the others violate it. Then, roughly speaking, the relative weights of these parts give us a criterion for the goodness of the symmetry.[10]

Going beyond the spectral distributions, we can study also the strength distributions for various excitation operators,[11] making thereby much more immediate contact with experiment. This would, for example, supply a way of studying cascade processes in highly excited systems, a subject also of direct experimental interest.

We mention also the possible extension to the case where the orbital states form a continuous, rather than discrete, set and to the case where the basis states have intrinsic correlations going beyond those supplied by any restricted orbital space.

These general remarks should indicate the utility of spectral distributions and show that partial widths of representations (and their extension to higher-order quantities) are the really essential ingredients of the subject. We now must proceed to methods for calculating such quantities. Let it be said at the outset that there does not as yet exist a general theory which can be applied to an arbitrary group structure. However, several important structures are well understood, as are also some features of the general case. It will turn out to be convenient to deal at first with total widths of representations, leaving until a little later the decomposition into partial widths (and similarly for the higher moments).

In the next section we consider, by the most elementary methods, a very simple case: that of averaging over all the states of m particles. In Sec. 4 we give a more general discussion introducing various concepts which will be of importance to us in later papers. The later sections of this

paper and all of the next (and these will not draw heavily on the results of Sec. 4) will be devoted to configuration distributions in the spherical shell model.

3. SCALAR DISTRIBUTION AS A SIMPLE EXAMPLE

By the m-particle *scalar* distribution we mean the spectral distribution averaged over all m-particle states. The appropriate decomposition of $\vec{\mathfrak{N}}$ is then $\vec{\mathfrak{N}} = \sum \vec{m}$. Let us first derive an elementary result for the *average* over $\vec{m}$ of the expectation value of a k-particle operator. This average we write as $\langle O(\vec{k})\rangle^{\vec{m}}$, and the corresponding *trace* as $\langle\langle O(\vec{k})\rangle\rangle^{\vec{m}}$. The particular k-particle operator which gives unity on states in which the single-particle states Nos. $1 \ldots k$ are filled and zero on states in which any of these are empty, obviously has a trace $\binom{N-k}{m-k}$, that number being the number of ways in which the $(m-k)$ "free" particles can be distributed over the $(N-k)$ "free" single-particle states. Other operators which differ only in specifying a different k subset have the same trace. The set of all such operators, supplemented by the set of nondiagonal k-particle operators [which, for example, convert $(1 \ldots m)$ into $(1 \ldots m-1,\ m+1)$] gives a basis for the general k-particle operator. These latter operators being traceless, we see then that, for the trace and the related average,

$$\begin{aligned} \langle\langle O(\vec{k})\rangle\rangle^{\vec{m}} &= \binom{N-k}{N-m} \langle\langle O(\vec{k})\rangle\rangle^{\vec{k}} , \\ \langle O(\vec{k})\rangle^{\vec{m}} &= \binom{m}{k} \langle O(\vec{k})\rangle^{\vec{k}} . \end{aligned} \tag{13}$$

The operators which we enounter will not in general have a specified particle rank; e.g., $O^2(\vec{k})$ has ranks $k, k+1, \ldots, 2k$, as long as $k \leq \frac{1}{2}N$. Rather than carry out the explicit decomposition by particle rank we can recognize that, since $\binom{m}{k}$ is a kth order polynomial in m, $\langle O\rangle^{\vec{m}}$ for an operator of maximum rank u will be a uth order polynomial in m. Writing such a polynomial as a linear function of its own values at $m = 0,\ 1,\ 2, \ldots, u$, we have then, for an operator of maximum rank u, that[4, 12]

$$\begin{aligned} \langle O\rangle^{\vec{m}} &= \sum_{t=0}^{u} \langle O\rangle^{\vec{t}} \prod_{\substack{y=0 \\ (\neq t)}}^{u} \frac{m-y}{t-y} \\ &= \sum_{t=0}^{u} (-1)^{t-u} \frac{m-u}{m-t} \binom{m}{u}\binom{u}{t} \langle O\rangle^{\vec{t}} \\ &= \sum_{t=0}^{u} (-1)^{t-u} \binom{m-t-1}{u-t}\binom{m}{t} \langle O\rangle^{\vec{t}} \\ &= \sum_{t=0}^{u} \binom{u-m}{u-t}\binom{m}{t} \langle O\rangle^{\vec{t}} , \end{aligned} \tag{14}$$

where the first form involves the usual Lagrange polynomials, and the other forms follow immediately from the first.[13] The last form demonstrates that for $m \leq u$ the result is simply an identity.

As a trivial application of Eq. (14), we have for the angular momentum,

$$\langle J^2\rangle^{\vec{m}} = -m(m-2)\langle J^2\rangle^{\vec{1}} + \binom{m}{2} \langle J^2\rangle^{\vec{2}} , \tag{15}$$

the first term then correcting for the fact that J^2 is not a pure two-body operator. For the usual case where the orbital space supplies a representation of the angular momentum group (defining therefore a set of spherical orbits), we have $\langle J^2\rangle^{\vec{N}} = 0$; then eliminating $\langle J^2\rangle^{\vec{2}}$ from Eq. (15) we have

$$\langle J^2\rangle^{\vec{m}} = \frac{m(N-m)}{(N-1)} \langle J^2\rangle^{\vec{1}} . \tag{16}$$

The result of Eq. (16) could have been written down immediately by using the fact that $\langle J^2\rangle^{\vec{m}}$ is a second-order polynomial in m which vanishes at $m = 0, N$. More generally, Eq. (14) is, as we have said, the equation which expresses the value for arbitrary m of the uth order polynomial in m as a linear function of its values at $m = 0, 1, \ldots u$; but from the linear independence of the m polynomials $\binom{m}{t}$ (or of the corresponding trace operators) it is obvious that we could choose any other $(u+1)$-dimensional set of m values (which we shall speak of as a "net") with which to define the polynomials. The solution for the new net is simple. If the net points are $t_1,\ t_2, \ldots, t_u$, then the new Lagrange polynomial for the net point t is

$$\prod_{\substack{i=1 \\ t_i \neq t}}^{u} \frac{m-t_i}{t-t_i} , \tag{17}$$

and with these we can express the trace of any u operator in terms of its traces for any $(u+1)$ particle numbers. We may say, incidentally, that the simplification in going from Eq. (15) to Eq. (16) has resulted from our choice of a net $(0, 1, N)$ simpler than the "elementary" net $(0, 1, 2)$. In general there is special interest in a net which is most economical with respect to the number of holes or particles involved; this is because the calculations required for the input quantities become increasingly complicated as the number of particles or holes increases. We achieve this economy by taking a two-segment net, one part proceeding upward from the origin, the other downward from the "plenum" state.[14] Taking these segments to be, respectively, $(t \leq u_1)$ and $(N - u_2 \leq t \leq N)$ where $u_1 + u_2 + 1 = u$, we find as the extension of the third form of Eq. (14) that[12]

$$\langle O\rangle^{\vec{m}} = \binom{N-m}{u_2+1}\sum_{t=0}^{u_1}(-1)^{t-u_1}\binom{N-t}{u_2+1}^{-1}\binom{m-t-1}{u_1-t}\binom{m}{t}\langle O\rangle^{\vec{t}} + \binom{m}{u_1+1}\sum_{t=N-u_2}^{N}(-1)^{t-u_2+N}\binom{t}{u_1+1}^{-1}\binom{t-1-m}{u_2-N+t}\binom{N-m}{N-t}\langle O\rangle^{\vec{t}}, \tag{18}$$

which gives $\langle O\rangle^{\vec{m}}$ as a linear combination of traces with ($t \leq u_1$) particles and ($t \leq u_2$) holes. If u is odd, then for maximum economy we would take $u_1 = u_2 = \frac{1}{2}(u-1)$, while if u is even we would take one of the limits to be $\frac{1}{2}u$, the other $\frac{1}{2}(u-2)$.

We have stressed that the scalar averaging results follow in a simple way from the properties of polynomials in particle number. Since the product of polynomials is itself a polynomial, it follows that the product of averages propagates by the same rule as does the average of a product, it being only necessary to take $u \geq$ (sum of particle ranks of factors). Thus we can deal with *central moments* or with *cumulants* in the same way as with the corresponding moments. We have then, for example, for the scalar centroid energy $\mathcal{E}(\vec{m})$ and the dispersion $\sigma^2(\vec{m})$ the results[12]

$$\mathcal{E}(\vec{m}) = \frac{m(m-1)}{N(N-1)}\mathcal{E}(\vec{N}) - \frac{(N-m)(m-1)}{N}\mathcal{E}(\vec{0}) + \frac{(N-m)m}{(N-1)}\mathcal{E}(\vec{1}), \tag{19}$$

$$\sigma^2(\vec{m}) = \frac{m(m-1)(m-2)(N-m)(N-m-1)}{(N-1)(N-2)(N-3)}\left[\frac{\sigma^2(\vec{N}-\vec{1})}{(N-m-1)} - \frac{(N-3)}{(m-1)}\sigma^2(\vec{1}) + \frac{(N-1)}{2(m-2)}\sigma^2(\vec{2})\right]. \tag{20}$$

In the first of these we have taken $u_1 = 1$, $u_2 = 0$, while in the second we have used $u_1 = 2$, $u_2 = 1$, along with the fact that the vacuum and plenum states are dispersion free. Both results could have been written down at sight.

As a simple example, consider the centroid energies in the (ds) shell, ($N = 24$). Reasonable interpretations of the low-lying level structure for $A = 16$, 17, 39, 40 enable us to evaluate the centroid energies for these cases ($m = 0$, 1, 23, 24) and, on the assumption[15] that H is of maximum rank 2, the question is whether the four centroids reasonably well satisfy Eq. (19). With the exception of the $A = 39$ $d_{5/2}$-hole energies (K^{39}, Ca^{39}) the assignments are all unambiguous. In each of the $A = 39$ nuclei three $\frac{5}{2}^+$ states are found[16] within a spread of 1 MeV centered at about 6-MeV excitation; we make the assumption that the $d_{5/2}$-hole strength is equally distributed among these. Then we find $\mathcal{E}(23) = -326.8$ MeV to be compared with the value -324.8 MeV found, via Eq. (19), from the other centroids. We would interpret this as satisfactory agreement (even though no convincing formal criterion for the goodness of agreement suggests itself). It is clear that this kind of simple analysis should precede any attempt to calculate, for example, effective interaction matrix elements by fits to empirical energy levels.

4. OPERATOR AVERAGING

We have used a simple combinatorial method to produce the results of the last section. While this kind of procedure would be adequate to deal with configuration distributions, that would not be so for more complicated cases. We therefore devote this section to a more formal (though still elementary) discussion in terms of operators, introducing thereby a number of important concepts.

We can interpret Eq. (13) as giving, for the trace of a k-body operator, a rule for propagation through the various subspaces $\vec{m}$ of $\vec{\mathfrak{N}}$. It tells us first that linear traces of k-body operators do propagate in a simple fashion and that, if we are interested only in such traces, only one significant piece of information distinguishes one k-body operator from another. Indeed we have, where n is the number operator,

$$O(\vec{k}) = \langle O(\vec{k})\rangle^{\vec{k}}\binom{n}{k} + \text{traceless parts}. \tag{21}$$

We then identify $\binom{m}{k}$ as the ($\vec{k} \to \vec{m}$) *propagation coefficient* for the average of a k-body operator, and $\binom{n}{k}$ as a *propagation operator*. For a quadratic trace we have seen that we need ($k+1$) pieces of information to distinguish the squares of k-particle operators, and similarly for other cases. It will be up to us, then, to calculate the traces which define, for a given moment, a complete set of pieces of "input" information.

The group structure involved in the trivial example of Eq. (14) is that of $U(N)$, the set of unitary transformations in the orbital space, and the m spaces are those which supply irreducible representations of $U(N)$. What is implied by the remark that $O(\vec{k})$ is a *k-body operator*? For one thing $O(\vec{k})$ vanishes in m spaces with $m < k$ [consistent with this, so does $\binom{m}{k}$]; beyond this the structure of $O(\vec{k})$ in spaces with $m > k$ is determined completely by its structure in the ($m = k$) space. Recalling now that an algebraist thinks of an operator as a transformation on a space, we see that the notion of a

k-body operator involves more than this. It implies specifying an algebraist's operator in the $(m=k)$ subspace together with a rule for propagating it into the other subspaces of $\vec{\mathfrak{N}}$. This general idea of *propagation* along a line (or more generally on a lattice) of representations is also of major importance to us.

For $O(\vec{k})$ the representation given by the subspace $\vec{k}$ is special and we might call it the *defining representation* of $O(\vec{k})$, this going along with the idea that the information about O is given to us in the $\vec{k}$ space. This would clearly be inadequate for an operator which is not number conserving. But in general we can think of any operator O as having a *quadratic structure*, since it may be expanded in terms of operators which connect one particular subspace with another. Thus we have, for the $U(N)$ case, $O=\sum_{\vec{k}\vec{k}'}O(\vec{k},\vec{k}')$, where $O(\vec{k},\vec{k}')$ produces a transformation $\vec{k}'\to\vec{k}$ and is defined in the subspace pair $(\vec{k},\vec{k}')$. Its behavior, when acting on a state of $\vec{m}\neq\vec{k}'$, is given by a propagation rule. Both the quadratic structure and the nature of the propagation rule become particularly clear in second quantization. For a general decomposition of $\vec{\mathfrak{N}}=\sum\vec{\alpha}$, corresponding for example to some given chain of groups, we have the corresponding operator expansion

$$O=\sum_{\vec{\alpha},\vec{\alpha}'}O(\vec{\alpha},\vec{\alpha}')\ , \tag{22}$$

and we would say that $O(\vec{\alpha},\vec{\alpha}')$ has the *defining representation pair* $(\vec{\alpha},\vec{\alpha}')$. For the diagonal case we shall continue to speak of the *defining representation* $\vec{\alpha}$.

A separate decomposition of O is by its tensorial behavior with respect to the groups under consideration, $O=\sum_{\vec{\gamma}}O^{\vec{\gamma}}$. We combine the two decompositions to get

$$O=\sum_{\vec{\alpha},\vec{\alpha}',\vec{\gamma}}O^{\vec{\gamma}}(\vec{\alpha},\vec{\alpha}')\ . \tag{23}$$

Since $O(\vec{\alpha},\vec{\alpha}')$ has the direct-product structure $\vec{\alpha}\times\vec{\alpha}'$, the allowed $\vec{\gamma}$'s are determined by the combination rule for $\vec{\alpha},\vec{\alpha}'$. For example, if we are dealing with $U(N)$, a k-body operator has $\vec{\alpha}=\vec{\alpha}'=\vec{k}$ and then it is well known that there are $(k+1)$ different representations $\vec{\gamma}$, those in fact with one- and two-columned Young shapes, $[N-\lambda,\lambda]$, with $\lambda=0,1,\ldots,k$. As another example, for the Coulomb interaction (defined in the isospin-one two-particle space) $\vec{\gamma}$ could define the isospin ranks 0, 1, 2; Eq. (23) then giving the usual scalar-vector-tensor separation.

Observe next that in the $U(N)$ case there is a natural ordering for the representations, defined by the fact that a k-body operator vanishes in m with $m<k$. The ordering is the trivial one $m=0,1,2,\ldots,N$ but the general idea of ordering is not trivial. For the $U(N)$ case the representations form a *fully ordered set* (or a *chain*), the ordering operation being that $\vec{\alpha}\geq\vec{\alpha}'$ if every operator defined in $\vec{\alpha}$ vanishes in $\vec{\alpha}'$. We see now that propagation proceeds in order along a chain. When we come to more complicated group structures we shall encounter the more subtle notion of a partially-ordered set, with a correspondingly more complicated propagation.

Equation (13) may be rewritten as

$$\langle O(\vec{k})\rangle^{\vec{m}}=\binom{m}{k}\binom{N}{k}^{-1}\langle O(\vec{k})\rangle^{\vec{N}}\ . \tag{24}$$

Thus, while for $k>0$ we cannot propagate from the vacuum representation (since the operator vanishes there), we *can* propagate from the plenum representation, which is just as simple and is indeed the hole-vacuum representation. The significant fact is that the plenum representation, giving only a highly nonfaithful representation for $O(\vec{k})$, is still useful, since it does carry the information about the linear trace of $O(\vec{k})$. We shall see later how a set of nonfaithful representations may be used as a *sieve* to decompose the moments of an operator.

Via a trivial example, we have introduced above the nontrivial notions of propagation, propagation coefficients and operators, defining-representation pairs, the linear and quadratic structure of operators, ordered sets of representations, and sieves. All of these are going, eventually, to be of importance to us.

We proceed now by introducing second-quantization forms for the operators and states of the system. This is not strictly necessary but it is highly advantageous. Corresponding to the N single-particle states which define the orbital space $\{N\}$ we introduce creation operators A_r and destruction operators $B_r=A_r^\dagger$, where $r=1,2,\ldots,N$. These satisfy the usual anticommutation relations,

$$\begin{aligned}&[A_r,B_s]_+=\delta_{rs}\ ,\\ &[A_r,A_s]_+=[B_r,B_s]_+=0\ .\end{aligned} \tag{25}$$

The normalized operator for m particles in state α is represented as $Z_\alpha(m)$. In a product (or Hartree-Fock) representation, a basis state $Z_\alpha(m)$ is a product of m A operators; more generally, it is a linear combination of such products. The operator $Z_\alpha(k)Z_{\alpha'}{}^\dagger(k)$ is a k-body operator which is defined by the single nonvanishing k-body matrix element $\langle k\beta|Z_\alpha(k)Z_{\alpha'}{}^\dagger(k)|k\beta'\rangle=\delta_{\alpha\beta}\delta_{\alpha'\beta'}$. Moreover, as α,α' run through the states of $\vec{k}$, the set of such quadratic objects gives a basis for the k-body operators. It follows then that the general expansion of a k-body operator $O(\vec{k})$ is

$$O(\vec{k}) = \sum_{\beta,\beta'} \langle k\beta|O(\vec{k})|k\beta'\rangle Z_\beta(k) Z_{\beta'}{}^\dagger(k) \ . \tag{26}$$

A general matrix element of $O(\vec{k})$ in m-particle states is

$$\langle m\alpha|O(\vec{k})|m\alpha'\rangle = \sum_{\beta\beta'} \langle k\beta|O(\vec{k})|k\beta'\rangle \times \langle Z_\alpha{}^\dagger(m) Z_\beta(k) Z_{\beta'}{}^\dagger(k) Z_{\alpha'}(m)\rangle_0 \ , \tag{27}$$

where $\langle\rangle_0$ denotes a vacuum expectation value (v.e.v.) which, of course, is entirely independent of the operator $O(k)$. Such a second-quantized representation makes explicit the defining properties of a k-body operator and its propagation, which we have discussed above; and similarly for more general operators.

The commutation rules (25) are invariant under the involution

$$\begin{aligned} A_r &\to B_r \equiv A_r(\mathrm{h}) \ , \\ B_r &\to A_r \equiv B_r(\mathrm{h}) \ , \end{aligned} \tag{28}$$

which, as indicated, defines holes to be fermions. This operation (applied in every element of the orbital space) we denote as $\tilde{}$. Thus we have

$$\begin{aligned} &\tilde{A}_r = B_r = A_r{}^\dagger = A_r(\mathrm{h}) \ , \\ &(A_r A_s)^T = B_r B_s = -(A_r A_s)^\dagger = A_r(\mathrm{h}) A_s(\mathrm{h}) \ , \end{aligned} \tag{29}$$

and for general state operators

$$\begin{aligned} \tilde{Z}_\alpha(m) &= (-1)^{\frac{1}{2}m(m-1)} Z_\alpha{}^\dagger(m) \equiv Z_\alpha(m_\mathrm{h}) \ , \\ \tilde{Z}_\alpha{}^\dagger(m) &= (-1)^{\frac{1}{2}m(m-1)} Z_\alpha(m) \equiv Z_\alpha{}^\dagger(m_\mathrm{h}) \ , \end{aligned} \tag{30}$$

these equations then defining for us a correspondence between hole and particle state operators. The essential equivalence between the operations $\tilde{}$ (^{T}) and † when applied to state operators with a definite number of particles is not maintained with more general operators and we have

$$\begin{aligned} Z_\alpha(k) Z_\beta{}^\dagger(k') &\to (-1)^{\frac{1}{2}(k+k'-1)(k-k')} Z_\alpha{}^\dagger(k) Z_\beta(k') \\ &= Z_\alpha(k_\mathrm{h}) Z_\beta{}^\dagger(k'_\mathrm{h}) \ . \end{aligned} \tag{31}$$

We see that in general $\tilde{O}$ may be said to be an operator with the same representation in the hole states as O has in particles. If for example O is a k-body operator [as it would be if $k = k'$ in (31)] then we shall call $\tilde{O}$ the corresponding k-hole operator. Then, reexpressing $\tilde{O}$ in normal form with respect to particles, we get a k-body operator which, to within a phase $(-1)^k$, is simply the adjoint[17] of O, along with terms of lower particle rank arising from commutation. In other words a k-hole operator is the sum (from $l = 0 \ldots k$) of l-body operators. The $l = k$ term does *not* vanish and is trivially related to the original operator. The $l < k$ terms may vanish; we shall see later the significance of such vanishings.

Since two state operators essentially commute,[18] as do their adjoints also, we have the result that

$$\langle Z_\alpha{}^\dagger(m) Z_\beta{}^\dagger(k) Z_{\beta'}(k) Z_{\alpha'}(m)\rangle_0 = \langle Z_\beta{}^\dagger(k) Z_\alpha{}^\dagger(m) Z_{\alpha'}(m) Z_{\beta'}(k)\rangle_0 \ , \tag{32}$$

which tells us that to an m-particle matrix element of a k-hole operator, there corresponds an equal k-particle matrix element of an m-hole operator (and similarly for non-number-conserving operators). Writing now, in correspondence with Eq. (26), the expansion of a k-hole operator, $\tilde{O}(\vec{k}) = O(\vec{k}_\mathrm{h})$, viz.,

$$O(\vec{k}_\mathrm{h}) = \sum_{\beta\beta'} \langle k_\mathrm{h}\beta|O(k_\mathrm{h})|k_\mathrm{h}\beta'\rangle Z_\beta{}^\dagger(k) Z_{\beta'}(k) \ , \tag{33}$$

we have for the $(\vec{m}, \vec{\alpha})$ trace

$$\langle\langle O(\vec{k}_\mathrm{h})\rangle\rangle^{\vec{m},\vec{\alpha}} = \sum_{\substack{\alpha\in\vec{\alpha} \\ \beta\beta'}} \langle k_\mathrm{h}\beta|O(\vec{k}_\mathrm{h})|k_\mathrm{h}\beta'\rangle \times \langle Z_\alpha{}^\dagger(m) Z_\beta{}^\dagger(k) Z_{\beta'}(k) Z_\alpha(m)\rangle_0 \ . \tag{34}$$

Let us now introduce the trace operator for the set $(\vec{m}, \vec{\alpha})$

$$\rho(\vec{m}, \vec{\alpha}) = \sum_{\alpha\in\vec{\alpha}} Z_\alpha(m) Z_\alpha{}^\dagger(m) \ . \tag{35}$$

This self-adjoint operator is the operator extension of the $(\vec{m}, \vec{\alpha})$ trace of the density matrix. It has the defining properties:
(i) $\rho(\vec{m}, \vec{\alpha})$ is an m-particle operator and therefore gives zero on all k-particle states with $k < m$.
(ii) $\rho(\vec{m}, \vec{\alpha})$ gives unity on all m-particle states in $(\vec{m}, \vec{\alpha})$ and zero on all states in $(\vec{m}, \vec{\alpha}')$ with $\vec{\alpha}' \neq \vec{\alpha}$.
In terms of these operators we have from Eqs. (32), (34) that[19]

$$\langle\langle O(\vec{k}_\mathrm{h})\rangle\rangle^{\vec{m},\vec{\alpha}} = \sum_{\beta\beta'} \langle k_\mathrm{h}\beta|O(\vec{k}_\mathrm{h})|k_\mathrm{h}\beta'\rangle \times \langle Z_\beta{}^\dagger(k) \tilde{\rho}(\vec{m}, \vec{\alpha}) Z_{\beta'}(k)\rangle_0 \ , \tag{36}$$

which gives the trace for an operator which is in *antinormal form*.

A simple and well-known device now enables us to do the same for a normal form operator, which is more interesting. It is clear that Z_α applied to the particle vacuum and $\tilde{Z}_\alpha$ applied to the hole vacuum (the plenum state for particles) give related states; these we define as complementary. Then

$$\begin{aligned} Z_{\alpha_c}(N-m)|0\rangle &= \tilde{Z}_\alpha(m)|N\rangle = \tilde{Z}_\alpha(m) Z(N)|0\rangle \ , \\ \langle 0|Z_{\alpha_c}{}^\dagger(N-m) &= \langle N|\tilde{Z}_\alpha{}^\dagger(m) = \langle 0|Z^\dagger(N)\tilde{Z}_\alpha{}^\dagger(m) \ , \end{aligned} \tag{37}$$

where we have chosen $\vec{\alpha}_c$, the $(N-m)$-particle basis set, to coincide with the complement of $\vec{\alpha}$, the m-particle basis set.[20]

The relationship between hole and particle v.e.v.'s

$$\langle Q\rangle_0 = \langle \tilde{Q}\rangle_{0_h} , \tag{38}$$

which follows from Eq. (28), when applied to the integrand operator of a matrix element, then leads to the result

$$\langle Z_\alpha{}^\dagger(m) K Z_{\alpha'}(m')\rangle_0 = \langle Z_{\alpha_c}{}^\dagger(N-m)\tilde{K} Z_{\alpha'_c}(N-m')\rangle_0 . \tag{39}$$

Thus, for a k-particle operator, we have

$$\begin{aligned}\langle\langle O(\vec{k})\rangle\rangle^{\vec{m},\vec{\alpha}} &= \sum_{\substack{\alpha\in\vec{\alpha}\\ \beta\beta'}} \langle k\beta|O(\vec{k})|k\beta'\rangle \\ &\quad\times\langle Z_\alpha{}^\dagger(m) Z_\beta(k) Z_{\beta'}{}^\dagger(k) Z_\alpha(m)\rangle_0 \\ &= \sum_{\beta\beta'} \langle k\beta|O(\vec{k})|k\beta'\rangle \\ &\quad\times\langle Z_\beta{}^\dagger(k)\tilde{\rho}(\vec{N}-\vec{m},\vec{\alpha}) Z_{\beta'}(k)\rangle_0 \\ &= \langle\langle\tilde{\rho}(\vec{N}-\vec{m},\vec{\alpha}) O(\vec{k})\rangle\rangle^{\vec{k}} ,\end{aligned} \tag{40}$$

where in the first step we have used the operator expansion of Eq. (26), in the second have used Eqs. (32), (35), and, in the last, either the reality of the matrix elements of O or the Hermiticity of ρ. Note that this result is derivable also from Eq. (36) via Eq. (39). For the corresponding compact form of Eq. (36) we use Eq. (39) and then

$$\langle\langle O(\vec{k}_{\vec{\pi}})\rangle\rangle^{\vec{m},\vec{\alpha}} = \langle\langle\rho(\vec{m},\vec{\alpha}) O(\vec{k}_{\vec{\pi}})\rangle\rangle^{\vec{N}-\vec{k}} . \tag{41}$$

We can think of the subspace $(\vec{m},\vec{\alpha})$ as one member in a subspace decomposition of $\vec{\mathfrak{N}}$. There are important decompositions of $\vec{\mathfrak{N}}$ for which it turns out that the trace operator for each subspace is diagonal with respect to subspaces and behaves like a multiple of unity in each one. If $\vec{\mathfrak{N}} = \sum(\vec{m},\vec{\alpha})$ is such a decomposition, we have then from Eq. (40) that

$$\begin{aligned}\langle\langle O(\vec{k})\rangle\rangle^{\vec{m},\vec{\alpha}} &= \sum_{\vec{\alpha}'} \langle k\alpha'|\tilde{\rho}(\vec{N}-\vec{m},\vec{\alpha})|k\alpha'\rangle\langle\langle O(\vec{k})\rangle\rangle^{\vec{k},\vec{\alpha}'} \\ &= \sum_{\vec{\alpha}'} \langle\tilde{\rho}(\vec{N}-\vec{m},\vec{\alpha})\rangle^{\vec{k},\vec{\alpha}'}\langle\langle O(\vec{k})\rangle\rangle^{\vec{k},\vec{\alpha}'},\end{aligned} \tag{42}$$

where, in the first form, α' is any state in $\vec{\alpha}'$. We see that in this case a subspace trace of $O(\vec{k})$ propagates from its defining representation throughout the entire lattice of subspaces with a propagating coefficient given by the matrix element indicated. An operator, then, which is traceless (or a multiple of unity) in each of the defining subspaces is traceless (or a multiple of unity) in all the subspaces. We shall describe this general situation, which is characteristic of the decomposition, as one of *simple propagation*. For the scalar distribution of Sec. 3, it should by this time be obvious that[21]

$$\rho(\vec{k}) = \binom{n}{k}, \quad \tilde{\rho}(\vec{k}) = \binom{N-n}{k} , \tag{43}$$

so that simple propagation does pertain in this case (as it will also in the case of configurations to be discussed in Sec. 5). The general reason for this should also be clear, namely that all m-particle states have equal standing, no preferred axes being specified in $\vec{m}$ by the operations considered. In these first papers our interest will be solely in cases which admit simple propagation, and in the discussion which follows here we make that assumption also.

The propagation coefficients have a symmetry which follows directly from Eq. (32), viz.,

$$\begin{aligned} d(\vec{k},\vec{\alpha}')\langle\tilde{\rho}(\vec{N}-\vec{m},\vec{\alpha})\rangle^{\vec{k},\vec{\alpha}'} &= \langle\langle\tilde{\rho}(\vec{N}-\vec{m},\vec{\alpha})\rangle\rangle^{\vec{k},\vec{\alpha}'} \\ &= \langle\langle\rho(\vec{k},\vec{\alpha}')\rangle\rangle^{\vec{m},\vec{\alpha}} \\ &= d(\vec{m},\vec{\alpha})\langle\rho(\vec{k},\vec{\alpha}')\rangle^{\vec{m},\vec{\alpha}} ,\end{aligned} \tag{44}$$

where, as always, $d(\vec{\gamma})$ is the dimensionality of $\vec{\gamma}$. Using this we have[22] (for the *average* instead of the trace)

$$\langle O(\vec{k})\rangle^{\vec{m},\vec{\alpha}} = \sum_{\vec{\alpha}'} \langle m\alpha|\rho(\vec{k},\vec{\alpha}')|m\alpha\rangle\langle O(\vec{k})\rangle^{\vec{k},\vec{\alpha}'} , \tag{45}$$

$$O(\vec{k}) \equiv \sum_{\vec{\alpha}'}\langle O(\vec{k})\rangle^{\vec{k},\vec{\alpha}'}\rho(\vec{k},\vec{\alpha}') , \tag{46}$$

where Eq. (46) displays a linear-trace equivalence. The operator $\rho(\vec{k},\vec{\alpha}')$ is then, in the sense of the discussion following Eq. (21), a propagation operator. It functions like a net-point Green's function in propagating, throughout the lattice, trace information given in the defining subspace $(\vec{k},\vec{\alpha}')$. Alternatively it may be regarded, *for fixed* k as a $(\vec{k},\vec{\alpha}')$ projection operator, since it satisfies the condition

$$\begin{aligned}\langle k\alpha|\rho(\vec{k},\vec{\alpha}')|k\alpha\rangle &= 1 \quad \text{if } \alpha\in\vec{\alpha}' \\ &= 0 \quad \text{if } \alpha\notin\vec{\alpha}' .\end{aligned} \tag{47}$$

If the operator with which we deal is not of definite particle rank [e.g., $O^2(\vec{k})$ which we would need for the second moment], we could decompose it into operators of definite rank, each part of which would then propagate via Eq. (45). Though we shall sometimes use this procedure, it is basically uneconomical to carry out a microscopic transformation of an operator solely for the purpose of evaluating a few traces. We may alternatively proceed as follows, which will be recognized as a natural extension of what we have already done in Sec. 3.

Suppose that the operator has maximum particle rank which is not greater than u; e.g., we would take $u=4$ for the square of a $(0+1+2)$-particle Hamiltonian. Then those terms in the defining expansion of the operator which are nondiagonal in representations cannot contribute to traces, because we are dealing with cases of simple propagation. Therefore the operator is defined on a *net of*

representations $(\vec{k}, \vec{\alpha})$ with $k=0, 1, \ldots, u$. Now, while a density operator $\rho(\vec{k}, \vec{\alpha}')$ does give $\delta(m,k)\delta(\vec{\alpha}, \vec{\alpha}')$ in any representation $(\vec{m}, \vec{\alpha})$ with $m \leq k$, it cannot vanish in all those representations of the defining net which have $m > k$. This follows from the fact that $\rho(\vec{k}, \vec{\alpha}')$, being a k-body operator whose defining trace does not vanish, must necessarily have a nonvanishing trace in states with $m > k$. Thus $\rho(\vec{k}, \vec{\alpha}')$ does not behave on the defining net like a Green's function. We therefore introduce a new set of density operators $\rho_u(\vec{k}, \vec{\alpha}')$,

$$\rho_u(\vec{k}, \vec{\alpha}') = \binom{u-n}{u-k}\rho(\vec{k}, \vec{\alpha}') = (-1)^{u-k}\binom{n-k-1}{u-k}\rho(\vec{k}, \vec{\alpha}'), \tag{48}$$

where, as always, n is the number operator. The n factor, being then a product of linear factors which give zero on all representations with $k < m \leq u$, forbids propagation from the "source point" $(\vec{k}, \vec{\alpha}')$ to any representation of the defining net. The $\rho_u(\vec{k}, \vec{\alpha}')$ are operators of maximum rank $\leq u$ satisfying

$$\rho_u(\vec{k}, \vec{\alpha}') \to \delta(m,k)\delta(\vec{\alpha}, \vec{\alpha}') \text{ on } (\vec{m}, \vec{\alpha}) \text{ if } m, k \leq u \tag{49}$$

and act collectively as a Green's function on the defining net.[23]

In terms of these operators we have, as an extension of Eq. (46),

$$O \equiv \sum_{(\vec{k}, \vec{\alpha}')} \langle O\rangle^{\vec{k}, \vec{\alpha}'}\rho_u(\vec{k}, \vec{\alpha}') , \tag{50}$$

the sum being over the defining net, and the operator being of maximum rank $\leq u$. The equation is valid for linear traces and follows from the fact that the right-hand side is of the correct maximum particle rank and, via Eq. (49), reproduces the defining traces of O. Then, corresponding to Eq. (45), we have

$$\langle O\rangle^{\vec{m}, \vec{\alpha}} = \sum_{(\vec{k}, \vec{\alpha}')} \langle m\alpha|\rho_u(\vec{k}, \vec{\alpha}')|m\alpha\rangle\langle O\rangle^{\vec{k}, \vec{\alpha}'} . \tag{51}$$

We may use Eq. (50) to expand the density operators themselves. Then for $t \leq u$ we have

$$\rho(\vec{t}, \vec{\gamma}) = \sum_{k=t}^{u} \sum_{\vec{\alpha}} \langle\rho(\vec{t}, \vec{\gamma})\rangle^{\vec{k}, \vec{\alpha}}\rho_u(\vec{k}, \vec{\alpha}) \tag{52}$$

and since $\langle\rho(\vec{t}, \vec{\gamma})\rangle^{\vec{t}, \vec{\gamma}'} = \delta_{\vec{\gamma}\vec{\gamma}'}$, we may rewrite this as[24]

$$\rho(\vec{t}, \vec{\gamma})\left[1 - \binom{u-n}{u-t}\right] = \sum_{k=t+1}^{u} \sum_{\vec{\alpha}} \langle\rho(\vec{t}, \vec{\gamma})\rangle^{\vec{k}, \vec{\alpha}}\rho_u(\vec{k}, \vec{\alpha}) . \tag{53}$$

Similarly we find

$$\tilde{\rho}(\vec{t}, \vec{\gamma}) = \sum_{k=0}^{t} \sum_{\vec{\alpha}} \langle\tilde{\rho}(\vec{t}, \vec{\gamma})\rangle^{\vec{k}, \vec{\alpha}}\rho_u(\vec{k}, \vec{\alpha}) , \tag{54}$$

and we have also the expansions ($\tilde{\rho}$ versus ρ and ρ versus $\tilde{\rho}_u$) which come from applying the operation $(\tilde{\ })$ to these equations.

It is worthwhile to have the inverse of Eq. (52), which would express a trace operator which acts as a Green's function on the net, in terms of trace operators for single representations. We can invert the equation by a process which will be recognized as that of an elementary sieve. Remember that, by construction, $\rho_r(\vec{k}, \vec{\alpha})$ and $\rho_s(\vec{k}, \vec{\alpha})$ $(k \leq r \leq s \leq u)$ coincide in the $(m \leq r)$-particle representations; $\rho_s(\vec{k}, \vec{\alpha})$, however, has higher-rank terms $(r < \text{rank} \leq s)$ whose function is to cancel the $\rho_r(\vec{k}, \vec{\alpha})$ traces which propagate into the $(m > r,\ m \leq s)$-particle domain. Then we have

$$\begin{aligned}\rho_u(\vec{k}, \vec{\alpha}) &= \rho(\vec{k}, \vec{\alpha}) + \sum_{r=k+1}^{u} O(r) \\ &= \rho(\vec{k}, \vec{\alpha}) - \sum_{\vec{\alpha}_1} \langle\rho_k(\vec{k}, \vec{\alpha})\rangle^{\vec{k}+\vec{1}, \vec{\alpha}_1}\rho(\vec{k}+\vec{1}, \vec{\alpha}_1) \\ &\quad + \sum_{r=k+2}^{u} O(r) ,\end{aligned} \tag{55}$$

where the last step comes from the vanishing of $\rho_u(\vec{k}, \vec{\alpha})$ in $(k+1)$-particle states (if $k+1 \leq u$). The first two terms on the right-hand side of this equation give $\rho_{k+1}(\vec{k}, \vec{\alpha})$; proceeding in order we find the desired inversion,

$$\rho_u(\vec{k}, \vec{\alpha}) = \rho(\vec{k}, \vec{\alpha}) - \sum_{t=k+1}^{u} \sum_{\vec{\beta}} \langle\rho_{t-1}(\vec{k}, \vec{\alpha})\rangle^{\vec{t}, \vec{\beta}}\rho(\vec{t}, \vec{\beta}) . \tag{56}$$

Combining Eqs. (50) and (56) yields a trace expansion of an operator O, of maximum rank $\leq u$, in terms of t-particle operators; with the aid of this we can make the trace decomposition of an operator whose traces are given on the elementary net into a set of operators each defined in a single subspace of that net. The result is

$$\begin{aligned}O &\equiv \sum_{k=0}^{u} \sum_{\vec{\alpha}} \Lambda(\vec{k}, \vec{\alpha})\rho(\vec{k}, \vec{\alpha}) , \\ \Lambda(\vec{k}, \vec{\alpha}) &= \langle O\rangle^{\vec{k}, \vec{\alpha}} - \sum_{t=0}^{k-1} \sum_{\vec{\beta}} \langle\rho_{k-1}(\vec{t}, \vec{\beta})\rangle^{\vec{k}, \vec{\alpha}}\langle O\rangle^{\vec{t}, \vec{\beta}} ,\end{aligned} \tag{57}$$

which we can recognize as the natural extension (for the more general lattice) of the usual trace separation of an operator according to its particle ranks. For that case, Eq. (57) gives immediately the result (easily derivable also by other methods)

$$\begin{aligned}\Lambda(k) &= \sum_{t=0}^{k} (-1)^{t-k}\binom{k}{t}\langle O\rangle^{\vec{t}} , \\ O &\equiv \sum_{k=0}^{u} \sum_{t=0}^{k} (-1)^{k-t}\binom{k}{t}\langle O\rangle^{\vec{t}}\binom{n}{k} .\end{aligned} \tag{58}$$

As a minor application we find the trace expansion of an l-hole operator to be

$$\tilde{O}(\vec{l}) \equiv \langle \tilde{O}(\vec{l}) \rangle^{\vec{N}-\vec{l}} \sum_{k=0}^{l} \binom{n}{k} \sum_{t=0}^{k} (-1)^{t-k} \binom{k}{t} \binom{N-t}{l}$$

$$= \langle \tilde{O}(\vec{l}) \rangle^{\vec{N}-\vec{l}} \sum_{k=0}^{l} (-1)^{k} \binom{N-k}{N-l} \binom{n}{k} , \qquad (59)$$

where we have used a combinatorial identity. A different derivation of this result is worthwhile. Since $\langle \rho(\vec{k}) \rangle^{\vec{N}} = \binom{N}{k}$, it follows that $\rho(\vec{k}) - \binom{N}{k}\tilde{\rho}(\vec{0})$ vanishes in $(\vec{N})$; it gives $\binom{N-1}{k} - \binom{N}{k} = -\binom{N-1}{k-1}$ in $(\vec{N} - \vec{1})$; thus, $\rho(\vec{k}) - \binom{N}{k}\tilde{\rho}(\vec{0}) + \binom{N-1}{k-1}\tilde{\rho}(\vec{1})$, which $\equiv \binom{N-2}{k-2}$ in $(\vec{N} - \vec{2})$, and vanishes in $(\vec{N})$ and $(\vec{N} - \vec{1})$. Continuing in this way, we have that

$$\rho(\vec{k}) = \sum_{t=0}^{k} (-1)^{t} \binom{N-t}{k-t} \tilde{\rho}(\vec{t}) , \qquad (60)$$

since the difference between the operators on both sides, being an operator of maximum hole rank k which vanishes in $(l \leq k)$-hole states, must necessarily vanish. The hole-particle adjoint operation $(\tilde{\ })$ applied to Eq. (60) will give the density-operator equivalent of Eq. (59). These combinatorial results are elementary and, in fact, are not of very great interest; but their extensions for more complicated lattices are not trivial at all (a point which, in a more general way, has been made by Rota[25]) and, in some cases, will be of considerable interest.

When there is simple propagation, we are now able to propagate the trace of an operator of mixed particle rank without recourse to the normal-form decomposition. To do this via Eq. (51) we need to calculate the input traces over the entire defining net, but for high k in particular this may be very difficult. We can, however, proceed to a new net for which the required input calculations are simpler; in particular, one which discards the high-number members of the defining net in favor of representations involving only a few holes. An elementary way to do this is to use Eq. (51) to eliminate elementary-net points on the right-hand side in favor of simple representations on the left, as we have already done for the simple scalar case in Sec. 3. We shall see later how this works out in practice for more complicated cases. We shall give also more elegant ways of proceeding which get around difficulties arising from the fact that not every net of the correct dimensionality carries all the necessary input information, this because of a failure of linear independence.[26] It might be noted that the defining net gives the simplest faithful array of representations for the operator being considered and that the simpler net does not then define a faithful array. But for traces of limited order, such faithfulness is not required and, as we shall see, the use of a nonfaithful array makes things often very much easier.

Finally, we mention a different way of looking at some of the things discussed above. We have in Eq. (27) written the matrix elements of an operator in terms of the vacuum expectation value of a quartic object. We can consider this v.e.v. as measuring the overlap of two quadratic objects. For example, the nonnegative quantity $\langle Z_\alpha^\dagger(m) Z_\beta^\dagger(k) Z_\beta(k) Z_\alpha(m) \rangle_0$ determines the normalization of the state produced by combining an m-particle and a k-particle system as indicated, while $\langle Z_\alpha^\dagger(m) Z_\beta(k) Z_\beta^\dagger(k) Z_\alpha(m) \rangle_0$ measures the amplitude with which the state (k, β) can be found in the state (m, α). It is easy to see that in each case we have $\langle\ \rangle \leq 1$ (consider the evaluation in a Hartree-Fock basis).

We are really interested in the combination of *subspaces* instead of states. A natural measure then of the "strength" with which two subspaces combine is

$$\mathfrak{a}(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}) = d^{-1}(\vec{m}, \vec{\alpha}) d^{-1}(\vec{k}, \vec{\beta}) \times \sum_{\substack{\alpha \in \vec{\alpha} \\ \beta \in \vec{\beta}}} \langle Z_\alpha^\dagger(m) Z_\beta^\dagger(k) Z_\beta(k) Z_\alpha(m) \rangle_0$$

$$= d^{-1}(\vec{k}, \vec{\beta}) \langle \tilde{\rho}(\vec{k}, \vec{\beta}) \rangle^{\vec{m}, \vec{\alpha}} , \qquad (61)$$

which incidentally gives us an upper limit on the propagation coefficients (since $\mathfrak{a} \leq 1$). The departure of $\mathfrak{a}$ from unity represents what is commonly called a "blocking effect." For the simple $U(N)$ case, Eq. (43) gives, for combining an m particle and k particle subspaces, that

$$\mathfrak{a}(\vec{m}; \vec{k}) = \binom{N}{k}^{-1} \binom{N-m}{k}$$

$$= \left(1 - \frac{m_>}{N}\right)\left(1 - \frac{m_> - 1}{N-1}\right) \cdots \left(1 - \frac{m_> - m_<}{N - m_<}\right) , \qquad (62)$$

where $m_>$ is the larger of (m, k) and $m_<$ the smaller. The "blocking effect" measured by $(1 - \mathfrak{a})$ is seen to be small, as expected, if we combine two subspaces each small compared with the total space available.

In the same way a measure for the probability of finding a subspace $(\vec{k}, \vec{\beta})$ in $(\vec{m}, \vec{\alpha})$ is

$$d(\vec{m}, \vec{\alpha}) \mathfrak{B}(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta})$$

$$= d^{-1}(\vec{k}, \vec{\beta}) \sum_{\substack{\alpha \in \vec{\alpha} \\ \beta \in \vec{\beta}}} \langle Z_\alpha^\dagger(m) Z_\beta(k) Z_\beta^\dagger(k) Z_\alpha(m) \rangle$$

$$= d(\vec{m}, \vec{\alpha}) d^{-1}(\vec{k}, \vec{\beta}) \langle \rho(\vec{k}, \vec{\beta}) \rangle^{\vec{m}, \vec{\alpha}} . \qquad (63)$$

The measure adopted here ensures a unit value for the measure of a space within itself and leads to

the simple result of Eq. (65) below. The normalization of $\mathfrak{B}$ is such as to give the simplest form for the symmetry properties which follow from Eq. (44); they are

$$\mathfrak{B}(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}) = \mathfrak{A}(\vec{N} - \vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}) = \mathfrak{A}(\vec{k}, \vec{\beta}; \vec{N} - \vec{m}, \vec{\alpha}) = \mathfrak{B}(\vec{N} - \vec{k}, \vec{\beta}; \vec{N} - \vec{m}, \vec{\alpha}) \ . \tag{64}$$

$\mathfrak{B}$ of course vanishes if $k > m$, and $\mathfrak{A}$ if $m + k > N$, and both quantities are bounded by unity. Indeed, they satisfy elementary sum rules arising from the the fact that $\sum_{\vec{\gamma}} \rho(\vec{t}, \vec{\gamma}) = \rho(\vec{t})$.

If we have simple propagation, then, on combining two spaces (i.e., taking the product of an orthonormal basis set in one space with a set in another), the states of an orthonormal basis for the resultant space appear with equal intensity; and, similarly, for the operation measuring one space in another. In this case, also, we have a very simple picture of the trace propagation. For an operator defined in a subspace $(\vec{k}, \vec{\beta})$, we have

$$\text{Trace of } O \text{ in } (\vec{m}, \vec{\alpha}) = [\text{Trace of } O \text{ in } (\vec{k}, \vec{\beta})] \times [\text{Measure of } (\vec{k}, \vec{\beta}) \text{ in } (\vec{m}, \vec{\alpha})] \ . \tag{65}$$

The $\mathfrak{A}$, $\mathfrak{B}$ quantities correspond to looking at the quartic object, whose vacuum expectation value is of interest to us, according to its [(12)(34)] structure rather than [1(23)4] which is natural when we think of density operators. When later we replace the *scalar* multiplication of the four objects by a *tensor* coupling, with subspaces and tensors defined by the group structure being considered, we shall be led naturally to decompose $\mathfrak{A}$ and $\mathfrak{B}$ according to the intermediate subspaces, viz.,

$$\begin{aligned} \mathfrak{A}(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}) &= \sum_{\vec{\gamma}} A(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}; \vec{m} + \vec{k}, \vec{\gamma}) \ , \\ \mathfrak{B}(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}) &= \sum_{\vec{\gamma}} B(\vec{m}, \vec{\alpha}; \vec{k}, \vec{\beta}; \vec{m} + \vec{k}, \vec{\gamma}) \ . \end{aligned} \tag{66}$$

The resultant quantities, as we shall see later, are vital for the decomposition of widths into partial widths. They have a considerably extended set of symmetry properties and sum rules. The relationship between the two kinds of decompositions of the quartic structure will be that of a Racah transformation involving, of course, the Racah algebra of the relevant group or set of groups.

5. CONFIGURATION DISTRIBUTIONS

The scalar distribution of Sec. 3 is always of interest, since it has to do with the distribution of the eigenstates themselves, but it tells us essentially nothing about the structure of the eigenstates. We thus turn to a more detailed decomposition of the $\mathfrak{N}$ space, that corresponding to configurations.

In the configuration or fixed-partition distribution we imagine a partitioning of the orbital set $\{N\}$ into l subsets, $\{N\} \to \{N_1, N_2, \ldots, N_l\} = \{[N]\}$, say,[27] in which $\sum N_i = N$, N_k being then the number of single-particle states in the kth subset. Such partitioning is naturally suggested by the orbitals of spherical or deformed shell models, but we may in fact have no shell model in mind at all. Corresponding to this partition we may distribute particles according to $m \to (m_1, m_2, \ldots, m_l) = [m]$, with $\sum m_i = m$, this arrangement defining a configuration and $[\vec{m}]$ then standing for a basis set for that configuration.

We observe that even a number-conserving operator may not conserve the separate numbers m_i. Operators which change configurations are of course traceless in m; among the m-conserving operators the simplest are those of the type $O([\vec{k}])$ which have definite particle ranks with respect to each subset of $\{N\}$. For these operators we have an immediate extension of Eqs. (13) and (43), viz.,

$$\langle O([\vec{k}]) \rangle^{[\vec{m}]} = \langle O([\vec{k}]) \rangle^{[\vec{k}]} \prod_i \binom{m_i}{k_i} \ , \tag{67}$$

$$\rho([\vec{m}]) = \prod_i \binom{n_i}{m_i} \ , \tag{68}$$

which will give the averages and trace equivalents for a general operator as long as its decomposition $O = \sum O([\vec{k}; \vec{k}'])$ is available.

What now is the extension which, without recourse to normal-form expansions, will enable us to deal with operators of indefinite (vectorial) particle rank? Just as we did before, in the transition from Eq. (13) to Eq. (14) or (46)–(50), we may introduce a set of Lagrange polynomials or trace operators orthogonal on a defining net. If we wish to deal with an operator O whose vectorial rank $\leq [u]$ (i.e., rank in the ith orbit $\leq u_i$), then it follows from the direct-product nature of the system that the density operator on the u-net factors according to the orbits, and we have

$$\begin{aligned} \rho_{[u]}([\vec{k}]) &= \prod_i \rho_{u_i}(k_i) \\ &= \prod_i (-1)^{u_i - k_i} \binom{n_i - k_i - 1}{u_i - k_i} \binom{n_i}{k_i} \ , \end{aligned} \tag{69}$$

the average of O being then given by the natural extension of Eq. (14).

This in fact is not very useful, for usually we shall deal with operators O which have a specified maximum *scalar* rank u. Then the maximum ranks in the separate orbits are also restricted to $\leq u$ but there is a correlation between them. With a $(0+1+2)$-body Hamiltonian in a two-orbit configuration, we have for example $[\vec{k}] = [\vec{2}, \vec{0}]$, $[\vec{1}, \vec{1}]$, $[\vec{0}, \vec{2}]$, but $[\vec{2}, \vec{1}]$ and $[\vec{2}, \vec{2}]$ would be ruled out. In

the $l=2$ case, then, we should take the $\binom{u+2}{2}$ dimensional *triangular* net ($t_1+t_2\leq u$) rather than the square net ($t_i\leq u$) appropriate to Eq. (69); this constitutes a major simplification, since the new net has fewer and simpler elements; and similarly for arbitrary l. We shall indicate the new density operators as $\rho_u([\vec{t}])$.

Consider as an example $l=2$, $u=5$, $[\vec{t}]=[\vec{1},\vec{2}]$ as shown in Fig. 2. We need an operator of (mixed) rank ≤ 5 which gives zero for all points on the net except for unity on $(\vec{1},\vec{2})$. Then noting that there are three varieties of linear factors [(0+1)-particle operators] which annihilate along a line we see that

$$\rho_5([\vec{1},\vec{2}])=\tfrac{1}{4}n_1n_2(n_2-1)(n-4)(n-5)\ . \tag{70}$$

A little consideration will show that the same kind of linear factoring is valid for all points of the net, for arbitrary u, and finally for an arbitrary dimensionality l. The result then, as may easily be verified, is

$$\rho_u([\vec{t}])=\binom{u-n}{u-t}\prod_i\binom{n_i}{t_i}=(-1)^{t-u}\binom{n-t-1}{u-t}\prod_i\binom{n_i}{t_i}\ , \tag{71}$$

which gives for the average

$$\langle O\rangle^{[\vec{m}]}=\sum_{t_1=0}^{u}\cdots\sum_{t_l=0}^{u}(-1)^{t-u}\binom{m-t-1}{u-t}\times\left[\binom{m_1}{t_1}\cdots\binom{m_l}{t_l}\right]\langle O\rangle^{[\vec{t}]},\quad (t\leq u), \tag{72}$$

where $t=\sum t_i$, $m=\sum m_i$. The $[\vec{m}]$ dependence of $\langle O\rangle^{[\vec{m}]}$ is, of course, that of a uth-rank polynomial in the l variables $m_1\ldots m_l$.

Once again, just as in the scalar case, the elementary net (the triangular net about the origin which constitutes the defining space for O) will usually not be convenient to deal with, because of the complexity of the necessary input traces. In the scalar case a "most economical" net and the corresponding density operators were easily found but, because of a failure of linear independence, this is not at all true in the present case. It has been shown by Kim[28] that a "most economical" lattice in the l-dimensional case derives from the elementary net by a kind of reflection-contraction process in which $[\vec{t}]\rightarrow[\vec{t}^*]$ where $t_i^*=(N_i-\frac{1}{2}t_i+\frac{1}{2})$ if t_i is odd, $t_i^*=\frac{1}{2}t_i$ if t_i is even. This replaces the triangular elementary net by a set of triangular nets, one at each corner, the largest of which corresponds to $\frac{1}{2}u$ or $\frac{1}{2}(u-1)$ according to whether u is even or odd. The general solution for ρ_u for this net is very complicated but in any case of interest we may numerically invert Eq. (72) to express the old input traces in terms of the new ones.

Instead of using this method we shall in the next sections use a normal-form decomposition of H^2 [propagating the separate parts via Eq. (67)] to express the configuration widths in terms of the Hamiltonian matrix elements, and shall give also a decomposition into partial widths. In a later paper a quite different solution for the width problem will be derived by use of a unitary-group decomposition of the Hamiltonian and expressed in terms of physically significant quantities. The entire structure of the width expressions will then become transparent.

6. SCALAR AND CONFIGURATION MOMENTS IN THE SPHERICAL SHELL MODEL

In this section we derive and discuss expressions, in terms of the Hamiltonian matrix elements, for the centroids and widths of the scalar and configuration spectral distributions. We are particularly interested in the case where the set of single-particle states corresponds to a number of spherical orbits and we work, therefore, in the usual shell-model or spherical-tensor representation in which both states and operators carry definite angular momentum (and isospin where that is relevant). Actually, since we do not now consider distributions for fixed angular momentum, this choice of representation is not at all essential and it is, in fact, a slightly restrictive one since, at first sight, it precludes a consideration of nonspherical orbits. This restriction however is more apparent than real, because it is clear from the discussions above that the centroids and widths must be expressible in terms of linear and quadratic traces in the matrix-element space, and the translation of such quantities from one representation to another is not difficult. We choose the explicit

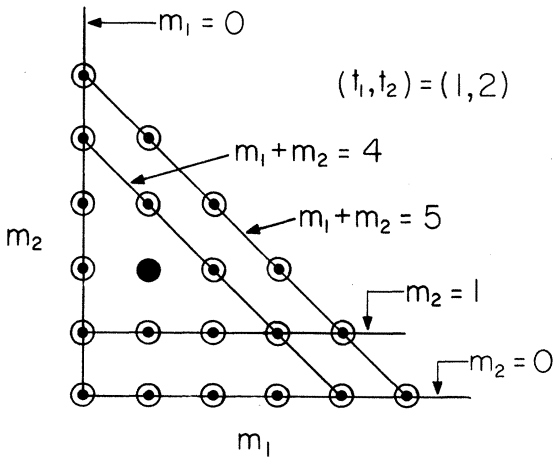

FIG. 2. Representation of the density operator in Eq. (70).

spherical basis because that will be particularly convenient for future work. In dealing with the propagation of the quadratic traces we shall use the normal-form method, leaving until later the application of other methods. The essential formal problem is then that of decomposing H and H^2 in an appropriate way and evaluating the N-state expectation value of the various parts.

We adopt a notation[29] which emphasizes the tensorial properties of the various quantities arising in the spherical shell model. Single-particle orbitals are characterized by principal quantum number, parity, angular momentum, and, where relevant, the isospin (whose value is $t=\frac{1}{2}$). We can for most purposes describe all these by a composite label r which, among other things, then defines the tensorial ranks. In the isospin formalism, the $2(2j_r+1)$ single-particle states corresponding to such an orbital are distinguished by their projection quantum numbers $(\mu_j, \mu_t)\equiv\mu$. The basic creation operator is A^r_μ which creates a normalized single-particle state

$$A^r_\mu|0\rangle \equiv \psi^r_\mu \ . \tag{73}$$

The destruction operator B^r_μ is related to the Hermitian conjugate of A^r_μ as

$$B^r_\mu = (-1)^{r+\mu}(A^r_{-\mu})^\dagger \ , \tag{74}$$

the phase being chosen to cause B^r_μ to transform as the μ component of a spherical tensor of rank r. The notation is a direct-product one so that in a (j, t) formalism we have, for example,

$$(-1)^r = (-1)^{j_r+t_r} = (-1)^{j_r+1/2} \ . \tag{75}$$

But we can also interpret the equations via a j formalism in which isospin does not occur (at least not as a tensorial rank) or even via a t formalism. In some cases it will be found advantageous to introduce more explicitly some of the single-particle state labels.

The normalized two-particle state is

$$-\zeta_{rs}(A^r\times A^s)^\Gamma_\mu|0\rangle \equiv |r, s; \Gamma, \mu\rangle \ , \tag{76}$$
$$\zeta_{rs}=1, \quad r\neq s \ ,$$
$$\zeta_{rs}=1/\sqrt{2} \ , \quad r=s \ ,$$

where $(\Gamma, \mu)\equiv(JT, \mu_J\mu_T)$ in an isospin formalism and the indicated $(\times)$ product defines the usual angular momentum coupling. The coupled commutation rules for the basic operators are then

$$(A^r\times A^s)^\Gamma + (-1)^{r+s-\Gamma}(A^s\times A^r)^\Gamma = 0 \ ,$$
$$(B^r\times B^s)^\Gamma + (-1)^{r+s-\Gamma}(B^s\times B^r)^\Gamma = 0 \ , \tag{77}$$
$$(A^r\times B^s)^\Gamma + (-1)^{r+s-\Gamma}(B^s\times A^r)^\Gamma = [r]^{1/2}\delta_{rs}\delta_{\Gamma 0} \ ,$$

where $[r]$ denotes the statistical weight of orbital r,

$$[r]=N_r=(2j_r+1)(2t_r+1)=2(2j_r+1) \tag{78}$$

in the (j, t) formalism. $\delta_{rs}=0$ unless r, s define the same orbital. It will be found convenient, allowing for the fact that there may be active orbits differing only in radial quantum number, to introduce the symbol $\hat{\delta}_{rs}$ which distinguishes between orbits only according to their tensorial rank

$$\hat{\delta}_{rs}=\delta(j_r, j_s) \qquad [\text{in } j \text{ or } (jt) \text{ formalisms}] \ . \tag{79}$$

For the Hamiltonian we take a $(0+1+2)$-particle scalar operator, the separate parts of which via Eq. (26) have the form

$$H(\vec{0}) = H_0 \ ,$$
$$H(\vec{1}) = \sum_{r,s}\epsilon_{rs}[r]^{1/2}(A^r\times B^s)^0 \ , \tag{80}$$
$$H(\vec{2}) = -\tfrac{1}{4}\sum_{rstu\Gamma}[\Gamma]^{1/2}\zeta_{rs}^{-1}\zeta_{tu}^{-1}W^\Gamma_{rstu}[(A^r\times A^s)^\Gamma\times(B^t\times B^u)^\Gamma]^0 \ .$$

The one- and two-body matrix elements of H, denoted by ϵ and W, respectively, have the following symmetry properties:

$$\epsilon_{rs}\equiv\langle r|H(1)|s\rangle = \epsilon_{sr} = \hat{\delta}_{rs}\epsilon_{rs} \ , \tag{81}$$

$$W^\Gamma_{rstu}\equiv\langle rs, \Gamma|H(2)|tu, \Gamma\rangle = (-1)^{r+s-\Gamma}W^\Gamma_{srtu} = (-1)^{t+u-\Gamma}W^\Gamma_{rsut} = (-1)^{r+s-t-u}W^\Gamma_{srut} = W^\Gamma_{turs} \ . \tag{82}$$

We shall sometimes write the diagonal single-particle energies ϵ_{rr} as ϵ_r.

Similarly, $H^2\equiv K$ is a $(0-4)$-particle operator[30]

$$H^2=\sum_{t=0}^{4}K(t) \tag{83}$$

and on carrying out the commutations required to put K into normal form, we find

$$K(\vec{0}) = (H_0)^2 , \tag{84}$$

$$K(\vec{1}) = \sum_{rs} \{2H_0[r]^{1/2}\epsilon_{rs} + \sum_t [r]^{1/2}\epsilon_{rt}\epsilon_{ts}\}(A^r \times B^s)^0 , \tag{85}$$

$$K(\vec{2}) = \sum_{rstu\Gamma} [\Gamma]^{1/2}(-\tfrac{1}{2}H_0\zeta_{rs}^{-1}\zeta_{tu}^{-1}W^\Gamma_{rstu} - \epsilon_{rt}\epsilon_{su} - \tfrac{1}{2}\sum_e \zeta_{rs}^{-1}\zeta_{te}^{-1}W^\Gamma_{rste}\epsilon_{eu}$$
$$- \tfrac{1}{2}\sum_e \zeta_{es}^{-1}\zeta_{tu}^{-1}\epsilon_{re}W^\Gamma_{estu} - \tfrac{1}{8}\sum_{ef} \zeta_{rs}^{-1}\zeta_{ef}^{-2}\zeta_{tu}^{-1}W^\Gamma_{rsef}W^\Gamma_{eftu})[(A^r \times A^s)^\Gamma \times (B^t \times B^u)^\Gamma]^0 , \tag{86}$$

$$K(\vec{3}) = \sum_{\substack{rstuef \\ \Gamma\Gamma'\Delta}} [\Delta]^{1/2}\{-\tfrac{1}{2}\zeta_{rs}^{-1}\zeta_{tu}^{-1}\epsilon_{ef}W^\Gamma_{rstu}\delta_{\Gamma\Gamma'}(-1)^{e+\Gamma-\Delta} + \tfrac{1}{4}\sum_g \zeta_{rs}^{-1}\zeta_{fg}^{-1}\zeta_{eg}^{-1}\zeta_{tu}^{-1}[\Gamma]^{1/2}$$
$$\times W^\Gamma_{rsfg}W^{\Gamma'}_{egtu}(-1)^{\Delta+\Gamma-e}W(\Gamma' ef\Gamma : g\Delta)\}\{[(A^r \times A^s)^\Gamma \times A^e]^\Delta \times B^f \times (B^t \times B^u)^{\Gamma'}]^\Delta\}^0 , \tag{87}$$

$$K(\vec{4}) = \sum_{\substack{rstuefgh \\ \Gamma\Gamma'\Delta}} \tfrac{1}{16}[\Delta]^{1/2}\zeta_{rs}^{-1}\zeta_{tu}^{-1}\zeta_{ef}^{-1}\zeta_{gh}^{-1}W^\Gamma_{rstu}W^{\Gamma'}_{efgh}\{[(A^r \times A^s)^\Gamma \times (A^e \times A^f)^{\Gamma'}]^\Delta \times [(B^t \times B^u)^\Gamma \times (B^g \times B^h)^{\Gamma'}]^\Delta\}^0 . \tag{88}$$

All orbital summations are unrestricted. The sumbol $W(\Gamma' ef\Gamma : g\Delta)$ in Eq. (87) is the usual Racah coefficient. It is clear *a priori*, and demonstrated in these equations, that the product $H(\vec{k})H(\vec{k}')$ (for $k \geq k'$) contributes to $K(\vec{k})$, $K(\vec{k}+\vec{1}), \ldots, K(\vec{k}+\vec{k}')$. Note also that the matrix elements of the k-particle part of $H(\vec{k})H(\vec{k})$ are those which arise from the usual matrix product in the k space, this coming about because the k space supplies a representation of $K(\vec{k})$ as well as of $H(\vec{k})$. Examples are the ϵ^2 terms in $K(\vec{1})$ and the W^2 terms in $K(\vec{2})$. The matrix elements of $K(\vec{k}+\vec{k}')$ arising from $H(\vec{k})H(\vec{k}')$ are those of a kind of direct-product matrix, examples being the ϵW terms in $K(\vec{3})$ and W^2 in $K(\vec{4})$. These terms, of course, arise from transforming the product to normal form but ignoring all the commutator contractions.

For the scalar centroid and width we use Eq. (24) for which the necessary input is the set of N-state values of $H(\vec{t})$ and $K(\vec{t})$. These we evaluate by the standard methods and we find

$$\langle H(\vec{0})\rangle^N = H_0 , \tag{89}$$

$$\langle H(\vec{1})\rangle^N = \sum_r N_r\epsilon_{rr} , \tag{90}$$

$$\langle H(\vec{2})\rangle^N = \tfrac{1}{2}\sum_{rs} A_{rsrs} , \tag{91}$$

$$\langle K(\vec{0})\rangle^N = H_0^2 , \tag{92}$$

$$\langle K(\vec{1})\rangle^N = \sum_r (2H_0N_r\epsilon_{rr} + \sum_k N_r\epsilon_{rk}\epsilon_{kr}) , \tag{93}$$

$$\langle K(\vec{2})\rangle^N = \sum_{rs}[H_0A_{rsrs} + N_rN_s\epsilon_{rr}\epsilon_{ss} - N_r\epsilon_{rs}\epsilon_{sr} + \sum_k (A_{rsrk}\epsilon_{ks} + \epsilon_{rk}A_{ksrs}) + \tfrac{1}{4}\sum_{kl} B_{rskl}] , \tag{94}$$

$$\langle K(\vec{3})\rangle^N = \sum_{rst}[N_t\epsilon_{tt}A_{rsrs} + \sum_k N_s^{-1}A_{rsrk}A_{tkts}\hat{\delta}_{sk} - A_{srst}\epsilon_{tr} - \epsilon_{tr}A_{rsts} - \tfrac{1}{2}\sum_k B_{rstk}] , \tag{95}$$

$$\langle K(\vec{4})\rangle^N = \sum_{rstu} (\tfrac{1}{4}A_{rsrs}A_{tutu} + \tfrac{1}{4}B_{rstu} - N_s^{-1}A_{rsrt}A_{tusu}\hat{\delta}_{st}) , \tag{96}$$

where the orbital summations are all unrestricted.

We have introduced here the quantities

$$A_{rstu} = \zeta_{rs}^{-1}\zeta_{tu}^{-1}\sum_\Gamma [\Gamma]W^\Gamma_{rstu} ,$$
$$B_{rstu} = \zeta_{rs}^{-2}\zeta_{tu}^{-2}\sum_\Gamma [\Gamma](W^\Gamma_{rstu})^2 , \tag{97}$$

which to within normalization may be regarded as deriving from a Γ averaging of the matrix elements of $H(\vec{2})$ and $[H(\vec{2})]^2$ between the two-particle states (r, s) and (t, u). In terms of these it is clear that

$$W_{rs} = (N_rN_s)^{-1}\sum_{J,T}[JT]W^{JT}_{rsrs} = (N_rN_s)^{-1}A_{rsrs} , \quad r \neq s \tag{98}$$

is the average two-body interaction between two nucleons in different orbits, r, s. When they are in the same orbit the average is

$$W_{rr} \equiv W_r = \binom{N_r}{2}^{-1}\sum_{JT}[JT]W^{JT}_{rrrr} = [N_r(N_r-1)]^{-1}A_{rrrr} . \tag{99}$$

Then, considering all the two-nucleon states, we have (for the trace instead of the average), writing $\mathcal{W}$ for the two-particle *matrix* of $H(\vec{2})$ and W for the over-all average interaction energy

$$\langle\langle H(\vec{2})\rangle\rangle^{\vec{2}} = \mathrm{Tr}(\mathcal{W}) = \binom{N}{2} W = \sum_{\substack{r,s \\ r<s}} N_r N_s W_{rs} + \sum_r \binom{N_r}{2} W_r = \tfrac{1}{2}\sum_{r,s} A_{rsrs} \ , \tag{100}$$

$$\langle\langle [H(\vec{2})]^2\rangle\rangle^{\vec{2}} = \mathrm{Tr}(\mathcal{W}\times\mathcal{W}) = \tfrac{1}{4}\sum_{rstu} B_{rstu} \ . \tag{101}$$

Finally, the following symmetry properties for the A's and B's follow immediately from Eq. (82).

$$A_{rsrs} = A_{srsr} \ , \tag{102}$$

$$A_{rstu} = A_{turs} = (-1)^{r+s-t-u} A_{srut} \ , \tag{103}$$

$$B_{rstu} = B_{srtu} = B_{rsut} = B_{srut} = B_{turs} \ . \tag{104}$$

The centroid of the complete scalar distribution now follows via Eq. (24) and is

$$\mathcal{E}(\vec{\mathrm{m}}) = \langle H\rangle^{\vec{\mathrm{m}}} = H_0 + \frac{m}{N}\sum_r N_r \epsilon_{rr} + \frac{m(m-1)}{N(N-1)}\,\tfrac{1}{2}\sum_{rs} A_{rsrs} \ . \tag{105}$$

For the dispersion we may do the same for $\langle H^2\rangle^{\vec{\mathrm{m}}}$ and then subtract the square of the centroid polynomial. Or equivalently we can recognize that $\sigma^2(\vec{\mathrm{m}})$ is the second moment (and similarly for the pth central moment) of

$$H - \sum_{k=0}^{2} \langle H(k)\rangle^{\vec{\mathrm{k}}} \binom{n}{k} = H - H_0 - \epsilon n - W\binom{n}{2} \ , \tag{106}$$

the subtracted term being simply the linear trace equivalent of H. The result is

$$\begin{aligned}\sigma^2(\vec{\mathrm{m}}) &= \langle H^2\rangle^{\vec{\mathrm{m}}} - (\langle H\rangle^{\vec{\mathrm{m}}})^2 \\ &= \frac{m}{N}Q + \frac{m(m-1)}{N(N-1)}(X+Y-Q) + \frac{m(m-1)(m-2)}{N(N-1)(N-2)}(Z-X-2Y) + \frac{m(m-1)(m-2)(m-3)}{N(N-1)(N-2)(N-3)}(Y-Z) \ ,\end{aligned} \tag{107}$$

which, as will be recognized from the m polynomials, exhibits separately the dispersions from the $(1-4)$-particle parts of H^2. Here

$$\begin{aligned}Q &= \sum_{rs} N_r (\epsilon_{rs})^2 - \frac{1}{N}\left(\sum_r N_r \epsilon_{rr}\right)^2 \\ &= \mathrm{Tr}(\epsilon\times\epsilon) - \frac{1}{N}\left[\mathrm{Tr}(\epsilon)\right]^2\end{aligned} \tag{108}$$

$$X = 2\sum_{rst} A_{rsrt}\,\epsilon_{ts} - \frac{2}{N}\left(\sum_r N_r \epsilon_{rr}\right)\left(\sum_{st} A_{stst}\right) \ , \tag{109}$$

$$\begin{aligned}Y &= \frac{1}{4}\sum_{rstu} B_{rstu} - \frac{1}{2N(N-1)}\left(\sum_{rs} A_{rsrs}\right)^2 \\ &= \mathrm{Tr}(\mathcal{W}\times\mathcal{W}) - \binom{N}{2}^{-1} (\mathrm{Tr}\mathcal{W})^2 \ ,\end{aligned} \tag{110}$$

$$Z = \sum_{rstu} N_s^{-1} A_{rsru} A_{tuts}\,\delta_{su} - \frac{1}{N}\left(\sum_{rs} A_{rsrs}\right)^2 \ , \tag{111}$$

where, in correspondence with $\mathcal{W}$ as used in Eqs. (101) and (110), ϵ in Eq. (108) is the one-particle matrix of $H(\vec{1})$. The terms Q and Y then have a simple significance, being the one- and two-particle matrix dispersions, i.e., the dispersions of the one- and two-particle Hamiltonians, each considered as a matrix operator in its defining space. The parameters X, Z involve less familiar "partial" matrix products. Observe that each of these four separate terms propagates in its own characteristic way, the Q and Y polynomials, for example, being proportional to $\binom{m}{k}\binom{N-m}{k}$ with $k=0$, 1, respectively. The significance of the new forms and of the partial products will become clear when we consider the unitary-group decompositions of the widths.

We turn now to configurations. In this case we need a further decomposition of H and H^2 in order to iso-

late those parts which are number conserving and have a definite rank in each orbit separately. The N-state expectation values of these operators are then the input [see Eqs. (24) and (67)]. The decomposition follows by inspection in Eqs. (80) and (85)–(88). Using $H(r^a s^b t^c \dots)$ to indicate that part of H which has particle ranks $a, b, c, \dots$ in orbits $r, s, t, \dots$, respectively, we see for example that

$$H(rs) = -\sum_{\Gamma} [\Gamma]^{1/2} W^{\Gamma}_{rsrs} [(A^r \times A^s)^{\Gamma} \times (B^r \times B^s)^{\Gamma}]^0 \ , \tag{112}$$

it being understood of course that $r \neq s$. The relevant N-state expectation values are then

$$\langle H(\vec{0}) \rangle^N = H_0 \ , \tag{113}$$

$$\langle H(r) \rangle^N = N_r \epsilon_{rr} \ , \tag{114}$$

$$\langle H(r^2) \rangle^N = \tfrac{1}{2} A_{rrrr} \ , \tag{115}$$

$$\langle H(rs) \rangle^N = A_{rsrs} \ , \tag{116}$$

$$\langle K(\vec{0}) \rangle^N = (H_0)^2 \ , \tag{117}$$

$$\langle K(r) \rangle^N = 2H_0 N_r \epsilon_{rr} + N_r \sum_k (\epsilon_{rk})^2 \ , \tag{118}$$

$$\langle K(r^2) \rangle^N = N_r (N_r - 1)(\epsilon_{rr})^2 + H_0 A_{rrrr} + 2\sum_k \epsilon_{rk} A_{rrrk} + \tfrac{1}{4} \sum_{kl} B_{rrkl} \ , \tag{119}$$

$$\langle K(rs) \rangle^N = 2N_r N_s \epsilon_{rr} \epsilon_{ss} - 2N_r (\epsilon_{rs})^2 + 2H_0 A_{rsrs} + 2\sum_k (\epsilon_{rk} A_{srsk} + \epsilon_{sk} A_{rsrk}) + \tfrac{1}{2} \sum_{kl} B_{rskl} \ , \tag{120}$$

$$\langle K(r^3) \rangle^N = (N_r - 2)\epsilon_{rr} A_{rrrr} + N_r^{-1} \sum_k (A_{rrrk})^2 \hat{\delta}_{rk} - \tfrac{1}{2} \sum_k B_{rrrk} \ , \tag{121}$$

$$\begin{aligned} \langle K(r^2 s) \rangle^N = {} & 2(N_r - 1)\epsilon_{rr} A_{rsrs} + N_s \epsilon_{ss} A_{rrrr} - 4\epsilon_{rs} A_{rrrs} + 2N_r^{-1} \sum_k A_{rrrk} A_{ksrs} \hat{\delta}_{kr} \\ & + N_s^{-1} \sum_k (A_{rsrk})^2 \hat{\delta}_{sk} - \sum_k B_{rsrk} - \tfrac{1}{2} \sum_k B_{rrsk} \ , \end{aligned} \tag{122}$$

$$\begin{aligned} \langle K(rst) \rangle^N = {} & 2N_r \epsilon_{rr} A_{stst} + 2N_s \epsilon_{ss} A_{rtrt} + 2N_t \epsilon_{tt} A_{rsrs} - 4\epsilon_{rt} A_{rsts} - 4\epsilon_{rs} A_{rtst} - 4\epsilon_{st} A_{srtr} \\ & - \sum_k (B_{rstk} + B_{rtsk} + B_{strk}) + 2N_r^{-1} \sum_k A_{ksrs} A_{ktrt} \hat{\delta}_{kr} + 2N_s^{-1} \sum_k A_{krsr} A_{ktst} \hat{\delta}_{ks} + 2N_t^{-1} \sum_k A_{krtr} A_{ksts} \hat{\delta}_{kt} \ , \end{aligned} \tag{123}$$

$$\langle K(r^4) \rangle^N = \tfrac{1}{4} B_{rrrr} + (\tfrac{1}{4} - N_r^{-1})(A_{rrrr})^2 \ , \tag{124}$$

$$\langle K(r^3 s) \rangle^N = B_{rrrs} + (1 - 2N_r^{-1}) A_{rrrr} A_{rsrs} - 2N_r^{-1} (A_{rrrs})^2 \hat{\delta}_{rs} \ , \tag{125}$$

$$\langle K(r^2 s^2) \rangle^N = \tfrac{1}{2} B_{rrss} + B_{rsrs} + \tfrac{1}{2} A_{rrrr} A_{ssss} + (1 - N_r^{-1} - N_s^{-1})(A_{rsrs})^2 - 4N_r^{-1} A_{rrrs} A_{rsss} \hat{\delta}_{rs} \ , \tag{126}$$

$$\begin{aligned} \langle K(r^2 st) \rangle^N = {} & B_{rrst} + 2B_{rsrt} + A_{rrrr} A_{stst} + 2(1 - N_r^{-1}) A_{rsrs} A_{rtrt} - 2N_s^{-1} (A_{rsrt})^2 \hat{\delta}_{st} \\ & - 4N_r^{-1} A_{rrrs} A_{rtst} \hat{\delta}_{rs} - 4N_r^{-1} A_{rrrt} A_{rsts} \hat{\delta}_{rt} \ , \end{aligned} \tag{127}$$

$$\begin{aligned} \langle K(rstu) \rangle^N = {} & 2(B_{rstu} + B_{rtsu} + B_{rust}) + 2(A_{rsrs} A_{tutu} + A_{rtrt} A_{susu} + A_{ruru} A_{stst}) - 4N_r^{-1} A_{srst} A_{rutu} \hat{\delta}_{rt} \\ & - 4N_r^{-1} A_{srsu} A_{rtut} \hat{\delta}_{ru} - 4N_r^{-1} A_{trts} A_{rusu} \hat{\delta}_{rs} - 4N_s^{-1} A_{rsrt} A_{sutu} \hat{\delta}_{st} \\ & - 4N_s^{-1} A_{rsru} A_{stut} \hat{\delta}_{su} - 4N_t^{-1} A_{rtru} A_{tsus} \hat{\delta}_{tu} \ . \end{aligned} \tag{128}$$

The centroid and dispersion polynomials are now formed just as in the scalar case. The terms in Eqs. (113)–(116) propagate via Eq. (65) to give the energy polynomial for the configuration $[\vec{m}] \equiv [\vec{m}_1, \vec{m}_2, \dots \vec{m}_l]$;

$$\mathcal{E}([\vec{m}]) = \langle H \rangle^{[\vec{m}]} = H_0 + \sum_r M_r(1) \times N_r \epsilon_{rr} + \sum_r M_r(2) \times \tfrac{1}{2} A_{rrrr} + \sum_{rs}{}' M_r(1) M_s(1) \times \tfrac{1}{2} A_{rsrs} \ , \tag{129}$$

where

$$M_r(k) = \binom{m_r}{k} \binom{N_r}{k}^{-1} = \frac{m_r (m_r - 1) \cdots (m_r - k + 1)}{N_r (N_r - 1) \cdots (N_r - k + 1)} \ , \tag{130}$$

with these polynomial quantities varying in value from 0 to 1 as the orbit fills. Equation (129) would follow immediately from our definitions of the average energies. For the dispersion we may similarly propagate the terms in Eqs. (117)–(128) and then subtract from the resultant polynomial the square of the centroid polynomial [Eq. (129)]. Alternatively, we may subtract from H its linear trace equivalent

$$H \to \mathcal{H} = H - H_0 - \sum_r \epsilon_{rr} n_r - \sum_r W_r \binom{n_r}{2} - \sum_{r<s} W_{rs} n_r n_s \ , \tag{131}$$

which is equivalent in matrix elements to

$$H_0 \to 0, \ \epsilon_{rr} \to 0, \quad W^{\Gamma}_{rrrr} \to W^{\Gamma}_{rrrr} - W_r \ , \qquad W^{\Gamma}_{rsrs} \to W^{\Gamma}_{rsrs} - W_{rs} \ . \tag{132}$$

The forms here, if not obvious, are derived from Eqs. (97) and (129). The second moment of the new operator is then simply the variance. The result is

$$\begin{aligned}
\sigma^2([\vec{m}]) = {} & \sum_r M_r(1)[N_r \sum_k (\epsilon_{rk})^2(1-\delta_{rk})] + \sum_r M_r(2)\{\tfrac{1}{4}\sum_{kl} B_{rrkl} - \tfrac{1}{2}[N_r(N_r-1)]^{-1}(A_{rrrr})^2 + 2\sum_k \epsilon_{rk} A_{rrrk}(1-\delta_{rk})\} \\
& + \sum_{rs}{}' M_r(1) M_s(1)\{\tfrac{1}{4}\sum_{kl} B_{rskl} - \tfrac{1}{2}[N_r N_s]^{-1}(A_{rsrs})^2 + 2\sum_k \epsilon_{rk} A_{srsk}(1-\delta_{rk}) - N_r(\epsilon_{rs})^2\} \\
& + \sum_r M_r(3)\{[N_r(N_r-1)]^{-1}(A_{rrrr})^2 - \tfrac{1}{2}\sum_k B_{rrrk} + N_r^{-1}\sum_k (A_{rrrk})^2 \hat{\delta}_{rk}(1-\delta_{rk})\} \\
& + \sum_{rs}{}' M_r(2) M_s(1)\{[N_r N_s]^{-1}(A_{rsrs})^2 - \sum_k B_{rsrk} - \tfrac{1}{2}\sum_k B_{rrsk} - 4\epsilon_{rs} A_{rrrs} + 2N_r^{-1}\sum_k A_{rrrk} A_{srsk}\hat{\delta}_{rk}(1-\delta_{rk}) \\
& + N_s^{-1}\sum_k (A_{rsrk})^2 \hat{\delta}_{sk}(1-\delta_{sk})\} + \sum_{rst}{}' M_r(1) M_s(1) M_t(1)[-\tfrac{1}{2}\sum_k B_{rstk} - 2\epsilon_{rt} A_{srst} \\
& + N_t^{-1}\sum_k A_{rtrk} A_{stsk}\hat{\delta}_{tk}(1-\delta_{tk})] + \sum_r M_r(4)\{\tfrac{1}{4}B_{rrrr} - \tfrac{1}{2}[N_r(N_r-1)]^{-1}(A_{rrrr})^2\} \\
& + \sum_{rs}{}' M_r(3) M_s(1)[B_{rrrs} - 2N_r^{-1}(A_{rrrs})^2\hat{\delta}_{rs}] + \sum_{rs}{}' M_r(2) M_s(2)\{\tfrac{1}{4}B_{rrss} + \tfrac{1}{2}B_{rsrs} \\
& - \tfrac{1}{2}[N_r N_s]^{-1}(A_{rsrs})^2 - 2N_r^{-1} A_{rrrs} A_{rsss}\hat{\delta}_{rs}\} + \sum_{rst}{}' M_r(2) M_s(1) M_t(1)[\tfrac{1}{2}B_{rrst} + B_{rsrt} - N_s^{-1}(A_{rsrt})^2\hat{\delta}_{st} \\
& - 4N_r^{-1} A_{rrrs} A_{trts}\hat{\delta}_{rs}] + \sum_{rstu}{}' M_r(1) M_s(1) M_t(1) M_u(1)(\tfrac{1}{4}B_{rstu} - N_t^{-1} A_{rtru} A_{stsu}\hat{\delta}_{tu}) \ .
\end{aligned} \tag{133}$$

The summation $\sum'$ indicates that terms with any two summation variables equal must be omitted; otherwise the summations are unrestricted. The product $\hat{\delta}_{rs}(1-\delta_{rs})$ designates a term which survives only when orbitals r and s are distinct from each other but differ only in their principal quantum number, such as the $1s$ and $2s$ orbitals. The origin of each term in Eq. (133) is clearly indicated by the polynomial factors. Thus terms $M_r(2)M_s(1)M_t(1)$ arise from that four-body part of H^2 which is a two-body operator in orbit r and a one-body operator in orbits s and t. The quantities $B_{rrrr} - \binom{N_r}{2}^{-1}(A_{rrrr})^2$ and $B_{rsrs} - [N_r N_s]^{-1}(A_{rsrs})^2$ which appear in Eq. (133) are proportional to the variance of the two-body interaction between a pair of nucleons in the same and different orbits, respectively. The configuration widths do not depend on the diagonal single-particle energies $\epsilon_{rr} \equiv \epsilon_r$, as is clear formally from Eqs. (132) and (133) and otherwise from the fact that an operator which is a multiple of unity in a subspace does contribute to the energy but cannot contribute to the dispersion. The same is clearly true of the partial width. There is an incipient paradox here; a partial width connecting two subspaces is unchanged if we move one of them so high up in energy that its effects on the other subspace become negligible. But the paradox disappears when we remember that the admixing intensities depend in the limit inversely as the square of the centroid differences.

A decomposition of the width into partial widths, whose importance we have already stressed, is achieved via an intermediate-state expansion

$$\sigma^2([\vec{m}]) = \sum_{[\vec{m}']} \sigma^2([\vec{m}];[\vec{m}']) = \sum_{\substack{[\vec{m}'] \\ \alpha \in [\vec{m}] \\ \beta \in [\vec{m}']}} |\langle [\vec{m}]\alpha | \mathcal{H} | [\vec{m}']\beta \rangle|^2 \ . \tag{134}$$

We may think of $[\vec{m}']$ as generated from $[\vec{m}]$ by the excitation of a particular number and type of particle-hole pairs; $[\vec{m}_1 + \vec{1}, \ \vec{m}_2 - \vec{1}, \ \vec{m}_3, \ldots, \vec{m}_t]$ is a particular 1p-1h excitation, and so on. We see easily then that, in Eq. (133), the terms B_{rrrr}, B_{rsrs}, $(A_{rrrr})^2$, and $(A_{rsrs})^2$ are due to the internal mixing of 0p-0h states; the terms $(\epsilon_{rs})^2$, $\epsilon_{rs}A_{rrrs}$, $\epsilon_{rs}A_{rtst}$, B_{rsss}, B_{rsts}, $(A_{rrrs})^2$, $(A_{rsrt})^2$, $A_{rrrt}A_{srst}$, and $A_{rtru}A_{stsu}$ are

due to the admixing of 0p-0h states with 1p-1h states; the terms B_{rrss}, B_{rrst}, and B_{rstu} are due to the admixing of 0p-0h and 2p-2h states.

We may thus decompose the variance into terms each of which involves intermediate states of a unique configuration. We now list these partial variances using the notation that, for example, $\sigma^2([\vec{m}]; r^{-2}s^{+1}t^{+1})$ arises from the process

$$[\vec{m}] \rightarrow [\vec{m}_1, \vec{m}_2, \ldots, \vec{m}_r - \vec{2}, \vec{m}_s + \vec{1}, \vec{m}_t + \vec{1}, \ldots, \vec{m}_l] \rightarrow [\vec{m}] \ ,$$

where, of course, the orbits r, s, t are distinct. We find

$$\sigma^2([\vec{m}]:0) = \sum_r [M_r(2) - 2M_r(3) + M_r(4)]\left[\frac{1}{4}B_{rrrr} - \frac{1}{4}\binom{N_r}{2}^{-1}(A_{rrrr})^2\right]$$

$$+ \sum_{rs}{}' [M_r(1)M_s(1) - 2M_r(2)M_s(1) + M_r(2)M_s(2)]\left[\frac{1}{2}B_{rsrs} - \frac{1}{2N_rN_s}(A_{rsrs})^2\right] \ , \tag{135}$$

$$\begin{aligned}
\sigma^2([\vec{m}]:r^{-1}s^{+1}) = {} & M_r(1)[1 - M_s(1)] \times N_r(\epsilon_{rs})^2 + M_r(2)[1 - M_s(1)] \times 2\epsilon_{rs}A_{rrrs} \\
& + M_r(1)[M_s(1) - M_s(2)] \times 2\epsilon_{rs}A_{rsss} + [M_r(2) - M_r(3)][1 - M_s(1)] \times \tfrac{1}{2}B_{rrrs} \\
& + M_r(1)[M_s(1) - 2M_s(2) + M_s(3)] \times \tfrac{1}{2}B_{rsss} + M_r(2)[M_s(1) - M_s(2)] \times 2N_r^{-1}A_{rrrs}A_{rsss}\hat{\delta}_{rs} \\
& + M_r(3)[1 - M_s(1)] \times N_r^{-1}(A_{rrrs})^2\hat{\delta}_{rs} + M_r(1)[M_s(2) - M_s(3)] \times N_r^{-1}(A_{rsss})^2\hat{\delta}_{rs} \\
& + M_r(1)[1 - M_s(1)]\sum_t{}'[M_t(1) - M_t(2)] \times B_{rtst} + M_r(1)[1 - M_s(1)]\sum_t{}' M_t(1) \times 2\epsilon_{rs}A_{rtst} \\
& + M_r(1)[M_s(1) - M_s(2)]\sum_t{}' M_t(1) \times 2N_r^{-1}A_{rsss}A_{rtst}\hat{\delta}_{rs} + M_r(2)[1 - M_s(1)]\sum_t{}' M_t(1) \\
& \times 2N_r^{-1}A_{rrrs}A_{rtst}\hat{\delta}_{rs} + M_r(1)[1 - M_s(1)]\sum_t{}' M_t(2) \times N_r^{-1}(A_{rtst})^2\hat{\delta}_{rs} \\
& + M_r(1)[1 - M_s(1)]\sum_{tu}{}' M_t(1)M_u(1) \times N_r^{-1}A_{rtst}A_{rusu}\hat{\delta}_{rs} \ ,
\end{aligned} \tag{136}$$

$$\sigma^2([\vec{m}]:r^{-2}s^{+2}) = M_r(2)[1 - 2M_s(1) + M_s(2)] \times \tfrac{1}{4}B_{rrss} \ , \tag{137}$$

$$\sigma^2([\vec{m}]:r^{-2}s^{+1}t^{+1}) = M_r(2)[1 - M_s(1)][1 - M_t(1)] \times \tfrac{1}{2}B_{rrst} \ , \tag{138}$$

$$\sigma^2([\vec{m}]:r^{-1}s^{-1}t^{+2}) = M_r(1)M_s(1)[1 - 2M_t(1) + M_t(2)] \times \tfrac{1}{2}B_{rstt} \ , \tag{139}$$

$$\sigma^2([\vec{m}]:r^{-1}s^{-1}t^{+1}u^{+1}) = M_r(1)M_s(1)[1 - M_t(1)][1 - M_u(1)] \times B_{rstu} \ . \tag{140}$$

The summation symbol $\sum'$ in Eq. (136) indicates that the summation variables are distinct from r and s. If we add together the terms from Eqs. (135)–(140) we reproduce the results of Eq. (133). The separate terms have certain obvious vanishings; for example, any r^{-2} term vanishes for a configuration with less than two particles in orbit r. It should be clear that the widths are unaffected by the $(H \rightarrow \mathcal{H})$ transformation of Eq. (131). The $(r^{-1}s^{+1})$ and $(r^{+1}s^{-1})$ terms involve the same matrix elements of H but are not equal, because of an asymmetry arising from different occupancies; a way will be described in a later paper in which this can be used to give an inductive method for partial widths when we deal with more complicated group symmetries.

A familiar result emerges if one asks for the change in the centroid energy due to the addition of a nucleon in the rth orbit. Calculating the difference $\Delta\mathcal{E}_r$ between $\mathcal{E}([\vec{m}_1, \vec{m}_2, \ldots, \vec{m}_r + \vec{1}, \ldots, \vec{m}_l])$ and $\mathcal{E}([\vec{m}_1, \vec{m}_2, \ldots, \vec{m}_r, \ldots, \vec{m}_l])$, one finds via Eqs. (98), (99), and (129) that

$$\Delta\mathcal{E}_r = \epsilon_{rr} + \sum_t m_t W_{tr} \ , \tag{141}$$

a result entirely to be expected. Similarly, on adding a pair of particles in the same or different orbits we find, in an obvious notation,

$$\begin{aligned}
\Delta\mathcal{E}_{rr} &= 2\Delta\mathcal{E}_r + W_r \ , \\
\Delta\mathcal{E}_{rs} &= \Delta\mathcal{E}_r + \Delta\mathcal{E}_s + W_{rs} \ .
\end{aligned} \tag{142}$$

7. MOMENT RENORMALIZATIONS

Shell-model calculations being feasible only in rather small spaces, we are forced to restrict ourselves,

usually, to dealing with a small set of configurations, a particular class of particle-hole states, or to a set of representation subspaces of a group which defines an approximate symmetry of H (this latter being an extension of the notion of configurations). In this section we cast the configuration polynomials into forms relevant to the first two types of restriction.[31] The idea is to consider the subspace embedded in a larger one, whose effects on the widths we then take account of by permitting transitions to intermediate states which lie outside the smaller subspace, this then generating a width external to the original subspace.

As a minor example, if we consider $(d_{5/2})^m$, firstly as a subspace with variance $\sigma^2(\vec{m})$, and secondly as a complete space with variance $\sigma^2([\vec{m}, \vec{0}])$ [the zero occupancy being for the $(d_{3/2}, s_{1/2})$ orbits], we have

$$\sigma^2([\vec{m}, \vec{0}]) = \sigma^2(\vec{m}) + P^3(\vec{m}) \ . \tag{143}$$

Since the external-width polynomial must involve at least one particle in $(d_{3/2}, s_{1/2})$, it can have no quartic terms in m, being then a third-order polynomial as indicated. In fact, since $\sigma^2(\vec{m})$ and $\sigma^2([\vec{m}, \vec{0}])$ are both known, the explicit form of the external-width polynomial can be easily written down.

For the general case we should take account also of orbits which are inert because they are filled. Then dividing our l orbits into l_A active orbits, l_E inert empty orbits, and l_F inert full orbits, we may rewrite the polynomials of Eqs. (129) and (133) for configuration centroids and dispersions. Depending on whether orbit r belongs to class A, E, or F, the single-orbit polynomial $M_r(m_r)$ is unchanged, zero, or unity; the dependence in Eqs. (129) and (133) on the occupancies of the inert orbits is thereby eliminated and the polynomials originally in l variables become polynomials in l_A variables. The algebraic form of the resulting renormalized width polynomial is complicated and we do not write it here. The energy polynomial becomes

$$\mathcal{E}([\vec{N}_F|\vec{m}_A|\vec{0}_E]) = H_0 + \sum_\alpha N_\alpha \bar{\epsilon}_{\alpha\alpha} - \tfrac{1}{2}\sum_{\alpha\beta} A_{\alpha\beta\alpha\beta} + \sum_r M_r(1)\times N_r \bar{\epsilon}_{rr} + \sum_r M_r(2)\times\tfrac{1}{2}A_{rrrr} + \sum_{rs}{}' M_r(1)M_s(1)\times\tfrac{1}{2}A_{rsrs} \ . \tag{144}$$

Here the symbols r, s, range over the active (A) orbits, and α, β over the inert filled (F) orbits. The $\bar{\epsilon}$ quantities are given by

$$\bar{\epsilon}_{ij} = (\epsilon_{ij} + N_i^{-1}\sum_\beta A_{\beta i\beta j})\hat{\delta}_{ij} \ , \tag{145}$$

where i, j refer to any of the orbits.

The energies defined by Eq. (144) may be regarded as "renormalized" in the sense of the above discussion, and similarly for the variances. If, in them, we put to zero all the coefficients which make reference to the inert orbits (F, E) we are left with the unrenormalized quantities which take no account at all of the inert orbits. The renormalization effects on the centroid energies are, of course, trivial but this is not at all so for the variances.

The single-particle ϵ parameters enter in the renormalized quantities only in the $\bar{\epsilon}$ quantities of Eq. (145), which are obviously the Hartree-Fock energies (as defined by the original orbits, no variation having been made to produce the optimal results). The condition that a closed-core state $[\vec{N}_F|\vec{0}_A|\vec{0}_E]$ can be an eigenstate of H is that

$$\sigma^2([\vec{N}_F|\vec{0}_A|\vec{0}_E]) = 0 = \sum_{\alpha k}(\bar{\epsilon}_{\alpha k})^2\delta_{\alpha k} + \tfrac{1}{4}\sum_{\alpha\beta kl} B_{\alpha\beta kl} \ , \tag{146}$$

where the explicit form comes via the operation defined above. Since each term here is positive definite [see Eq. (97) for B], it must vanish separately. The vanishing of the $\bar{\epsilon}_{\alpha k}$ implies zero single-particle nondiagonal energies involving an occupied and an unoccupied orbit (the usual Hartree-Fock condition) while the vanishing of $B_{\alpha\beta kl}$ would imply the absence of two-particle–two-hole excitations in this representation. The energy of the HF state is then the centroid energy

$$\mathcal{E}([N_F|0_A|0_E]) = \sum_\alpha N_\alpha \bar{\epsilon}_{\alpha\alpha} - \tfrac{1}{2}\sum_{\alpha\beta} A_{\alpha\beta\alpha\beta} \ , \tag{147}$$

the usual result. Thus, if a HF calculation has been performed the quantity $(\frac{1}{4}\sum_{\alpha\beta kl} B_{\alpha\beta kl})^{1/2}$ computed in the HF basis is the width of the distribution of the HF ground state over the actual eigenstates of the system, and thus represents a measure of how close the HF ground state is to an eigenstate of the complete Hamiltonian. The HF energies also have the expected interpretation, as single-particle and single-hole energies, in terms of the differences between centroids. We have

$$\bar{\epsilon}_{rr} = \mathcal{E}([N_F|r^{+1}|0_E]) - \mathcal{E}([N_F|0_A|0_E]) , \tag{148}$$

$$\bar{\epsilon}_{\alpha\alpha} = \mathcal{E}([N_F|0_A|0_E]) - \mathcal{E}([\alpha^{-1}|0_A|0_E]) \tag{149}$$

in an obvious notation.

Finally we turn to the particle-hole truncation scheme in which one treats a subset of normally filled orbits as a vacuum whose excitations give the various particle-hole states. We could go back to the original Hamiltonian, make p$\rightleftharpoons$h transformations for the orbits filled in the vacuum, and then proceed just as above. It is often simpler, however, to introduce polynomials for holes instead of particles. The basic transformation (for the density operators) is given by Eq. (60) and this in turn gives for the polynomials of Eq. (130) the result

$$M_\alpha(k) = \sum_{t=0}^{k} (-1)^t \binom{k}{t} \tilde{M}_\alpha(t) , \tag{150}$$

where

$$\tilde{M}_\alpha(t) = \binom{h_\alpha}{t} \binom{N_\alpha}{t}^{-1} , \tag{151}$$

$h_\alpha = (N_\alpha - m_\alpha)$ being the number of holes in orbit α. We then find for a configuration $[\vec{h}|\vec{m}]$, with h holes distributed over the hole orbits and m particles over the particle orbits, that

$$\begin{aligned}\mathcal{E}([\vec{h}|\vec{m}]) = \mathcal{E}([\vec{0}|\vec{0}]) &+ \sum_r M_r(1) \times N_r \bar{\epsilon}_{rr} - \sum_\alpha \tilde{M}_\alpha(1) \times N_\alpha \bar{\epsilon}_{\alpha\alpha} + \sum_r M_r(2) \times \tfrac{1}{2} A_{rrrr} \\ &+ \sum_\alpha \tilde{M}_\alpha(2) \times \tfrac{1}{2} A_{\alpha\alpha\alpha\alpha} + \sum_{rs}{}' M_r(1) M_s(1) \times \tfrac{1}{2} A_{rsrs} + \sum_{\alpha\beta}{}' \tilde{M}_\alpha(1) \tilde{M}_\beta(1) \times \tfrac{1}{2} A_{\alpha\beta\alpha\beta} - \sum_{\alpha r} M_r(1) \tilde{M}_\alpha(1) \times A_{r\alpha r\alpha} ,\end{aligned} \tag{152}$$

where the particle-hole vacuum energy $\mathcal{E}([\vec{0}|\vec{0}])$ is given in terms of previously defined particle matrix elements, by Eq. (148). In particular, we find for the (1p-1h) and (2p-2h) configurations, written in terms of the average interaction energies of Eqs. (98) and (99),

$$\begin{aligned}&\mathcal{E}([\alpha^{-1}|r^{+1}]) - \mathcal{E}([0|0]) = \bar{\epsilon}_{rr} - \bar{\epsilon}_{\alpha\alpha} - W_{r\alpha} , \\ &\mathcal{E}([\alpha^{-2}|r^{+2}]) - \mathcal{E}([0|0]) = 2\bar{\epsilon}_{rr} - 2\bar{\epsilon}_{\alpha\alpha} + W_{rr} + W_{\alpha\alpha} - 4W_{r\alpha} .\end{aligned} \tag{153}$$

These intuitively obvious results, when coupled with the corresponding results for widths (which derive in the same way but whose explicit forms we do not give) will be of consequence in studying the structure of nuclei near closed shells. Renormalizations, as discussed in the first part of this section, will also be significant here.

8. SUMMARY AND FINAL REMARKS

We have discussed the essential ideas involved in the application of spectral-distribution methods to nuclear structure (and, indeed, to other many-particle systems). The distributions are characterized by their moments, expectation values of powers of the Hamiltonian averaged over subsets of states, and these become the central elements of the theory. A new technique, that of propagation throughout the lattice of subsets, has been introduced for the evaluation of moments in a certain class of cases, and in particular to write the configuration moments as polynomials in occupation numbers. These have been rearranged in ways corresponding to common vector-space truncations used in spectroscopic calculations, this focussing attention upon the difference between truncations of the operator whose moments are being considered and truncation of powers of the operator; the first of these is equivalent to a restriction of the space in a detailed calculation, while the second goes beyond that. Having explicit polynomials whose coefficients are Hamiltonian integrals, we shall be able, for example, to see which parts of the interaction are dominant in various parts of the total space. We have indicated a number of domains in which moment methods may be usefully applied; the following paper and others in the future will be concerned with that. It may turn out that a valuable use of these methods will be in the development of a kind of perturbation theory, based on moments, which will permit the extension of finite-space calculations.

Since we cannot look forward to dealing with high-order moments, it will be a requirement on the subspaces and operators with which we deal that the distributions be well described by a few low-order moments, this in turn requiring that they be close to normal. The experience has been that this is liable to be an excellent assumption, although a satisfactory theoretical justification for

it is not presently available. We rely instead on detailed study of examples, some of which have already been given[32] and others of which are given in the next paper. A very important aspect of the moment methods is that they display the explicit dependence of the quantities of interest on the Hamiltonian parameters and structure, at the same time reducing a highly nonlinear matrix problem to one whose nonlinearities are of low order; basic to this procedure is the assumption of near normality which in turn implies that the higher cumulants (which, for example, determine fluctuations in the distributions) carry only little of the interesting physics.

We mention finally that besides giving applications of the methods above, future papers will describe new methods which are particularly relevant for dealing with group symmetries and more complex representation subspaces, and will also discuss strength distributions for various processes.

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[1]I. Talmi and I. Unna, Ann. Rev. Nucl. Sci. 10, 353 (1960); A. de-Shalit, in *Nuclear Physics, Proceedings of the International School of Physics, "Enrico Fermi," Course XXIII,* edited by V. F. Weisskopf (Academic Press Inc., New York, 1963).

[2]G. E. Brown, *Unified Theory of Nuclear Models and Nucleon Forces* (North-Holland Publishing Company, Amsterdam, The Netherlands, 1967), 2nd ed.; M. Baranger, in *Nuclear Structure and Nuclear Reactions, Proceedings of the International School of Physics, "Enrico Fermi," Course XL,* edited by M. Jean and R. A. Ricci (Academic Press Inc., New York, 1969).

[3]I. Kelson and C. A. Levinson, Phys. Rev. 134, B269 (1964); G. Ripka, in *Advances in Nuclear Physics,* edited by M. Baranger and E. Vogt (Plenum Press, Inc., New York, 1968), Vol. 1; D. Rowe, Rev. Mod. Phys. 40, 153 (1968).

[4]J. B. French, in *Nuclear Structure,* edited by A. Hossain (North-Holland Publishing Company, Amsterdam, The Netherlands, 1967), and earlier references given therein. See also P. Löwdin, Rev. Mod. Phys. 39, 259 (1967).

[5]States regarded as remaining inert, either filled or empty, would not usually be counted in $\{N\}$. In some cases some of the subsets of $\{N\}$ would be better describable in terms of holes, in which case we could use m to indicate the number of active fermions, noting, of course, that this number does not necessarily remain constant and that H is not necessarily fermion-number conserving. Modifications to look after these things will be simple.

[6]The point of this is that we could instead define H to be the projection into $\vec{\mathfrak{N}}$ of an operator defined in the general many-fermion-Hilbert space. Then we would have a notational ambiguity when writing H^p. As things stand now we proceed as if single-particle states outside the orbital space $\{N\}$ did not "exist." Of course, the relationship between projections of powers of H and powers of projections of H is the heart of the matter as far as general many-body problems are concerned, and we shall approach this later by considering $\{N\}$ to be a subspace of a larger orbital space $\{N'\}$.

[7]C. E. Porter, *Statistical Theories of Spectra: Fluctuations* (Academic Press Inc., New York, 1965).

[8]For representations of different dimensionalities, the partial-width matrix is not symmetrical, as shown by Eq. (12). But this simply corresponds to the fact that, if the dimensionalities are very different, the smaller representation could be completely fragmented, thereby losing its identity, without this having any appreciable effect on the individual states of the larger representation.

[9]J. Griffin, Phys. Rev. Letters 17, 478 (1966).

[10]J. B. French, Phys. Letters 26B, 75 (1967).

[11]J. B. French and L. S. Hsu, Phys. Letters 25B, 75 (1967).

[12]J. B. French, Phys. Letters 23, 248 (1966).

[13]Remember that $\binom{a}{b}$ is defined for a negative as well as positive, and

$$\binom{-a}{b} = (1)^b \binom{a+b-1}{b} = (-1)^{a+b} \binom{-b-1}{-b-a} .$$

[14]I.e., the N-particle state (in which all single-particle states are filled). We borrow the term from L. C. Biedenharn.

[15]In such light nuclei, and when we span a large domain of A we must expect variations in the effective interactions due, among other things, to nuclear size effects. Taking input data from both ends of the domain tends to minimize the effects which these variations have on the calculated centroid energies; whether this is a good thing or bad is another matter.

[16]S. Hinds and R. Middleton, Nucl. Phys. 84, 651 (1966).

[17]We assume that we deal with real vector spaces of operators so that the matrix elements in Eq. (26) are real.

[18]I.e., commute or anticommute depending upon the particle numbers involved.

[19]Note carefully that the m-hole trace operator $\tilde{\rho}(\vec{m}, \vec{\alpha}) = \sum Z_\alpha^\dagger(m) Z_\alpha(m)$ is not at all the same as the $(N-m)$-particle operator.

[20]The subscript c is then redundant and we shall usually omit it. Note, as a point of notation, that $Z_{\alpha_c}(k)$ is a state operator for k particles, *not* for $(N-k)$. Note also that $Z_{\alpha_c}(N-m) \neq \tilde{Z}_\alpha(m) Z(N)$; we do have though that $Z_{\alpha_c}(N-m)$ is the lowest-rank part [the $(A)^k$ part] in the normal expansion of $\tilde{Z}_\alpha(m) Z(N)$.

[21]Equations (42) and (43) will reproduce the elementary result of Eq. (13). A combinatorial derivation of Eq. (43)

will be found both simple and instructive.

[22]If the subspace decomposition allows simple propagation, Eqs. (45) and (46) are valid for all operators $O(\vec{k})$. It is easily seen that if this should not be so, we would still have propagation of traces for those operators whose form is that of Eq. (46), behaving as a multiple of unity in every subspace. This should be remembered for those equations ahead in this section which are written for operators O. On the other hand, equations written explicitly for density operators [e.g., Eq. (52)] are valid for arbitrary (disjoint) decompositions.

[23]While the density operator ρ is analogous to the elementary Green's function of electrostatics which gives potentials in terms of charges, ρ_u corresponds to the more sophisticated function which gives potentials in terms of surface potentials.

[24]The right-hand side of Eq. (53) involves "higher" subspaces (with respect to particle number) than $(\vec{t},\vec{\gamma})$ itself, but if we take $t \geq N/2$, these higher subspaces are, of course, simpler. Even so, Eq. (53) does not yield an inductive method for constructing the ρ operators, since $\rho(\vec{t},\vec{\gamma})$ appears on both sides.

[25]G. C. Rota, Z. Wahrscheinlichtkeitstheorie 2, 340 (1964).

[26]The criterion for linear independence of a net is that the determinant of the propagating coefficients should not vanish. It follows from Eq. (49) that the defining net is linearly independent.

[27]Square brackets define a "vector" in l dimensions. Note that $\{N\} \equiv \vec{1}$ and $\{[N]\} \equiv [\vec{1}]$. For a $[\vec{k}'] \rightarrow [\vec{k}]$ operator, as in Eq. (22), we shall often write $O([\vec{k};\vec{k}'])$, and shall as well often write $O([\vec{k};\vec{k}])$ as $O([\vec{k}])$.

[28]J. Kim, private communication.

[29]J. B. French, in *Many-Body Description of Nuclear Structure and Reactions, Proceedings of the International School of Physics, "Enrico Fermi," Course XXXVI, 1966,* edited by C. Bloch (Academic Press Inc., New York, 1966).

[30]We write $K \equiv H^2$ to avoid an ambiguity. According to our notation $H^2(t)$ should stand for $[H(t)]^2$, the squares of the t-particle part of H, while $K(t)$ is the t-particle part of the square of H.

[31]More complex group structures will be considered in later papers.

[32]F. S. Chang, J. B. French, and K. F. Ratcliff, Phys. Letters 23, 251 (1966).

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Applications of Spectral Distributions in Nuclear Spectroscopy*

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The energy moments of spectral distributions are used to investigate the structure of spectroscopic calculations. Eigenvalue distributions are used to predict energy spectra, which are compared with the results of matrix diagonalization. The nature of the corresponding eigenvectors is similarly analyzed. The propagation of moments for scalar and configuration distributions is illustrated throughout the *sd* shell. These scalar moments are then used to estimate the trend in theoretical binding energies for these nuclei and in turn are compared with empirical data. Finally, we investigate the dependence of the energy and wave function of the ground state of O^{16} upon the vector space underlying a theoretical calculation. The unrenormalized Kuo-Brown matrix elements are employed in this analysis, and the role of multiple particle-hole excitations is discussed.

I. INTRODUCTION

The concepts of spectral distributions, of operator averaging, and the propagation of such averages through a sequence of subspaces have been the subject of recent investigations.[1-6] In this paper we apply these ideas to a number of examples that are closely related to conventional nuclear spectroscopy. The techniques which we develop below are founded on the moments of spectral distributions, i.e., the averages of powers of the Hamiltonian over various subspaces of the complete many-particle space. One may adopt various attitudes towards these moments. They may be regarded as measures of the average behavior of the Hamiltonian in various subspaces and then be used to study various formal problems. Alternatively they may be used in a fashion that is complementary to conventional spectroscopy in which one sets up and diagonalizes the Hamiltonian matrix in a representation generated by a finite number of single-nucleon states. This latter attitude is adopted in this paper. The spectral moments are used to make predictions of spectroscopic details for spaces that are too large for conventional matrix analysis. The general quality of these predictions may be assessed by working in smaller spaces in which comparison with exact diagonalization is