STATISTICAL SPECTROSCOPY

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ABSTRACT

A review is made of some recent developments in statistical spectroscopy.

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Instead of solving the equations of motion, as one does by matrix diagonalization, one can apply standard methods of statistical mechanics, adapted to the finite direct-product (shell-model) spaces encountered in spectroscopy. In place of the partition function it is better to calculate (as a function of the system parameters) the eigenvalue density, which is its inverse Laplace transform and carries therefore the same information; it is moreover directly measureable for parameter values relevant to the system.

In a many-particle asymptotic limit, through the action of a central-limit theorem (CLT) the smoothed (fluctuation-free) density for all realistic Hamiltonians takes on a characteristic form[1] defined by a few moments (traces of low powers of H, in particular the centroid and variance). Secular deviations from the characteristic form can be calculated similarly. On the other hand the fluctuations (deviations from the smoothed form) cannot be treated in this way but are calculated instead by averaging over an ensemble of Hamiltonians[2]. The observable fluctuations, such as those found in slow-neutron reactions, are of a relatively simple type, describable[3] in terms of a two-point correlation function. It should be noted that the statistical operations used involve both spectral averaging and ensemble averaging. The success of the former is due to the great power of the CLT, even for interacting particles, which gives a large-scale rigidity to the smoothed density; the success of the latter is due to an ergodic behavior of the ensembles used and a remarkable microscopic (level-to-level) rigidity of the spectrum, first discussed by Dyson and Mehta[4], but whose origins go back to the level repulsion of von Neumann and Wigner[5]. These mechanisms are effective over the entire periodic table and over the complete spectrum even into the ground-state domain (as is observed both empirically[6] and by Monte-Carlo calculations, and the reason for which is by now well understood).

In conventional statistical mechanics it is essential that the ensemble be ergodic so that the results of ensemble averaging can be taken as identical with the results of time averaging (along the phase-space orbit of the system). Similarly here the equivalence of the fluctuation results with those which would emerge from spectral averaging (if that could be done) requires an ergodic behavior of the ensemble. This behavior which has in the past been observed in Monte-Carlo calculations has recently[7] been proved analytically for the standard ensembles. The ergodicity which obtains is very strong and "locally generated" so that the ensemble results are relevant to averaging over only a small segment of the spectrum, exactly what is called for in applications.

Shell-model spaces admit many symmetries, the most important of which correspond to subgroups of the basic group U(N) of unitary transformations in the space spanned by the single-particle states, N in number. A corresponding partitioning of the model space according to irreducible representations of the subgroup, or set of subgroups, gives both increased accuracy

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in the calculations and methods for studying the goodness of the symmetries. Partitioning of the model space gives rise to partitioning of the moment traces and hence to a representation of the density as a *linear* superposition of subspace densities (which will in general no longer correspond individually to eigenvalue densities). Linearity here does *not* imply that the subspaces are treated independently, which would be a very bad approximation; the interaction between subspaces shows up in lowest order in the fact that the variance for one distribution has contributions from excitations which connect that one with any other. We find indeed a hierarchical classification of the interactions, the maximum complexity depending on the order of the moments which are needed to fix the distributions.

The smoothed level density, and its decomposition by symmetries (configuration, isospin, angular momentum and others) are of major interest in themselves. Approximate binding energies and low-lying spectra derive from the density via a correspondence between the smoothed distribution function, defined for a density ρ by $F(x) = \int_{-\infty}^{x} \rho(x')dx'$, and the "staircase" function which represents the exact distribution. Many calculations of these kinds have been made[8,9].

Other quantities come by parametric differentiation and related operations on the density function. For the expectation value of an operator G

$$d(m)\langle E|G|E\rangle = \rho^{-1}(E)T_r^{(m)}\{G\delta(H-E)\} = -\rho^{-1}(E)\left[\frac{\partial F_\alpha(E)}{\partial\alpha}\right]_{\alpha=0} d(m) \qquad (1)$$

which derives[10] from the response of the system under $H \to (H + \delta\alpha \cdot G)$. Here F_α is the distribution function for the Hamiltonian $(H + \alpha G)$ and all densities ρ are normalized to unit integral. A natural expansion of the intermediate form here in terms of the orthonormal polynomials $P_\mu(E)$, defined by the density as weight function so that $\int P_\mu(E)P_\nu(E)\rho(E)dE = \delta_{\mu\nu}$, gives an expansion which is strongly convergent "to within fluctuations"

$$\langle E|G|E\rangle = d^{-1}(m)\sum_\mu P_\mu(E)\cdot T_r^{(m)}\{GP_\mu(H)\} \xrightarrow{CLT} d^{-1}(m)\left[T_r^{(m)}(G) + \frac{(E-\bar{E})}{\sigma^2} T_r^{(m)}G(H-\bar{E})\right] \qquad (2)$$

where $T_r^{(m)}$ is the trace over the d(m)-dimensional space. In the last form $\bar{E},\sigma^2$ are the spectral centroid and variance and we have taken the CLT limit which then gives linearity in the energy as the characteristic form for smoothed expectation values. One finds similarly that transition strengths are asymptotically bilinear in the energies (linear both in the starting and final energies). These results have been used in the calculation of occupancies[11], spin-cut-off factors[8,12], β-decay strengths[13] and in sum rules for electromagnetic transitions[10,14]; modifications of them are being used for studying effective interactions[15]. Strength and expectation-value fluctuations are treated via ensemble averaging which leads to the Porter-Thomas distribution and various extensions of it. Finite-response results for the density are also of interest, while infinitesimal response for the ensemble average of the product of two densities leads very directly to a theory for the (two-point) energy-level fluctuations[3].

The linear asymptotic form[2] for the expectation value follows immediately from the fact that the density (since it has a characteristic form) strongly resists shape deformations as we test its response by $H \to H + \alpha G$. But, ignoring the centroid whose "action is very simple",we see then that

everything then is determined asymptotically by a variance (a number of them for a partitioned space). The variance however defines a norm and hence a unitary geometry in which operator magnitudes are expressed in terms of the standard unitary norm

$$||G||^2 = d^{-1} T_r^{(m)}(G^+G) \tag{3}$$

The effectiveness of this geometry, which gives precise definitions of orthogonality, projection (e.g. how much Q·Q is contained in H acting in a given space) and so forth, is then guaranteed by the CLT. The linear form in (2) then simply transcribes into the energy domain a model-space scalar product, or correlation coefficient, of the two operators G and (H-E). Many of the other forms encountered in statistical spectroscopy have similar direct geometrical interpretations. These geometrical considerations have been recently applied[16] to constructing Casimir-operator models for realistic Hamiltonians.

Since all of the relevant information in the spectroscopic space is expressed in terms of many-particle traces, the question arises of how such traces may be calculated. For the simplest possible case, that of a k-body operator in an unpartitioned m-particle space, one might guess that

$$\left[\text{Trace}^{(m)}\, G(k)\right] \sim \left[\text{Trace}^{(k)}\, G(k)\right] \times \tag{4}$$
$$\times\left[\text{no. of ways in which a k-particle subspace } \{k\} \text{ can be realized in } \{m\}\right]$$

in which the first factor is the single necessary piece of "input" information, while the second (whose value is $\binom{N-k}{N-m}$) *propagates* that piece of information to the more complicated spaces. This is indeed the correct result. An extension of it applies moreover in immensely more complicated cases, in subspaces defined by U(N) subgroups, and to operators of mixed particle rank and non-scalar nature. As long as the subspaces are defined in terms of group representations a factoring analogous to that in (4) obtains[17] and propagates the input information to the parts of the model space where it is needed. The propagators themselves are traces of operators which, by construction, are scalars with respect to the subgroup (or the smallest subgroup in the case of a subgroup chain) so that the problem of explicitly constructing them reduces to a much studied group-theoretical problem, that of cataloging and constructing the polynomial invariants. In some cases this is a simple operation, in others not so; but in all cases there appear to be physically significant approximations (for "dilute" systems for example). The methods used indeed appear simpler than those used heretofore by the group theorists so that statistical spectroscopy makes a contribution in that mathematical domain.

These methods are not applicable for fluctuations, for which however the propagation seems extremely simple. The results from the simplest ensembles seem to apply everywhere except in the presence of conserved symmetries or strong collectivities, so that the fluctuations carry very little information. This no longer seems surprising but there is in fact no real understanding of why it should be true.

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