2-17-1975

Polynomial expansions for excitation strengths

J. P. Draayer
University of Rochester

J. B. French
University of Rochester

V. Potbhare
University of Rochester

S. S.M. Wong
University of Toronto

Recommended Citation

Draayer, J., French, J., Potbhare, V., & Wong, S. (1975). Polynomial expansions for excitation strengths. *Physics Letters B, 55* (3), 263-266. https://doi.org/10.1016/0370-2693(75)90595-X

POLYNOMIAL EXPANSIONS FOR EXCITATION STRENGTHS*

J. P. Draayer, J. B. French, V. Potbhare

Department of Physics and Astronomy,

University of Rochester, Rochester, N.Y. 14627

and

S. S. M. Wong

Department of Physics,

University of Toronto, Toronto, Canada

MASTER

Rapidly convergent expansions for the strength function of an excitation in a many-particle model space are given in terms of orthogonal polynomials defined by the state or partial state densities of the system. Convergence is assured in a wide range of circumstances by the operation of a central limit theorem. Level-to-level fluctuations are in many cases small, their automatic elimination in the statistical smoothing generated by truncating the series then leading to only small errors.

DISCLAIMER

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

The microscopic strength function (BE2, spectroscopic factor, etc.) associated with an excitation operator O is defined as

$$R(W',W) = \left| \langle W'|O|W \rangle \right|^2 \qquad (1)$$

where $|W\rangle$, $|W'\rangle$ are Hamiltonian eigenstates with energies W, W' (additional quantum numbers being suppressed for convenience). Depending on the nature of the excitation, the initial and final states may be taken as belonging to the same model subspace (electromagnetic transitions between states of the same spin and parity for example), or different ones (as with particle transfer). The direct evaluation of $R(W',W)$ has not been feasible, except in special cases, because of the complexity of the wave functions required; in most cases the same has been true for the sum rules associated with O, which determine strength moments as expectation values of moment operators, $M_p = O^+H^PO$,

$$M_p(W) = \langle W|M_p|W \rangle = \sum_{W'} R(W',W)(W')^P . \qquad (2)$$

Here M_o is the total strength originating with eigenstate $|W\rangle$, M_1/M_o is its centroid, and so on.

We introduce in this paper a polynomial expansion for $R(W',W)$ which is rapidly convergent for a wide range of excitation operators and model spaces, even for spaces of indefinitely large dimensionality, and which nowhere requires the explicit construction of model eigenstates. Basically $R(W',W)$ is derived by testing statistically the response[1] of the system, as measured by its state density, when the Hamiltonian is modified by adding to it an appropriate function of the

excitation operator[+]. Shape deformations of the densities (which give rise to polynomials in the strength expansion of order 2 and higher) are however inhibited by the operation, in the model space, of a central limit theorem[3] (which essentially fixes the shape). The higher the polynomial order the stronger the inhibition; hence convergence! The polynomials of order 0,1 which arise from the translation of the density and a change of scale,are uninhibited and as a consequence the strengths in the central region of the spectra are linear in the energies, as then also are the sum-rule quantities $M_p(W)$. The linearity for the low-order sum rules in particular often extends over the entire spectra.

The eigenstate density, the strength moments, and the strength itself can all be expressed in terms of traces over the model space. Writing $<G>^m = d^{-1}(m) \times \text{Trace } (G)$ where $d(m)$ is the dimensionality of the m-particle space, and normalizing the density to unity, $\int \rho(x)dx = 1$, we have by simple manipulations

$$\rho(W) = d^{-1}(m) \sum_i \delta(W_i - W) = d^{-1}(m) \text{ Trace } \delta(H-W) = <\delta(H-W)>^m \quad (3)$$

$$\rho(W)M_p(W) = <0^+ H^p 0 \delta(H-W)>^m \quad (4)$$

$$\rho(W')R(W',W)\rho(W) = <0^+ \delta(H-W') 0\delta(H-W)>^m \quad (5)$$

Associated with the non-negative-definite density $\rho(W)$ is a unique set of orthonormal polynomials $P_\mu(W)$ which satisfy closure and are defined[4] in terms of the density moments $M_\nu = <H^\nu>^m = \int \rho(W)W^\nu dW$;

[+]A quite different response theory which does not make use of statistical averaging methods has been used by Bertsch and Tsai[2].

we have

$$\int P_\mu(W) \; P_\nu(W) \; \rho(W)dW = \delta_{\mu\nu} \tag{6}$$

$$\rho(W) \sum_\mu P_\mu(H) \; P_\mu(W) = \delta(H-W) \tag{7}$$

$$[D_\mu D_{\mu-1}]^{\frac{1}{2}} \; P_\mu(W) \;\; = \;\; \begin{vmatrix} 1 & M_1 & \cdots & M_\mu \\ M_1 & M_2 & \cdots & M_{\mu+1} \\ \vdots & \vdots & & \vdots \\ M_{\mu-1} & M_\mu & \cdots & M_{2\mu-1} \\ 1 & W & \cdots & W^\mu \end{vmatrix} \tag{8}$$

where D_μ is the determinant of (8) with each W^ν replaced by $M_{\mu+\nu}$.
The first two polynomials, for example, are simply $P_o(W) = 1$ and
$P_1(W) = (W-E)/\sigma$ where $E = M_1$ is the energy centroid and $\sigma = \{M_2 - M_1^2\}^{\frac{1}{2}}$
is the width. The moments M_ν, $0 \le \nu \le 2\mu$ suffice to define uniquely
all polynomials through order μ. For a Gaussian density distribution
the polynomials are Hermite; thus for $\rho(W) = (2\pi\sigma^2)^{-\frac{1}{2}}\exp[-(W-E)^2/2\sigma^2]$,
$P_\mu(W) = (\mu!)^{-\frac{1}{2}} \text{He}_\mu[(W-E)/\sigma]$ where $\text{He}_\mu(z) = 2^{-\mu/2} H_\mu(z/\sqrt{2})$. For a
discrete density distribution the number of polynomials is finite and
equal to the number of distinct eigenvalues. In what follows, all
distributions will be written as if continuous; a transcription to a
discrete formalism can be made by inspection.

Using (7) in (4,5) yields polynomial expansions, the first of which
we write for a general operator K, not necessarily the moment operator M_p,

$$K(W) = \sum_\mu <K \; P_\mu(H)>^m \; P_\mu(W) \tag{9}$$

$$R(W',W) = \sum_{\mu,\nu} <0^+ \; P_\mu^\dagger(H) \; 0 \; P_\nu(H)>^m \; P_\mu^\dagger(W')P_\nu(W) \tag{10}$$

Both results are formally exact and have the characteristic convergence of a Fourier expansion. Using (10) to evaluate $\int R(W',W)P_\mu(W')\rho(W')dW'$ gives (9) with $K = O^\dagger P_\mu(H)O$, the polynomial-moment operator.[+] Geometrically the expansion (9) amounts to projecting K along directions defined by the polynomial operators $P_\mu(H)$ which are orthogonal with respect to the (Euclidean) norm supplied by the trace. The polynomials defined by ρ are the natural ones for this expansion because the density enters into the traces which define the moments; expansions in terms of other polynomial sets are possible (and that in terms of Hermite polynomials has already been given[1]) but, using them leads in (9) to a ratio of the two defining densities which is often difficult to deal with.

Alternatively, (9) may be deduced from the first-order change in the density which is generated when $H \rightarrow H + \alpha K$. Then, as indicated above, the convergence follows from the convergence of the density to Gaussian[3] as particle number increases. This convergence has been proved by showing: (1) that for reasonable ensembles of k-body interactions the ensemble-averaged density goes rapidly to Gaussian as particle number increases; and (2) that, while members of the ensemble do not give the same spectra, the member-to-member density deviations, and hence the deviations from the ensemble average, go to zero in the same limit. If the W',W spaces are distinct we encounter two polynomial sets as indicated, deriving from the two densities. Note

---

[+]At this stage we can, by integrating separately over the ranges $W' \leq W$ and $W' \geq W$, decompose the sum-rule quantities into exothermic and endo-thermic parts which is often required in the analysis of data, always in the treatment of cascades.

that, by using (9), we can rewrite (10) in terms of polynomial-weighted linear combinations of sum-rule quantities, so that we can infer from the rapid convergence of the single series a corresponding convergence for the double one.

Since the polynomials oscillate more and more rapidly as their order increases, truncation of the series expansions is equivalent to a statistical smoothing of $K(W)$ and $R(W',W)$. The first two terms of (9) for example,

$$K(W) \approx <K>^m + <K(H-E)/\sigma>^m (W-E)/\sigma , \qquad (11)$$

give a representation of $\hat{K} = K - <K>^m$ in terms of $<\hat{K}(H-E)>^m = <K(H-E)>^m$ which, when divided by $\{<\hat{K}^2>^m\}^{1/2}\sigma$ can either be interpreted geometrically as the cosine of the angle between the two operators, or statistically as a correlation coefficient. If the operators are uncorrelated $K(W)$ is constant over the spectrum, and, if strongly correlated or anti-correlated, it rises or falls rapidly as the energy increases (the rates in all cases being proportional to the correlation coefficient).

The technical problem in making use of (9,10) is the evaluation of traces. The densities and the polynomials are defined by the moments $<H^\nu>^m$, the former by a Gram-Charlier series, and the latter via (8). Analytic results and programs for these moments are presently available up to fourth order; it would usually not be profitable to go much beyond this in the G.C. series. In principle, moments of this order determine the polynomials only up to second order; in practice one can usually go to fourth order by assuming a vanishing of the higher-order cumulants. Some results and programs are available also for the

strength moments. For single-nucleon transfer, present results are adequate for certain sum-rules up to third or fourth order and almost adequate for strengths to second order ($\mu_{max} = \nu_{max} = 2$ in (7)). For two-nucleon transfer and electromagnetic or other hole-particle excitations only first order is available. But modest extensions of these limits are feasible and are now being undertaken. A very helpful feature which has shown up in the detailed examples so far considered is that both the secular energy variation, and fluctuations about the secular average, are much milder for renormalized moments, such as the centroid M_1/M_o, than for the moments themselves, so that good accuracy in M_o, which is the easiest to achieve, is well rewarded.

Even with this simplification a problem remains in calculating terms of high-enough order to achieve accuracy in large model spaces, including the accuracy required for determining the ground state energies so as to properly locate things in the spectra. A straightforward solution is provided by configuration partitioning of the space, this leading to expansions which should be effective in spaces of arbitrarily large dimensionality and over the whole range of the spectrum including the ground-state domain. Under a partitioning of the single-particle space into "orbits" (which need not be spherical) the m-particle space decomposes into configurations defined, as usual, by assigning numbers of particles to the various orbits, $m \to \sum \underline{m}$ say, where $\underline{m} \equiv [m_1, m_2, \ldots]$ defines a configuration. The trace which defines $R(W', W)$ decomposes similarly; and the density also. Moreover, the excitation operator may be decomposed into parts, each of which connects any state in one configuration only with states of one other. We write $O = \sum O$ (q)

where $q \equiv [q_1, q_2 \ldots]$, with q_i specifying the number of particles which O creates in the i'th orbit; in most cases O is presented to us already in this form. We have now, for the proper trace $(= d(m) < \quad >^m)$

$$<<O^+ \delta(H-W') O \delta(H-W)>>^m = \sum_{\underline{m}, \underline{q}} <<O^+(q) \delta(H-W') O \delta(H-W)>>^{\underline{m}} \qquad (12)$$

in which there is a configuration decomposition of both spaces, that for the W' space deriving from $\underline{m} \times \underline{q} = \underline{m}' = (\underline{m} + \underline{q})$. Since a configuration density is to some extent localized in the spectrum we are led naturally to introduce orthonormal polynomial sets for each configuration and to use the appropriate pair for each $(\underline{m}, \underline{q})$ term in (12). Since a given term is now not required to give results over the entire spectra, much lower polynomial orders are adequate, and, since for the same order, configuration traces are no harder to evaluate than the "scalar" ones, everything becomes remarkably simpler. In practice it should be almost always satisfactory to use Gaussian densities and (Hermite) polynomials up to and including second order. The resulting strength function is now

$$R(W', W) = \sum_{\underline{m}, \underline{m}'} \gamma(\underline{m}', \underline{m}; W'W) \sum_{\mu, \nu} < O^+(\underline{m}' - \underline{m}) P_\mu^{\underline{m}'}(H) O P_\nu^{\underline{m}}(H) >^{\underline{m}} P_\mu^{\underline{m}'}(W') P_\nu^{\underline{m}}(W)$$

$$\gamma(\underline{m}', \underline{m}; W'W) = d(\underline{m}) \rho^{\underline{m}'}(W') \rho^{\underline{m}}(W) / d(m) \rho'(W') \rho(W) \qquad (13)$$

in which γ is the natural branching ratio. This result is also formally exact and can be written in a variety of ways. It exhibits interesting correlation structure. Its lowest-order terms give the most elementary schematic treatment of the strengths; increasing the order, and allowing for more intermediate excitations, we can see, where that is relevant,

the build-up of collectivity. The sum rules follow from an integration on (13) or by a configuration decomposition of (10). We leave for a more detailed treatment, and for the applications, a discussion of the fluctuations which we have eliminated by truncating the polynomial series, as well as the multipole extension of the polynomial theory which gives results for the strength connecting states of specified (J,T).

References

1. F. S. Chang and J. B. French, Phys. Lett. 44B (1973) 131.

2. G. F. Bertsch and S. F. Tsai, to be published in Physics Reports.

3. J. K. Mon, Princeton University Thesis, 1973; A. Gervois, Nucl. Phys. A184 (1972) 507; J. B. French, Rev. Mex.Fís. 23 (1974) 189, and references therein.

4. H. Cramer, Mathematical Methods of Statistics, (Princeton, 1946); G. Szego, Orthogonal Polynomials, (American Mathematical Society Colloquium Publications, Vol. XXIII, 1939).