SOME STATISTICAL ASPECTS OF SHELL-MODEL CALCULATIONS

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Initially the growth of the dimensionality of the shell-model configuration spaces was rather modest, but recently we have seen how the possibilities of the modern computers have rapidly led to model spaces of immense size. Nevertheless these spaces are the result of some truncation procedure, or should one say truncation choice since usually a firmly grounded recipe for the truncation is lacking.

As an alternative to the detailed microscopic approach to nuclear spectroscopy it was suggested by J.B. French [1] to consider spectral distributions instead. Inspection of the results of large-scale shell-model calculations showed that, e.g., the eigenvalue distributions can be represented in good approximation by Gaussians. It must be remarked that for a system of m noninteracting particles the Gaussian eigenvalue distribution is a direct consequence of the central limit theorem for large values of m.

When the (smoothed) eigenvalue density, $\rho(E)$, is well approximated by a Gaussian distribution, only a few of its lower moments should suffice for a description. Thus it is desirable to have at one's disposal methods to calculate these few moments without a complete diagonalization, or rather a complete evaluation, of the energy matrix.

The first moment or centroid

$$M_1 = \int \rho(E)\, E\, dE = \frac{1}{N}\sum_{j=1}^{N} \int \phi_j^*(\vec{r})\, H\, \phi_j(\vec{r})\, d\vec{r} = \frac{1}{N}\sum_{j=1}^{N} \langle \phi_j | H | \phi_j \rangle \qquad (1)$$

yields no problems as it is given essentially by the trace of the Hamiltonian H in an arbitrary set of basis functions $\phi_j(\vec{r})$ $(j = 1, 2, \ldots, N)$:

For an evaluation of the second moment or rather the variance

$$\sigma^2 = \int\rho(E)\ (E-M_1)^2\ dE = \frac{1}{N}\sum_{j=1}^{N} \langle\phi_j|(H-M_1)^2|\phi_j\rangle =$$

$$= \frac{1}{N}\sum_{j,k=1}^{N} \langle\phi_j|(H-M_1)|\phi_k\rangle\ \langle\phi_k|(H-M_1)|\phi_j\rangle \tag{2}$$

one needs, however, the complete energy matrix.

For a truncation of the configuration space spanned by the state vectors $\phi_j(\vec{r})$ ($j = 1, 2 \ldots, N$) one divides the configuration space into a model space P and a neglected space Q, and tries to find or to construct effective operators to be used in space P. For this procedure to be successful it is necessary that the influence of space Q on the processes considered (and described in space P) is weak.

The total width of the energy density, σ, can be divided into an internal width σ_P and an external width σ_Q according to the equations

$$\sigma_P^2 = \frac{1}{N}\sum_{\substack{j\epsilon P\\ k\epsilon P}} \langle\phi_j|(H-M_1)|\phi_k\rangle\ \langle\phi_k|(H-M_1)|\phi_j\rangle \tag{3}$$

and

$$\sigma_Q^2 = \frac{1}{N}\sum_{\substack{j\epsilon P\\ k\epsilon Q}} \langle\phi_j|H|\phi_k\rangle\ \langle\phi_k|H|\phi_j\rangle,\ \text{which imply} \tag{4}$$

$$\sigma^2 = \sigma_P^2 + \sigma_Q^2. \tag{5}$$

For a proper truncation, e.g., the ratio σ_Q/σ should be small [2]. Also, from the density $\rho_\alpha(E)$, defined by its moments in eqs.(1) and (2) and evaluated for a particular subspace α, one can derive [3] a measure for the relative contribution of that subspace to the energy spectrum below some energy E.

Moreover, the internal and external widths may indicate a way to renormalize the effective interaction in the model space.

Hence it would be extremely useful for the practice of shell-model calculations to have a feasible algorithm for the computation of the width σ and partial widths σ_P and σ_Q, that avoids a numerical evaluation of the complete energy matrix $<\phi_j|H|\phi_k>$ and that can be used in the customary j-j coupling scheme.

And, if one continues wishful thinking, a truncation procedure that also takes into account the strength distribution of electromagnetic transitions, divided over P-space and Q-space, could avoid the introduction of large effective charges or the strong renormalization of magnetic transition operators.

Not everything turns Gaussian, however, in large-scale shell-model calculations. The distribution of the amplitudes of the eigenvector components of a large-scale shell-model Hamiltonian is strongly peaked near the region of small values of the amplitudes and the shape is certainly not Gaussian, but more complicated.

Let the eigenvector ψ_i of the Hamiltonian H be expanded in the basis $\{\phi_\alpha\}$ $(\alpha = 1,2,\dots,N)$

$$\psi_i = \sum_{\alpha=1}^{N} c_{\alpha i}\, \phi_\alpha \quad (i = 1,2,\dots,N). \tag{6}$$

For a fixed eigenvector ψ_i one can plot the values of the amplitudes $|c_{\alpha i}| = |<\phi_\alpha|\psi_i>|$ against the values of the diagonal matrix elements $H_{\alpha\alpha} = <\phi_\alpha|H|\phi_\alpha>$. One then observes a secular variation $\overline{|c_{\alpha i}|}$ and fluctuations of the actual values of the amplitudes $|c_{\alpha i}|$ about the average. These fluctuations can be described in terms of the Porter-Thomas assumption: the coefficients $c_{\alpha i}$ show locally, i.e. for some small neighbourhood of $H_{\alpha\alpha}$, a normal distribution with zero mean.

The distribution of the diagonal matrix elements $H_{\alpha\alpha}$ is given in good approximation by a Gaussian

$$\rho_o(H_{\alpha\alpha}) = \frac{N}{\sigma_o\sqrt{2\pi}} \exp\left[-\frac{(H_{\alpha\alpha}-E_o)^2}{2\sigma_o^2}\right]. \tag{7}$$

Let the secular variation of the values $|c_{\alpha i}|$ as a function of $H_{\alpha\alpha}$ be denoted by $\rho_r(H_{\alpha\alpha})$, then by the use of the technique of parametric differentiation $^{4)}$ one can prove that the product $\rho_r(H_{\alpha\alpha})\rho_o(H_{\alpha\alpha})$ can be approximated by a Gaussian distribution

$$\rho_r(H_{\alpha\alpha})\rho_o(H_{\alpha\alpha})\equiv\rho_1(H_{\alpha\alpha}) = \frac{M_o}{\sigma_1\sqrt{2\pi}} \exp\left[-\frac{(H_{\alpha\alpha}-E_1)^2}{2\sigma_1^2}\right] \tag{8}$$

with the moments, centroid and variance given by

$$M_p = \sum_\alpha |c_{\alpha i}|(H_{\alpha\alpha})^p \qquad (p = 0,1,2), \tag{9}$$

$$E_1 = \frac{M_1}{M_o}, \tag{10}$$

$$\sigma_1^2 = \frac{M_2}{M_o} - \left(\frac{M_1}{M_o}\right)^2 . \tag{11}$$

As the parameters N, E_o, σ_o, M_o, E_1 and σ_1 can be derived from the energy matrix $H_{\alpha\alpha}$, eqs.(7) and (8) fix the function $\rho_r(H_{\alpha\alpha})$.

Since the magnitudes of the amplitudes, $|c_{\alpha i}|$, are assumed to show a distribution

$$\rho(|c_{\alpha i}|) = \frac{2}{\sigma\sqrt{2\pi}} \exp\left[-c_{\alpha i}^2/2\sigma^2\right], \tag{12}$$

one obtains the condition for the width

$$\sigma = \frac{\sqrt{\pi}}{2}\,\rho_r(H_{\alpha\alpha}). \tag{13}$$

Now one can determine the number of amplitudes $|c_{\alpha i}|$ smaller than some value, say Γ, in the interval $\{H_{\alpha\alpha}, H_{\alpha\alpha}+\Delta H_{\alpha\alpha}\}$

$$\rho_o(H_{\alpha\alpha})\Delta H_{\alpha\alpha}\int_0^{\Gamma}\frac{2}{\pi\rho_r(H_{\alpha\alpha})}\exp\left[-\frac{x^2}{\pi\rho_r^2(H_{\alpha\alpha})}\right]dx. \tag{14}$$

Integration of the integrand of eq.(14) over all values of $H_{\alpha\alpha}$ then leads to the frequency function of the amplitudes $|c_{\alpha i}|$

$$F(|c_{\alpha i}|) = \frac{\sqrt{2}}{\pi\sqrt{\pi}}\frac{N}{\sigma_o n_r}\times$$

$$\times\int_{-\infty}^{\infty} dE\,\exp\left[-\frac{(E-E_o)^2}{2\sigma_o^2}+\frac{(E-E_r)^2}{2\sigma_r^2}-\frac{|c_{\alpha i}|^2}{\pi n_r^2}\exp\left[\frac{(E-E_r)^2}{\sigma_r^2}\right]\right] \tag{15}$$

with

$$n_r = \frac{\sum_\alpha |c_{\alpha i}|\sigma_o}{N\sigma_1}\exp\left[(E_1-E_o)^2/2(\sigma_o^2-\sigma_1^2)\right], \tag{16}$$

$$E_r = \frac{\sigma_o^2E_1-\sigma_1^2E_o}{\sigma_o^2-\sigma_1^2}, \tag{17}$$

$$\sigma_r^{-2} = \sigma_1^{-2}-\sigma_0^{-2}. \tag{18}$$

Comparison of eq.(15) with the results of an exact counting for the lowest three $J^\pi=1^+$ states of ^{22}Na and of the lowest three $J^\pi=\frac{1}{2}^+$ states of ^{25}Mg shows excellent agreement. The basis states are taken in the j-j coupling scheme to span the full sd-shell, which leads to dimensions 243 and 1434, respectively. The two-body interaction is the MSDI. It is pointed out that no parameters are fitted to obtain these results [5].

There is disagreement, however, with results obtained by Whitehead et al.[6]. They used a different approach and considered ensembles of Hamiltonians that preserved two-body selection rules. Instead of the function $F(|c_{\alpha i}|)$given in eq.(15) they obtained a modified Bessel function K_o. Their calculations were performed in the m-scheme, though, and they used a different interaction.

References

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