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Information entropy, chaos and complexity of the shell model eigenvectors

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Abstract

The energies and wave functions of stationary many-body states are analyzed to look for the signatures of quantum chaos. Realistic shell model calculations are performed in the JT -scheme for 12 particles in the sd -shell. Local level statistics are in perfect agreement with the GOE predictions whereas the eigenvectors show evidence for non-complete energy dependent chaoticity. The information entropy of individual eigenvectors turns out to be a convenient measure of degree of complexity of individual wave functions. We discuss the representation dependence and the sensitivity to the interaction strength. The exceptional role of the mean field basis is stressed.

Quantum chaos in many-body systems was studied mostly from the viewpoint of level statistics which displays a clear relation to the notion of classical chaos [1–3]. Presumably much more information could be obtained from an analysis of the wave functions and transition amplitudes, see [4] and references therein. Here one expects to encounter the transition from the simple picture of almost independent elementary excitations to extremely mixed compound states which would display new specific features as, for example, the so-called dynamic enhancement of weak interactions [5].

To perform such an analysis and to check various hypotheses concerning complicated quantum dynamics, one needs a rich set of data which would allow one to make statistically reliable conclusions. The realistic nuclear shell model is one of the most promising

candidates for studying this largely unknown structure of quantum chaotic states [6–12] in a many-body system. Similar studies have been performed recently for the levels of a heavy atom [13] but in this case the matrix dimension is less by an order of magnitude than in modern shell model calculations.

Statistical spectroscopy [6–9] being developed in parallel to the random matrix methods predicted a “local” Gaussian distribution of the components of generic wave functions. As was tested with realistic shell model eigenfunctions by Brown and Bertsch [10], the states in the region of high level density show the expected behavior. The change of this distribution as a function of excitation energy carries information on the process of the mixing of simple shell model configurations by the residual interaction. In what follows we first test the “standard” signatures of

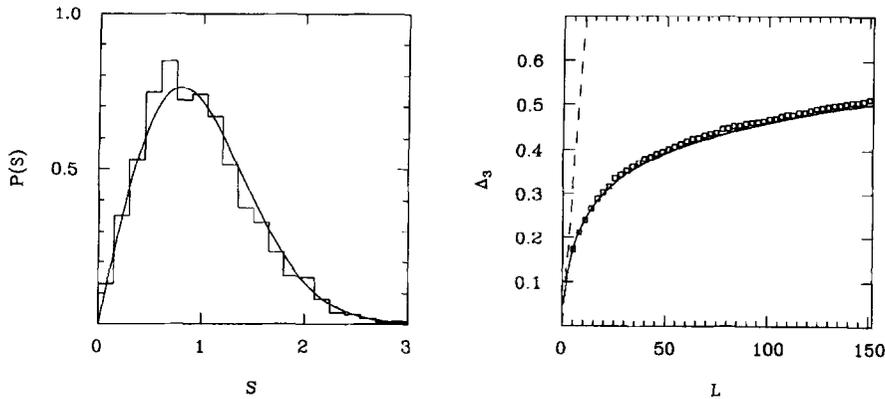


Fig. 1. Unfolded distribution of the nearest neighbor spacings, $P(s)$, left, and the rigidity of the spectrum, Δ_3 , right, for 2^+0 states.

quantum chaos in level statistics. Then we analyze the wave functions from the viewpoint of their complexity using the information entropy and moments of the amplitude distribution to quantify this complexity and establish its evolution along the spectrum. This is the first such study for nuclear levels, and it sheds new light on the quantitative way in which individual nuclear wave functions change from regular to chaotic as a function of excitation energy. The analysis of wave functions, contrary to spectral measures of chaos, is representation-dependent. Our results confirm the idea of the singular role of the mean field basis.

We studied the behavior of the basis-state amplitudes of the shell model eigenvectors produced in the JT -scheme for 12 particles in the sd shell. Our model Hamiltonian describing a many-body system of valence particles within a major shell contains a one-body part, which is due to an existing core (e.g. ^{16}O for the sd shell) and a two-body antisymmetrized interaction of the valence particles

$$H = \sum_{\mu} \epsilon_{\mu} a_{\mu}^{\dagger} a_{\mu} + \frac{1}{4} \sum V_{\mu\nu\lambda\rho} a_{\mu}^{\dagger} a_{\nu}^{\dagger} a_{\lambda} a_{\rho}. \quad (1)$$

In our calculations the Wildenthal interaction [14] was used along with the well known procedure to project out of the m -scheme the states with correct values of the total angular momentum J and isospin T [15]. As was stressed in [10], the projection is necessary in order to reach valid conclusions. The JT -projected states $|k\rangle$ are used to build the matrix of the many-body Hamiltonian, $H_{kk'} = \langle JT; k | H | JT; k' \rangle$, which is then diagonalized producing the eigenvalues E_{α} and the eigenvectors

$$|JT; \alpha\rangle = \sum_k C_k^{\alpha} |JT; k\rangle. \quad (2)$$

They represent the object of our investigation.

The matrix dimension for the $J^{\pi}T = 2^+0$ states is 3273. The density of states steeply increases along with excitation energy, reaches its maximum and then decreases again for the highest energy. This high-energy behavior, as well as the approximate symmetry with respect to the middle of the spectrum, are artificial features of models with finite Hilbert space in contrast to actual many-body systems.

The extreme theoretical limit of chaotic quantum dynamics can be described by the Gaussian orthogonal ensemble (GOE) of random matrices. We will compare our results which are purely dynamical (no random elements) with average predictions of the GOE. Fig. 1 shows the standard quantities which define the chaoticity of a quantum system [3,4], the “unfolded” distribution of the nearest neighbor spacings $P(s)$ and the spectral rigidity $\Delta_3(L)$, for this class of states¹. The solid lines in both parts of the figure describe the results expected for the GOE. The dashed line on the right corresponds to the Poisson level distribution which is characteristic of an integrable system.

¹ For the analysis of $P(s)$ we used all levels except for 15 lowest and 15 highest ones. This restriction which does not really matter for $P(s)$ is related to our procedure of determining the mean local level spacing by averaging over the energy interval including 15 levels on both sides of a given level. In order to study the spectral rigidity $\Delta_3(L)$ at large L , the corresponding average [4] was taken over intervals $[-L/2, L/2]$ with the center located further than by 150 levels from the edges of the spectrum.

The closeness of $\Delta_3(L)$ to the random matrix results even for very large values of L is remarkable. Previous to this study the largest value of L considered was less than 100 [11]. Thus, the level statistics manifest generic chaotic behavior.

We next look to the structure of the wave functions which could reveal in more detail how close to chaoticity we are. In the GOE there are no correlations between the eigenvalues and the components of the wave functions. Therefore complexity of the eigenvectors is uniform along the spectrum. Any realistic system reveals correlation of complexity with excitation energy. The specific dependence on the excitation energy reflecting the process of stochastization is of special interest. In what follows we study the properties of individual eigenstates (no averaging is carried out) which display both local chaotic distributions of the amplitudes in Eq. (2) which agrees with the predictions of statistical spectroscopy and a regular evolution of complexity along the spectrum.

An alternative (and complementary) way of the analysis is connected with studying fluctuations of the components of the wave functions in comparison with corresponding fluctuations in the GOE. This can be done with the aid of “unfolding” of those components [16] similar to the treatment of the energy spectra. This procedure partially destroys the information on the correlations between wave functions and eigenvalues. In the current study in contrast we use the “raw” data on the eigenfunctions expressed in the model basis.

The appropriate quantities to measure the degree of complexity of a given eigenstate $|\alpha\rangle$, Eq. (2), with respect to a given basis are, for instance, the information entropy [17,18] (it was used also for studying the structure of states coupled to continuum [19]),

$$S^\alpha = - \sum_k |C_k^\alpha|^2 \ln |C_k^\alpha|^2, \quad (3)$$

or the moments of the distribution of amplitudes $|C_k^\alpha|^2$. The second moment determines the number of principal components (NPC) of an eigenvector $|\alpha\rangle$,

$$(\text{NPC})^\alpha = \left(\sum_k |C_k^\alpha|^4 \right)^{-1}. \quad (4)$$

In the GOE all basis states are completely mixed so that the resulting eigenvectors are totally delocalized

and cover uniformly the N -dimensional sphere of radius 1 [4,20,21]. The GOE distribution function is invariant with respect to orthogonal transformations of the basis. Gaussian fluctuations with zero mean, $\overline{C_k^\alpha} = 0$, and width $\overline{|C_k^\alpha|^2} = 1/N$ lead, in the limit $N \gg 1$, to the average values $\ln(0.48N)$ and $N/3$ for the quantities (3) and (4) respectively. Here N is the total dimension of the model space. In reality, the incomplete mixing of basis states determined by specific properties of the Hamiltonian can coexist with the GOE-type level correlations. The latter appear [10,22] when typical mixing matrix elements reach the order of magnitude comparable with the mean level spacing. This however is not sufficient for complete mixing and delocalization. Moreover, the distribution of amplitudes is strongly basis-dependent.

The left upper part of Fig. 2 presents the $\exp(S^\alpha)$ quantity of Eq. (3) calculated for the 2^+0 states with the use of the original shell model projected basis $|k\rangle$. On the x -axis are the eigenstates numbered in order of their energies. This simple “numbered” scale is similar to the “unfolding” procedure described for example by Brody et al. [4]. The solid line represents the average GOE result ($0.48N$). One observes a very smooth semicircle-type behavior and a 12% deviation from the GOE even for the maximum entropy in the middle of the spectrum. Let us remind that we do not “unfold” the components of the wave functions.

It is interesting to study the role of single-particle energies (see Eq. (1)) for the chaotic behavior of the amplitudes. The upper right part of Fig. 2 shows the $\exp(S^\alpha)$ quantity for the 2^+0 states for the same Hamiltonian but with all single particle energies, ϵ_μ in Eq. (1), set to zero. In this degenerate case the average GOE limit (solid line) is attained and the chaotic regime extends over a larger part of the spectrum. At smaller statistics, the similar conclusion was obtained in [10].

To further quantify these effects, we look to the distribution $P(l_S)$ of $l_S^\alpha = \exp(S^\alpha)/0.48N$. One can interpret l_S^α as a delocalization length N^α/N , a fraction of the total original basis set covered by an eigenvector $|\alpha\rangle$. In the chaotic limit the distribution is expected to be shaped around $l_S = 1$. The lower left panel of Fig. 2 presents the results for the values of l_S calculated for the normal Hamiltonian and shown on the upper left panel. Here the limit of $l_S = 1$ is not reached. On

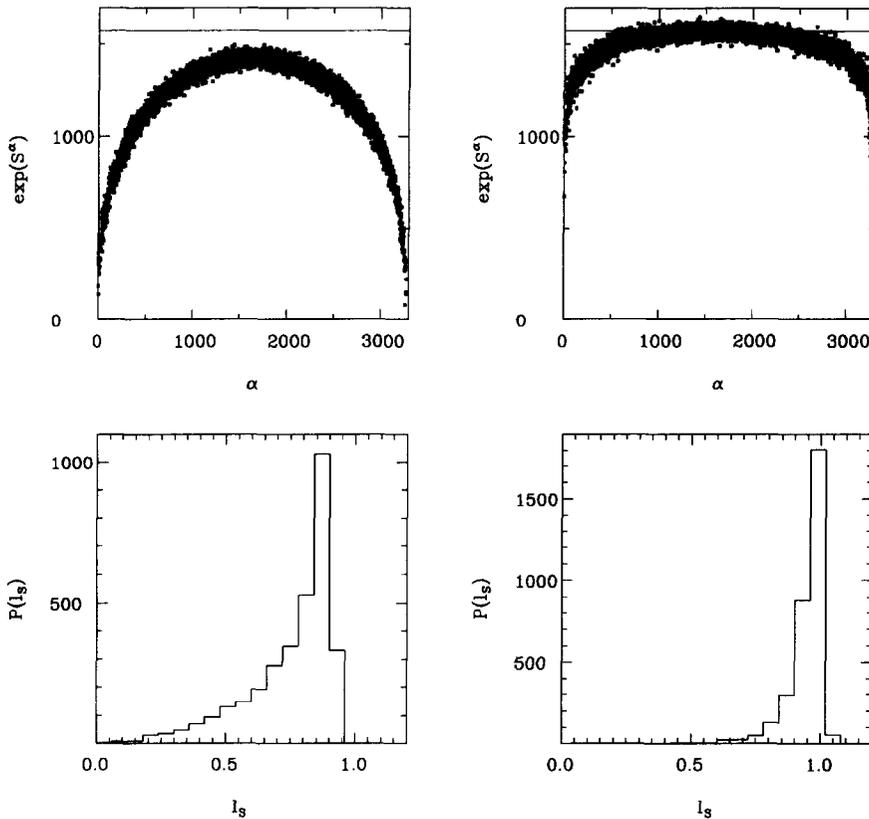


Fig. 2. Left panel: exponential of entropy (upper part), and the distribution of $l_S = (\exp S)/0.48N$ for 2^+ states calculated with the full Hamiltonian of the model (lower part); right panel: the same quantities for the degenerate model with $\epsilon_\mu = 0$.

the other hand, for degenerate single-particle orbitals (upper and lower panels on the right side), the distribution of localization lengths is more narrow and the full chaotic limit is reached. This is related to the fact that the mean field in general tends to smooth out the chaotic aspects of many-body dynamics [23].

The number of principal components (4) computed for the same basis behaves in a similar way gradually increasing from the edges of the spectrum to the middle, Fig. 3 (left). Even the most complicated states are shifted down from the GOE limit of complete mixing. However, for the ratio $(\exp S^\alpha)/(\text{NPC})^\alpha$ one obtains the results in the right part of Fig. 3. For a Gaussian distribution of amplitudes C_k^α of a given eigenvector $|\alpha\rangle$, the ratio $(\overline{\exp S})/(\overline{\text{NPC}})^\alpha$ of average quantities would be given by the universal (N -independent) random matrix result equal to 1.44 (solid line). The flattened region close to this numerical value indicates

that our large deterministic Hamiltonian matrix actually exhibits self-averaging (ergodic) properties and the chaotic dynamics, even if not complete, extends far beyond the region nearby the maximum of the information entropy.

In a given basis, the eigenstates are characterized by a typical delocalization length $N^\alpha/N < 1$ and by a Gaussian distribution of the amplitudes C_k^α with zero mean value and variance $(N^\alpha)^{-1}$ which agrees with statistical spectroscopy [7,9]. This length cancels in the ratio $\exp(S^\alpha)/(\text{NPC})^\alpha$ for the majority of states in the middle of the spectrum. The flatness of the ratio, as compared to strong α -dependence of $\exp(S^\alpha)$ and $(\text{NPC})^\alpha$ separately, indicates the existence of the local chaotic properties scaling with N^α . The edge regions with this ratio larger than 1.44 clearly correspond to relatively weakly mixed states with a reduced NPC. We note the very narrow dispersion of points in Figs.

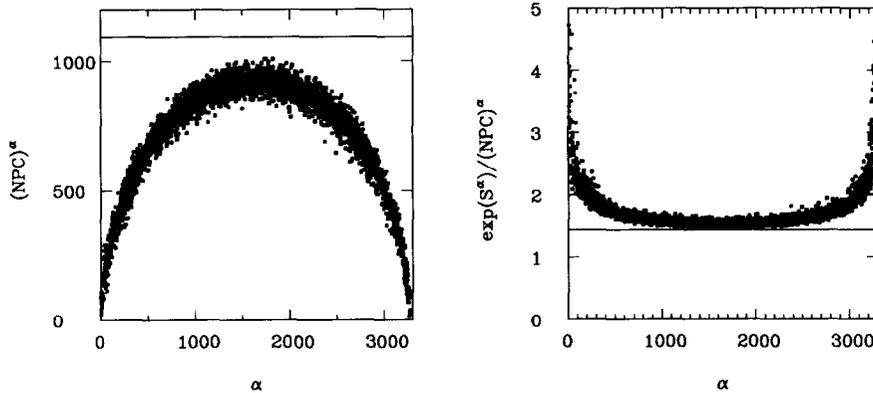


Fig. 3. The number of principal components, Eq. (4), of 2^+0 states (left), and the ratio $\exp(S^\alpha)/(NPC)^\alpha$ for the same states (right).

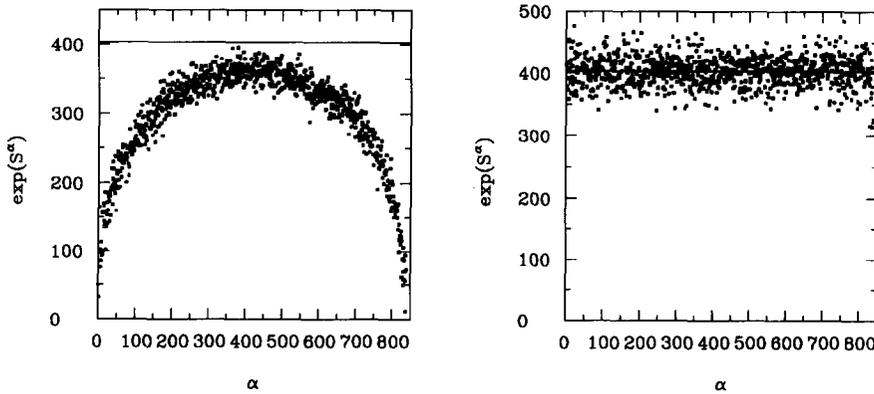


Fig. 4. Entropy of 0^+0 states in the shell model basis (left), and in the basis of the eigenvectors of the $SU(3)$ Hamiltonian (right).

2 and 3 for our measures of complexity. This dispersion scales $\propto \sqrt{N^\alpha}$ and agrees with the magnitude of fluctuations expected for the local GOE.

Using the same tools we also analyzed the $J^\pi T = 0^+0$ states of the model (the dimension of this subspace is 839) and obtained very similar results, see Fig. 4 (left).

Another important aspect is the above mentioned basis dependence of the signatures of complexity. Certainly, the eigenbasis itself shows no complexity at all: in this basis $C_k^\alpha = \delta_{\alpha k}$ so that $S^\alpha = 0$ and $(NPC)^\alpha = 1$. To demonstrate that the basis dependence is physically significant and informative we show the entropies S^α for 0^+0 stationary states calculated in a standard JT -projected shell model basis, Fig. 4 (left), and in the eigenbasis of the $SU(3)$ Hamiltonian [24], Fig. 4 (right). Similar to 2^+0 states, Fig. 3 (left), the shell

model basis reveals the smooth semicircle-type evolution of complexity along the spectrum.

The $SU(3)$ Hamiltonian is well known [24] as a reasonable model for describing collective nuclear properties. It was also used in statistical spectroscopy [8] for evaluating strength distributions. We see, Fig. 4 (right), that the information entropy of actual eigenvectors in the $SU(3)$ basis indicates the limiting chaoticity uniformly over the spectrum. The $SU(3)$ model is capable of accounting for collective trends concentrated supposedly in a small number of low-lying rotational bands. But, in sharp contrast to the shell model with the realistic spherical mean field, this basis turns out to be uncorrelated to degree of complexity of exact states. Actually, a totally random basis unrelated to the mean field of the problem gives the same GOE pattern as Fig. 4 (right).

The mean field basis is in some sense exceptional since it can be shown that the mean field itself is generated by averaging out the most chaotic components of many-body dynamics [23]. Therefore it provides us with the best separation of coherent and random dynamics and can be considered as a preferential representation for our purpose. We have already mentioned smooth behavior and narrow dispersion (low level of “noise”) for the measures of chaoticity calculated with the use of the mean field basis for the individual states which are close in energy but apparently can have very different intrinsic structure. It is remarkable that the “natural” choice of the shell model basis sheds a detailed light on the global and local chaotic properties of the wave functions in the many-body system with strong interaction. Using the mean field representation as a reference point, one acquires the possibility to describe the degree of chaoticity in terms of thermal excitations of quasiparticles. We hope to pursue this analogy further in a separate publication.

In conclusion, we have studied the chaotic properties of a many-body quantum system which consists of 12 valence particles interacting in the *sd*-shell. The standard signatures of chaos, nearest neighbor spacing distribution and spectral rigidity, are in agreement with the GOE results. With no random elements in the problem, chaos appears as a result of strong mixing between shell model configurations. But the level statistics alone are not sensitive enough to describe the process of stochastization. The information entropy or moments of the $|C_k^\alpha|^2$ distribution like (NPC) are much more suited to reveal these details. Arguments are given in support of local chaos characterized by a Gaussian distribution of the components of the wave functions with the variance related to the localization length. This length grows as the level density increases but does not reach the GOE limit. The effect of the core (given by the single-particle energies) diminishes the maximal degree of chaoticity which can be obtained when the system consists of interacting valence particles only. Our signatures of complexity are basis-dependent, they reflect mutual properties of the eigenbasis of the problem and the original “simple” basis $|k\rangle$. The basis dependence can give additional physical information. The important question of spreading widths of original simple states and the relation of our results to statistical spectroscopy [6–9] is not fully understood. Work in this direction is under progress.

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