

Shell-Model studies of chaos and statistical properties in nuclei

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Abstract. Shell-model calculations with realistic empirical interactions constitute an excellent tool to study statistical properties of nuclei. Using large-scale shell-model calculations in pf -shell nuclei, we study how the onset of chaos depends on different properties of the nuclear interaction and on excitation energy. We make use of classical random matrix theory and other theoretical developments based on information theory and time series analysis. We show that besides energy-level statistics, other statistical properties like the complexity of wave functions are fundamental for a proper determination of the dynamical regime of nuclei. Important deviations from GOE are observed in level fluctuations and in the complexity of wave functions.

1. Introduction

Beyond detailed nuclear spectroscopy, the statistical properties of nuclei are important not only in nuclear physics, but also in astrophysics. For example, statistical spectroscopy methods generated by many-body chaos and two-body random matrix ensembles provide useful information on Gamow-Teller strength sums and beta decay rates for stellar evolution and supernovae. For a recent review of these topics, as well as quantum chaos in Hamiltonian systems, see Gómez *et al.* [1]. We refer to this paper for references and a more detailed account of the topics of the present paper. In this work we discuss statistical properties related to chaos in nuclei and will try to give an answer to a simple question: *to what extent is nuclear motion chaotic?* We discuss experimental and theoretical results and conclude that there is no simple answer to this question. It depends on which nuclei and which excitation energy region we are talking about.

It is well known that real and complex systems are usually not fully ergodic and neither are they integrable. The chaotic orbits only occupy a certain part of its phase space. For quantum stationary systems with a classical analog, there is abundant evidence showing a clear relationship between the fluctuation properties of their energy levels and the large time scale behavior of the classical analog. The pioneering work of Berry and others, especially Bohigas *et al.* [2] lead to an important and concise statement known as the BGS conjecture: *the spectral properties of simple systems known to be ergodic in the classical limit follow very closely those*



of the Gaussian orthogonal ensemble (GOE) of random matrices. During many years it has been mainly supported by many numerical calculations, and more recently an analytical proof was obtained as well by Heusler *et al.* [3]. The idea is generalized to quantum systems without a classical limit, and thus a quantum system is considered chaotic if its fluctuation properties agree with those of random matrix theory (RMT). In this case the distribution of the nearest-neighbor spacings is given to a good approximation by the Wigner surmise. It corresponds to the existence of linear repulsion between adjacent levels. On the contrary, integrable systems lead to level fluctuations that are well described by the Poisson distribution, i.e., levels behave as if they were uncorrelated.

The information on regular and chaotic nuclear motion available from experimental data is rather limited, because the analysis of energy levels requires the knowledge of sufficiently large pure sequences, i.e., consecutive level samples all with the same quantum numbers (J, π, T) in a given nucleus. The situation is clear above the one-nucleon emission threshold, where a large number of neutron and proton $J^\pi = 1/2^+$ resonances are identified. The agreement between this Nuclear Data Ensemble (NDE) [4] and the GOE predictions is excellent. In the low-energy domain, however, it is rather difficult (if not impossible) to get large enough pure sequences. For this reason, even if the data coming from different nuclei are conveniently scaled and gathered, the conclusions are less clear. There is some evidence that, at low energy, the spectral fluctuations are close to GOE predictions in spherical nuclei while they deviate towards the Poisson distribution in deformed nuclei.

In order to get a deeper understanding of what happens in the low-energy region we can use the interacting shell model. Using large-scale shell-model calculations in pf -shell nuclei with a realistic empirical interaction, we study how the onset of chaos depends on different properties of the nuclear interaction and on excitation energy. We make use of classical random matrix theory and other theoretical developments based on information theory and time series analysis. We compare the results of sd and pf nuclei and find that they are quite different in particular nuclei. We will also show that some simple statistics, like the nearest-neighbor spacing distribution, can sometimes become misleading by itself and one has to look at other energy-level statistics, as well as other statistical properties like the complexity of wave functions, for a proper determination of the dynamical regime of nuclei.

2. Statistics used to assess quantum chaos

The first step in the study of spectral fluctuations is the unfolding of energy levels. Fluctuations are somehow defined as the departure of the actual level density from a local uniform density. For this reason, and because of the exponential-like increase of the nuclear density, it is essential to eliminate this secular variation. It should be noted that unfolding the spectrum is a difficult task when the exact form of the smooth density is not known, which is often what happens in complex quantum systems. See Gómez *et al.* [5] for a discussion on this point.

We consider three spectral statistics for the unfolded energy levels: the nearest neighbor level-spacing distribution $P(s)$, the average spectral rigidity $\Delta_3(L)$ of Dyson and Mehta [6, 7], and the power spectrum P_k^δ of the δ_n statistic. Both $P(s)$ and $\Delta_3(L)$ are well known and have been extensively used as a measure of chaos in quantum systems. Therefore we will give only a brief description of δ_n .

Apart from the comparison with random matrix behavior, there is an alternative approach to the analysis of spectral fluctuations of quantum systems which is based on the power spectrum of the energy level fluctuations [8]. There is an analogy between a discrete time series and a quantum energy spectrum, if time t is replaced by the energy E of the quantum states. In time series analysis, fluctuations are usually studied by means of the power spectrum of the signal.

We define the statistic δ_n as a signal,

$$\delta_n = \sum_{i=1}^n (s_i - \langle s \rangle) = \varepsilon_{n+1} - \varepsilon_1 - n, \quad n = 1, 2, \dots, N-1, \quad (1)$$

where $s_i = \varepsilon_{i+1} - \varepsilon_i$, ε_i are the unfolded levels, and the average values $\langle s \rangle = 1$ and $\langle \varepsilon_n \rangle = n$ have been used.

Thus δ_n represents the deviation of the n th excited level from its expected mean value. The discrete power spectrum of this signal is given by

$$P_k^\delta = \left| \hat{\delta}_k \right|^2 = \left| \frac{1}{\sqrt{N}} \sum_{n=1}^N \delta_n \exp\left(\frac{-2\pi i k n}{N}\right) \right|^2 \quad (2)$$

where $\hat{\delta}_k$ is the Fourier transform of δ_n , and N is the size of the series.

The first quantum spectra analyzed by this method were the levels of several nuclei calculated using the interacting shell model. It turned out that P_k^δ behaved very accurately as $1/k$. Then the analysis was performed for the basic random matrix ensembles GOE, GUE and GSE [8] and for a quantum billiard with chaotic classical limit. In all the cases the result was the same, namely the power spectrum of δ_n behaved as $1/k$. This led to the conjecture that *quantum chaos is characterized by $1/f$ noise*. Thus, without need to refer to any other systems, like random matrices, there is an intrinsic property that characterizes quantum chaos: A quantum system is considered chaotic if its spectral fluctuations are characterized by $1/f$ noise [8]. An analytical proof of this behavior for all the classical random matrix ensembles, independently of the symmetries of the system, was given by Faleiro *et al.* [9]. On the contrary, regular quantum systems exhibit Poisson statistics and $1/f^2$ noise.

Finally, apart from energy spectra, one should pay attention to the wave functions. The complexity of states can be measured by means of the information entropy S^{inf} . For any state of the basis $S^{inf} = 0$, and it takes the maximum value, $\ln(N)$, for a uniformly distributed state. For GOE matrices $S^{inf} = \ln(0.48N)$. The information entropy measures, somehow, the degree of delocalization of a certain state with regard to the mean-field basis. However, to avoid the dependence on the dimension N , the normalized localization length $l_{loc} = \exp(S^{inf})/0.48N$ is often used instead of the information entropy.

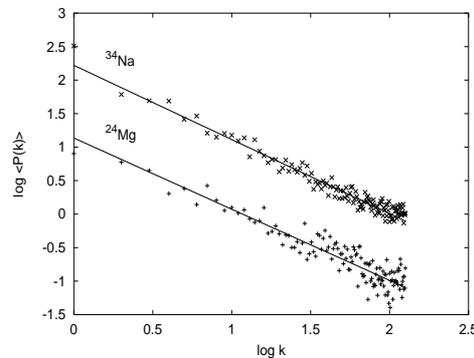


Figure 1. Average power spectrum of the δ_n function for ^{24}Mg and ^{34}Na , using 25 sets of 256 levels from the high level density region. The plots are displaced to avoid overlapping.

3. Shell-model calculations of chaotic properties in pf -shell nuclei

Large-scale shell-model calculations provide very long pure and complete sequences of energy levels. This makes possible the study of both short-range and long-range spectral correlations and in general the statistical analysis is quite reliable. Most shell-model calculations for statistical purposes have been done for nuclei in the sd shell and in the pf shell. We point out some of the most important theoretical results, focusing mostly on the pf shell, as these calculations are more recent and, because of the large dimensionalities of pf shell matrices, it becomes possible to study the dependence of the statistical properties on the excitation energy, angular momentum, pairing and isospin, for example. Results for the sd shell were summarized in the excellent review about shell model and many-body quantum chaos by Zelevinsky *et al.* [10]. The onset of the chaotic behavior in atomic nuclei is a question that has not been fully clarified experimentally as yet. We simply do not have sufficient experimental data. On the theoretical side this issue has been explored thoroughly using shell-model calculations. Early studies of level fluctuations in shell-model energy spectra showed a general agreement with GOE. This is indeed a remarkable result that has been known but has remained unexplained for many years. The many-body matrix elements of the nuclear shell-model Hamiltonian are certainly not random, as in GOE. Instead, all of them arise from the fairly well known nucleon-nucleon interaction. To understand the chaotic behavior of nuclei and to compare the results with RMT one needs to take into account the properties of realistic empirical shell-model interactions. See Section 6.2.1 of Gómez *et al.* [1] for a discussion on this point.

All theoretical work in the sd shell seems to indicate that nuclei present a strongly chaotic behavior, even in the proximity of the ground state. The spectral statistics $P(s)$ and $\Delta_3(L)$ follow closely the predictions of RMT [10]. Moreover, the power spectrum of δ_n for nuclei in this mass region clearly exhibits $1/f$ noise. This is illustrated by Fig. 1, which shows the results for a typical stable sd -shell nucleus, ^{24}Mg , with matrix dimensionalities up to $N \simeq 2000$; and for a very exotic nucleus, ^{34}Na , with N up to about 5000, in the sd proton and pf neutron shells. The shell-model calculations have been performed using the USD interaction [11] for ^{24}Mg , and the interaction described in [12] for ^{34}Na . Clearly, the power spectrum of δ_n follows closely a power law. We may assume the simple functional form $\langle P_k^\delta \rangle = 1/k^\alpha$.

A least squares fit to the data of Fig. 1 gives $\alpha = 1.11 \pm 0.03$ for ^{34}Na , and $\alpha = 1.06 \pm 0.05$ for ^{24}Mg [8]. Thus we clearly observe the existence of $1/f$ noise in these nuclei.

Turning now to pf -shell nuclei, we find a more diversified picture of spectral fluctuations. The shell-model calculations for pf -shell nuclei have been performed using the KB3 interaction [13]. Fig. 2 shows the $P(s)$ distribution for a very large number of levels in ^{52}Ca and ^{52}Sc [14]. After unfolding the spectrum for all the levels with the same $J^\pi T$, all the nearest neighbor level spacings for different $J^\pi T$ in a nucleus are gathered together. In ^{52}Ca all the J^π from 0^+ to 12^+ , $T = T_z$ states are included, giving in total 11981 states. In ^{52}Sc the dimensionalities are much larger, and only the $J^\pi = 0^+$, 11^+ and 12^+ , $T = T_z$ states were considered, giving a total of 11493 states. These large numbers of levels provide excellent statistics and we see that the agreement of $P(s)$ with GOE predictions is excellent, as could be expected. However, the $\Delta_3(L)$ behavior in the same nuclei is somewhat surprising, especially for the 0^+ states.

As Fig. 3 shows, in ^{52}Sc the $\Delta_3(L)$ statistic follows GOE up to large L values, but in ^{52}Ca it clearly deviates from GOE for stretches larger than $L \simeq 10$. Therefore, contrary to what the $P(s)$ results suggested, nuclear motion in ^{52}Ca cannot be considered to be very chaotic. As discussed in [14] and [1], several effects contribute to deviations from GOE in Ca isotopes. There are only active neutrons in the pf shell for Ca isotopes. For the 0^+ states, states of different seniority are included in the same sequence of levels, thus this approximate symmetry is not taken into account and that causes deviations towards Poisson, especially in the ground state region. More generally, for all J values there is a common feature in Ca isotopes. The residual n - n interaction is much weaker than the residual p - n interaction, and therefore the residual

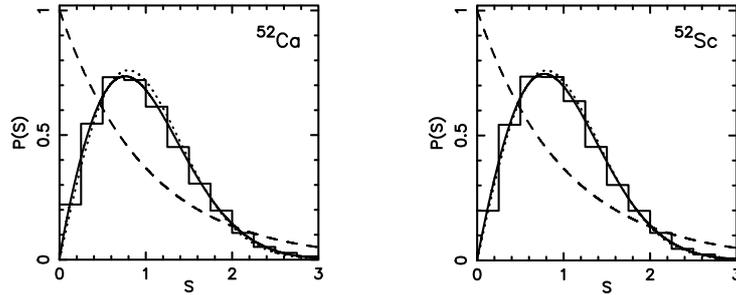


Figure 2. Nearest neighbor spacing distribution $P(s)$ for ^{52}Ca , $J^\pi = 0^+ - 12^+$, $T = 6$ states (left) and for ^{52}Sc , $J^\pi = 0^+, 11^+, 12^+$, $T = 4$ states (right). The dotted and dashed curves represent the GOE and Poisson $P(s)$ values, respectively.

interaction in Ca isotopes disturbs the ordered mean field motion much less than in other nuclei with valence protons and neutrons. In fact, a comparison of spectral statistics in the ^{46}Ca , ^{46}Sc and ^{46}Ti isobars shows strong deviations from GOE in ^{46}Ca , especially at low excitation energy. The simple presence of a proton in ^{46}Sc makes a great difference towards GOE, and this effect is enhanced in ^{46}Ti , in which the number of possible p - n configurations is even larger. Thus it can be concluded that chaos in nuclei has a strong isospin dependence [14, 1].

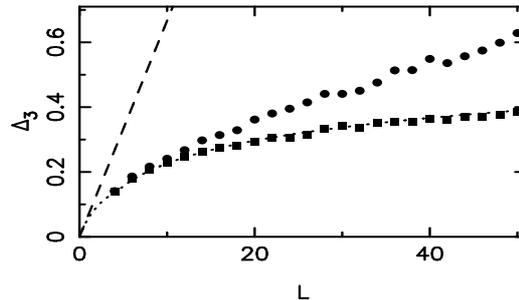


Figure 3. Average $\Delta_3(L)$ for all the $J^\pi = 5^+$, $T = T_z$ levels of ^{52}Ca (dots) and ^{52}Sc (squares). The dotted and dashed curves represent the GOE and Poisson $\Delta_3(L)$ values, respectively.

Finally we look at the complexity of wave functions. Fig. 4 compares the localization length l_{loc} for the 2^+ states in ^{28}Si [10] and in ^{46}Ti [1]. In both cases the number of levels is very large, providing good statistics. In both cases the behavior of $P(s)$ and $\Delta_3(L)$ are very close to GOE. We recall that $\exp(S^{inf})$ is the same as l_{loc} , except for a constant numerical factor. However, it is seen that in the region of largest density of states, the values in ^{28}Si are very close to the GOE limit, but in ^{46}Ti the maximum information entropy is about 65% of the GOE limit. Similarly, calculations for the $J^\pi T = 1^+ 2$ ($N = 2051$) states of ^{46}Sc and the $J^\pi T = 6^+ 5$ ($N = 2042$) states of ^{50}Ca , show that at the maximum density of states, l_{loc} is about 60% of the GOE value in ^{46}Sc , and about 40% in ^{50}Ca [14]. These results are consistent with the results for $\Delta_3(L)$, showing the existence of isospin dependence of chaos in nuclei, as well as the large deviations from GOE in nuclei like Ca isotopes in which all the valence particles are neutrons.

4. Conclusions

Large scale shell-model calculations with realistic empirical interactions provide long sequences of pure $J^\pi T$ states which facilitate reliable calculations of statistical nuclear properties. In

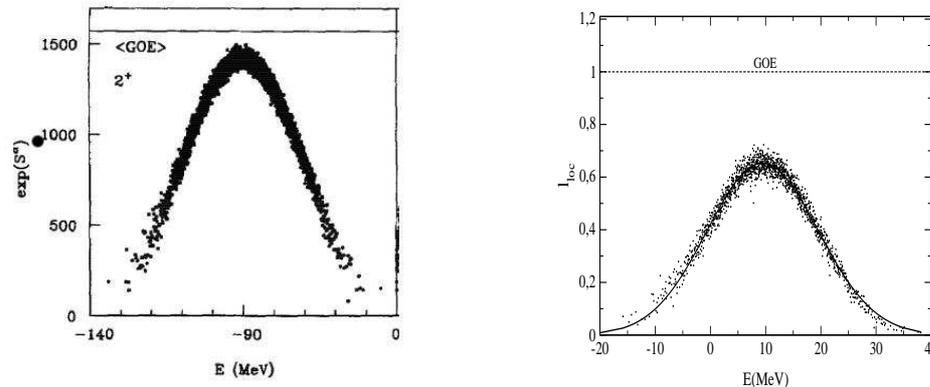


Figure 4. Comparison of the normalized localization length $l_{loc} = \exp(S^{inf})/0.48N$ as a function of excitation energy for the $J^\pi T = 2^+0$ states of ^{28}Si (left) [10] and for the $J^\pi T = 2^+1$ states of ^{46}Ti (right) [1]. In the figure on the left the information entropy S^{inf} is called S^α .

particular, in pf shell nuclei the sequences of states with the same $J^\pi T$ quantum numbers are very large and it has been possible to observe on the one hand the onset of chaos as the excitation energy increases, and on the other the onset of chaos as the strength of the residual interaction increases for fixed A , i. e., as the number of possible p - n configurations for the valence nucleons increases. In all the investigated nuclei, level fluctuations deviate from GOE in the lower part of the spectrum, and even when the full spectrum is taken into account for Ca isotopes the $\Delta_3(L)$ statistic clearly deviates from GOE for $L \geq 10$. The analysis of shell-model wave functions shows that the localization length l_{loc} in pf -shell nuclei is clearly smaller than the GOE value ($l_{loc}(\text{GOE}) = 1$), and again a clear isospin dependence is observed for isobaric nuclei. We conclude that it is necessary to study the behavior of different spectral statistics, including short range and long range level correlations, as well as the complexity of wave functions, in order to get a clear picture and assess the degree of chaos in nuclei. In particular, it is clear that the results for the $P(s)$ distributions alone are not sufficient for a reliable assessment. Finally, we conclude that the deviations from GOE observed in our shell-model calculations in pf -shell nuclei make sense. After all, the nuclear interaction gives two-body matrix elements which are far from random, and the shell model configurations lead to nuclear wave functions with some components more important than others, especially, but not only, in the ground state region. On the contrary, in GOE the amplitudes of the wave function are more uniformly distributed.

References

- [1] Gómez J M G, Kar K, Kota V K B, Molina R A, Relaño A and Retamosa J 2011 *Phys. Rep.* **499** 103-226.
- [2] Bohigas O, Giannoni M J and Schmit C 1984 *Phys. Rev. Lett.* **52** 1.
- [3] Müller S, Heusler S, Braun P, Haake F and Altland A 2004 *Phys. Rev. Lett.* **93** 014103.
- [4] Haq R U, Pandey A and Bohigas O 1982 *Phys. Rev. Lett.* **48** 1086.
- [5] Gómez J M G, Molina R A, Relaño A and Retamosa J 2002 *Phys. Rev. E* **66** 036209.
- [6] Dyson F J and Mehta M L, 1963 *J. Math. Phys.* **4** 701.
- [7] Mehta M L, 2004 *Random Matrices*, Academic Press, 3rd ed.
- [8] Relaño A, Gómez J M G, Molina R A, Retamosa J and Faleiro E 2002 *Phys. Rev. Lett.* **89** 244102.
- [9] Faleiro E, Gómez J M G, Molina R A, Muñoz L, Relaño A and Retamosa J 2004 *Phys. Rev. Lett.* **93** 244101.
- [10] Zelevinsky V, Brown B A, Frazier N and Horoi M 1996 *Phys. Rep.* **276** 85.
- [11] Wildenthal B H 1983 *Prog. Part. Nucl. Phys.* **11** 5.
- [12] Poves A and Retamosa J 1994 *Nucl. Phys. A* **571** 221.
- [13] Poves A and Zuker A 1981 *Phys. Rep.* **70** 4.
- [14] Molina R A, Gómez J M G and Retamosa J 2000 *Phys. Rev. C* **63** 014311.