Quantum chaos in $A=46–50$ atomic nuclei

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Abstract: The spectral statistics of low–lying states of several $fp$ shell nuclei are studied with realistic shell–model calculations. For Ca isotopes, we find significant deviations from the predictions of the random–matrix theory which suggest that some spherical nuclei are not as chaotic in nature as the conventional view assumes.

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In recent years many authors have shown great interest in the fluctuation properties of energy levels. It is well known that the fluctuation properties of quantum systems with underlying classical chaotic behaviour and time–reversal symmetry agree with the predictions of the Gaussian Orthogonal Ensemble (GOE) of random matrix theory, whereas quantum analogs of classically integrable systems display the characteristics of the Poisson statistics [1].

One of the best systems for the study of quantum chaos is the atomic nucleus, which was studied in pioneer work [2] and has been the subject of many investigations [3]. In atomic nuclei, the fluctuation properties of experimental energy levels are best studied in the domain of neutron and proton resonances near the nucleon emission threshold, where a large number of levels of the same spin and parity in the same nucleus are present, and an excellent agreement with GOE predictions has been found [2]. In the ground state region, however, the samples of consecutive experimental levels of the same spin and parity in any one nucleus are quite small. Therefore it is more difficult to calculate reliable mean values and fluctuations of statistics such as energy level spacings. In order to circumvent this difficulty, in recent years [4–6] statistical analyses of experimental low energy levels have combined data from a large range of excitation energies and angular momenta of a nucleus or a set of nuclei. Such analyses have provided evidence suggesting that spherical nuclei show level spectra close to GOE predictions and deformed nuclei show strong deviations from GOE behaviour. In a recent analysis [7] of level spacings close to the yrast line of deformed nuclei with $Z = 62–75$ and $A = 155–185$, the average level spacing for states with the same spin and parity was calculated for the total ensemble instead of for individual nuclei. The level spacing fluctuations obtained are quite close to the Poisson distribution, showing evidence of regular motion, although it is possible that this Poisson behaviour may be related to a hidden symmetry in the $K$ quantum number. In general it seems quite clear that the available experimental data are insufficient to establish the borderlines in mass number, excitation energy, etc., between order and chaos in nuclei.
Theoretical work, especially realistic shell model calculations, should help to establish the domains of chaos in nuclei. The statistical analyses of shell–model energy spectra and wave functions have been mainly concentrated on the sd shell region, and a very chaotic behaviour has been found for these nuclei [8–11]. However, recent shell–model calculations by Bae et al. [12] have shown that for nuclei of mass $A = 212$ shell–model spectra display features of regular motion in some cases. The main reason for this seems to be the relatively small values of the residual interaction matrix elements as compared to the average spacing between neighboring single–particle levels in heavy nuclei.

In this work, we undertake the statistical analysis of the shell–model energy levels in the $A = 46–50$ region. Exact calculations are performed in the $(f_{7/2},p_{3/2},f_{5/2},p_{1/2})$ shell–model space, assuming a $^{40}$Ca inert core [13]. The diagonalizations are performed in the $m$–scheme using a fast implementation of the Lanczos algorithm with the code ANTOINE [14]. For a fixed number of valence protons and neutrons we calculate the energy spectrum for projected total angular momentum $J$ and total isospin $T$. The interaction we use is a minimally modified Kuo–Brown realistic force with monopole improvements [15].

We calculate the $T = T_z$ states from $J = 0$ to $J = 9$ for all the combinations of 6 active nucleons, i.e. $^{46}$V, $^{46}$Ti, $^{46}$Sc, and $^{46}$Ca, and also for $^{48}$Ca and $^{50}$Ca. Table 1 shows the $m$–scheme dimensions and the largest dimensions in the JT scheme of the isotopes analyzed.

Since we are looking for deviations from chaotic features, we are mainly interested in the low–lying levels, up to a few MeV above the JT yrast line. Let us consider the energy levels up to 4, 5 and 6 MeV above the yrast line, and calculate the fluctuations around the average spacing between neighboring levels. In this range of energies, the level spectrum can be mapped into unfolded levels with quasi–uniform level density by using the constant temperature formula. In order to guarantee that the results up to different energies are unaffected by the unfolding procedure, the unfolding is performed using always the whole set of levels up to 6 MeV, for each JT set in the nucleus. In some cases, the resulting
number of levels is too small, e.g. 3 levels for \( J = 0 \) in \(^{46}\text{Ca}\), and then we use a larger set of levels for the calculation of the mean level spacing as a function of energy. The mean level density can be assumed to be of the form

\[
\bar{\rho}(E) = \frac{1}{T} \exp \left[ \frac{(E - E_0)}{T} \right],
\]

where \( T \) and \( E_0 \) are constants. For fitting purposes it is better to use not \( \bar{\rho}(E) \) but its integral \( \bar{N}(E) \). We write

\[
\bar{N}(E) = \int_0^E \bar{\rho}(E')\,dE' + N_0 = \exp \left[ \frac{(E - E_0)}{T} \right] - \exp \left[ -\frac{E_0}{T} \right] + N_0.
\]

The constant \( N_0 \) represents the number of levels with energies less than zero. Following Shriner et al. [5], we consider Eq. 2 as an empirical function to fit the data and let \( N_0 \) take non–zero values. The parameters \( T \), \( E_0 \) and \( N_0 \) that best fit \( N(E) \) are obtained by minimizing the function:

\[
G(T, E_0, N_0) = \int_{E_{\text{min}}}^{E_{\text{max}}} [N(E) - \bar{N}(E)]^2\,dE,
\]

where \( N(E) \) is the number of levels with energies less than or equal to \( E \). The energies \( E_{\text{min}} \) and \( E_{\text{max}} \) are taken as the first and last energies of the level sequence. As an example, Fig. 1 illustrates the fit to the integrated level density \( N(E) \) for the \( J^\pi T = 6^+1 \) levels of \(^{46}\text{Ti}\).

The spectral statistic \( P(s) \) is used to study the local fluctuations of the energy levels [16,17]. \( P(s) \) is the distribution of nearest–neighbour spacings

\[
s_i = \bar{N}(E_{i+1}) - \bar{N}(E_i)
\]

of the unfolded levels. It is obtained by accumulating the number of spacings that lie within the bin \((s, s + \Delta s)\) and then normalizing \( P(s) \) to unity.

For quantum systems whose classical analogs are integrable, \( P(s) \) is expected to follow the Poisson limit, i.e. \( P(s) = \exp (-s) \). On the other hand, quantal analogs of chaotic systems exhibit the spectral properties of GOE with \( P(s) = (\pi/2)s \exp (-\frac{\pi}{4}s^2) \) [1,2].

The distribution \( P(s) \) is the best spectral statistic to analyze shorter series of energy levels and the intermediate regions between order and chaos. In order to quantify the
chaoticity of $P(s)$ in terms of a parameter, it can be compared for example to the Brody or the Berry–Robnik distributions, which are adequate for the description of intermediate situations between order and chaos. Although each of these distributions have some advantage in limiting cases [18], they are very similar in a particular case like ours. We use here the Brody distribution [19], given by

$$P(s, \omega) = \alpha (\omega + 1) s^{\omega} \exp (-\alpha s^{\omega+1}),$$

with

$$\alpha = (\Gamma(\frac{\omega + 2}{\omega + 1}))^{\omega+1}.$$  \hspace{1cm} (5)

This distribution interpolates between the Poisson distribution ($\omega = 0$) of integrable systems and the GOE distribution ($\omega = 1$) of chaotic ones, and thus the parameter $\omega$ can be used as a simple quantitative measure of the degree of chaoticity.

In order to obtain more meaningful statistics, $P(s)$ is calculated using the unfolded level spacings of the whole set of $J = 0$–9 levels for fixed $T$ up to a given energy limit above the yrast line. The number of $J = 0$–9 spacings below 4, 5 and 6 MeV range from 42, 66 and 105 in $^{46}$Ca, to 86, 149 and 231 in $^{46}$Ti, respectively.

Table 2 shows the best fit Brody parameter $\omega$ of the $P(s)$ distribution for the $J = 0$–9 set of level spacings in the $A = 46$ nuclei up to 4, 5 and 6 MeV above the yrast line. Clearly, $^{46}$V, $^{46}$Ti and $^{46}$Sc are chaotic for these low energy levels, but there is a considerable deviation from GOE predictions in $^{46}$Ca, which is a single closed–shell nucleus. In view of the peculiarity of this nucleus, we performed calculations for $^{48}$Ca and $^{50}$Ca, and obtained again strong deviations toward regularity, as the values of Table 2 show. Thus, for the Ca isotopes we find the same kind of phenomenon obtained by Bae et al. [12] in the heavy single–closed nuclei $^{212}$Rn and $^{212}$Pb, namely that low–lying states deviate strongly from chaoticity toward regularity.

To obtain a better estimate of the Brody parameter, we can combine spacings of different nuclei. In Fig. 2 (a) we plot $P(s)$ for $^{46}$V+$^{46}$Ti+$^{46}$Sc, and in Fig. 2 (b) for $^{46}$Ca+$^{48}$Ca+$^{50}$Ca, up to 6 MeV above the yrast lines. The number of level spacings is
now sufficiently large to yield meaningful statistics and we see that Ca isotopes are not very chaotic at low energy, in contrast to other nuclei in the same region.

Concerning the energy dependence of $\omega$ in the low energy region, for individual nuclei we see fluctuations which may be due to the fact that some of the samples of levels are not very large. Table 2 shows the results for $^{46}$V+$^{46}$Ti+$^{46}$Sc and $^{46}$Ca+$^{48}$Ca+$^{50}$Ca. For these larger sets of levels, fluctuations are reduced, and the energy dependence of $\omega$ is seen to be small in the 4–6 MeV range, although the chaoticity increases slightly with the excitation energy.

Since the semi–closed nuclei are quite regular for the low–lying levels, compared with other neighboring nuclei, it is interesting to find out in the framework of the model the chaoticity at higher excitation energies. Therefore we have calculated the whole spectrum for $^{46}$Ca, unfolding the levels with the local density method [3]. Different $J$ values were combined to improve the $P(s)$ statistics. The value of $\omega$ increases rather smoothly with the excitation energy end point, and we obtain $\omega = 0.72, 0.83$ and $0.88$ for levels below 12, 16 and 20 MeV, respectively. We do not find significant differences in $\omega$ for different $J$ values in $^{46}$Ca when they are analyzed separately.

Why are Ca isotopes less chaotic than their neighbors? We observe that the two–body matrix elements of the proton–neutron interaction are, on average, larger than those of the proton–proton and neutron–neutron interactions. Consequently the single–particle mean–field motion in nuclei with both protons and neutrons in the valence orbits suffers more disturbance and is thus more chaotic.

It should be noted that an analysis [20] of experimental energy levels below 4.3 MeV excitation energy in the semi–magic nucleus $^{116}$Sn yields a near–neighbor spacing distribution which is intermediate between GOE and Poisson, with $\omega = 0.51 \pm 0.19$. This result is consistent with the theoretical findings of Bae et al. [12] for $^{212}$Rn and $^{212}$Pb, and our present results for Ca isotopes.

The energy spectra of all these nuclei are the result of the interaction of like nucleons,
and we conclude that this residual interaction is relatively weak and, at least for low energy levels, it only partially destroys the regular motion of nucleons generated by the nuclear mean field.

We can ask ourselves why do all shell–model calculations give chaotic features for \textit{sd} shell nuclei, without any significant deviations towards regularity. First, it should be noted that most of these calculations include a large number of states, up to excitation energies far above the nucleon emission threshold. This is, for example, the case of the \textsuperscript{22}O calculations of Bae \textit{et al.} [12], which include the full set of levels for several \textit{J} values and obtain \( \omega = 0.96 \). Second, we notice that Ormand and Broglia [10] obtained a GOE–like distribution for the first two spacings of each spectrum for a set of \textit{sd} shell nuclei. However, these nuclei have valence protons and neutrons and are thus similar to the case of \textsuperscript{46}V, \textsuperscript{46}Ti and \textsuperscript{46}Sc, for which we also find chaotic behaviour. We conclude that no regular features have been found in the \textit{sd} shell region because single–closed nuclei have a very small configuration space for these nuclei and thus too few low–lying levels for statistical analysis, and also because the disturbance of single–particle motion by the two–body interaction is greatest in light nuclei, where the range of the single–particle orbits is not much larger that the range of the nuclear force.

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Matrix dimensions in the $m$ scheme and maximum dimensions in the $JT$ scheme for the analyzed isotopes.

|                | $^{46}$V | $^{46}$Ti | $^{46}$Sc | $^{48}$Ca | $^{50}$Ca |
|----------------|---------|---------|---------|---------|---------|
| $m$-scheme dimension | 121 440 | 86 810 | 30 042 | 3 952 | 12 002 | 17 276 |
| largest dim. $J^+T$ | $4^0$ | $4^1$ | $4^2$ | $4^3$ | $4^4$ | $4^5$ |
| $J^+T$ dimension   | 4 750  | 8 026  | 3 783  | 615    | 1 755  | 2 468  |
Table 2

Brody parameter $\omega$ for the nearest neighbour level spacings distribution for $0 \leq J \leq 9$, $T = T_z$ states up to 4, 5 and 6 MeV above the yrast line in the analyzed nuclei.

| Energy   | $^{46}$V | $^{46}$Ti | $^{46}$Sc | $^{48}$Ca | $^{50}$Ca | $^{46}$V+$^{46}$Ti+$^{46}$Sc | $^{46}$Ca+$^{48}$Ca+$^{50}$Ca |
|----------|----------|----------|----------|----------|----------|-----------------------------|-----------------------------|
| $\leq 4$ MeV | 1.14    | 0.90    | 0.81    | 0.41    | 0.58    | 0.67            | 0.92            | 0.56            |
| $\leq 5$ MeV | 1.10    | 0.81    | 0.96    | 0.53    | 0.58    | 0.69            | 0.93            | 0.60            |
| $\leq 6$ MeV | 0.93    | 0.94    | 0.99    | 0.51    | 0.66    | 0.62            | 0.95            | 0.61            |
Figure Captions

Figure 1: Best fit of the constant temperature formula to the integrated level density for $J^\pi T = 6^+ 1$ of $^{46}$Ti.

Figure 2: $P(s)$ distribution for low-lying levels of $fp$ shell nuclei with $0 \leq J \leq 9$: (a) $^{46}$V, $^{46}$Ti and $^{46}$Sc; (b) $^{46}$Ca, $^{48}$Ca and $^{50}$Ca. The dotted, dashed and solid curves stand for GOE, Poisson, and Brody distributions, respectively.