Spectral statistics of calcium isotopes from realistic shell-model calculations

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The spectral statistics of calcium isotopes are studied with realistic shell-model calculations. For these nuclei, there are significant deviations from the predictions of the random-matrix theory. In particular, we observe an order-chaos transition when the excitation energy is increased and a clear quantum signature of the breaking of integrability when the single-particle energy spacings are decreased. [S0556-2813(98)04910-3]

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I. INTRODUCTION

As is well known, the fluctuation properties of quantum systems with underlying classical chaotic behavior 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 features of the Poisson statistics [1]. The nearest-neighbor spacing distribution of energy levels provides a good signature of regular or chaotic motion. However, in real nuclei long and complete sequences of states of the same spin and parity are very difficult to obtain experimentally. The main exceptions are the neutron and proton resonances, which show a very chaotic behavior of atomic nuclei above the nucleon emission threshold [2]. For low-lying nuclear energy levels the data are much more scarce, but the analysis of the available experimental level sequences suggests [3] that spherical nuclei, and especially the light ones, are rather close to GOE behavior, while strong deviations are mostly found in deformed nuclei. This may be related to the possible existence of states of different K quantum numbers in the level sequences studied. However, the experimental data available are insufficient to establish the borderlines in mass number, excitation energy, etc., between order and chaos in nuclei [4].

The nuclear shell model, with a realistic interaction and large configuration space, is one of the best theoretical approaches to the study of nuclear spectra.The model provides large sets of exact energy levels and wave functions in truncated space, and their statistical analysis can give information on the features and borderlines of the transition from regular to chaotic dynamics in nuclei. The statistical analysis of shell-model energy spectra and wave functions has mainly concentrated on the sd shell region and chaotic behavior has been found for these nuclei both near the yrast line and at higher energies [5]. Recently we studied the spectral statistics of shell-model low-lying states of several fp shell nuclei, using a realistic interaction [6]. For Ca isotopes, we found 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.

The aim of this paper is to perform a more detailed statistical analysis of the shell-model energy levels of Ca isotopes, in order to study whether an order to chaos transition can be observed, and how it depends on variables such as excitation energy, angular momentum, and single-particle energy spacings.

II. ANALYSIS OF ENERGY SPECTRA

The nuclear shell-model Hamiltonian, in second-quantization notation, can be written as

$$H=\sum_{\alpha}\ \epsilon_{\alpha}a_{\alpha}^{+}a_{\alpha}+\frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\delta\gamma\rangle a_{\alpha}^{+}a_{\beta}^{+}a_{\gamma}a_{\delta}, \quad (1)$$

where the labels denote the accessible single-particle states, ϵ_{α} is the corresponding single-particle energy, and $\langle\alpha\beta|V|\delta\gamma\rangle$ is the two-body matrix element of the nuclear residual interaction.

We follow the standard approach to obtain the eigenvalues of the shell-model Hamiltonian. Exact calculations for several nuclei are performed in the $(f_{7/2},\ p_{3/2},\ f_{5/2},\ p_{1/2})$ configuration space, assuming a ^{40}Ca inert core. The construction and diagonalization of large shell-model matrices are performed using a modified version of the computer code ANTOINE [7]. For a fixed number of valence protons and neutrons we calculate the energy spectrum for total angular momentum J and total isospin T. The interaction is a minimally modified Kuo-Brown realistic force with monopole improvements [8]. Coulomb effects are not included.

To analyze the energy level fluctuations, it is necessary to consider only levels which have the same symmetries. In our case this means the same number of nucleons and the same total angular momentum, parity and isospin. The level spectrum is then mapped onto unfolded levels with quasi-uniform level density. The suitable unfolding procedure depends on the region of the spectrum to be analyzed.

TABLE I. Brody parameter ω for the nearest-neighbor level spacing distribution for $0 \leqslant J \leqslant 9$, $T = T_z$ states up to 4, 5, and 6 MeV above the yrast line in the analyzed nuclei.

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

For the low-lying levels, we use an unfolding procedure based on the constant temperature formula [3]. The mean level density can be assumed to be of the form

$$\overline{\rho}(E) = \frac{1}{T}\exp[(E-E_0)/T], \tag{2}$$

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

$$\overline{N}(E) = \int_0^E \overline{\rho}(E')dE' + N_0 = \exp[(E-E_0)/T] - \exp[-E_0/T] + N_0. \tag{3}$$

The constant N_0 represents the number of levels with energies less than zero. We consider this equation as an empirical function to fit the data and let N_0 take nonzero values. The parameters T, E_0, and N_0 that best fit $N(E)$ are obtained by minimizing the function

$$G(T,E_0,N_0) = \int_{E_{\min}}^{E_{\max}} [N(E) - \overline{N}(E)]^2 dE, \tag{4}$$

where $N(E)$ is the number of levels with energies less than or equal to E. The energies $E_{\min}$ and $E_{\max}$ are taken as the first and last energies of the level sequence.

We have compared this unfolding method with the standard local unfolding method [9]. Provided that the number of energy levels is not too small, the two procedures give similar results in the low-energy region, but the constant temperature level density is smoother and is preferable in the ground-state region. When the analysis includes many levels or the full spectrum, we use the local unfolding or a Gaussian function because, as is well known, due to the finite size of the shell model basis, the eigenvalues are generally Gaussian distributed.

In our opinion, the $P(s)$ distribution of the nearest-neighbor spacings $s_i = \overline{N}(E_{i+1}) - \overline{N}(E_i)$ of the unfolded levels is the best spectral statistic to study the fluctuations of the short-range correlations. To quantify the chaoticity of $P(s)$ in terms of a parameter, we compare it to the Brody distribution

$$P(s,\omega) = \alpha(\omega+1)s^{\omega}\exp(-\alpha s^{\omega+1}), \tag{5}$$

with

$$\alpha = \left(\Gamma\left[\frac{\omega+2}{\omega+1}\right]\right)^{\omega+1}. \tag{6}$$

This distribution interpolates between the Poisson distribution ($\omega = 0$) of regular systems and the Wigner distribution ($\omega = 1$) of chaotic ones (GOE). The parameter ω can be used as a simple quantitative measure of the degree of chaoticity [10]. We note that $P(s)$ can also be compared to the Berry-Robnik distribution [11] but, although the Brody and Berry-Robnik distributions have some advantage in limiting cases [12], they are very similar for the cases investigated in this work.

The long-range correlations between energy levels are characterized by the Δ_3 statistic, defined for the interval $[a,a+L]$ in the cumulative level density as

$$\Delta_3(L) = \frac{1}{L}\ \min_{A,B}\int_a^{a+L} [\overline{N}(E) - AE - B]^2 dE. \tag{7}$$

For a stretch $[a,b]$, the value of $\Delta_3(L)$ is obtained as the average Δ_3 over overlapping intervals $[a,L]$, $[a+L/2,a+3L/2]$, $[a+L,a+2L]$, . . . , covering the whole stretch $[a,b]$. In the Poisson limit, $\Delta_3(L) = L/15$. In the GOE limit, $\Delta_3 \sim L/15$ for small L, while $\Delta_3 \sim \pi^{-2}\ln L$ for large L.

III. DISCUSSION OF NUMERICAL RESULTS

We start the analysis of energy spectra looking at the lowest energy region, up to a few MeV above the yrast line. The main problem in this region is that the number of energy levels of the same symmetry is too small for a reliable statistical analysis. But having at our disposal the whole energy spectrum, we can use a sufficiently large set of levels to determine the secular behavior of the level density (2) and perform the unfolding procedure for each symmetry class of states. Moreover, in order to obtain more meaningful statistics, after the unfolding we can combine the level spacings of different J in a nucleus, or even of different nuclei, to calculate the $P(s)$ distribution.

TABLE II. Centroids $\overline{V}_{2j,2j'}$ of the nn and pn two-body matrix elements of the KB3 interaction in the *fp* shell.

	$\overline{V}_{77}$	$\overline{V}_{73}$	$\overline{V}_{75}$	$\overline{V}_{71}$	$\overline{V}_{33}$	$\overline{V}_{35}$	$\overline{V}_{31}$	$\overline{V}_{55}$	$\overline{V}_{51}$	$\overline{V}_{11}$
nn	−0.24	0.20	0.07	0.16	−0.52	−0.02	−0.37	0.05	0.06	−0.25
pn	−0.95	−0.54	−0.93	−0.61	−1.12	−0.47	−1.21	−0.53	−0.35	−0.87

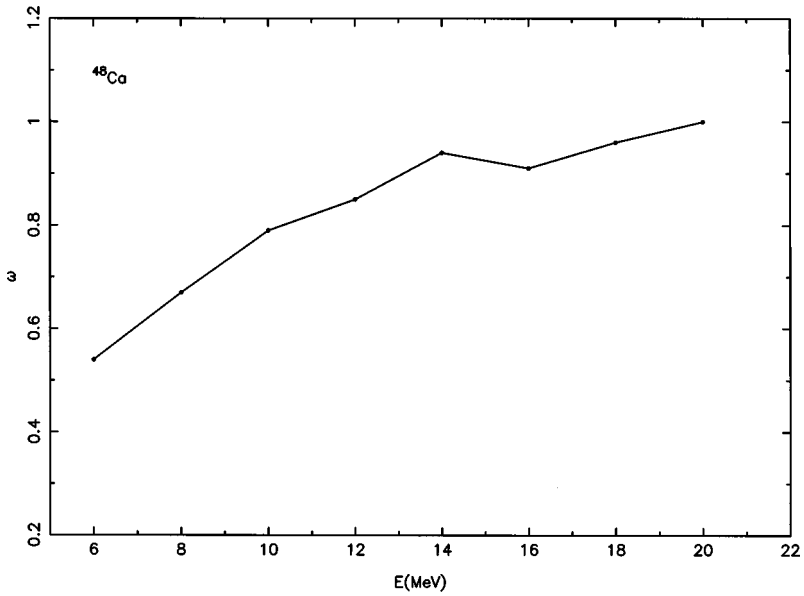


FIG. 1. Energy dependence of the Brody parameter ω in ^{48}Ca. All levels up to an energy E above the yrast line are included for each J value.

Table I shows the best fit Brody parameter ω 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. The number of spacings up to 6 MeV ranges from 105 in ^{45}Ca to 231 ^{46}Ti. 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 we again obtained strong deviations toward regularity.

A better estimate of the Brody parameter is obtained combining spacings of different nuclei. Table I shows the results for ^{46}V+^{46}Ti+^{46}Sc and ^{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.

A plausible interpretation of this peculiar property of Ca isotopes can be done in terms of the strength of the residual interaction. Generally, the nucleon motion would be regular in a spherical mean field and it is the residual interaction that induces chaotic nuclear motion. But the neutron-neutron force is much weaker than the proton-neutron force and thus in Ca isotopes, which only have neutrons in the valence orbits, the regular motion is less disturbed by the residual interaction than in neighboring nuclei with both protons and neutrons in the valence orbits. The average nn and pn residual interactions can be estimated from the centroids. If the two particles are in orbits j and k, the centroid of the two-body matrix elements is defined as

$$\overline{V}_{jk}=\begin{cases}\dfrac{\sum_{(J)}(2J+1)V^{nn,J}_{jkjk}}{\sum_{(J)}(2J+1)}, & nn,\\[2ex] \dfrac{\sum_{J}(2J+1)V^{pn,J}_{jkjk}}{\sum_{J}(2J+1)}, & pn.\end{cases} \tag{8}$$

The sum over (J) for nn indicates that only even J are allowed when the two neutrons are in the same orbit.

Table II contains the centroids of the KB3 interaction in the fp shell. The $\overline{V}_{jk}$ are all atractive for pn, however, for nn not only are they smaller in absolute value, but some of them are atractive and others are repulsive. The centroids for the whole fp shell become $\overline{V}^{pn}=-0.74$ MeV and $\overline{V}^{nn}=0.00$ MeV. Thus the average nn residual interaction is clearly very weak in Ca isotopes.

Returning to Table I, the combined data of ^{46}Ca+^{48}Ca+^{50}Ca show that the chaoticity increases slightly with excitation energy up to 6 MeV. It is generally believed that states at higher energy, in the high density region, should be much more chaotic in nature. Thus, calcium isotopes offer the possibility to study the energy dependence of the chaoticity in the framework of the shell model.

We have calculated the $P(s)$ distribution and the Brody parameter up to a fixed value of the excitation energy above the yrast lines from 6 to 20 MeV. We use the local unfolding method and include all levels with $J=0-11$. We find that the chaoticity increases rather smoothly with energy. This is illustrated in Fig. 1 for ^{48}Ca. It is necessary to include levels up to about 14 MeV to get $\omega>0.9$.

Table III shows the Brody parameter ω for the whole spectrum of the analyzed Ca isotopes, which range from ^{44}Ca to ^{50}Ca. We see that the lightest Ca isotopes are not fully chaotic even when the whole energy spectrum is taken into account.

For the heavier calcium isotopes the number of states is very large, e.g. 17 276 for ^{50}Ca. Therefore, it is possible to analyze separately the spectra for different J values with good statistics. We do not find any significant dependence on

TABLE III. Brody parameter ω for the nearest-neighbor level spacing distribution for Ca isotopes. All levels for each J value are included.

^{44}Ca	^{45}Ca	^{46}Ca	^{47}Ca	^{48}Ca	^{49}Ca	^{50}Ca
0.69	0.75	0.99	0.98	0.95	1.00	0.87

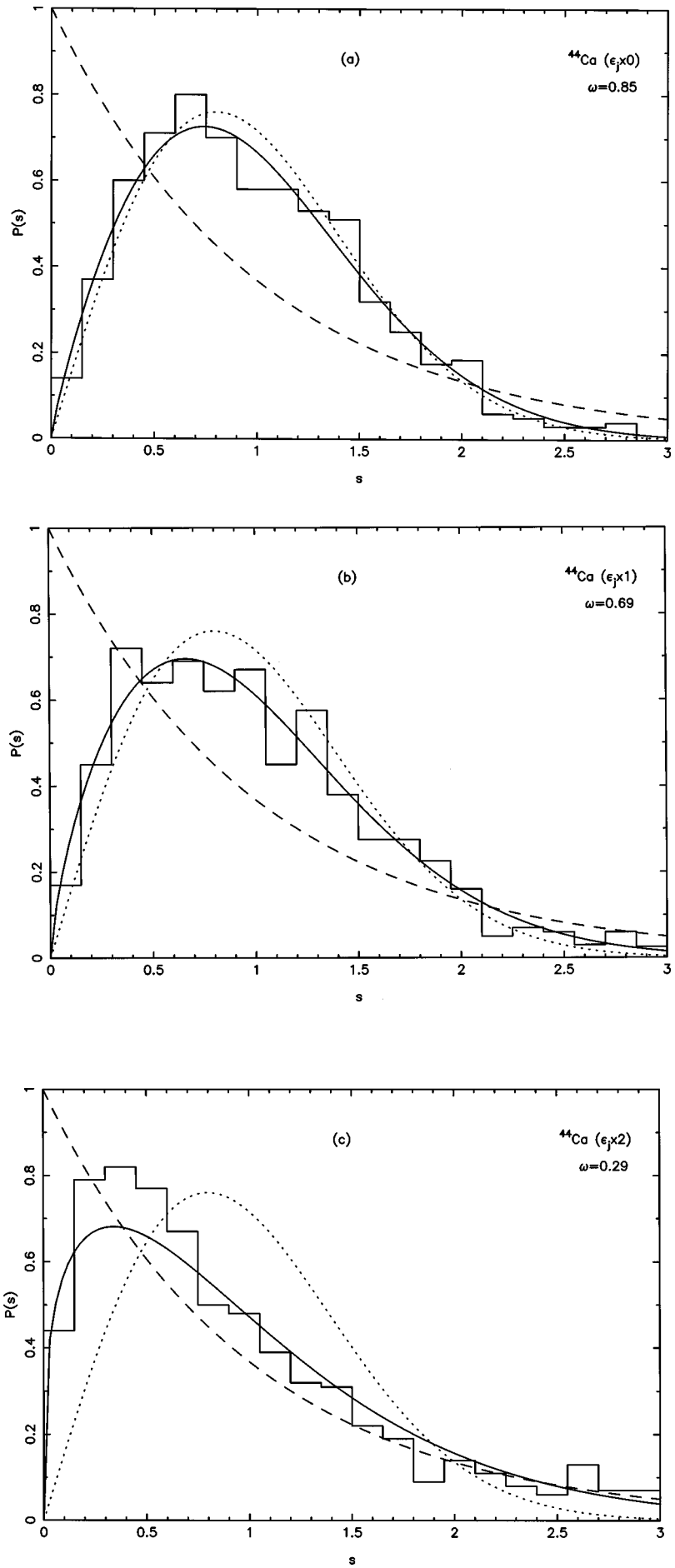
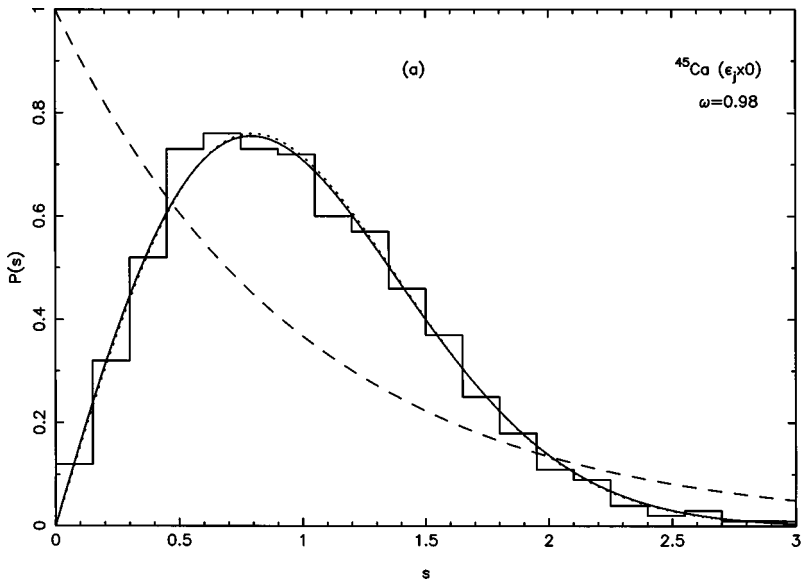
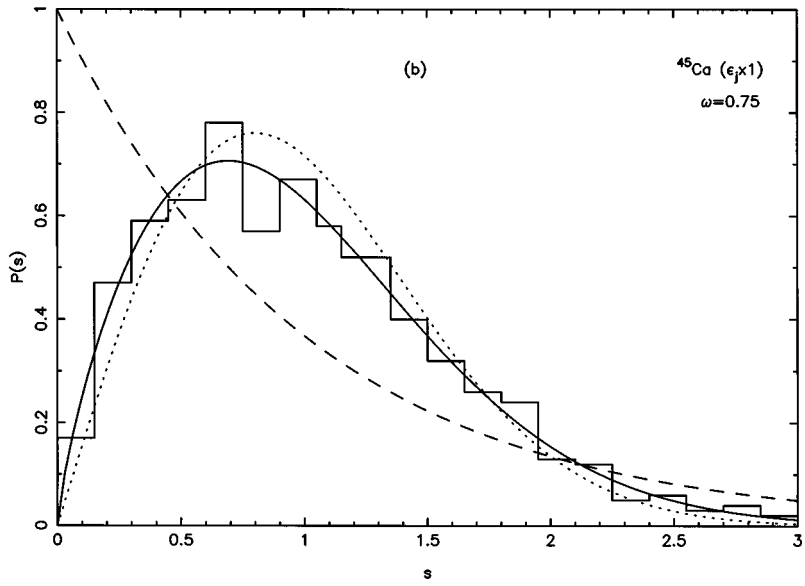


FIG. 2. $P(s)$ distribution for ^{44}Ca. All levels for each J value are included. The single-particle energies are (a) degenerate; (b) normal; (c) double spaced. The dotted, dashed, and solid curves stand for GOE, Poisson, and best fit Brody distributions, respectively.





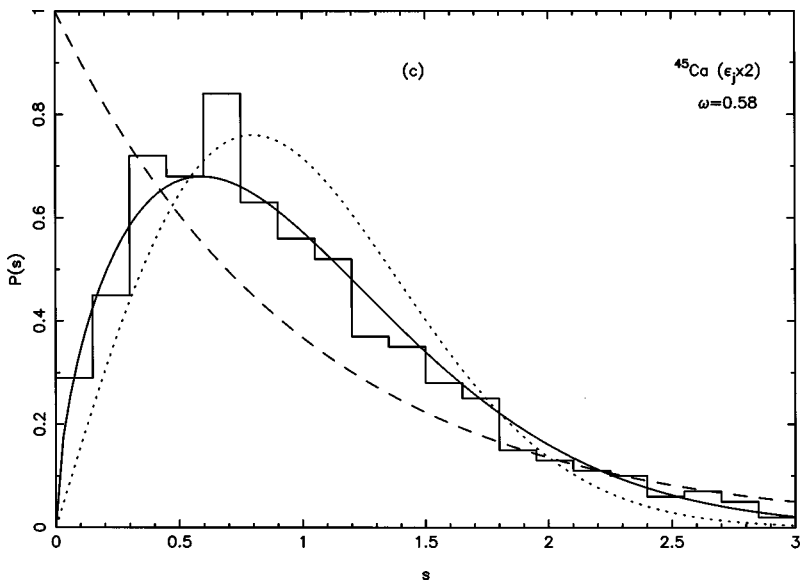


FIG. 3. The same as Fig. 2 for ^{45}Ca.

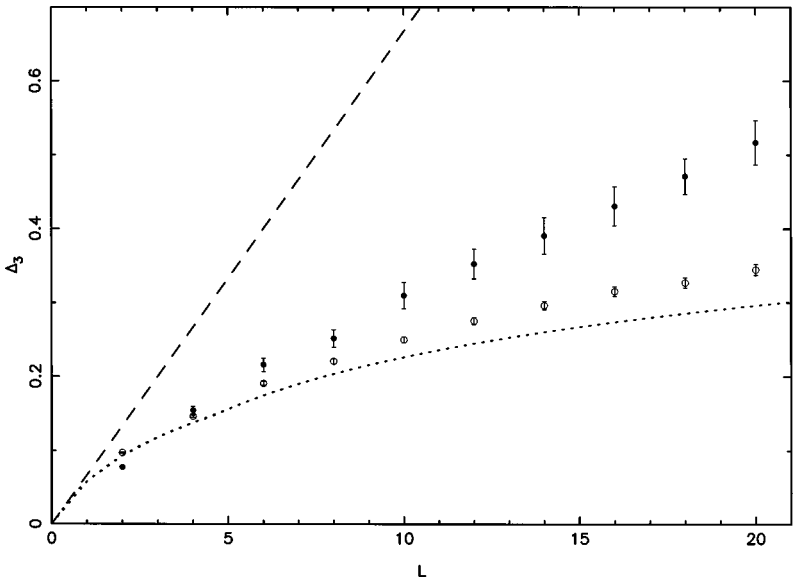


FIG. 4. Average Δ_3 for the $J=0-9$ energy levels of ^{48}Ca up to 10 MeV (filled circles) and 20 MeV (empty circles) excitation energy above the yrast line.

angular momentum, except for $J=0$ where we find $\omega \simeq 0.8$ both for ^{48}Ca and ^{50}Ca. This is probably related to the fact that the pairing interaction, which preserves the seniority quantum number, is more effective for the $J=0$ states.

Another important aspect is the effect of the one-body Hamiltonian on the $P(s)$ distribution. The single-particle motion in the spherical mean field is regular, while the nuclear two-body residual interaction is strongly nonlinear. Figure 2 shows how the fluctuation properties of nuclear energy levels in ^{44}Ca change when the single-particle spacings are changed. We consider three cases. In (a) the $f_{7/2}$, $p_{3/2}$, $f_{5/2}$, and $p_{1/2}$ single-particle levels are all degenerate, in (b) the experimental single-particle energies are used, and in (c) the single-particle spacings are multiplied by a factor of 2. The realistic residual interaction is the same in all cases. The $P(s)$ distribution includes all the nuclear levels, separately unfolded for each J value. For degenerate single-particle levels Fig. 2(a) clearly shows chaotic dynamics in ^{44}Ca, but when the single-particle spacings are increased, there is a transition towards regularity and in case (c) the motion is seen to be quasiregular.

Figure 3 shows a similar calculation for ^{45}Ca. The same kind of chaos to order transition is observed when single-particle spacings increase, but for every set of single-particle spacings ^{45}Ca is more chaotic than the corresponding case in ^{44}Ca. This confirms the trend observed in Table III, suggesting that the quantum signatures of regular motion observed for Ca isotopes in the ground state region are still present at high excitation energy for the lightest isotopes, but chaoticity quickly increases with the number of valence neutrons.

Let us now consider the Δ_3 statistic. We calculate Δ_3 for a set of levels with fixed J and then compute the average Δ_3 of several J values in a given nucleus, in order to improve statistics. Figure 4 shows the average Δ_3 for all $J=0-9$ in ^{48}Ca, calculated for energy levels up to 10 and 20 MeV above the yrast line. It is seen that the chaoticity increases with excitation energy towards the GOE behavior, but up to 10 MeV Δ_3 still is quite far from the GOE limit. All this is in agreement with the trend previously observed in Fig. 1 for the $P(s)$ dependence on exitation energy in the same nucleus.

Figure 5 illustrates the Δ_3 dependence on the single-

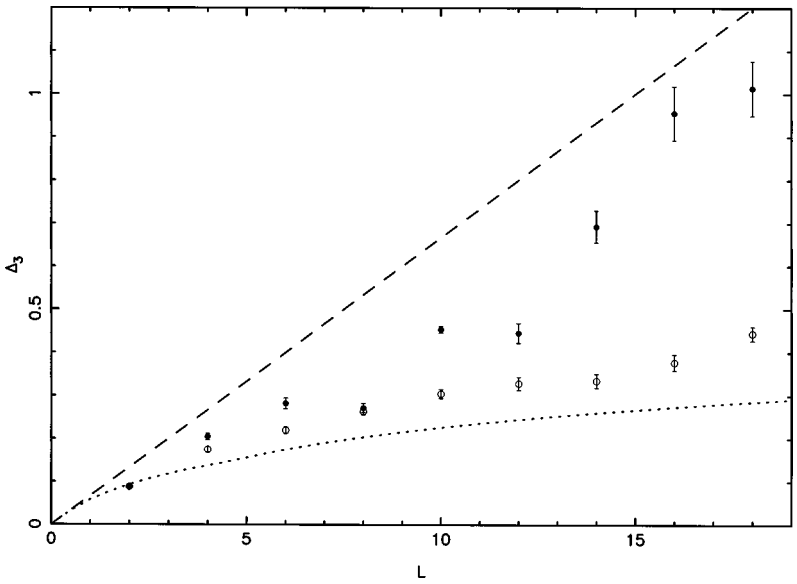


FIG. 5. Average Δ_3 for all the $J=0-9$ energy levels of ^{44}Ca, calculated using the normal single-particle energies (empty circles) and double spaced single-particle energies (filled circles).

particle energy spacing. The average Δ_3 of all $J=0-9$ in ^{44}Ca, for the whole energy spectrum, is plotted for normal (experimental) spacing and for double spacing of single particle energies. Since the number of states is now much smaller than in ^{48}Ca, the results for ^{44}Ca are not so smooth. However, it is clearly seen that for normal spacing Δ_3 is closer to the GOE behavior, although it is not fully chaotic, and for double spacing it is closer to the Poisson limit for large L. Thus we find that the chaoticity of Ca isotopes, measured in terms of the Δ_3 statistic, is strongly dependent on the single particle energy spacings. It confirms the results that we obtained from the analysis of the $P(s)$ distribution.

IV. CONCLUSIONS

The study of spectral statistics in nuclei using experimental data and nuclear models shows that nuclear motion is mostly chaotic. However, the success of nuclear models in the detailed description of nuclear properties, especially in the ground state region, provides inequivocal evidence of the existence of some regular motion in nuclei. Thus, it is interesting to localize the regions of regular motion as a function of variables such as mass, shape, excitation energy, etc., in nuclei, and to analyze as well how the different parts of the interaction influence the regular or chaotic features of nuclear motion.

In this paper the spectral statistics of Ca isotopes have been studied in detail using exact shell-model calculations in the fp shell with the realistic interaction KB3. These nuclei are especially interesting because the nearest-neighbor spacing distribution $P(s)$ of low-lying energy levels shows significant deviations from GOE predictions, in contrast to other neighboring nuclei which show fully chaotic spectral distributions.

The analysis of level spacings up to a given excitation energy, based on the $P(s)$ and Δ_3 statistics, shows that the chaoticity of Ca isotopes increases smoothly with the excitation energy end point. However, even when the whole energy spectrum is included, the lighter isotopes ^{44}Ca and ^{45}Ca are not fully chaotic, and the order to chaos transition is progressive as the number of active particles increases.

In the heavier Ca isotopes studied, the number of energy levels is very large and it is possible to analyze with good statistics the energy levels of a single J value. For example, in ^{50}Ca the dimension of many Hamiltonian matrices exceeds one or two thousand for fixed J. We do not find significant differences in the $P(s)$ distribution for different J values, except perhaps for $J=0$, for which we obtain a Brody parameter somewhat smaller than for other J values. This is probably related to the pairing component of the interaction and the aproximate conservation of the seniority quantum number.

Finally, the relationship of fp shell single-particle energy spacings to fluctuation properties of energy spectra have been studied. A clear chaos to order transition is observed as the single-particle spacings are increased. In the lighter Ca isotopes we obtain chaotic behavior for degenerate single-particle states and quasiregular motion when the single-particle spacings are twice the experimental values. Thus, it seems that the main reason for the substantial deviations from chaoticity obtained in Ca isotopes is that the relatively weak strength of the neutron-neutron interaction is not able to destroy the regular single-particle mean-field motion completely. But in the neighboring nuclei with both protons and neutrons in valence orbits, the stronger proton-neutron interaction seems to be sufficent to destroy the regular mean-field motion.

ACKNOWLEDGMENT

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