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Localization in $2p1f$ nuclear shell-model wavefunctions

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Abstract

For the study of complexity and chaos in many-particle nuclear wavefunctions in large shell-model basis spaces, the localization length related to the number of principal components is calculated for several Ca, Sc and Ti isotopes, and compared to the predictions of the embedded Gaussian orthogonal ensemble. The large dimensionalities involved, up to many thousands, ensure good statistics, and the agreement is very good in the chaotic region of the spectra. The localization length of shell-model wavefunctions in Ca isotopes is much smaller than in Sc, showing a strong isospin dependence of nuclear chaos, in good agreement with previous results based on energy level fluctuation properties.

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1. Introduction

The study of the eigenvector amplitudes of many-fermion systems and the construction of information entropy, number of principal components and similar measures for the study of complexity and chaos in the system is of great current interest. Firstly the investigation of Izrailev [1] and then results from detailed nuclear shell-model studies by Zelevinsky and collaborators [2,3] established the importance of these measures. It also became clear that the Gaussian orthogonal ensemble (GOE) of random matrices is totally inadequate to explain the strong energy dependence of these quantities.

On the other hand the study of statistical spectroscopy in nuclei long ago [4–9] developed the embedded Gaussian orthogonal ensemble (EGOE), and in the last few years it has been realized that this ensemble is well suited for the study of chaos in quantum mechanical many-particle systems. Kota ans Sahu [10] derived expressions for the information entropy and the number of principal components for EGOE and made numerical tests for their goodness [11].

The predictions of EGOE for strength sums of nuclear excitation operators and their agreement with the results from shell-model calculations in large $2p1f$ and $2s1d$–$2p1f$ spaces has been looked into recently

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in detail [12–14]. It was found that the agreement is very good in the chaotic regime of the nuclear motion. In this Letter we look into complementary aspects of such shell-model studies, i.e., agreement with EGOE predictions of the measures of complexity and chaos. In the process we develop possible correction terms to the EGOE expressions for application to large but finite dimensional systems. We also find realistic estimates of how much of the two-body interaction is needed to generate chaos for a $(1+2)$-body Hamiltonian, and hence find the applicability of EGOE through this study of wavefunction amplitudes. Section 2 introduces the measures of complexity and give their EGOE expressions and methods for further improving them. Section 3 gives the results in a number of $2p1f$ shell-model examples with very large dimensional Hamiltonian matrices and justifies the applicability of EGOE in these systems. Section 4 ends with a discussion and some conclusions.

2. EGOE results

2.1. Localization length in wavefunctions

In the nuclear shell model one has m fermions distributed over N single-particle states with a $(1+2)$-body interaction Hamiltonian. This Hamiltonian is written as

$$H = h(1) + V(2), \tag{1}$$

where $h(1)$ is the one-body mean-field part and $V(2)$ is the residual interaction. For the GOE (Gaussian orthogonal ensemble) one has a random real symmetric matrix (with invariance under orthogonal transformations) for the Hamiltonian in the m-particle space, whereas the two-body random ensemble (TBRE) is generated by defining the Hamiltonian as a random matrix in the two-particle space and then propagating it to the ${}^{N}C_{m}$ dimensional m-particle space by using its direct product structure. The TBRE is a GOE in the two-particle state and is called EGOE(2); we refer to [15] for details. When one adds a one-body part to this Hamiltonian, as in Eq. (1), it is often called EGOE$(1+2)$.

For large shell-model spaces one can define the normalized eigenfunction $\psi_E = |E\rangle$ in terms of the normalized mean field basis $\phi_k = |k\rangle$, i.e.,

$$|E\rangle = \sum_k C_k^E |k\rangle, \tag{2}$$

where C_k^E are the amplitudes in the expansion. Then, as a measure for the degree of the complexity of individual wavefunctions, one can define the information entropy S^{info} as

$$S_E^{\text{info}} = -\sum_k \left|C_k^E\right|^2 \ln\left|C_k^E\right|^2, \tag{3}$$

and the localization length $l_H(E)$ as

$$l_H(E) = \exp\left[S_E^{\text{info}}\right]/0.48\,d. \tag{4}$$

For GOE, the value of $S^{\text{info}} = \ln(0.48\,d)$ is independent of energy. Thus $l_H(E) = 1$ for GOE. The factor 0.48 arises from the assumption (well verified by many numerical calculations) that the local strength fluctuations for EGOE(2) are well described by the Porter–Thomas distribution [10]. One can also define the participation ratio or number of principal components, NPC, as

$$(\text{NPC})_E = \left[\sum_k \left|C_k^E\right|^4\right]^{-1}. \tag{5}$$

Its value for GOE, $(\text{NPC})_E = d/3$, is again independent of energy.

We now discuss the predictions of EGOE for these quantities. First of all we note that with m particles in N states there is an underlying $U(N)$ group structure, and with respect to this group one can write the part $V^{[0]}$ of $V(2)$ that generates the mean-field basis state energies E_k as the sum of a unitary scalar $V^{[0],0}$ and irreducible parts with ranks 1 and 2, $V^{[0],1}$ and $V^{[0],2}$. Calculations for typical sd and fp shell interactions show that the norm of $V^{[0],2}$ is less than 5% of the full $V(2)$ [16]. Thus, as $V^{[0],2}$ is usually very small in size, $V^{[0],0} + V^{[0],1}$ added to $h(1)$ gives an effective one-body mean-field part h. The location of the configuration centroids is generated by this effective one-body operator, while their spreading is due to the two-body operator $V^{[0],2}$. The effective one-body part is denoted as H_k in the following expressions. The Hamiltonian H_k generates the centroids E_k of the strength functions $F_k(E) = \langle\delta(H-E)\rangle^k = \sum_{E'} |C_k^E|^2 \delta(E-E')$, and σ_H^2 is the variance of the energies E_k. Similarly $\epsilon_H =$

$(d)^{-1}\sum_k \langle k|H|k\rangle$ is the centroid of both E and E_k energies, while σ_k is the variance of $F_k(E)$ and has the form given below. Using these quantities one can define the bivariate correlation coefficient ζ_{H,H_k} as

$$\zeta_{H,H_k} = \frac{\langle H H_k\rangle^m}{\sqrt{\langle H^2\rangle^m \langle H_k^2\rangle^m}} = \sqrt{\left(1 - \frac{\overline{\sigma_k^2}}{\sigma_H^2}\right)},$$

$$\sigma_H^2 = \frac{1}{d}\sum_{k,k'} \left|\langle k|H|k'\rangle\right|^2 - \left[\frac{1}{d}\sum_k \langle k|H|k\rangle\right]^2,$$

$$\overline{\sigma_k^2} = \frac{1}{d}\sum_{k\neq k'} \left|\langle k|H|k'\rangle\right|^2,$$

$$\sigma_H^2 - \overline{\sigma_k^2} = \sigma_{E_k}^2 = \frac{1}{d}\sum_k (E_k - \epsilon_{H_k})^2,$$

$$E_k = \langle k|H|k\rangle, \qquad \epsilon_{H_k} = \frac{1}{d}\sum_k E_k. \tag{6}$$

The EGOE formula for l_H, with $\widehat{E} = (E - \varepsilon_H)/\sigma_H$, is [11]

$$l_H(E) = \sqrt{1-\zeta_{H,H_k}^2}\exp\left(\frac{\zeta_{H,H_k}^2}{2}\right) \times \exp\left(-\left(\frac{\zeta_{H,H_k}^2 \widehat{E}^2}{2}\right)\right) \times \left(1 - \frac{1}{8}\left[\frac{(\delta\sigma^2)}{\sigma_H^2}\right]^2 Y(E)\right),$$

$$Y(E) = \frac{1}{(1-\zeta_{H,H_k}^2)^2} \times \left\{\left(1-\zeta_{H,H_k}^2\right)^2\left(\widehat{E}^2-1\right)^2 + 4\zeta_{H,H_k}^2\left(1-\zeta_{H,H_k}^2\right)\widehat{E}^2 + 2\zeta_{H,H_k}^4\right\},$$

$$\frac{(\delta\sigma^2)}{\sigma_H^2} = \left\{\overline{\sigma_k^2}\right\}^{-1}\left(1-\zeta_{H,H_k}^2\right) \times \left[(d)^{-1}\left\{\sum_k \left(\sigma_k^2 - \overline{\sigma_k^2}\right)^2\right\}\right]^{1/2}. \tag{7}$$

For details we refer to [15] and [10].

In Eq. (7) the last factor involving $Y(E)$ becomes 1 when $Y(E) = 0$, and the expression for the localization length becomes Gaussian in energy. So non-zero $Y(E)$ gives improvement over the Gaussian. Alternately one can introduce correction terms to the Gaussian in two different ways. Firstly one can make an Edgeworth-type expansion multiplying the Gaussian by a polynomial with a few low order terms, given by

$$l_H(E) = \sqrt{1-z^2}\exp\left(\frac{z^2}{2}\right)\exp\left(-\frac{z^2\widehat{E}^2}{2}\right) \times \left(1 + U\widehat{E} + V\widehat{E}^2\right), \tag{8}$$

where z is the correlation coefficient that we previously called ζ_{H,H_k}, and U and V are the coefficients of the linear and quadratic terms. Secondly, in another formalism, the expectation value of an operator K in a state with energy E is given by a polynomial expansion in E as

$$\langle E|K|E\rangle = \sum_\nu \left\langle K P_\nu(H)\right\rangle P_\nu(E), \tag{9}$$

where $\langle\cdots\rangle$ denotes average in the m-particle space and $P_\nu(x)$ are the orthogonal polynomials with the density $\rho_m(E)$ as the weight function. Under EGOE, as the density of states for the Hamiltonian H as well as the one for the perturbed Hamiltonian $H_\alpha = H + \alpha K$ tend to Gaussians, only the first two terms in the expansion (9) are unhindered [7]. The higher terms give decreasingly small correction terms. So one can use this expansion with the operator for the localization length as K and get an expression for $l_H(E)$.

2.2. Wavefunction structure for a regular to chaotic transition of the Hamiltonian

For a specific $(1+2)$-body Hamiltonian, the EGOE results mentioned above are good only in the domain of chaos. The chaotic regime sets in at an energy of a few MeV above the ground state region. There are attempts to estimate this energy analytically for particular forms of the Hamiltonian, as well as numerically ([14] and references therein). One can also study the problem in a different way, i.e., by studying the properties of the Hamiltonian $H_\lambda = h(1) + \lambda V(2)$ as a function of the parameter λ. One finds a crossover value λ_c of λ, such that for $\lambda > \lambda_c$ there is onset of chaos where one observes GOE level fluctuations in many-particle ($m \gg 1$) spaces. Clearly the ordered particle motion in the mean field $h(1)$ will be destroyed by a sufficiently strong two-body residual interaction. One can find that for $h(1)$ having average spacing Δ, λ_c turns out to be of the order of the ratio of the spacing between m-particle mean-field basis states, that are di-

rectly coupled to the two-body interaction, and Δ. For such studies we refer to [18,19].

On the other hand, through explicit construction of the measures of complexity numerically, one can slowly increase λ from zero, to see where the localization length and other similar quantities start matching with the EGOE predictions. One can also investigate how the λ_c evaluated this way compare with the λ_c obtained from the study of the spacing distribution, i.e., the nearest neighbor spacing and the Δ_3 statistic. The next section describes such studies.

3. Shell-model results

Shell-model calculations for a number of nuclei with different (J, T) values in the $2p1f$ shell (hereafter called pf shell) were carried out using the modern shell-model code NATHAN [17]. The single-particle energies considered (defined by the one-body part $h(1)$ of the Hamiltonian H) are 0.0, 2.0, 4.0 and 6.5 MeV for the $f_{7/2}$, $p_{3/2}$, $p_{1/2}$ and $f_{5/2}$ orbits, respectively, and the two-body effective interaction $V(2)$ is the well established KB3 interaction [17]. From now on this $H = h(1) + V(2)$ is simply called the KB3 interaction.

In Fig. 1 we present the results for the localization length as a function of energy for the $J = 2$, $T = 1$ states of the nucleus ^{46}Ti, which has a large dimension of 6338. The figure gives the exact shell-model result along with three different forms of predictions. The shell-model values exhibit small oscillations close to a smooth, nearly Gaussian shape. This exact calculation is compared to EGOE predictions as follows. (i) The EGOE Gaussian form of expression (7) with $Y(E) = 0$, that shows a good agreement with shell model. One finds that the inclusion of non-zero $Y(E) = 0$ in Eq. (7) makes very little change in the previous results. (ii) The EGOE Gaussian form with polynomial correction terms multiplying the Gaussian, as given by Eq. (8). It is seen that one achieves further improvement, particularly near the spectrum ends. We note here that the coefficients z, U and V in this expansion are actually calculated by best fit to the shell-model values. So this result really checks the applicability of the method and is not a prediction without diagonalization. (iii) The EGOE polynomial expansion form given by (9). It is taken up to the fourth order,

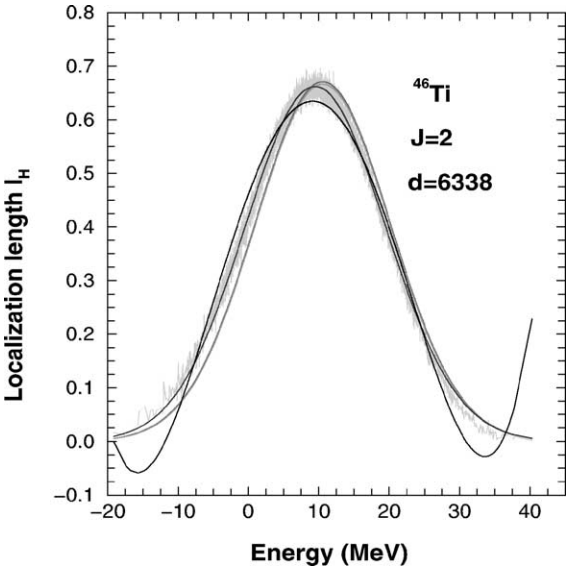

Fig. 1. Localization length l_H as a function of energy in MeV for ^{46}Ti($J = 2$, $T = 1$). The brown curve is the exact shell-model result, while the red and green curves are the EGOE predictions, as given by Eq. (7), with $Y(E) = 0$ and $Y(E) \neq 0$, respectively. The blue curve is the EGOE with polynomial corrections terms, as given by Eq. (8), and the black curve is the polynomial expansion given by Eq. (9).

Table 1
Shell-model valence space dimensionality d, and values of the parameters z, U and V used in Figs. 1 and 2. In the last column we also give the value of the correlation coefficient ζ_{H,H_k} calculated directly from the shell-model matrix elements

Nucleus	d	z	U	V	ζ_{H,H_k}
^{46}Sc($J = 0,\ T = 2$)	692	0.932	−0.118	0.064	0.905
^{46}Sc($J = 1,\ T = 2$)	2042	0.924	−0.105	0.043	0.910
^{46}Ti($J = 0,\ T = 1$)	1514	0.902	−0.100	0.032	0.891
^{46}Ti($J = 1,\ T = 1$)	4105	0.899	−0.099	0.045	0.892
^{46}Ti($J = 2,\ T = 1$)	6338	0.898	−0.094	0.037	0.893
^{48}Sc($J = 0,\ T = 3$)	2958	0.914	−0.063	0.032	0.900
^{48}Sc($J = 1,\ T = 3$)	8590	0.911	−0.057	0.030	0.900
^{50}Sc($J = 0,\ T = 4$)	5986	0.906	−0.025	0.028	0.900

and it shows excellent agreement in the central region, but strong deviations near the two ends.

Fig. 2 gives results similar to those of Fig. 1, but for all the $T = T_z$ eight cases considered, i.e., ^{46}Sc($J = 0$), ^{46}Sc($J = 1$), ^{48}Sc($J = 0$), ^{48}Sc($J = 1$), ^{50}Sc($J = 0$), ^{46}Ti($J = 0$), ^{46}Ti($J = 1$) and ^{46}Ti($J = 2$). The dimensions of the shell-model spaces, the correlation coefficient z, and the U and V coefficients for all the cases are given in Table 1. The

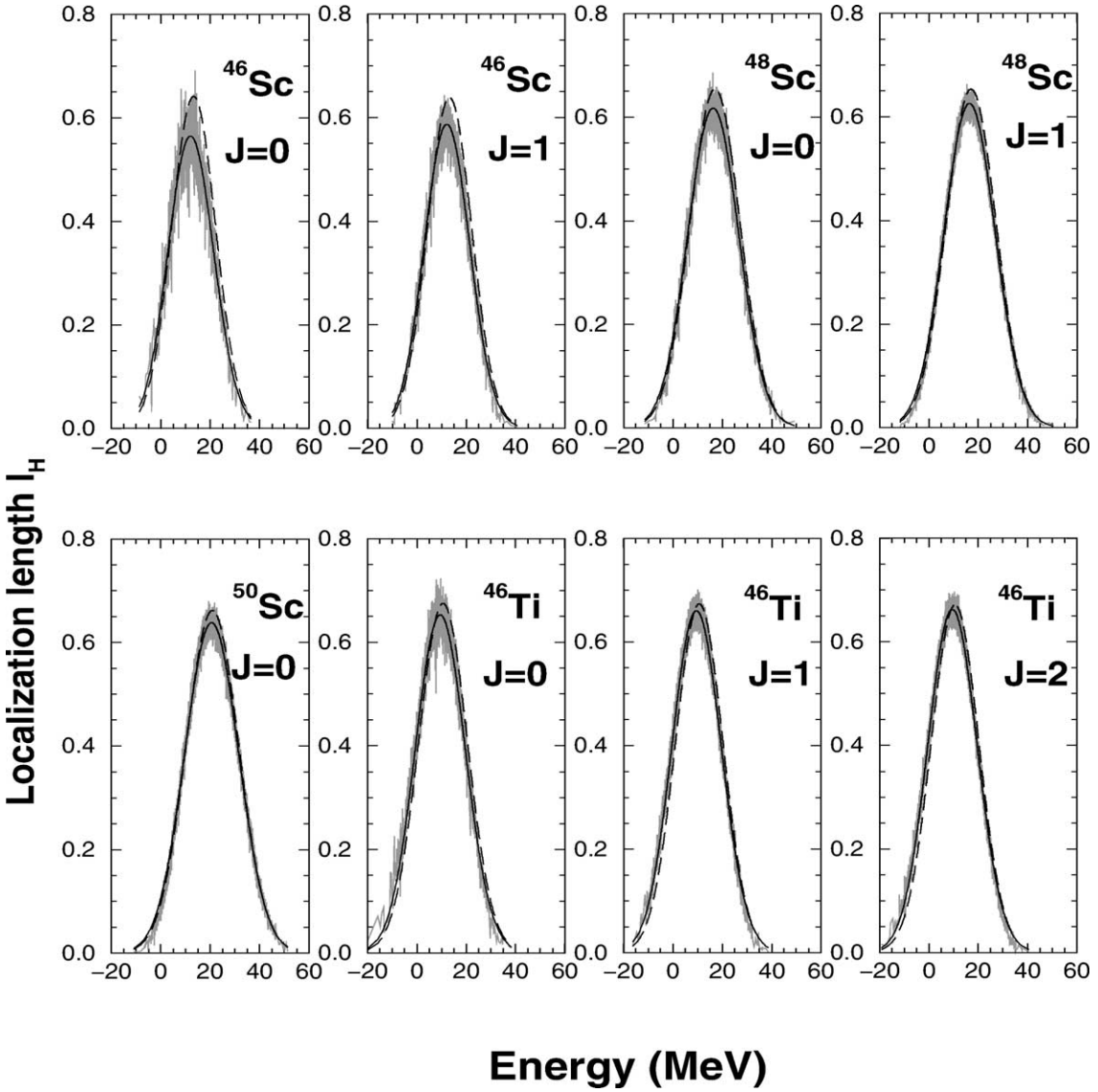

Fig. 2. Same as Fig. 1 for different J states in several Sc and Ti isotopes. Here the green curve represents the exact shell-model result, the black long dashed line is the EGOE prediction with $Y(E) = 0$, and the solid line is the EGOE prediction with polynomial correction terms.

general features for all those cases are similar to those of ^{46}Ti($J = 2$). One observes that as the dimension increases, the agreement of the EGOE with the shell model shows gradual improvement.

Fig. 3 gives the behavior of the localization length for the nucleus ^{46}Sc($J = 1,\ T = 2$) when the Hamiltonian is slowly changed from the one-body form to the full $(1 + 2)$-body Hamiltonian through the parameter λ. Results are shown for $\lambda = 0$, 0.1, 0.3, 0.5, 0.7 and 1.0. Along with the shell-model fluctuating curves, one sees here the dashed curve which is the Gaussian form in energy, i.e., Eq. (7) with $Y(E) = 0$, and the continuous curve which is the Gaussian with the polynomial corrections of Eq. (8). Actually, these curves are those with the best fit values of z, U and V, i.e., 0.905, -0.118 and 0.064, respectively. We observe that for $\lambda = 0.5$ or more the polynomial correction curve gives good agreement with the shell model.

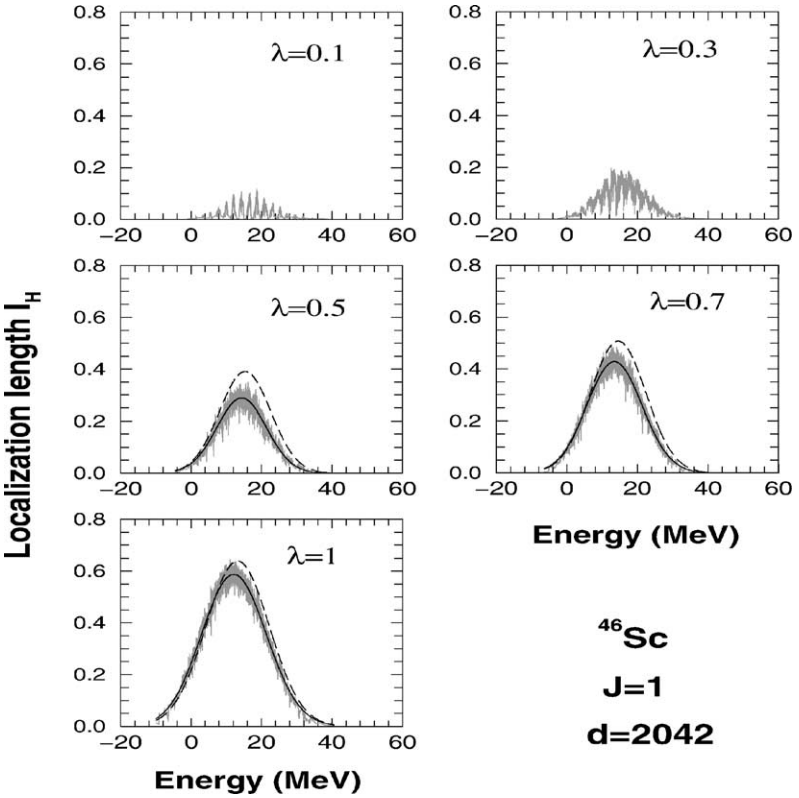

Fig. 3. Localization length l_H for ^{46}Sc($J = 1$, $T = 1$), as a function of λ, the strength parameter multiplying the two-body interaction. The value $\lambda = 0$ corresponds to the mean-field Hamiltonian and $\lambda = 1$ gives the full $(1 + 2)$-body Hamiltonian.

This feature is in agreement with the observed behavior of the spectral rigidity parameter Δ_3 for energy spectra [12].

In Fig. 4 the localization length averaged over all energy states with fixed J is plotted as a function of the J values. This is done for four nuclei ^{46}Sc, ^{48}Ca, ^{50}Ca and ^{52}Ca. One finds that ^{46}Sc shows a marked different behavior than the other three. The fact that l_H is larger for ^{46}Sc than for the three Ca isotopes is consistent with previous results [20,21], which showed that the usual level fluctuation statistics, like the nearest neighbor spacing distribution $P(s)$ and Δ_3, are closer to the Poisson limit in Ca isotopes than in other nuclei with active protons and neutrons. In this sense we may say that Ca isotopes are less chaotic than other neighboring nuclei. This is especially true for the low energy spectrum. As discussed below, there are two reasons for this behavior: (i) the residual n–n interaction is weaker than the n–p interaction,

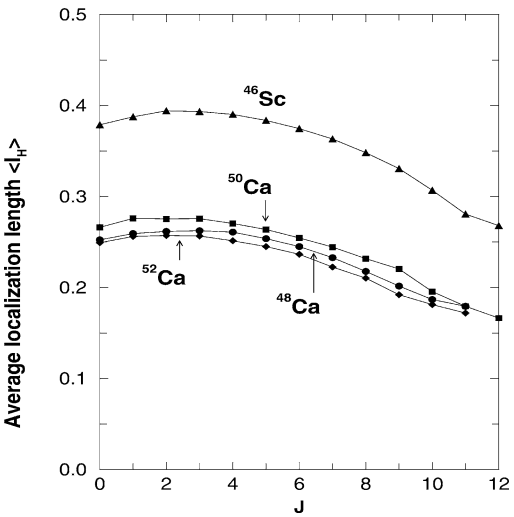

Fig. 4. Average localization length as a function of the angular momentum J, showing the marked difference of ^{46}Sc from Ca isotopes.

and (ii) seniority is to a large extent a good quantum number in Ca isotopes.

4. Discussion and conclusions

In this Letter we have studied the localization length l_H for nuclear shell-model wavefunctions in large $2p1f$ spaces, looking for a better understanding of the onset of chaos in nuclei. The large dimensionalities involved, up to $d = 8590$, guarantee good statistics and therefore reliable results. The values of l_H as a function of energy were compared with predictions of the EGOE theory, obtaining very good agreement in the chaotic, central region of the energy spectra, while some deviations are observed in the ground state region.

The important question of how much of the two-body interaction is needed to generate chaos was also studied using an order-to-chaos transition Hamiltonian depending on a strength parameter λ. One finds that the localization length gives results similar to those obtained from previous studies of Δ_3 for energy spectra, i.e., that nuclear motion becomes chaotic for $\lambda \geqslant 0.5$, meaning that a half of the realistic residual interaction is sufficient for the onset of chaos.

Finally, looking at the average localization length $\langle l_H \rangle$, it is seen that there is a strong isospin dependence of chaos in nuclei. Single close-shell nuclei like Ca isotopes have much smaller localization lengths than other nuclei. When only one of the neutrons is replaced by a proton, there is a sudden increase of chaoticity, which is observed by a strong increase of localization lengths, and by a Δ_3 behavior much closer to GOE. The reasons for this sudden change of chaoticity from Ca to Sc isotopes have been discussed in previous papers [21]. One of the reasons is that the $T = 0$ two-body residual interaction is much stronger than the $T = 1$ interaction. The strong $T = 0$ interaction in Sc isotopes destroys the ordered mean field motion of the nucleons much more than the weaker $T = 1$ part. Since Ca isotopes only have $T = 1$ interaction, because they only have active neutrons outside the closed shell core, the nuclear motion becomes more regular. This effect applies to the whole energy spectrum and to all the wave functions, and therefore to the localization lengths. The second reason applies especially to the ground state region. In Ca isotopes there is an approximate symmetry associated to the pairing force among valence neutrons, and this symmetry is not taken into account in the statistical analysis. This mixing of states belonging to different symmetries gives rise to Poisson like statistics. On the other hand, the presence of a proton in Sc isotopes destroys this symmetry, and therefore we do not mix different symmetry states in the statistical analysis of energy level and wave function fluctuations.

We note that the construction of localization lengths for transition strength distributions and their study for electromagnetic, Gamow–Teller and other transitions is also important and will provide valuable additional information on chaotic features. With this regard, we also note that very recently it has been conjectured that $1/f$ noise is a fundamental property characterizing the spectral fluctuations of chaotic quantum systems [22]. We plan to address these issues in future work and see how they compare with predictions based on more traditional statistics.

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