

# Energy fluctuations of pseudointegrable systems with growing surface roughness

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The eigenfrequencies of two-dimensional systems with fractal boundaries and with nonscaling rough boundaries are calculated numerically by the Lanczos algorithm and analyzed by means of level statistics. The systems are pseudointegrable and the fluctuations of their eigenvalue spectra show a global statistical behavior between the Poisson and the Wigner distributions. With increasing irregularity of the boundary, the systems approach the Wigner limit and the results seem to depend only on the genus number of the geometry and not on details, such as the asymptotic shape of the geometry, the type of roughness (scaling or nonscaling), and the boundary conditions (Neumann or Dirichlet). No transition between localized and extended states is found in fractal drums.

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## I. INTRODUCTION

The vibrational behavior of geometrically irregular objects has been a subject of considerable interest. This interest arises from both a fundamental and a practical point of view, because many systems with strongly irregular geometries exist in nature. Their physical properties, such as, e.g., their vibrational or electronic behavior, differ in many cases from those of their regular counterparts. Fractal geometry [1] permits a description of many irregular systems as well-defined geometrical objects, if the physical properties of the considered objects are due to the hierarchical character of their geometry [2].

Here, we are interested in the vibrational and electronic behavior of surface fractals (“fractal drums”) [3]. These are normal Euclidean systems, whose boundaries have fractal shapes. Their vibrational excitations have been referred to as “Dirichlet fractinos” or “Neumann fractinos,” depending on their boundary conditions. Their energy spectra and localization properties are clearly distinct from those of systems with smooth boundaries. This has been demonstrated by numerical simulations [4–6] as well as by experiments on liquid crystal films [6] and on acoustic cavities [7]. Among other things, we are interested in the localization properties of fractal drums, which are most important when applied to real systems. For example, the nanostructures in porous silica can be modeled to some extent by fractal drums under Dirichlet boundary conditions,  $\Psi = 0$ , along the boundary. In this case, the relevant electron states are localized, in the sense that they occupy only a small portion of the total system volume. This leads to a broadening of the band gap and could explain the observed luminescence of porous silica [8]. When considering the vibrational modes in irregular macroscopic fractal-shaped acoustic cavities and membranes, it was also found that localization effects have important consequences for the acoustic behavior. When this localization is enhanced, viscous damping is increased [7,9].

In this paper, the electronic and vibrational properties of fractal drums are studied by the methods of level statistics, which is an important tool in quantum chaos. We concentrate on those fractal drums that have been used earlier in Refs. [4–9]. First, we want to see if the states that occupy only

some percent of the total system are really localized, i.e., if their localization lengths approach a constant when the system size is increased. Second, fractal drums are so-called pseudointegrable systems [10,11] (see below), which are geometrically intermediate between regular and chaotic systems. Although pseudointegrable systems have attracted a lot of attention in recent years [12–14], up to now, only relatively simple pseudointegrable systems have been investigated. These systems showed comparatively small surface roughness. The boundaries were nonfractal and no localized states occurred. For a particular pseudointegrable geometry, where the chaotic Sinai shape was approached by a certain number of corners, it was found numerically that with growing surface roughness the systems showed more and more chaotic behavior [14]. The analysis was restricted to the low-frequency spectrum and it is not yet clear if the results are also valid in the regime where the wavelengths are small enough to resolve the edges. In this paper we want to investigate the energy fluctuations of the whole high-energy spectrum and see if details of the geometry, like, e.g., the fractal shape or the asymptotic shape of the system, have some specific consequences or if the behavior of the level statistics depends solely on the number of edges. For this purpose, several pseudointegrable systems of various geometries are compared to the fractal drums. The paper is organized as follows. In Sec. II, the model systems and the various geometries are explained. In Sec. III, the density of states of the fractal drums is shown. Finally, in Sec. IV, the level statistics results for the fractal drums and several other systems under Dirichlet and Neumann boundary conditions are compared and discussed.

## II. MODEL SYSTEMS

Let us consider a membrane that lies in the  $xy$  plane and vibrates in the  $z$  direction. When the restoring forces are considered as scalar, the vibrations of this membrane are described by the Helmholtz equation

$$\Delta \Psi_n(x,y) = -\frac{\omega_n^2}{c^2} \Psi_n(x,y), \quad (1)$$

where  $\Psi_n(x,y)$  is the  $n^{\text{th}}$  eigenfunction,  $\epsilon_n \equiv \omega_n^2$  the corresponding eigenvalue, and  $c$  the sound velocity of the membrane. This equation has the same form as the stationary Schrödinger equation with zero potential  $V=0$  inside the drum. Therefore, under Dirichlet boundary conditions, which refer to infinite potential on the boundary it can also describe an electron in an infinite potential well. In this case, one has to replace  $\omega_n^2/c^2$  by  $2\mu E_n/\hbar^2$ , where  $\mu$  is the electron mass and  $E_n$  the energy eigenvalue.

For the numerical calculations, Eq. (1) is discretized on a square lattice. At each lattice point  $i$ , we put identical masses  $m$ , which are coupled by linear nearest-neighbor springs  $k$ . The discretized form of Eq. (1) can be written as ( $c^2 = k/m$ )

$$\frac{k}{m}[\Psi_n(i+1,j) + \Psi_n(i-1,j) + \Psi_n(i,j+1) + \Psi_n(i,j-1) - 4\Psi_n(i,j)] = -\omega_n^2\Psi_n(i,j), \quad (2)$$

where the neighbor terms  $\Psi_n(i\pm 1,j)$ ,  $\Psi_n(i,j\pm 1)$  are the values of the discretized eigenfunction  $\Psi_n$  at neighboring sites of  $\Psi_n(i,j)$ . Equations (1) and (2) are connected by a second order Taylor expansion of the neighbor terms. This problem can be reduced to the diagonalization of a symmetric matrix, which is carried out by the Lanczos algorithm [15], a numerical procedure to compute eigenvalues and eigenvectors of sparse  $N \times N$  matrices by reducing them iteratively to a tridiagonal form, for which effective algorithms exist. The eigenvalues of several rough geometries are calculated numerically over the whole frequency range under Dirichlet and Neumann boundary conditions and their spectra are analyzed systematically by means of level statistics. In Fig. 1 the fractal drums under study are shown; they are characterized by their boundaries. Here, the same boundaries as in Refs. [4–9] are used. To obtain the fractal drums, the generator [cf. Fig. 1(a)] is applied several times to two different sides of a regular square. As a result, we get nonsymmetric fractal drums of different generations  $\nu$  (with  $\nu$  up to 3 in this work) and therefore different stages of surface roughness. For the study of the localization properties, larger drums are also studied, as shown in Fig. 1(c) for the first generation. In Fig. 2 simpler systems with varying geometry and surface roughness are shown that are studied for comparison. For technical reasons to do with the Lanczos algorithm, all systems are unsymmetric.

All systems considered are pseudointegrable and thus intermediate between chaotic and regular (integrable) systems. The term ‘‘pseudointegrable’’ can best be described when looking at the related billiard problem. There, we consider a particle that moves freely in the  $xy$  plane inside the considered system and that is elastically reflected at the boundaries. Pseudointegrable billiards have many features of integrable systems, and the additional property of ‘‘beam splitting.’’ Like integrable systems, pseudointegrable systems have polygon enclosures whose angles are rational multiples of  $\pi$ . Unlike integrable systems, neighboring trajectories in pseudointegrable billiards can split at certain singular points. An example is the salient corners of the drum as illustrated in

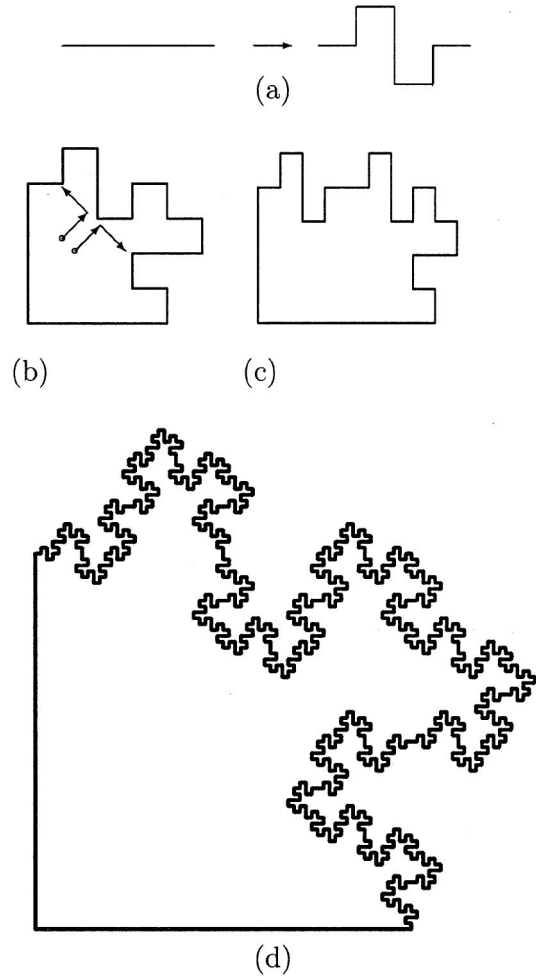


FIG. 1. (a) The fractal generator. (b) and (c) fractal drum and large fractal drum of first generation. (d) Fractal drum of third generation. (The large fractal drum of the third generation is not shown for technical reasons.) In (b) the principle of beam splitting at a salient corner is illustrated: Depending on whether a particle arrives on the left- or on the right-hand side of the corner, it is reflected in two different directions. The fractal dimension of the perimeter is  $D_f = \ln 8/\ln 4 = 3/2$ .

Fig. 1(b). The spectral fluctuations of the related eigenvalue problem are described by Poisson statistics for integrable systems and by Wigner statistics for chaotic systems (see below), whereas pseudointegrable systems are intermediate between the two.

The geometry of rational polygon billiards with angles  $\pi n_i/m_i$ ,  $i = 1, \dots, k$ , can be described by the genus number [10,11]

$$g = 1 + \frac{M}{2} \sum_{i=1}^k \frac{n_i - 1}{m_i}, \quad (3)$$

where  $M$  is the least common multiple of the  $m_i$ . The trajectories of a particle in a polygon billiard are restricted to a two-dimensional surface in phase space. For an integrable billiard,  $g = 1$  and the trajectories lie on an invariant torus in phase space, while for pseudointegrable billiards,  $g > 1$  and

is equal to the number of holes in this surface. The systems in [14] had values of  $g \leq 20$ , whereas in this work systems with  $g$  up to 1000 are considered.

Fractal drums show several bands of quasidegeneracies, which correspond to surface states that seem to be localized in the sense that their wave amplitudes occupy only some percent of the system size. This is a common feature of deterministic fractals, which should not exist in random fractals and were described in [16]. On the other hand, pseudointegrable systems are expected to show level repulsion as an inherent feature [10–12], which is not in line with localization. In this sense, fractal drums are more complicated than other pseudointegrable systems and it is not clear at all if their spectra are completely described by the genus number  $g$  or if other features like scaling surface roughness, localization, or the asymptotic shape of the system play a role.

### III. DENSITY OF STATES

All drums of the  $\nu$ th generation are constructed, starting from a discretized square of length  $L_{\text{gen}} = Z_{\text{gen}}a$ , which can be considered as a fractal drum of zeroth order. Here,  $a$  is the lattice constant and  $Z_{\text{gen}}$  counts the segments per side. All drums of the same  $L_{\text{gen}}$  possess the same area. In order to discuss the results on a single frequency scale, we normalize them by  $\omega_0 = \sqrt{2}\pi c/L_{\text{gen}}$ , which is the fundamental frequency of a square membrane of side length  $L_{\text{gen}}$  under Dirichlet boundary conditions:

$$\Omega_{n,\nu}^2 \equiv \frac{\omega_{n,\nu}^2}{\omega_0^2} = \frac{\omega_{n,\nu}^2}{2\pi^2 c^2/L_{\text{gen}}^2}. \quad (4)$$

In the calculations,  $m$ ,  $k$ ,  $a$ , and thus the sound velocity  $c = \sqrt{k/m}$  are set to unity.

An approximation for the integrated density of states (IDOS)  $N(\Omega^2)$  is given by Weyl's conjecture [17–19], which therefore also serves as an estimation, if the computed eigenvalues are reasonable. For a two-dimensional system, the first term of Weyl's conjecture is proportional to the surface of the membrane ( $\sim \Omega^2$ ), and the second term is proportional to the perimeter  $L_\Gamma$ . The higher-order terms contain, e.g., contributions of holes and corners of the system. With these terms, Weyl's conjecture can be written in our units as

$$N(\Omega^2) = (\pi/2)\Omega^2 \pm (\sqrt{2}L_\Gamma)/(4L)\Omega + N_{\text{corner}} + (\text{higher-order terms}), \quad (5)$$

where in the second term the  $+$  applies for Neumann and the  $-$  for Dirichlet boundary conditions. According to [18] the contributions for corners of angles  $\pi/2$  and  $3\pi/2$  yield  $N_{\text{corner}}(\pi/2) = 1/16$  and  $N_{\text{corner}}(3\pi/2) = -5/144$ , which is non-negligible for the third-order drums. Note that Eq. (5) cannot be used for real mathematical fractals with infinite perimeter, where the second term has to be replaced by a term proportional to  $\Omega^{D_f}$  with the Minkowski dimension  $D_f$  of the perimeter [17,19]. Note also that Weyl's formula was

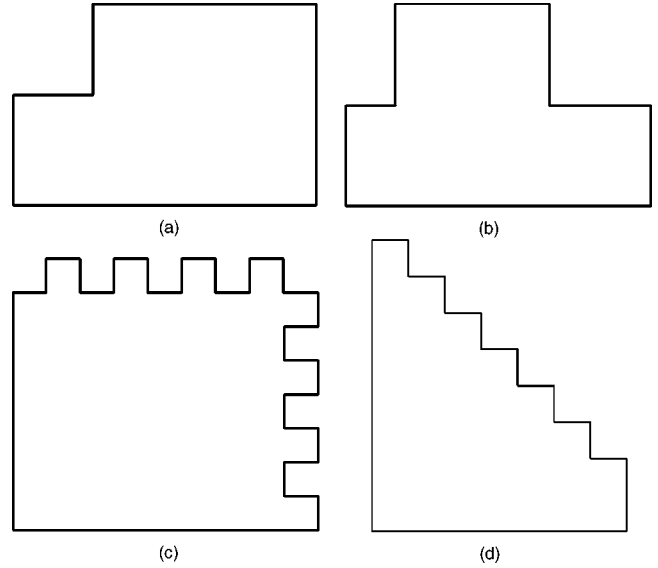


FIG. 2. Geometries of the pseudointegrable systems that are calculated for comparison: (a) and (b) simple systems, (c) rough structures, and (d) step structures. The systems of (c) and (d) are calculated for different stages of surface roughness.

derived for continuous and not for discrete systems. A partial theoretical analysis of the spectrum of a discrete system has been proposed by Fisher [20], but does not lead to an equivalent of Weyl's formula for discrete lattices. This means that the comparison of our numerical results with Weyl's formula is only an approximation, particularly in the limit of high frequencies, where the discrete nature of the lattice becomes especially important.

Figure 3 shows the computed IDOS  $N(\Omega^2)$  for the systems of  $L_{\text{gen}} = 256$  and  $\nu = 1$  and 3 for about the lowest 3000 eigenvalues under Dirichlet and Neumann boundary conditions. The results are compared to Weyl's approximation including the corner terms. Despite the discrete character of the systems, the coincidence with Weyl's formula is good, indicating the applicability of the Lanczos algorithm. With increasing length of the boundaries,  $N(\Omega^2)$  increases under Neumann and decreases under Dirichlet boundary conditions. There are, however, several steplike increases in the IDOS at special frequencies, which cause deviations from Weyl's formula and can be better seen in the insets of Fig. 3, where the IDOS is displayed for several selected intervals. The increases are caused by an accumulation of surface states, that are "quasidegenerate." For the low-frequency spectrum of symmetric drums under Neumann boundary conditions, this has already been described in [5]. Figure 3 shows that quasidegeneracies also exist in nonsymmetric drums, under Dirichlet conditions, and also for higher frequencies. Surface states are situated close to the boundary in small pores. As there are many very similar small pores along the boundary (even if not equivalent under a symmetry operation), there exist many eigenmodes with very similar energy. This effect arises at several different energy values, corresponding to several length scales in the fractal geometry, and is much stronger under Neumann boundary condi-

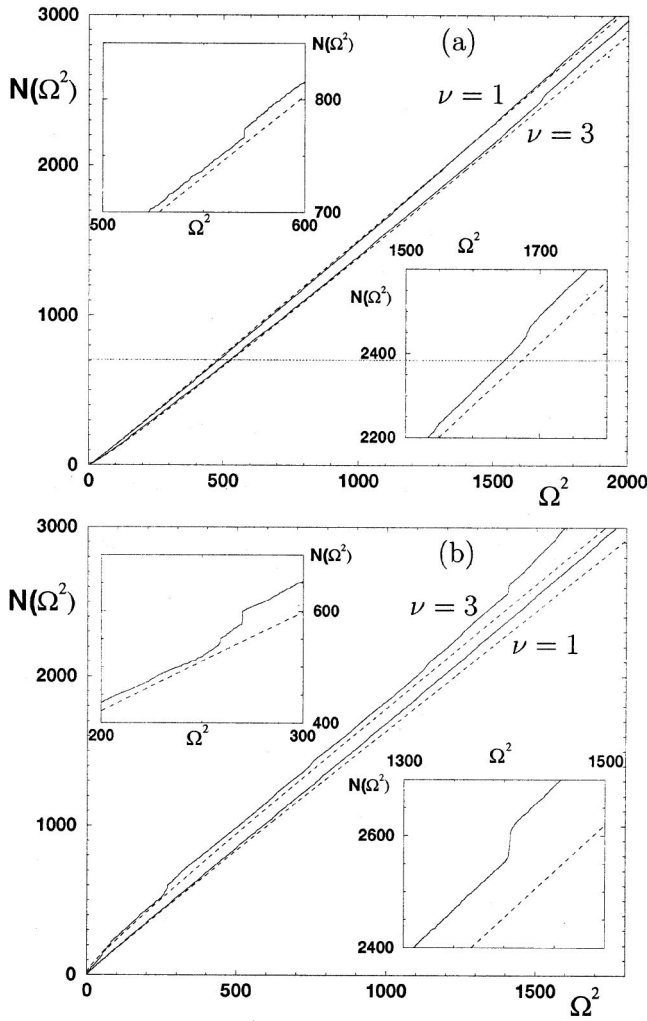


FIG. 3. Integrated density of states (IDOS) for fractal drums of  $\nu=1$  and  $\nu=3$  with (a) Dirichlet and (b) Neumann boundary conditions, plotted versus the normalized eigenvalues  $\Omega^2 = \omega^2 / \omega_0^2$  according to Eq. (4). The solid lines show the numerical results and the dashed lines refer to Weyl's formula. The insets show the step-like increases in the IDOS for several selected frequency intervals.

tions, which can vibrate freely. However, smaller steplike increases are also visible under Dirichlet conditions. The quasidegeneracies are not included in Weyl's formula (which is smooth) and might be due to higher-order terms.

#### IV. LEVEL STATISTICS

Level statistics is a powerful tool for determining if a system shows regular (integrable) or chaotic behavior. First, the probability  $P(s)$  of finding two consecutive eigenvalues with a given distance  $s$  is considered. Here,  $s$  is the normalized distance,  $s = (\Omega_n^2 - \Omega_{n-1}^2) / \Delta$ , where  $\Omega_n^2$  is the  $n$ th eigenvalue and  $\Delta$  is the mean eigenvalue spacing in the considered frequency range. Normalization or “unfolding” makes  $s$  independent of details of the considered system, like, e.g., its microscopic size. Details of the unfolding are explained in [21,22]. For systems of infinite size, two char-

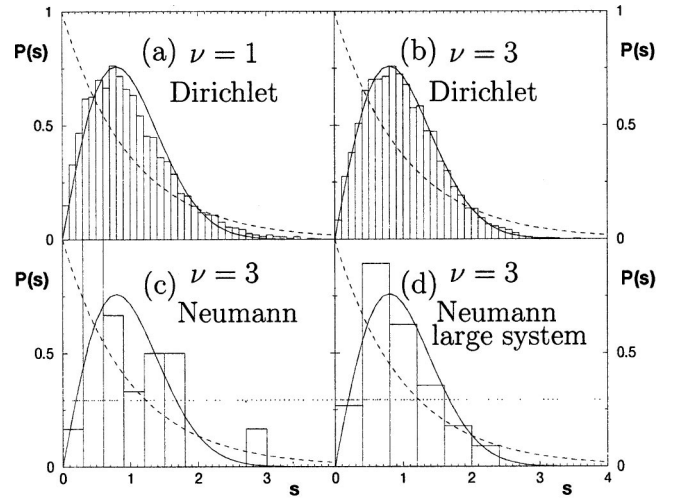


FIG. 4. Level statistics histograms  $P(s)$  for fractal drums of different boundary conditions and fractal generations, plotted versus the normalized distance  $s$  between two consecutive eigenvalues. (a) First generation, Dirichlet boundary conditions, (b) third generation, Dirichlet boundary conditions, (c) third generation, surface states under Neumann boundary conditions (about 20 quasidegenerate surface states around  $\Omega^2 \approx 1400$ ), (d) surface states under Neumann boundary conditions for about 30 states of the large system of the third generation. The theoretical Poisson and Wigner distributions are indicated by a dashed and a full line, respectively.

acteristic limiting situations can be distinguished. For chaotic systems with extended states, the level spacing distribution  $P(s)$  shows the universal random matrix theory result, which is well approximated by the Wigner surmise  $P_W(s) = (\pi/2)s \exp[-\pi s^2/4]$ . For regular systems or for localized states, on the other hand, it shows the Poisson behavior for uncorrelated eigenvalues,  $P_P(s) = \exp[-s]$ . Localized states are uncorrelated (at infinite system size) and therefore always approach the Poisson distribution with increasing system size. Therefore, level statistics is often used to distinguish between localized and extended states in disordered systems [23]. It is instructive to apply this method to fractal drums.

The results are shown in Fig. 4. In Figs. 4(a) and 4(b),  $P(s)$  for fractal drums of the first and third generations under Dirichlet boundary conditions is shown for about 10 000 eigenstates in the frequency range of  $1000 \leq \Omega^2 \leq 7000$ . There are no qualitative differences from the Neumann case, which is therefore not shown. For the first generation, the behavior is intermediate between the Wigner and the Poisson distributions. This can best be seen in the range of larger distances  $s > 2$ , where the values of the histograms lie between  $P_P(s)$  and  $P_W(s)$ . It can be recognized that the distribution approaches the Wigner distribution when passing from the first to the third generation. In Figs. 4(c,d), we look at the surface states  $\Omega^2 \approx 1400$  of  $\nu=3$  under Neumann boundaries. As they occupy only a small portion of the total system, they could be uncorrelated and thus obey the Poisson distribution. Indeed, even if this histogram contains only 20 states, and should be considered as preliminary, we can see that it looks much more similar to the Poisson distribution



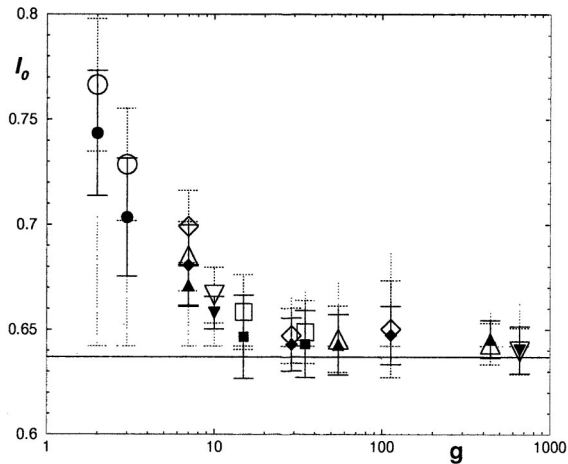


FIG. 5. The dimensionless second half moments  $I_0$  (averaged over 15 intervals throughout the whole frequency spectrum) for several different system geometries under Dirichlet (open symbols, dotted error bars) and Neumann (filled symbols, straight lines as error bars) boundary conditions are plotted versus the genus number  $g$  of the systems. The different symbols indicate the geometries of Figs. 1 and 2: fractal drums (triangles up), large fractal drums (triangles down), rough structures (squares), step structures (diamonds), and simple structures (circles).

than the global histogram of the system. However, this behavior is not maintained when we increase the system size. The same surface states of the larger drum (as explained in Fig. 1) show a distribution  $P(s)$ , that is changed toward the Wigner distribution. This indicates that the surface states—even if they occupy only some percent of the system size—grow with the system and are therefore not really localized states. For a final conclusion, a better statistics should be achieved.

Instead of comparing the histograms, it is easier to calculate the second half moments  $I_0 = \frac{1}{2} \langle s^2 \rangle = \frac{1}{2} \int_0^\infty s^2 P(s) ds$ , which lie between the two limiting values  $I_0^{\text{Wigner}} \approx 0.637$  and  $I_0^{\text{Poisson}} = 1$  [23]. This enables us to decide if the statistics is closer to Wigner or closer to Poisson by comparing just one number  $I_0$ . This has been done for all systems of Figs. 1 and 2 for about 15 separate energy intervals throughout the whole high-energy spectrum where in the first interval  $\Omega^2 \approx 3000$  (corresponding to level numbers around 5000) and in the last interval  $\Omega^2 \approx 25\,000$  (close to the end of the spectrum). Each interval contained about 500–1500 eigenstates. In all systems,  $I_0$  fluctuated with  $\Omega^2$  around a mean value, but, apart from fluctuations, it showed no frequency dependence in the considered frequency range. Therefore, in Fig. 5, the average  $I_0$  for each system under Dirichlet (open symbols) and under Neumann (filled symbols) boundaries is plotted versus the genus number  $g$ . The Wigner limit is indicated by a straight line. Systems with small genus numbers  $g$  show intermediate behavior, in agreement with recent results of a numerical analysis on triangular billiards under Dirichlet boundary conditions [24], where systems with small  $g$  were found to obey a semi-Poisson statistics with  $I_0 = 0.75$ . For increasing  $g$ , the results here provide strong evidence

that the values of  $I_0$  of all systems considered move from the Poisson toward the Wigner limit in quite the same way, which is described solely by  $g$ . For  $g > 20$ , the Wigner limit lies inside the error bars (which are estimated by the fluctuations of  $I_0$  between different frequency intervals). For Neumann boundary conditions,  $I_0$  shows slightly smaller values than in the Dirichlet case, but this effect is inside the error bars.

The fractal drums of third order show no size dependence, i.e., the values of  $I_0$  are the same for the smaller and the larger drums in all considered frequency intervals (apart from fluctuations around the mean value). This is also an indication that no transition between localized and extended states occurs. For the first generation, the values of  $I_0$  for the larger drum already lie close to the Wigner limit, whereas the  $I_0$  for the smaller drum are clearly higher. This size effect reflects the larger number of corners of the larger drum and therefore only occurs for intermediate systems with small  $g$ . It is not related to localization.

The approach of  $I_0$  toward the Wigner limit with increasing  $g$  is remarkable, as—contrary to the systems considered in [14] which approached the Sinai billiard with increasing surface roughness—the geometries of the systems here do *not* converge to the geometry of chaotic systems. So, for the pseudointegrable systems considered here, with right angles but for very different asymptotic shapes and different types of surface roughness (scaling or nonscaling),  $I_0$  approaches the Wigner limit in a similar way as a function of the genus number  $g$ . It will be interesting to investigate the extent to which this  $g$  dependence is general and holds for all pseudointegrable systems.

## V. CONCLUSIONS

The eigenvalues of two-dimensional pseudointegrable fractal drums have been investigated numerically by the Lanczos algorithm and analyzed by means of level statistics in the high-energy limit. For this purpose, the eigenvalue distribution  $P(s)$  and the respective second half moments  $I_0$  were calculated, which have clearly defined values in the Poisson and in the Wigner limit. This calculation was done for many energy intervals throughout the spectrum for level numbers  $\geq 5000$ . Comparing different system sizes, no transition between localized and extended states was found. Even if there exist many modes whose amplitudes are large only in a very small section of the system, they seem to grow when the system size is increased, and show level repulsion. Then it was investigated if the level statistics of the fractal drums is closer to the Wigner or to the Poisson limit. For comparison, several different pseudointegrable systems of various geometries with nonscaling surface roughness were analyzed as well. Systems with small surface roughness were found to show intermediate behavior, in essential agreement with [24]. With increasing irregularity of the boundary, the  $I_0$  of the systems here approaches the Wigner limit. The approach seems to depend only on the genus number  $g$ , because complicated fractal drums as well as simple systems with nonscaling surface roughness fall onto the same seemingly universal curve. Also, there are no qualitative differ-

ences between Neumann and Dirichlet boundary conditions and it seems unimportant if the asymptotic geometry with more and smaller corners approaches a chaotic shape or not.

It should be emphasized that only systems with right angles were considered and it will be instructive to extend this analysis to different ones and to see to what extent this  $g$  dependence is general. The systems, considered even with large genus numbers  $g$ , are not chaotic and it will also be interesting to perform different tests, such as, e.g., the level dynamics under a change of a wall or the behavior of the

wave functions, to see, if this approach to chaotic behavior is also found for other quantities.

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