Misleading signatures of quantum chaos

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The main signature of chaos in a quantum system is provided by spectral statistical analysis of the nearest-neighbor spacing distribution $P(s)$ and the spectral rigidity given by the $\Delta_3(L)$ statistic. It is shown that some standard unfolding procedures, such as local unfolding and Gaussian broadening, lead to a spurious saturation of $\Delta_3(L)$ that spoils the relationship of this statistic with the regular or chaotic motion of the system. This effect can also be misinterpreted as Berry's saturation.

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Quantum chaos has been an active research field since the link between energy level fluctuations and the chaotic or integrable properties of Hamiltonian systems was conjectured [1,2], providing one of the fundamental signatures of quantum chaos [3,4] in atoms, molecules, nuclei, quantum dots, etc. The secular or smooth behavior of the level density is a characteristic of each quantum system, while the fluctuations relative to this smooth behavior are related to the regular or chaotic character of the motion in all quantum systems. To achieve the separation of the smooth and fluctuating parts, the energy spectrum is scaled to a sequence with the same local mean spacing along the whole spectrum. This scaling is called *unfolding* [5]. Although this can be a nontrivial task [6], the description of the unfolding details of calculations is usually neglected in the literature.

In this paper we show that, contrary to common assumptions, the statistics that measure long-range level correlations are strongly dependent on the unfolding procedure utilized, and some standard unfolding methods give very misleading results in regard to the chaoticity of quantum systems. Long-range level correlations are usually measured by means of the Dyson and Mehta Δ_3 statistic [5]. On the other hand, we find that short-range correlations, characterized by the nearest-neighbor spacing distribution $P(s)$, are not very sensitive to the unfolding method.

Let us consider a rectangular quantum billiard with a size ratio $a/b=\pi$. This is a well known example of a regular system. In general, for regular systems level fluctuations behave like in a sequence of uncorrelated energy levels, and the $\Delta_3(L)$ statistic increases linearly with L. However, it was shown by Berry [7] that the existence of periodic orbits in the phase space of the analogous classical system leads to a saturation of $\Delta_3(L)$ for L larger than a certain value L_s, related to the period of the shortest periodic orbit. Figure 1 shows the Δ_3 behavior for a sequence of 8000 high energy levels of the mentioned quantum billiard, calculated with two different unfolding procedures. The mean level density for this system is given by the Weyl law [8]. Using this density to perform the unfolding, Δ_3 follows the straight line of level spacings with Poisson distribution, characteristic of regular systems. In this example, Berry's saturation takes place at $L_s \simeq 750$, that is outside the figure. Let us suppose now that the law giving the mean level density of the system was unknown. Then, a standard method to obtain the local mean level density at energy E is to calculate the average density of a few levels around this energy. Using this method one obtains a very different behavior, namely, Δ_3 flattens strongly at $L \simeq 20$, and afterwards Δ_3 is close to the Gaussian orthogonal ensemble (GOE) line characteristic of chaotic systems. The latter behavior is not at all related to the Berry saturation, that takes place at much higher L in this case, as mentioned above. Instead, it is a spurious effect due to inappropriate unfolding of the level spectrum, and it implies that strong long-range correlations have been improperly introduced by the procedure.

This first example illustrates the problem that can arise with some reasonable unfolding methods currently used in quantum chaos calculations [9–13]. In order to understand its origin we shall analyze different unfolding procedures. The principal difficulty in the unfolding is the correct characterization of the mean level density function $\overline{\rho}(\alpha,E)$, where α stands for some parameters defining the functional form of $\overline{\rho}$. Having this function, the mean accumulated level density is given by

$$\overline{N}(\alpha,E)=\int_{-\infty}^{E}\overline{\rho}(\alpha,E')dE'. \tag{1}$$

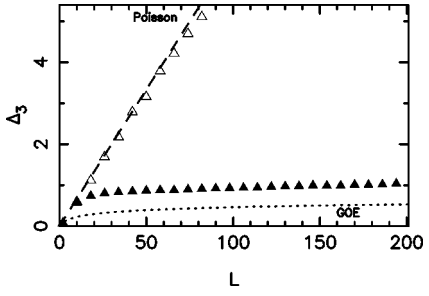

FIG. 1. Comparison of the Δ_3 statistic for a rectangular quantum billiard using two unfolding procedures. Open triangles correspond to the smooth unfolding using the Weyl law, and filled triangles correspond to the local unfolding method. The dashed line is the Poisson limit and the dotted line is the GOE limit.

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The parameters α are determined finding the values α_0 for which the smooth function $\overline{N}(\alpha_0,E)$ is closest to the step function $N(E)$ that gives the true number or levels up to energy E. An alternative procedure, which often gives better results, consists on assuming a functional shape for $\overline{N}(\alpha,E)$, or expanding it in some basis functions, and fit it to $N(E)$.

The *unfolded energy levels* are given by

$$\varepsilon_i = \overline{N}(\alpha_0, E_i). \tag{2}$$

These dimensionless variables constitute a quasiuniform spectrum with constant mean level density equal to 1. The unfolded spacing sequence is then

$$\{s_i = \varepsilon_{i+1} - \varepsilon_i\}, \tag{3}$$

and the nearest-neighbor spacing distribution $P(s)$ is well suited to study the short-range spectral correlations [5].

The Δ_3 statistic is used to investigate the long-range correlations. It is defined for the interval $[a,a+L]$ in the cumulative level density as

$$\Delta_3(a,L) = \frac{1}{L}\min_{A,B}\int_a^{a+L} [\mathcal{N}(\varepsilon) - A\varepsilon - B]^2 d\varepsilon, \tag{4}$$

where $\mathcal{N}(\varepsilon)$ is the step function that gives the true number or unfolded levels up to ε. The function $\Delta_3(L)$, averaged over intervals, measures the deviations of the quasiuniform spectrum from a true equidistant spectrum. Therefore $\Delta_3(L)$ is related to the *spectral rigidity*. When $\Delta_3(L)$ is nearly flat, the rigidity is strong [2]. In the limiting case of a harmonic oscillator, the spectrum is completely rigid and $\Delta_3(L)$ is constant and close to zero. For GOE spectra, the levels are strongly correlated and $\Delta_3(L) \sim \ln L$. By contrast, for Poisson spectra the levels are uncorrelated, the spectrum is *soft*, and $\Delta_3(L)$ increases linearly with L.

For some systems a natural unfolding procedure exists, because $\overline{\rho}(E)$ (we drop the index α from now on) is known from an appropriate statistical theory or by a well checked empirical ansatz. For example, $\overline{\rho}(E)$ is a semicircle for large GOE matrices [5], it often has Gaussian form with Edgeworth corrections for large nuclear shell-model matrices [5], and follows the Weyl law in quantum billiards [8]. In all those cases it is possible to unfold the level spectrum properly, but it should be noted that it is a delicate operation. If the calculated mean level density $\overline{\rho}(E)$ is not accurate enough, the unfolding procedure will introduce accumulated errors in $\mathcal{N}(\varepsilon)$ in Eq. (4), leading for large L to a spurious increase of $\Delta_3(L)$ above the true value. For example, in most nuclear shell-model spectra, a Gaussian density without Edgeworth corrections will provide distorted results of this kind for $L>50$. In general, this effect can hide any Berry saturation in a system.

In the present paper, we deal mainly with systems where there is no natural choice for the mean level density function. In those cases, the local value of $\overline{\rho}(E)$ is usually estimated from a set of neighboring levels. The simplest method, called *local unfolding*, has been widely used [9–12]. The mean level density is assumed to be approximately linear in a window of v levels on each side of E_i, and is given by

$$\overline{\rho}_L(E_i) = \frac{2v}{E_{i-v} - E_{i+v}}, \tag{5}$$

where L stands for local unfolding. More sophisticated is the *Gaussian broadening* method [8,13]. The level density $\rho(E) = \Sigma_i \delta(E - E_i)$ is substituted by an average level density

$$\overline{\rho}_G(E) = \frac{1}{\sigma\sqrt{2\pi}} \sum_i \exp\left\{ -\frac{(E-E_i)^2}{2\sigma^2} \right\}, \tag{6}$$

where G stands for Gaussian broadening. The sum runs over all the energy levels, but only those satisfying $|E - E_i| \lesssim \sigma$ do significantly contribute to $\overline{\rho}_G(E)$. Although these two methods are different, both depend on a parameter v or σ that measures, in a real or effective way, how many neighboring levels are used to calculate the local mean density.

The atomic nucleus is an example of a quantum system more complex than the quantum billiard. In most nuclei, level fluctuations are in agreement with GOE predictions at all energies, showing that the motion is chaotic. However, it has recently been observed that single closed shell nuclei are less chaotic than expected [11,14]. One of the most regular nuclei at low energy is ^{52}Ca. Analysis of the shell-model level spectrum [14] shows that the nearest-neighbor spacing distribution $P(s)$ is close to the Poisson limit (the Brody parameter [5] is $\omega = 0.25$) for levels up to 5 MeV above the yrast line. As the excitation energy is increased, $P(s)$ approaches the spacing distribution of a chaotic system. Nevertheless, other statistics indicate that the dynamics is still not fully chaotic. The $\Delta_3(L)$ statistic is very sensitive to the dynamical regime of motion, and therefore it is generally considered to be a reliable statistic to detect chaos in quantum systems. However, we shall now show that its L dependence can be very misleading if local unfolding or similar methods are used.

Consider the full pf shell-model spectrum of ^{52}Ca. If we perform a careful global unfolding, using for $\overline{\rho}(E)$ an Edgeworth expansion up to fourth order around a Gaussian form [5], the resulting $\Delta_3(L)$ is close to the GOE limit for very small L values, but it increases linearly instead of logarithmically for larger L values, as can be seen in Fig. 2. We have checked that this behavior is not spurious, i.e., it is not the effect of cumulative errors mentioned above. Besides unfolding with the global mean density, we determined $\overline{N}(E)$ directly using an expansion in Chebyshev polynomials and fitting it to the cumulative step function $N(E)$. This unfolding method gave a result very similar to the open triangles shown in Fig. 2. Thus, except for very small L values, the spectral rigidity is intermediate between those of GOE and Poisson limits, giving a clear signature of nonchaotic motion in this semimagic nucleus.

On the other hand, when the Edgeworth expansion around a Gaussian form fails to reproduce the smooth global shell-model level density, as it happens sometimes [11], local unfolding or Gaussian broadening are current methods to deter-

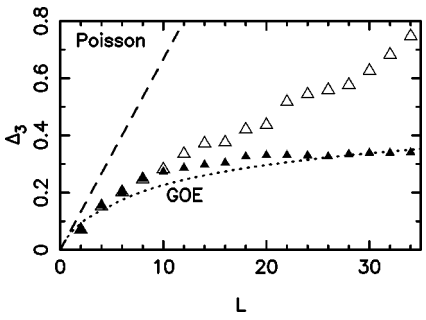

FIG. 2. Δ_3 for the complete $J=10$ level sequence of a shell-model calculation for ^{52}Ca in the pf shell. For smooth unfolding made by an Edgeworth expansion in the cumulants, the result (open triangles) lies between Poisson (dashed line) and GOE (dotted line) limits. Filled triangles correspond to local unfolding with a $2v=10$ window.

mine the local mean level density. Figure 2 also shows the results using local unfolding with $v=5$ in ^{52}Ca. The Δ_3 statistic follows closely the line obtained with the smooth unfolding up to $L\simeq 2v$, but for larger L it saturates to a roughly constant value. This is the same behavior that was observed in the quantum billiard system described above. Moreover, since the Δ_3 values are rather close to the GOE limit when $v=5$ is used, it follows that ^{52}Ca is a fully chaotic system, i.e., we arrive to a wrong conclusion.

This example is then very enlightening. First, it illustrates that, contrary to common practice, the $\Delta_3(L)$ statistic should be calculated up to high L values, because otherwise one can miss relevant information on the system dynamics. Second, it shows the problems that can arise when the mean level density function is not known and one has to rely on local unfolding. For small L values, up to $L\simeq 10$, the results are essentially independent of the unfolding method, and the $\Delta_3(L)$ statistic indicates that the system is quite chaotic. For larger L values, the locally unfolded spectrum seems to be fully chaotic. On the contrary, the globally unfolded spectrum reveals strong deviations from the GOE limit. This signal of nonchaotic motion in ^{52}Ca is realistic and fully in agreement with the behavior of the wave function localization lengths [14].

To avoid any uncertainties on the real behavior of the mean level density $\overline{\rho}(E)$, and therefore on the calculated level fluctuations, we can study GOE and Poisson level spectra, the paradigmatic cases of chaotic and regular systems, respectively. We consider a GOE matrix with dimension $N=10\,000$, and compare the spectral fluctuations obtained by three different methods: Smooth unfolding made with the semicircle law, local unfolding, and Gaussian broadening unfolding. As Fig. 3 shows, all these methods yield almost indistinguishable results for the $P(s)$ distribution, and in perfect agreement with the Wigner surmise. The behavior of the short-range correlations is not affected by the method of unfolding.

However, Fig. 4 shows a completely different scenario for the Δ_3 behavior of a GOE energy level spectrum. For the smooth unfolding, the spectral rigidity behaves as predicted

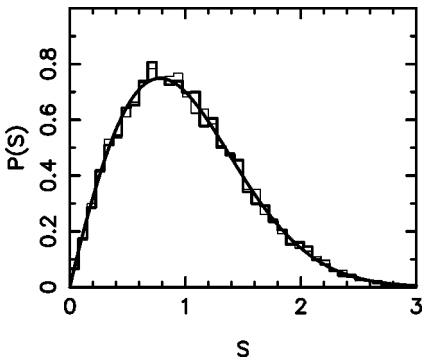

FIG. 3. Comparison of the nearest-neighbor spacing distribution $P(s)$ for an $N=10\,000$ GOE level spectrum, calculated with different unfolding methods. The thin line histogram is obtained for local unfolding with $2v=18$, and the thick line histogram for global unfolding with the semicircular mean level density. The Gaussian broadening unfolding method (not shown for figure clarity) gives very similar results as well. The solid line is the Wigner surmise.

by GOE, up to very large L values. The local unfolding was performed using two different windows, with $v=9$ and $v=21$. The calculated Δ_3 coincides now with GOE predictions only up to $L\simeq 2v$, then it leaves the GOE trend and saturates to a constant value. The Gaussian broadening unfolding was performed for $\sigma=1$ MeV and $\sigma=2$ MeV. In the central part of the spectrum these values correspond to windows containing about 10 and 20 states, respectively. Therefore, the effective number of states that affect the average level density is about the same as in the local unfolding case. Again, we see the same Δ_3 saturation for L values greater than the window used in the unfolding.

Similarly, Fig. 5 shows the spectral rigidity for 10 000 energy levels generated with Poisson statistics and a uniform density $\overline{\rho}(E)=1$. The smooth unfolding gives Δ_3 values close to Poisson predictions, but local unfolding with $v=2$, 9, and 21, leads again to the same saturation behavior observed in previous cases for $L\gtrsim 2v$. In fact, for the small window with four spacings, the Δ_3 of the Poisson spectrum closely follows GOE predictions.

Looking for deeper insight into the spurious Δ_3 satura-

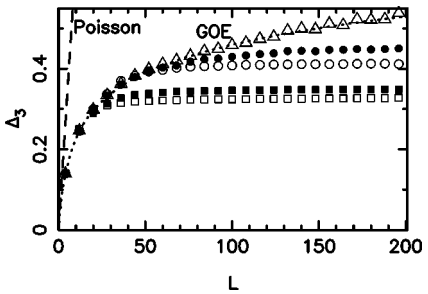

FIG. 4. Comparison of the spectral rigidity for an $N=10\,000$ GOE level spectrum, calculated with different unfolding methods. Open triangles correspond to the smooth unfolding. Filled circles and squares correspond to the local unfolding with window size $2v=42$ and $2v=18$, respectively. Open circles and squares to the Gaussian broadening unfolding for $\sigma=2$ and $\sigma=1$ MeV, respectively.

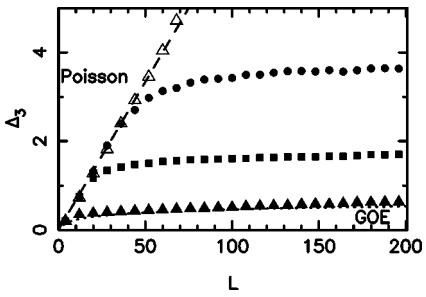

FIG. 5. Comparison of the spectral rigidity for a Poisson sequence of 10 000 levels with uniform density, using several unfolding procedures. Open triangles correspond to the smooth unfolding. Filled circles, squares, and triangles correspond to the local unfolding with window size $2v=42$, $2v=18$, and $2v=4$, respectively.

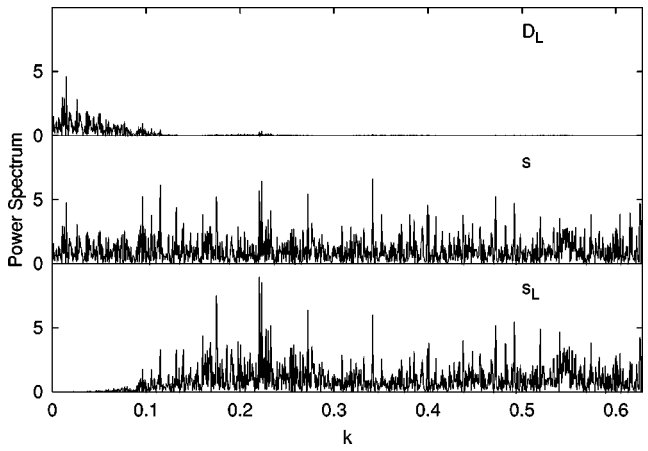

FIG. 6. Comparison of the power spectrum for the level spacing sequences D_L, s, and s_L, of 10 000 uncorrelated levels with uniform density. The locally unfolded spacings s_L are calculated with a window of size $2v=42$ that corresponds to $k_0=0.15$.

tion, we may consider the sequence of nearest level spacings as a physical signal, and apply Fourier analysis techniques to its study. The index i in Eq. (3) is considered as the analog of a discrete time, and s_i is the value of the signal at this time. Obviously, the analogy is only formal and the discrete time is dimensionless. The Fourier analysis is performed by means of a fast Fourier transform. The frequencies obtained are $k=2\pi n/d$, where n is an integer and d is the total number of spacings. Frequencies beyond the Nyquist frequency, reached at $n=d/2$, have no physical meaning.

We have chosen a system with Poisson statistics and uniform level distribution to illustrate the idea, because the smooth density in this case is constant. Therefore, the fundamental assumption of the local unfolding method, namely, that the mean density is approximately linear within a window, is exactly fulfilled. From the real nearest-neighbor level spacing sequence S, we obtain: (a) the average spacing sequence D_L calculated with the local constant density of Eq. (5) for $v=21$, (b) the sequence of smoothly unfolded spacings s, and (c) the sequence of locally unfolded spacings s_L. Since for this spectrum $\overline{\rho}(E)=1$, we have mean spacing $D=1$ and therefore $s=S$.

Figure 6 displays the power spectrum of these three sequences for frequencies up to $k=0.6$. For D_L, it has a maximum near $k=0$ and decreases smoothly afterwards, becoming zero at some threshold frequency $k_0=\pi/v$. However, this behavior is a spurious effect, because the real mean spacing D is constant and consequently its power spectrum is zero for all frequencies $k\neq 0$. Therefore the local unfolding procedure introduces spurious low frequency components into the D_L signal. Comparing the power spectra of D_L and s, it is seen that they are very similar at low frequencies, except for the damping of the former. The power spectra of s and s_L are also very similar, except that the low frequency components are missing in the latter. These results clarify the deficiencies of local unfolding. It becomes apparent that the procedure is filtering out low frequency fluctuations from the spectrum s, and improperly including them in D_L. Moreover, by reducing or eliminating fluctuations of frequency smaller than k_0, the procedure is introducing long-range correlations with wavelengths greater than $2v$. As this fluctuation reduction is progressive, the spurious long-range correlations become stronger as L increases beyond the window size $2v$. It is precisely this phenomenon what has previously been detected by the Δ_3 statistic, namely, the strong long-range correlations leading to a saturation of the Δ_3 are observed for $L\gtrsim 2v$.

In summary, we have shown that the correct behavior of Δ_3 is strongly modified by some commonly used unfolding procedures when the exact shape of the mean level density is not known. Methods such as local unfolding or Gaussian broadening introduce spurious long-range correlations in the unfolded level spectrum, leading to a saturation of $\Delta_3(L)$. In these methods the $\overline{\rho}(E)$ is calculated from the levels inside an energy window around E. The spurious behavior of the Δ_3 statistic is observed for L larger than the window size. In general it gives misleading signatures of quantum chaos, and for small windows the behavior of Δ_3 may be close to the GOE limit. Furthermore, the spurious saturation of Δ_3 can easily be misinterpreted as Berry's saturation.

For systems intermediate between regular and chaotic, the traditional spectral statistics $P(s)$ and $\Delta_3(L)$ for small L values may be close to the GOE limit, and strong deviations of Δ_3 from GOE predictions only appear for larger L values. Thus if the local mean level density is not known from a statistical theory or a good empirical ansatz, the analysis of energy level fluctuations based on local unfolding or similar methods will not lead to correct conclusions on the system dynamics. In many cases it will be very convenient to go beyond level statistics and study properties of the wave functions, such as localization length, transition strengths and transition strength sums [15], to have a reliable overview of statistics related to quantum chaos.

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[1] M.V. Berry and M. Tabor, Proc. R. Soc. London, Ser. A **356**, 375 (1977).
[2] O. Bohigas, M.J. Giannoni, and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984).
[3] O. Bohigas and M.J. Giannoni, in *Mathematical and Computational Methods in Nuclear Physics*, edited by J.S. Dehesa, J.M.G. Gómez, and A. Polls (Springer-Verlag, Berlin, 1984).
[4] H.J. Stöckmann, *Quantum Chaos* (Cambridge University Press, Cambridge, England, 1999).
[5] T.A. Brody, J. Flores, J.B. French, P.A. Mello, A. Pandey, and S.S.M. Wong, Rev. Mod. Phys. **53**, 385 (1981).
[6] T. Guhr, A. Müller-Groeling, and H.A. Weidenmüller, Phys. Rep. **299**, 189 (1998).
[7] M.V. Berry, Proc. R. Soc. London, Ser. A **400**, 229 (1985).
[8] F. Haake, *Quantum Signatures of Chaos* (Springer-Verlag, Heidelberg, 2001).
[9] J.B. French and S.S.M. Wong, Phys. Lett. **35B**, 5 (1971).
[10] V. Paar, D. Vorkapic, K. Heyde, A.G.M. van Hees, and A.A. Wolters, Phys. Lett. B **271**, 1 (1991).
[11] M.S. Bae, T. Otsuka, T. Mizusaki, and N. Fukunishi, Phys. Rev. Lett. **69**, 2349 (1992).
[12] H. Meyer, J.C. Angles d'Auriac, and J.M. Maillard, Phys. Rev. E **55**, 5380 (1997).
[13] H. Bruus and C.A. d'Auriac, Phys. Rev. B **55**, 9142 (1997).
[14] R.A. Molina, J.M.G. Gómez, and J. Retamosa, Phys. Rev. C **63**, 014311 (2001).
[15] J.M.G. Gómez, K. Kar, V.K.B. Kota, J. Retamosa, and R. Sahu, Phys. Rev. C **64**, 034305 (2001).