Statistical measures of chaos in quantum systems

Per Persson [1] and Sven Åberg[1,2]

[1] *Department of Mathematical Physics, Lund Institute of Technology, P.O. Box 118, S-221 00 Lund, Sweden*
[2] *Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831*

(Received 16 December 1994)

A simple model, based on random matrix theory, is utilized for the description of energy levels and level dynamics in mixed regular and chaotic quantum systems. We find that different types of level statistics, such as nearest neighbor distributions, long-range correlations, wave function analysis, curvature distributions, etc., show dramatically different sensitivity to the "chaoticity parameter." Differences between long-range and short-range fluctuation measures are explained in terms of localization of the wave functions.

PACS number(s): 05.45.+b, 05.40.+j, 03.65.−w, 24.60.Lz

I. INTRODUCTION

Random matrix theory plays an import role in the study of quantum signatures of chaos, "quantum chaos," see, e.g., [1]. By performing level statistical analyses of the quantum levels of several simple systems, such as the hydrogen atom in a strong magnetic field, quantum billiards, etc., one has been able to identify the transition from order to chaos in the classical system as a subsequent change of the fluctuation properties of the corresponding quantum system from Poisson (completely uncorrelated spectrum) to GOE (Gaussian orthogonal ensemble), see, e.g., [2,3]. This kind of evidence led Bohigas *et al.* to conjecture [4] that the quantum mechanical version (in the semiclassical limit) of a classically chaotic system has fluctuations which depend only on the underlying symmetry of the physical problem, and implies a universal behavior of the "chaotic" quantum system. Chaotic systems with time reversal symmetry generically show fluctuations which follow GOE statistics.

By considering the motion of eigenvalues under the change of an external parameter other types of correlations of the quantum system may be studied (see, e.g., [5]). These types of correlations are complementary to those that can be obtained from a static spectrum, and may have a direct relation to experimental quantities, such as the magnetic susceptibility or the dynamic moment of inertia in nuclear physics. In Refs. [6] and [7] the possibility was discussed to relate these two measurable quantities to quantum chaos.

The GOE is based on random matrix theory (RMT) that was originally developed by Wigner for the description of the structure of highly excited atomic nuclei. From the RMT several properties have been derived concerning the behaviour of fluctuations of the energy spectrum and the eigenfunctions (see [8,10,9,2]). Recently, it has become clear that also level dynamical distributions are universal, see, e.g., [11, 12]. One basic question we discuss in this paper is if we can conclude that a quantum system can be described by GOE when we have found that, for example, the nearest neighbor energy-spacing distribution follows a GOE distribution. That is, if observing GOE properties of one kind of statistical measure implies that also other kinds of statistical measures give GOE. This question is certainly quite relevant since it is common to draw conclusions about the full system from one kind of statistical measure only. With a limited stretch of energy levels, as may be the case if the analysis is based on experimental data, it may be impossible to perform, for example, a reasonable long-range correlation analysis (such as the Δ_3 statistics [13]).

In Sec. II we propose a simple model of a general (time reversal) quantum system based on RMT, that can describe a smooth transition from "order" (Poisson) to "chaos" (GOE) through the variation of one parameter, a "chaoticity parameter." In addition, dynamics is introduced into the model through an explicit (linear) dependence of the Hamiltonian on an external parameter which can be considered as a "time" variable. The aim of the paper is then to study how different statistical measures behave as the "chaoticity parameter" is changed (Sec. III). In Sec. III A we study how the level density changes, while local fluctuation measures, such as the nearest neighbor energy-spacing distribution (NND) and the stiffness of the spectrum (Δ_3 statistics and its variance), are studied in Sec. III B. The distribution of wave function components is considered in Sec. III C, and the distribution of energy level curvatures is studied in Sec III D. Finally, in Sec. IV we summarize and discuss the obtained results.

II. A RANDOM MATRIX MODEL

The starting point and original motivation for the introduction of random matrix models is a complicated quantum mechanical system. The complexity may arise due to an underlying classical chaotic dynamics, in a few-body or many-body system, and one aim is to describe the quantum signs of this. In order to mimic the transition from "order" to "chaos" in the quantum system we propose the following random matrix model:

$$\mathbf{H}(I) = \mathbf{H}_0 + \Delta\mathbf{H}_1 + I\mathbf{A}, \tag{1}$$

where

$$(\mathbf{H}_0)_{ij} \in \delta_{ij} G\left(0, \sqrt{\frac{2}{N}}\right), \tag{2}$$

$$(\mathbf{H}_1)_{ij} \in (1-\delta_{ij}) G\left(0, \sqrt{\frac{1}{N}}\right), \tag{3}$$

$$(\mathbf{A})_{ij} \in \delta_{ij} G\left(0, \sigma_A \sqrt{\frac{1}{N}}\right), \tag{4}$$

i.e., $\mathbf{H}(I)$ constitutes an ensemble of N-dimensional random matrices where $\mathbf{H}_0$ and $\mathbf{A}$ are diagonal and $\mathbf{H}_1$ is nondiagonal, all with Gaussian distributed real matrix elements with mean value m and standard deviation $\sigma, G(m,\sigma)$. The two parameters Δ and σ_A determine the properties of the system. Throughout the paper we shall choose σ_A=1. By choosing the "chaoticity parameter," Δ, in the interval [0,1] we may study the smooth transition from Poisson to GOE. At Δ=0 we have $\mathbf{H}(0) \equiv \mathbf{H}^{\text{Poisson}}$ and at Δ=1 $\mathbf{H}(0) \equiv \mathbf{H}^{\text{GOE}}$. The external parameter, I, describes "time," but it could as well describe other variables such as angular momentum, strength of an external magnetic field, or an (intrinsic) quadrupole deformation parameter of a deformed atomic nucleus. For a given choice of $\mathbf{H}_0$, $\Delta\mathbf{H}_1$ and $\mathbf{A}$, the time variable, I, is subsequently varied.

The eigenvalue problem

$$\mathbf{H}\phi_i = E_i\phi_i \tag{5}$$

is solved by numerical diagonalization of an ensemble of $N \times N$ matrices (as a standard we shall take N=400). When $\Delta = 0$ the energy spectrum, $E_i(I)$, corresponds to a set of unperturbed bands. All bands correspond to states with different sets of good quantum numbers, and are straight lines with sharp crossings when plotted vs I. The subsequently added interaction, $\Delta\mathbf{H}_1$, corresponds to a residual interaction which acts between all the bands and breaks all the good quantum numbers. In the classical analog the Hamiltonian function $H_0 + IA$ is integrable, while all constants of motion are destroyed by ΔH_1 for $\Delta \neq 0$. Due to the KAM theorem chaos is expected to set in smoothly in the classical system as the value of Δ is increased from zero.

In general, the slopes $\partial E_i/\partial I$ correspond to "velocities," but could as well correspond to (the negative of) rotational frequencies (if I is the angular momentum), quadrupole moments (if I is a quadrupole deformation parameter), etc. The parameter, σ_A, controls the dispersion in slope, i.e., in velocity. The curvatures, $\partial^2 E_i/\partial I^2$, correspond to "accelerations," but could also correspond to $-1/J^{(2)}$, where $J^{(2)}$ is the dynamical moment of inertia (if I is the angular momentum), the magnetic susceptibility (if I is the magnetic field strength), etc.

III. STATISTICAL MEASURES

In this section we perform a numerical study of the statistical properties of energy eigenvalues and eigenfunctions of the ensemble of Hamiltonians described by our simple model, Eqs. (1)–(4). We typically let the ensemble be represented by 30–50 matrices, over which the calculated properties are averaged. As mentioned above, we choose the matrix sizes to be N = 400, and usually, in order to avoid truncation effects, only the central 60% of the spectrum is used. In general, we shall study the static properties of the levels and their wave functions at I=0. When the statistical properties of the eigenvalues are studied, a renormalization is first performed so that the average level density everywhere is equal to 1. We use the method of Fourier transformations developed in [14]. Definitions of the different statistical measures can be found, e.g., in [2], where also approximative analytical expressions for the limiting distributions (corresponding to full GOE or Poisson) can be found. If necessary, we use, however, numerical expressions deduced within the present model for $\mathbf{H}(0;\Delta = 0)$ and $\mathbf{H}(0;\Delta = 1)$.

A. Level density

The level density obtained in RMT is a global property, and is usually not given any significance in the application of the theory in describing (generic) fluctuation properties of quantum chaotic systems.

In the two limits, Poisson and GOE, simple expressions exist for the level density in the limit $N \to \infty$, namely the Gaussian distribution as imposed by Eq. (2),

$$\rho(E) = \frac{N}{4\pi} e^{-\frac{1}{4}NE^2}, \tag{6}$$

and the Wigner semicircle,

$$\rho(E) = \frac{1}{2\pi}\sqrt{4 - E^2}, \tag{7}$$

for Δ=0 and Δ=1, respectively. The N independence of the Wigner semicircle level density is due to our choice of N dependence of matrix elements in Eqs. (2) and (3). The transition between the two level density limits occurs around $\Delta \approx 0.1$, see Fig.1. With a total distribution

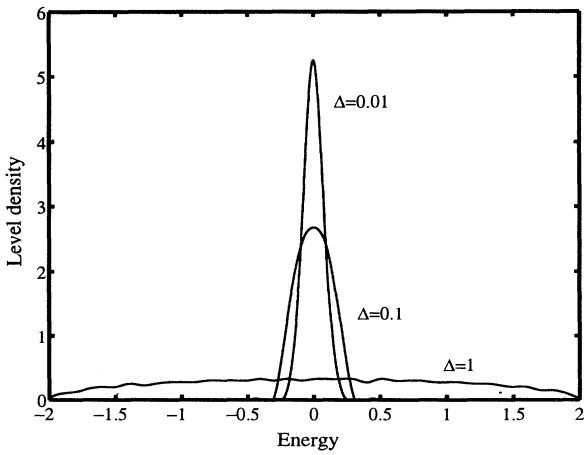

FIG. 1. Level density vs excitation energy or level number for different Δ values. Note the drastic change from narrow Gaussian to (Wigner) semicircle as Δ approaches 1.

width of the order of $N^{-1/2}$ [Eq. (6)] and N^0 [Eq. (7)], we obtain an average energy-level distance, $\overline{d} \sim N^{-3/2}$ and $\sim N^{-1}$, respectively. Or, in other words, the two distribution limits correspond to the average level densities, $\overline{\rho} \sim N^{3/2}$ and $\overline{\rho} \sim N$. For intermediate Δ values we find that the mean level density is well reproduced by an interpolation between the two limits as

$$\overline{\rho}(\Delta, N) \approx \frac{N^{3/2}}{4\Delta\sqrt{N} + 7N^{-\frac{3}{2}\Delta}}. \quad (8)$$

B. Energy fluctuations

From several calculations (see, e.g., [15, 16]) it seems as if GOE properties appear when the size of the perturbation (i.e., the size of the nondiagonal matrix elements) on an average is of the size of the mean level spacing of the unperturbed energy levels (i.e., the average distance between the diagonal matrix elements). In the model above (at I=0) this is obtained when

$$\Delta \frac{1}{\sqrt{N}} \sim \sqrt{\frac{2}{N}} \frac{1}{N} \Rightarrow \Delta \sim \frac{1}{N}, \quad (9)$$

which implies that the GOE properties are expected at much smaller values of Δ than what corresponds to the full GOE. For N=400 we thus expect the GOE properties already when $\Delta \approx 0.02$ [with proper constants inserted in Eq. 9]. Notice that with this argument GOE properties are expected for an infinitely small Δ value in the limit $N \to \infty$. Also notice that the relevant parameter is neither N nor Δ but rather the product $N\Delta$ [15].

In Fig. 2 the nearest neighbor energy-spacing distributions are shown for some different values of Δ. As expected, the GOE curve is reproduced for $\Delta \gtrsim 0.02$. If, on the other hand, we study the Δ_3 statistics [Fig. 3(a)] or quite similarly the variance of the Δ_3 statistics [Fig. 3(b)], for $\Delta = 0.02$ the corresponding GOE curve is followed up to a maximum value, $L_{\max} \approx 20$, of the correlation distance, L, in the energy spectrum. For larger L values both Δ_3 and Var(Δ_3) deviate from the GOE behavior. When Δ is decreased the GOE curve is followed up to a smaller $L_{\max}$ value, etc. In Fig. 4 the $L_{\max}$ values are shown as a function of the "chaoticity parameter," Δ.

Obviously, the GOE character of the spectrum is fulfilled over a limited range in energy only. The reason for this finite range of the GOE correlations is that the wave functions are rather localized for small Δ values [16]. The spread of the wave function on basis states is shown in Fig. 5 for some different values of Δ. For small Δ values only a few components are involved in the wave function. For larger Δ values the number of components increases and also the spreading width increases. Two distant wave functions do not show any overlap in their basis state components, and therefore cannot show any other correlations than those of completely regular, unmixed wave functions.

The localization length, or spreading width of the wave functions, Γ_μ, initiated by $\Delta\mathbf{H}_1$ can be estimated using Fermi's Golden Rule,

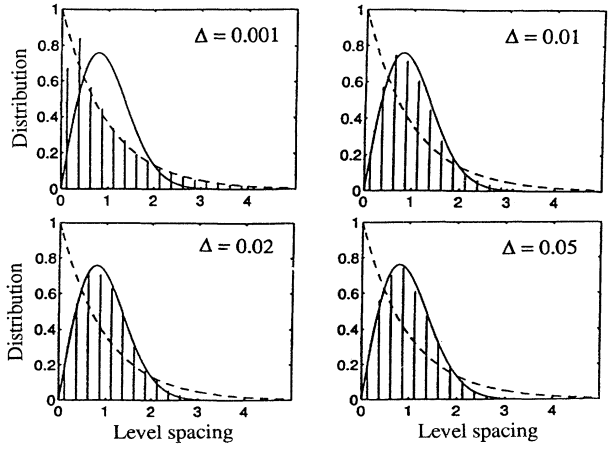

FIG. 2. Nearest neighbor distributions for different values of the mixing parameter Δ. The GOE (solid line) and Poisson (dashed line) limits are shown for comparison.

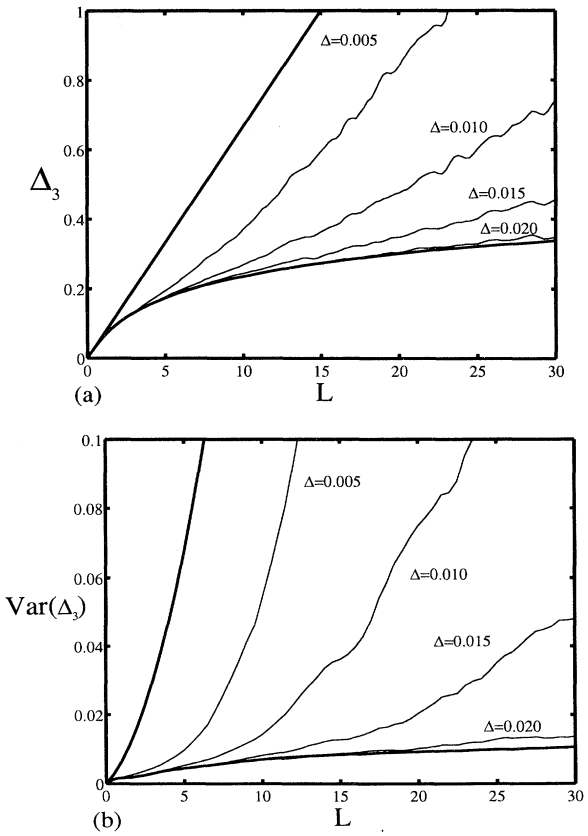

FIG. 3. (a) Δ_3 statistics and (b) the variance of Δ_3 for different values of the mixing parameter Δ. The GOE and Poisson limits are shown for comparison.

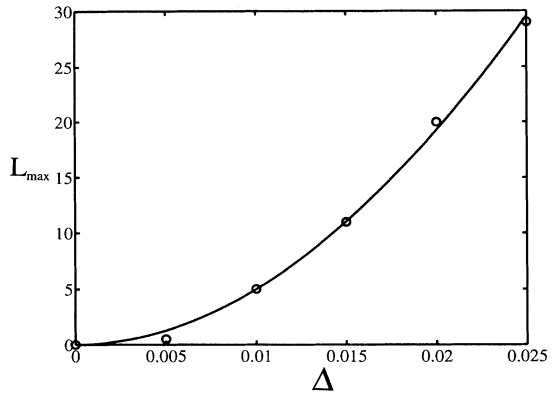

FIG. 4. $L_{\max}$ as a function of Δ deduced from the variance of Δ_3 (circles) and from Eq. (12) (solid line).

$$\Gamma_\mu \approx 2\pi\bar{\rho}_0\overline{\langle(\Delta\mathbf{H}_1)^2\rangle} \approx 2\pi\bar{\rho}_0\frac{\Delta^2}{N}. \tag{10}$$

When the mutual energy distance between two wave functions is larger than, say $2.5\Gamma_\mu$, there are no GOE correlations. This gives

$$L_{\max} \approx 2.5\bar{\rho}\Gamma_\mu \approx 5\pi\bar{\rho}_0\bar{\rho}\frac{\Delta^2}{N}. \tag{11}$$

By inserting the expression for the mean level density from Eq. (8), $\overline{\rho_0} = \bar{\rho}(0)$ and $\bar{\rho} = \bar{\rho}(\Delta)$, we obtain a relation between $L_{\max}$ and Δ ,

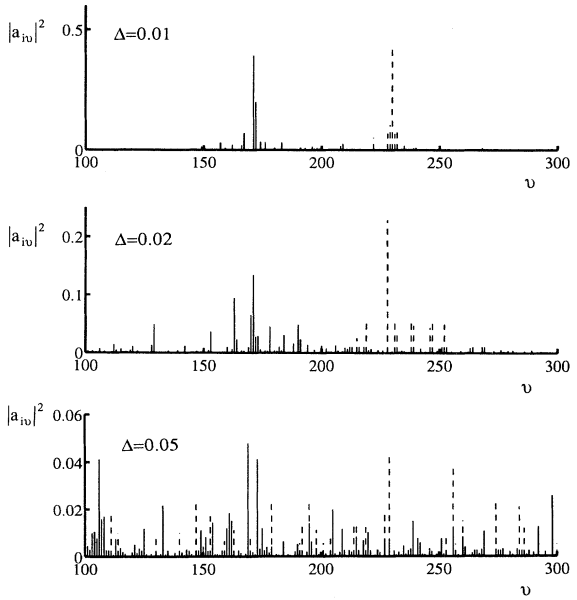

FIG. 5. The spread of the wave function on basis states. Two different wave functions, $\phi_i = \sum_\nu a_{i\nu} \mid \nu\rangle$, corresponding to state i=170 (solid lines) and i=230 (dashed lines) are shown for three different Δ values.

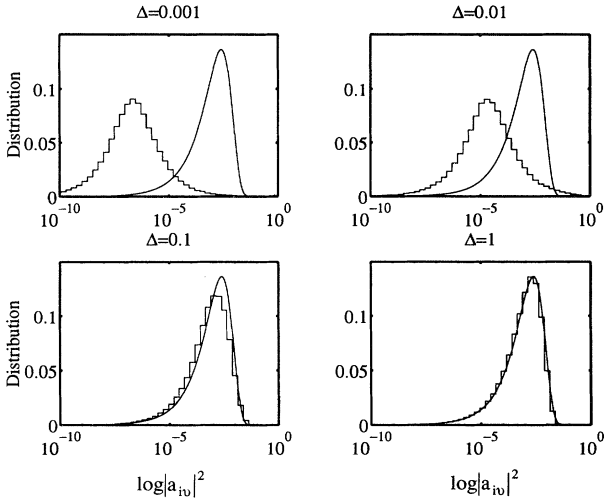

FIG. 6. Distribution of wave function components for different Δ values. The solid line shows the Porter-Thomas distribution.

$$L_{\max} \approx \frac{5\pi}{7}\Delta^2N^2\frac{1}{4\Delta\sqrt{N}+7N^{-\frac{3}{2}\Delta}}, \tag{12}$$

that excellently reproduces the calculated values, see the solid curve in Fig. 4. For much larger Δ values than shown in Fig 4, $L_{\max}$ obviously deviates from this estimate; a saturation of the localization length sets in that is connected with the finite size of the matrices.

C. Wave function fluctuations

In Fig. 6 it can be seen that the square of the wave function components follows the Porter-Thomas distribution (i.e., the size of the wave function components is Gaussian distributed) when $\Delta \gtrsim 0.1$. This means that the GOE limit is reached at considerably larger Δ values than for which, e.g., the corresponding NND follows the GOE curve [16]. Not until the wave functions are completely delocalized will the wave function components be Gaussian distributed over all basis states. This transition is global rather than local and is connected with the change of the level density from a narrow Gaussian peak to the much broader Wigner semicircle distribution as was discussed in Sec. III A (see Fig. 1).

D. Level dynamical properties

The motion of energy levels in the quantum mechanical system described by $\mathbf{H}(I)$ may be studied by letting the external parameter I vary. One may then define and study new statistical properties that describe the dynamics of the system. One such dynamical feature that can be obtained from the energy-level spectrum, E_i vs I, is the curvature.

Already in 1974 Pomphrey [17] emphasized the con-

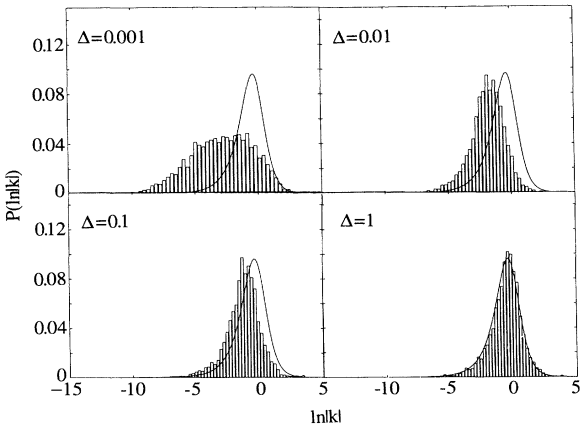

FIG. 7. Curvature distributions for four different values of the mixing parameter, Δ=0.001, 0.01, 0.1, and 1. As a comparison the expression for the generic curvature distribution [Eq. (14) with ν=1] is shown in each figure. The curvatures are scaled and plotted on a logarithmic scale.

nection between large curvatures in the energy spectrum and chaotic motion in the corresponding classical system. Later on expressions could be derived for the tail of the curvature distribution [18, 19],

$$P(K) \sim |K|^{-\nu+2}, \tag{13}$$

asymptotically valid for large curvatures. Here K is the calculated curvature, $K = d^2E/dI^2$, and ν depends only on the underlying symmetry of the system, ν=1, 2, and 4 for GOE, GUE (Gaussian unitary ensemble), and GSE (Gaussian symplectic ensemble), respectively. Based on numerical experiments and led by simplicity, Zakrzewski and Delande [11] subsequently proposed an expression for the full curvature distribution of a quantum chaotic spectrum,

$$P(k) = C_\nu(1 + k^2)^{-(\frac{\nu}{2}+1)}, \tag{14}$$

where C_ν is a normalization constant (=1/2 for ν=1), k is the scaled curvature, $k = K[\pi\rho\langle(dE/dI)^2\rangle]^{-1}$, where ρ is the level density. Since in our model the average slope $\langle(dE/dI)\rangle$=0 we have $\langle(dE/dI)^2\rangle=\sigma_\omega^2$, where σ_ω is the average dispersion in slope. Note that the scaled curvature distribution depends only on the symmetry class. The expression for the full curvature distribution, Eq. (14), has recently been proven rigorously for all three symmetry classes by von Oppen [12].

From our model [Eqs. (1)–(4)] we may calculate the curvature distribution also for mixed systems, and in Fig. 7 scaled curvature distributions are shown for Δ=0.001, 0.01, 0.1, and 1. The curvatures were numerically calculated as finite differences. In these calculations the step size, δI, was chosen small enough that the second derivatives were independent of δI. As is seen in Fig. 7 the generic distribution is not obtained until $\Delta \approx 1$, i.e., when the model corresponds to full GOE.

IV. SUMMARY AND DISCUSSION

Based on a random matrix model we have studied different kinds of statistical measures for eigenvalues, eigenfunctions, as well as the curvature distribution obtained from the level dynamics. Intermediate distributions between Poisson and GOE have been studied, and for each case the transition to the generic GOE distribution has been identified.

An important summarizing conclusion from the present study is that if a spectrum analysis, of, e.g., the nearest neighbor energy-level distribution, shows GOE properties, one may not assume automatically that all other properties connected with GOE are fulfilled. This suggests carefulness in drawing conclusions about quantum chaos based on established GOE properties of some statistical measures.

We have shown that different types of level statistics, such as nearest neighbor distributions (NND), Δ_3 statistics, wave function analysis, curvature distributions, etc., show dramatically different sensitivity to the "chaoticity parameter," Δ, that interpolates our random matrix model between regularity (Poisson) and chaos (GOE). At a rather small Δ value, approximately corresponding to the situation when the nondiagonal matrix elements are of the same size as the level spacing between the diagonal matrix elements, the energy-level fluctuations show GOE properties. This is particularly obvious for the NND. For the long-range correlations like Δ_3 statistics, Σ_2, and the variance of Δ_3, the GOE properties also appear for such small Δ values, but only over a finite stretch of energy levels. These differences between long-range and short-range fluctuation measures could be understood in terms of a localization of the wave functions. (See also the discussion on band random matrices and on the kicked rotor in [20], as well as the discussion on a RMT model in [15].) Expressing the localization length of the wave functions through Fermi's Golden Rule we could obtain a relation between the length of these correlations, $L_{\max}$, and the size of the perturbation, Δ. Consequently, by obtaining $L_{\max}$ from a Δ_3 analysis based on a stretch of measured energy states, one may obtain indirectly an estimate of the average size of the residual interaction that is responsible for breaking the quantum numbers related to the studied (unperturbed) energy levels.

The chaotic features of the system are thus far from being global for $\Delta \ll 1$, but rather, we may have an energy spectrum where eigenstates show (translational invariant) local chaos.

At much larger Δ values the wave function components become Gaussian distributed, and the wave functions become completely delocalized. This is connected with a rather drastic decrease in the level density, approaching the Wigner semicircle distribution. Both the level density and the wave function component distribution are mainly to be considered as global (rather than local) properties.

Recently it has been realized that also the motion of eigenvalues (level dynamics) shows universality. We concentrated on one statistical property, the distribution of curvatures, which is a measurable quantity for many sys-

tems. Not until the chaoticity parameter, Δ, is (approximately) equal to 1, i.e., the model is more or less identical to GOE, does the distribution of curvatures saturate and coincide with the generic distribution [Eq. (14)]. In our study this is thus the strongest requirement on the spectrum properties to be of GOE character. For some physical systems the curvature may be experimentally deduced, as, for example, the magnetic susceptibility. In the case of a rapidly rotating atomic nucleus the variable I may be considered as the angular momentum and, as was mentioned above, the curvature then corresponds to the negative and inverse of the dynamical moment of inertia. This is a physical property that can be measured also for quite excited states [21]. However, due to the quantum mechanical feature of angular momentum, the dynamical moment of inertia is obtained as a finite difference (with step size $2\hbar$ in angular momentum). We have therefore tested the sensitivity on stepsize in calculating the curvature distributions. It was found that the curvature distribution for small Δ values becomes quite different for a large stepsize (say δI=0.5) than for a small stepsize ($\delta I<10^{-4}$), while it is rather independent of the stepsize for Δ=1. This seems to imply a generic curvature distribution [Eq. (14)] also for curvatures obtained by finite size differences.

ACKNOWLEDGMENTS

This project was supported by the Swedish Natural Science Research Council (NFR) and the Joint Institute for Heavy Ion Research (JIHIR) in Oak Ridge. The JIHIR has as member institutions the University of Tennessee, Vanderbilt University, and the Oak Ridge National Laboratory; it is supported by the members and by the Department of Energy through Contract No. DE-FG05-87ER40361 with the University of Tennessee.

[1] F. Haake, *Quantum Signatures of Chaos* (Springer Verlag, Berlin, 1992).
[2] O. Bohigas, in *Chaos and Quantum Physics*, Proceedings of Les Houches Summer School, 1989, edited by M.-J. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1991), p. 87.
[3] A. Hönig and D. Wintgen, Phys. Rev. A **39**, 5642 (1989).
[4] O. Bohigas, M. Giannoni, and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984).
[5] K. Nakamura, *Quantum Chaos: A New Paradigm of Nonlinear Dynamics* (Cambridge University Press, Cambridge, 1993).
[6] K. Nakamura and H. Thomas, Phys. Rev. Lett. **61**, 247 (1988).
[7] A.J.S. Traiber, A.J. Fendrik, and M. Bernath, J. Phys. **A 23**, L305 (1990).
[8] C.E. Porter, *Statistical Theories of Spectra: Fluctuations*, edited by C.E. Porter (Academic Press, New York, 1965).
[9] T.A. Brody, J. Flores, J.B. French, P.A. Mello, A. Pandey, and S.S.M. Wong, Rev. Mod. Phys. **53**, 385 (1983).
[10] M.L. Mehta, *Random Matrices*, 2nd ed. (Academic Press, New York, 1991).
[11] J. Zakrzewski and D. Delande, Phys. Rev. E **47**, 1650 (1993).
[12] F. von Oppen, Phys. Rev. Lett. **73**, 798 (1994); Phys. Rev. E **51**, 2647 (1995).
[13] The Δ_3 function is defined as $\Delta_3(L) = \langle (1/L) \min_{A,B} \int_S^{S+L} [V(\xi) - A\xi - B]^2 d\xi \rangle_S$ where $N(\xi)$ is the number of unfolded energy levels below ξ.
[14] P. Persson, M. Sc. theses, Lund-MPh-94/07, Lund 1994; and (unpublished).
[15] T. Guhr and H.A. Weidenmüller, Ann. Phys. (N.Y.) **193**, 472 (1989).
[16] S. Åberg, Prog. Part. Nucl. Phys. **28**, 11 (1992).
[17] N. Pomphrey, J. Phys. B **7**, 1909 (1974).
[18] P. Gaspard, S.A. Rice, and K. Nakamura, Phys. Rev. Lett. **63**, 930 (1989).
[19] P. Gaspard, S.A. Rice, H.J. Mikeska, and K. Nakamura, Phys. Rev. A **42**, 4015 (1990).
[20] F.M. Izrailev, Phys. Rep. **196**, 299 (1990).
[21] O. Andersson *et al.*, Phys. Rev. Lett. **43**, 687 (1979).