Uncovering the Transition from Regularity to Irregularity in a Quantum System

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For a model quantum system the distributions of the spacings between adjacent levels in specified intervals of the energy spectrum are fitted by the Brody distribution. This analysis displays for the first time the expected transition from regularity to irregularity, in terms of a smooth increase of the parameter of the Brody distribution from 0 to 1.

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The number of publications on the interrelation between classical systems comprising stochastically unstable trajectories and the corresponding quantum systems has swollen enormously.[1–21] The wide popularity of the phrase "quantum chaos" used to circumscribe the presumed quantal effects should, however, not gloss over its vagueness. Indeed, the various manifestations of the well defined classical chaos do not transform in an unequivocal manner when passing to quantized systems.[2–5] It seems to be more appropriate to adopt the terms "regular" and "irregular" as introduced by Percival[6] to distinguish the quantal manifestations of quasiperiodic and ergodic classical motion. Various techniques such as the method of avoided crossings,[5,7,22] the investigation of the sensitivity of energy eigenvalues to perturbations,[6b,8,9] the statistical analysis of fluctuations in the spectral sequences,[10–15,23] the structure of the eigenvectors,[10,16,17] and others[18,19] have been employed to make the terms "regular" and "irregular" more precise. The lack of rigor of these tests and the unanswered question of their equivalence, however, represent a challenge for future work.

A powerful method to distinguish between regular and irregular spectral sequences is based on the distribution of nearest-neighbor spacings (NNS). With use of semiclassical arguments a continuous NNS distribution function has been derived for regular sequences[20] and conjectured for irregular ones.[14] In the generic regular case the energy eigenvalues are distributed randomly leading to a Poisson-type distribution function.[20] An irregualr spectrum occurs when the energy levels are correlated resulting in a repulsion of adjacent levels. Therefore, the NNS distribution function peaks at a finite value and exhibits the typical features of a Wigner function.[14] The analysis of the NNS distributions of several quantal spectra ensures the significance of these criteria for both purely regular[10,20] and purely irregular systems.[10,11,15]

Many classical systems are known which behave quasiperiodically at low energies and chaotically at high energies. Typically, for increasing energy one observes a gradual occupation of the phase space with irregular trajectories as evidenced by the gradual disappearance of the stability islands in the Poincaré surfaces of section.[1,3,8,9] However, the existence and the details of such a transition from regularity to irregularity in quantal systems have not yet been analyzed. Here we investigate the distribution of the energy eigenvalues of a specific quantum system uncovering thereby a smooth transition of the NNS histograms from a Poisson-type to a Wigner-type behavior as we increase the energy.

We consider a model system of two harmonic oscillators with equal frequencies coupled by a quartic term in the coordinates[9]

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + 4k\hat{q}_1^2\hat{q}_2^2,$$
$$\hat{H}_i = \tfrac{1}{2}(\hat{p}_i^2 + \hat{q}_i^2); \quad i = 1, 2. \tag{1}$$

Its classical analog shows a transition from quasiperiodicity to chaos. For $k = 0.0125$ the transition regime $15 \lesssim E \lesssim 50$ has been found.[9] Compared with the frequently studied Hénon-Heiles system the present model potential does not allow for dissociation and, therefore, makes the calculation of an arbitrarily large number of discrete eigenstates possible.

The numerical effort of diagonalizing the Hamiltonian (1) can be greatly reduced by exploiting its C_{4v} symmetry. In our calculation we confine ourselves to totally symmetric eigenstates. Arranging the secular matrix in an optimal manner we are able to obtain a sufficiently large part of the eigenvalue spectrum converged. We use the method of Jacoby rotations[24] to transform the banded secular matrix to a tridiagonal one which is diagonalized subsequently by a standard routine.[25] For a matrix dimension of 4095 we need ~5 h computation time on an IBM 370/168 utilizing thereby almost all of the core.

In order to perform a statistical analysis of a given spectral sequence appropriately it is exceedingly important to have a *constant average spacing* between neighboring energy levels[26] since global variations of the state density can falsify the fluctuation measures considerably. Various unfolding procedures are known to decompose a given spectrum into secular variations and fluctuations.[26,27] Here we have used cubic spline for smoothing with an appropriate number of knots to describe the secular variations of the integrated level density of the spectrum of H [Eq. (1)] in a given energy interval. A second important point is the necessity of large data sets in order to obtain reasonable fluctuation measures. For each energy interval investigated we consider ~ 200 energy levels as a lower limit for a reliable statistical test.

The distributions of the spacings between adjacent levels of the unfolded spectral sequence are displayed as histograms in Fig. 1 for specified energy intervals. The abscissa is in units of D which is the average spacing between adjacent levels in the respective energy interval. Here a value of the coupling parameter of $k=0.005$ has been chosen. An obvious trend from a Poisson-type distribution in the low-lying energy interval [Fig. (1a)] to Wigner-type distributions in the high-energy regime [Figs. 1(b) and 1(c)] can be seen. We are able to approximate the histograms conveniently by a continuous distribution function $P_q(S)$ specified by the parameter q:

$$P_q(S)=\alpha S^q \exp(-\beta S^{1+q}); \qquad (2)$$
$$\alpha=(1+q)\beta,$$
$$\beta=\{D^{-1}\Gamma[(2+q)/(1+q)]\}^{1+q}.$$

For $q=0$ $P_q(S)$ recovers the Poisson distribution $P_0(S)=(1/D)\exp(-S/D)$, and for $q=1$ the Wigner distribution $P_1(S)=(\pi S/2D^2)\exp(-\pi S^2/4D^2)$. It was introduced first by Brody[28] in order to fit NNS histograms obtained from nuclear spectra. The respective values of q displayed in Fig. 1 for the different energy intervals have been calculated by a least-squares fit.

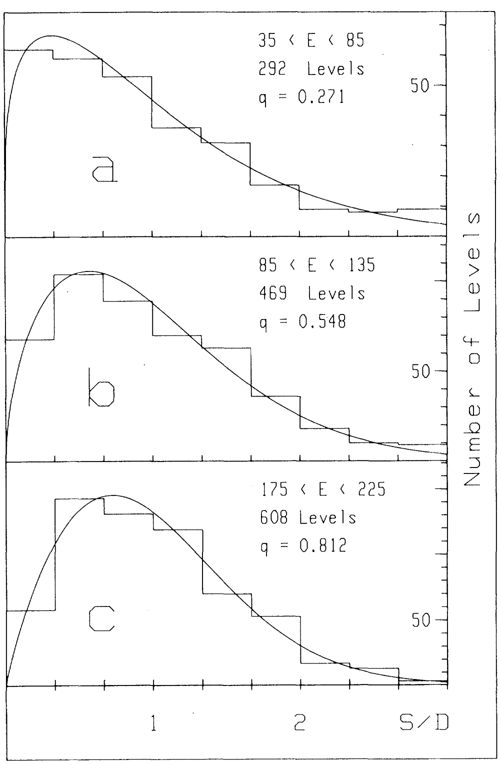

FIG. 1. Nearest-neighbor-spacing histograms for energy levels of the Pullen-Edmonds Hamiltonian [Eq. (1)] with $k=0.005$. The results for three different energy intervals are shown. In each case a best-fitting Brody distribution [Eq. (2)] specified by the parameter q is also shown.

Having observed the transition from regularity to irregularity for a specific Hamiltonian we now vary the coupling parameter k. Figure 2 shows in its upper part the variation of the q parameters with energy for different values of k [Eq. (1)]. For their computation we used energy intervals of length 50 whose centers are the abscissae of the respective data points. A continuation of the curves to the right would require more converged eigenvalues. However, it is evident that q will tend to unity as the energy and/or the value of the coupling parameter k increase. The curves have been truncated at the left-hand side, since the histograms for low-lying energy intervals exhibit the anomalies characteristic of systems of harmonic oscillators as analyzed thoroughly by Berry and Tabor.[20]

In order to elucidate the functional dependence of the Brody parameter q on the energy E and the coupling parameter k we employ the scaling property of the classical Hamilton function

$$H(k;p_1,q_1,p_2,q_2) = (1/k)\,H(1;p_1\sqrt{k},\ q_1\sqrt{k},\ p_2\sqrt{k},\ q_2\sqrt{k}), \qquad (3)$$

where $H(k;\,p_1,q_1,p_2,q_2)$ is the classical Hamilton function corresponding to the quantum mechanical Hamiltonian $\hat{H}$ of Eq. (1). It means that the classical dynamics depends solely on the product kE. Therefore, we have plotted in Fig. 2(b) the Brody

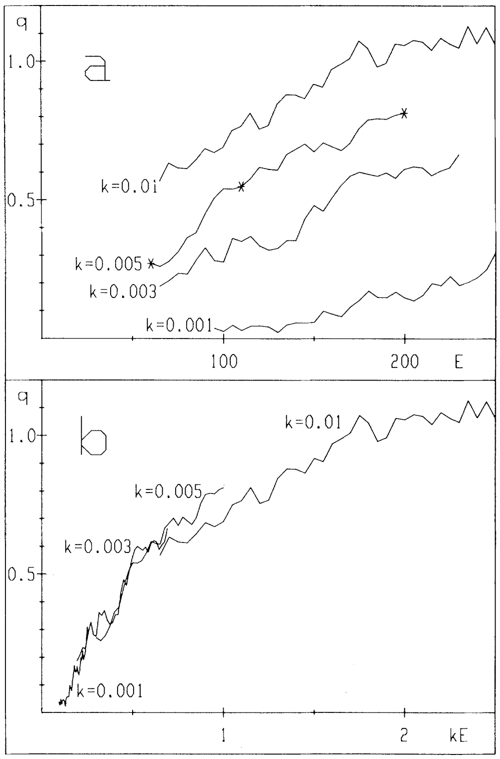

FIG. 2. (a) Brody parameter q [Eq. (2)] as a function of the energy for different values of the coupling constant k in the model Hamiltonian [Eq. (1)]. The three stars in the $k = 0.005$ curve mark the centers of the energy intervals of Fig. 1. (b) Representation of the functional dependence $kE \to q(kE)$ constructed from the four curves in (a).

parameters q versus kE. It should be emphasized that the scaling in Eq. (3) is feasible classically, but not quantum mechanically because of the appearance of Planck's quantum. Interestingly, all four curves in Fig. 2 appear on this scale approximately as sections of a single monotonically increasing function $q(kE)$. Small values of kE define the regular regime characterized by values of q close to zero, i.e., Poisson-type NNS distributions.[20] For large values of kE the value of q approaches unity thus implying Wigner-type distributions. Such distributions are characteristic of irregular spectral sequences[14] and have also been found in many other physical systems of sufficient complexity.[13,23,24,29] In our system the transition region between these two limiting cases is steadily and smoothly bridged by the proposed curve $q(kE)$. This result was of course not unexpected and could also have been obtained by fitting our level spacings to any other one-parameter family of distributions which smoothly interpolate between the Poisson and Wigner distributions, and we do not wish to claim that the Brody distributions have any theoretical basis. It should be noted that the width of the transition regime probably depends on the length of the energy intervals used in our calculation. Nevertheless, Fig. 2(b) unravels the transition from regularity to irregularity in the quantum system considered [Eq. (1)] in a rather convincing manner. We consider this analysis to be the first of this kind. Interestingly, the transition regime derived from the classical studies of Pullen and Edmonds[9] for this system $(0.2 \lesssim kE \lesssim 0.6)$ is consistent with our findings.

Further fluctuation measures such as the Δ statistics[23] or correlation coefficients between spacings[23] present themselves as further indicators of regularity and irregularity. For the transition to irregularity we find evidence that such quantities converge to certain constants. Interestingly, the values of these constants agree with the fluctuation measures derived for random matrix ensembles.[23] The simulation of irregularity by random matrix techniques is expected to further elucidate the quantal manifestations of classical chaos.

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