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LETTER TO THE EDITOR

On the connection between irregular trajectories and the distribution of quantum level spacings

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Abstract. For a model system the distribution of spacings between adjacent levels in specified intervals of the energy spectrum are compared with a semiclassical distribution. This distribution (Berry and Robnik) depends on the size of the phase space volume filled with irregular trajectories. Good agreement is found between quantal and semiclassical spacing distributions. In particular, the transition from regularity to irregularity observed in the quantum calculation (Haller *et al*) is well reproduced by the semiclassical results.

In classical Hamiltonian systems there exists a well defined distinction between regular (quasiperiodic) and irregular (chaotic) motion (Berry 1978). Considerable effort has been devoted to defining and observing irregularity (Percival 1973) for quantal systems, but the phrase 'quantum chaos' refers to a still rather undefined phenomenon. Evidence of irregularity, however, can be found in, for example, the nodal pattern of the wavefunctions (McDonald and Kaufman 1979, Stratt *et al* 1979), the overlap of the eigenvectors with those of a zero-order Hamiltonian (Nordholm and Rice 1974, Hose and Taylor 1982); the sensitivity of energy eigenvalues to small perturbations (Pomphrey 1974, Percival 1977, Pullen and Edmonds 1981) and via the statistical analysis of fluctuations in spectral sequences (McDonald and Kaufman 1979, Buch *et al* 1982, Haller *et al* 1984). Here we concentrate on the last phenomenon and will show that (at least for the Hamiltonian investigated) there exists a strong correlation between the distribution of nearest-neighbour level spacings and the size of the phase space volume filled with irregular trajectories.

The level spacing distribution of a completely regular (i.e. integrable) system assumes a Poisson-like form in the semiclassical limit (Berry and Tabor 1977). A completely irregular system, on the other hand, shows a Wigner-like level spacing distribution as found by many numerical experiments (see e.g. McDonald and Kaufman 1979) as well as conjectured by Pechukas (1983). A mixture of these two distributions should be observed if the corresponding classical system has regions of both regularity and irregularity. Berry and Robnik (1984) conjectured that the energy levels consist of two separate sequences, one being Poisson distributed, the other being Wigner distributed. The relative weight of these two distributions is assumed to be the Liouville measure of the region in phase space filled with regular and irregular trajectories, respectively. The superposition of the two level sequences, neglecting any interaction between them, yields the distribution

$$P(q, S) = \exp[-(1-q)S + \tfrac{1}{4}\pi q^2 S^2]\{1 - q^2 + \tfrac{1}{2}\pi q^3 S - (1-q^2)R(qS)\} \qquad (1)$$

where

$$R(z) = 1 - e^{\pi z^2/4}\,\mathrm{erfc}(\sqrt{\pi}z/2)$$
$$= \int_0^\infty e^{-\pi t^2/4}(1 - e^{-\pi t^2/2})\,\mathrm{d}t. \tag{2}$$

In (1) S denotes the level spacing (the average level spacing being normalised to unity) and q denotes a parameter which allows $P(q, S)$ to interpolate between the Poisson distribution ($q = 0$)

$$P(0, S) = e^{-S}, \tag{3a}$$

and the Wigner distribution ($q = 1$)

$$P(1, S) = \tfrac{1}{2}\pi S\, e^{-\pi S^2/4}. \tag{3b}$$

The parameter q is amenable to classical mechanics. It is the Liouville measure of the irregular region divided by the measure of the energy shell:

$$q = \left(\int \mathrm{d}\boldsymbol{\gamma}\,\delta(H(\boldsymbol{\gamma}) - E)\chi(\boldsymbol{\gamma})\right)\Big/\left(\int \mathrm{d}\boldsymbol{\gamma}\,\delta(H(\boldsymbol{\gamma}) - E)\right) \tag{4}$$

where $\boldsymbol{\gamma} = (x_1, \ldots, x_F, p_1, \ldots, p_F)$ denotes a point in phase space. (We are assuming F degrees of freedom.) The symbol χ denotes the characteristic function on the irregular phase space volume, i.e. $\chi(\boldsymbol{\gamma}) = 1(0)$ if an irregular (regular) trajectory runs through the phase space point $\boldsymbol{\gamma}$.

It is the aim of this letter to clarify if there is indeed such a simple direct connection between the quantal level spacing distribution and classical mechanics. For this purpose we consider a model system of two harmonic oscillators with equal frequencies coupled by a quartic term in the coordinates

$$H = \tfrac{1}{2}(p_x^2 + p_y^2 + x^2 + y^2) + 4kx^2y^2. \tag{5}$$

Pullen and Edmons (1981) were the first to study this Hamiltonian both classically and quantally. The quantal aspect of the present investigation, i.e. the diagonalisation of large secular matrices and the evaluation of the nearest-neighbour distributions $P(S)$, was discussed by some of us previously (Haller *et al* 1984). In that article we have shown that the system (5) exhibits a gradual transition from a Poisson-like level spacing distribution to a Wigner-like distribution if the energy (or the coupling constant k) is increased. Such a system is especially suitable for studying a possible connection to classical mechanics. The Brody distribution (Brody 1973) which was used by us (Haller *et al* 1984) is very convenient to analyse the transition from regularity to irregularity, but it has no relation to classical mechanics in contrast to distribution (1) which is studied here.

In the following we shall discuss the classical part of the problem and shall begin by making a few technical remarks. While running the trajectories we found that the usual all purpose integrators are not able to retain sufficient accuracy if the trajectory is run for a long time. We have, therefore, written a special routine (Meyer 1984) which takes advantage of the simple analytic structure of the particular equations of motion to be integrated. The truncation error of the new algoirthm is of 20th order (!) in the step size.

The stability matrix (see e.g. Benettin *et al* 1979)

$$M_{ij}(t) = \partial\gamma_i(t)/\partial\gamma_j(0) \tag{6}$$

is integrated simultaneously with each trajectory. From this stability matrix we define the Lyapunov function (Benettin *et al* 1976)

$$\lambda(t) = \ln(\|M(t)\|)/t \tag{7}$$

where $\|\cdot\|$ denotes the euclidean norm. For a regular trajectory it can be shown that $\lambda(t)$ tends to zero (like $\ln(\beta t)/t$) if time goes to infinity. For irregular trajectories it is generally believed that $\lambda(t)$ converges to some finite value ('exponentially separating neighbouring trajectories'). At the end of each trajectory it was checked whether $\lambda(t)$ was below or above some carefully chosen threshold. This enabled us to distinguish regular from irregular trajectories.

In order to determine the ratio q appearing in (1) we considered the surface of section (Hénon and Heiles 1964), i.e. the cut through the phase space which is characterised by the constraints $y=0$ and $H(x, y, p_x, p_y) = E$. The surface of section was divided into rectangular cells of width $\Delta x = \Delta p_x = (2E)^{1/2}/100$. We then run trajectories for 50 to 250 'periods' and decided—aided by the Lyapunov number—whether a particular trajectory was regular or irregular. All cells touched by the trajectory were assigned to belong to the regular or irregular regime, respectively. We continued to run trajectories until each cell was touched by a least one trajectory.

Next we define q_S as the ratio of the number of cells belonging to the irregular regime divided by the total number of (energetically accessible) cells. Except for the discretisation error this ratio is given by

$$q_S = \frac{\int \mathrm{d}x \int \mathrm{d}p_x\, \theta(E - H(x, 0, p_x, 0))\chi(x, 0, p_x, p_y(x, p_x))}{\int \mathrm{d}x \int \mathrm{d}p_x\, \theta(E - H(x, 0, p_x, 0))} \tag{8}$$

where θ denotes the step function and where p_y denotes the positive root of the implicit equation $E = H(x, 0, p_x, p_y)$. The ratio q_S can be related to q by recognising that q_S is given by a phase space integral (Meyer 1984)

$$q_S = \left(\int \mathrm{d}\gamma\, \delta(H(\gamma) - E)\nu(\gamma)\chi(\gamma)\right) \Big/ \left(\int \mathrm{d}\gamma\, \delta(H(\gamma) - E)\nu(\gamma)\right) \tag{9}$$

where $\nu(\gamma)$ denotes the average frequency with which the trajectory, started at the phase space point γ, hits the surface of section

$$\nu = \lim_{t\to\infty} t^{-1} \int_0^t \mathrm{d}t'\, \dot{y}(t')\theta(\dot{y}(t'))\delta(y(t')). \tag{10}$$

Comparing (9) with (4) one notices that $q_S = q$ if ν is constant, or, more generally, if the average of ν over all irregular trajectories on the energy shell equals the average of ν over all regular ones. The latter assumption was found to be satisfactorily obeyed for the system under investigation and we have identified q with q_S.

The fraction q thus obtained is shown in figure 1 (full curve). It depends solely on the product kE as can be shown by a simple analysis of the equations of motion. The curve shown in figure 1 should be, of course, perfectly smooth. The kinks in the curve are due to the discretisation error introduced by the finite area of the cells of the surface of section. The points shown in figure 1 represent the quantum q-values found by fitting equation (1) to the level spacing distribution obtained by diagonalising the Hamiltonian (5). The different symbols denote different coupling strengths, k, of the quantum calculations. One observes a good overall agreement between the fitted q-values and the fraction of phase space filled with irregular trajectories. In particular, the transition energy is correctly predicted by classical mechanics.

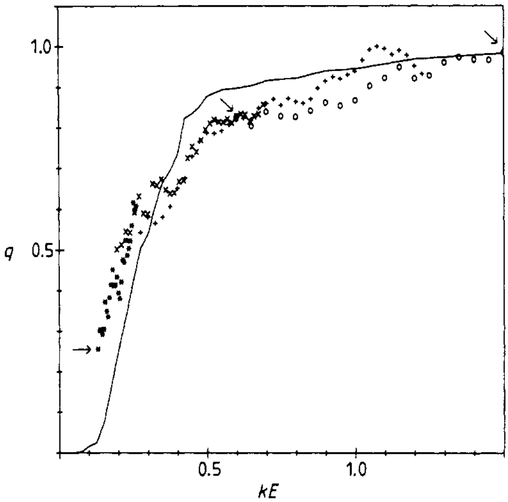

Fig. 1. The full line represents the fraction of classical phase space filled with irregular trajectories (cf (4)). The points give the values obtained by fitting the distribution (1) to the numerically evaluated quantal distributions (compare with Haller *et al* 1984). The different symbols stand for different couplings strengths k: $*$, 0.001; $\times$, 0.003; $+$, 0.005; $\bigcirc$, 0.01, respectively. The three arrows indicate the three particular distributions shown in figure 2.

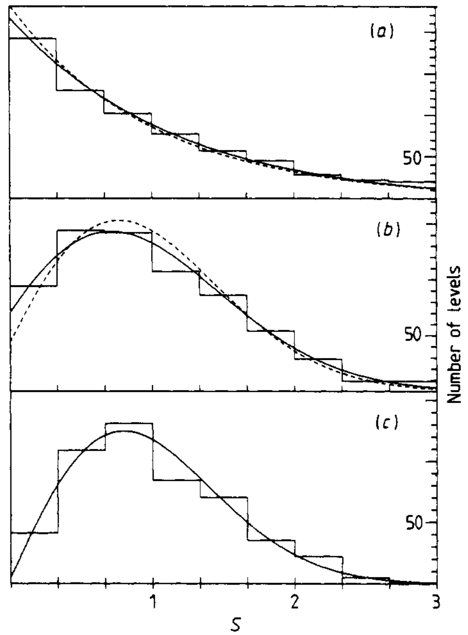

Figure 2. The numerically evaluated quantal level spacing distribution (histogram) in comparison with the distribution (1). The parameter q, determining the form of the distribution (1), is obtained by fitting this distribution to the histogram (full curve and (a) $q=2.60$, (b) $q=0.830$, (c) $q=0.987$) or by classical mechanics via (4) (broken curve and (a) $q=0.046$, (b) $q=0.898$, (c) $q=0.986$). The product kE was evaluated by choosing the centre of the energy interval out of which the energy levels were taken to represent the energy of this interval. (a) $kE=0.13$, $105<E<155$, 699 levels; (b) $kE=0.6$, $175<E<225$, 679 levels; (c) $kE=1.5$, $125<E<175$, 500 levels.

To clarify our procedure, we give in figure 2 three examples. The numerically evaluated level spacing distribution (histogram) and the distribution (1) where the parameter q is obtained by a least squares fit to the histogram (full line) and by classical mechanics (broken curve) are shown for comparison. Figure 2(a) demonstrates that the large deviations shown in figure 1 at small q-values are not significant. This can be understood by recognising that the power expansion of the distribution (1) starts with q^2 rather than with q

$$P(q,S)=\mathrm{e}^{-S}\{1-q^2(1-2S+S^2/2)+\mathrm{O}(q^3S)\}. \tag{11}$$

A chi-squares statistical analysis (Abramowitz and Stegun 1964) of our data has shown that virtually all the deviations of the classically predicted level spacing distribution from the quantum one are within the statistical uncertainty of the latter. Although deviations from the 'classically predicted' level spacing distribution are to be expected because of quantum effects (in particular interaction between the two different sequences due to tunnelling through dynamical barriers), we are not able to definitely identify such deviations because of the limited number of levels available.

In conclusion we would like to remark that although the phrase 'quantum chaos' has no *precise* meaning we feel that we have demonstrated that, at least for the example studied here, there is a very strong correlation between a classical measure of chaos, the fraction of phase space filled with irregular trajectories, and a well defined property of quantal systems, the nearest-neighbour spacing distribution of energy levels.

A few words of caution may be appropriate at this point. Firstly, only eigenvalues belonging to a single symmetry class of the point group are to be considered if the Hamiltonian has geometrical symmetries. Secondly, we emphasise that the secular variation of the energy levels has been carefully removed by an unfolding procedure (Haller *et al* 1983, 1984, Brody *et al* 1981) before evaluating the level spacing distribution. Thirdly, only levels out of specified energy intervals are considered. In particular, we never considered the few *lowest* eigenvalues of the spectrum. The lowest quantum states are always likely to behave anomalously, e.g. show a very regular nodal pattern even for completely irregular systems (Shapiro *et al* 1984).

While deriving the distribution (1) it was assumed that classical irregular motion implies quantum level repulsion (i.e. a Wigner-like distribution) and that classical regular motion implies quantum level clustering (i.e. a Poisson-like distribution). The first implication is almost certainly correct (Berry 1984). The second implication, however, does not always hold. For example, the 'desymmetrised square torus billiard' studied by Richens and Berry (1981) shows level repulsion, but does not show exponentially separating neighbouring trajectories. More important is probably the oscillator anomaly thoroughly discussed by Berry and Tabor (1977). These authors showed that the level spacing distribution becomes anomalous if the energy levels are (approximately) equal to the levels of a set of uncoupled harmonic oscillators. More generally, the anomaly is expected to occur if the energy levels of an integrable system do not depend on the two quantum numbers n and m individually (we are assuming two degrees of freedom for the sake of simplicity), but rather depend on a *linear* combination of the quantum numbers

$$E_{nm} = f(n + bm) \tag{12}$$

where f denotes some smoothly increasing function and b some positive number. The anomalous distributions may, for low resolution, roughly look Wigner-like, although the system is completely regular. We also observed these anomalous distributions when we set the coupling constant k, appearing in our model Hamiltonian (5), to a too small number. For $kE \geqslant 0.13$, however, the anomaly is broken.

Benjamin *et al* (1984) have recently discussed some level spacing distributions obtained with the algebraic Hamiltonian method. This Hamiltonian possess by construction very special constants of motion. In view of equation (12) we believe that some of their results are merely a demonstration of the above mentioned oscillator anomaly.

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