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LETTER TO THE EDITOR

A note on the level spacings distribution of the Hamiltonians in the transition region between integrability and chaos

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Abstract. It is well known that there is no strict universality of the spectral fluctuations of quantum Hamiltonians whose classical counterparts undergo the transition from integrability to complete chaos. I discuss the level spacings distribution P(S), and explain why the semiclassical formulae of Berry and Robnik cannot be correct for small S. There is no global universality of P(S) for nearly integrable systems, but the approach to the integrability as the perturbation parameter ε goes to zero can be universal. This is reflected in the fact that the slope dP/dS at S = 0 for small ε is universally inversely proportional to ε . I give two models in terms of two-dimensional random matrices, one of them being based on maximum entropy considerations. I also point out the connection to the statistics of zeros of random functions, and discuss the numerical evidence.

The quantum energy levels of a Hamiltonian H fluctuate around the mean spectral staircase and such spectral fluctuations obey universal laws for a few universality classes of Hamiltonians (see, e.g., Bohigas and Giannoni 1984). In the random matrix theories the classification is in terms of the symmetries (Porter 1965), which has been recently extended by Robnik and Berry (1986) and further generalised by Robnik (1986). Thus for Hamiltonians without spin, one must distinguish between the systems with an antiunitary symmetry (which generalises the concept of time reversibility) and systems without such a symmetry. The representation matrix of the Hamiltonian is real symmetric in the former case, and is complex Hermitian for systems with broken antiunitary symmetry. The random matrix theory of spectral fluctuations deals with random matrices whose elements are statistically independent and their distribution is assumed invariant with respect to the orthogonal or unitary transformations, for the first and for the second class respectively. It follows (see, e.g., Porter 1965) from these two assumptions that the distribution of the matrix elements must be Gaussian, hence the names for the two classes of infinite random matrices: Gaussian orthogonal ensemble (GOE) and Gaussian unitary ensemble (GUE). Originally the results of the random matrix theories were meant to apply to sufficiently complex systems (many coupled degrees of freedom), for which a statistical approach is not only very natural but also the only feasible one. However, it has been one of the major advances in the non-linear dynamics of quantum systems to demonstrate that Hamiltonian systems with only a few freedoms and such that their classical counterparts have chaotic dynamics everywhere in phase space (ergodicity) generically display spectral fluctuations which are correctly described either by GOE or GUE statistics (Bohigas et al 1984, Seligman et al 1985, Pechukas 1984, Berry 1985, Yukawa 1985, Berry and Robnik 1986), depending on whether the Hamiltonian does or does not have antiunitary symmetry (Robnik and Berry 1986, Robnik 1986).

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These are two of three coherent classes each of which conforms to its own universal law of spectral fluctuations. The remaining class consists of those systems with integrable classical counterparts, and they have generically Poisson statistics irrespective of their symmetries (Berry and Tabor 1977). Recently Casati *et al* (1985) discovered some departures from exact Poisson statistics, but they still report evidence for the universality. For the discussion of the statistical significance of these and similar results see Feingold (1985) and Casati *et al* (1986).

One might add to this list a fourth class consisting of nearly integrable systems which do have some universal aspects of their spectral fluctuations which we discuss in this letter. Although this class consists of truly generic systems in the intermediate region of transition from integrability to chaos (Robnik 1984, Meyer *et al* 1984, Seligman *et al* 1984, Yukawa 1985, Ishikawa and Yukawa 1985), it is not coherent enough to display a complete universality in the spectral fluctuations. It is very important to keep in mind that these are systems whose classical counterparts are *not* ergodic but have mixed dynamics in the classical phase space in the sense of the KAM theorem. The transition from an integrable Hamiltonian by perturbing it is generally a smooth one (*not* a 'phase transition' of the spectral statistics which occurs for instance when an integrable Hamiltonian is made ergodic). This has been demonstrated numerically by Robnik (1984) and independently by Meyer *et al* (1984), Seligman *et al* (1984), Ishikawa and Yukawa (1985), Terasaka and Matsushita (1984), and by Seligman *et al* (1985) and Wintgen and Friedrich (1987).

The semiclassical theory of level spacings of such systems has been given by Berry and Robnik (1984), but the predicted P(S) cannot be correct for small S, because the assumption of statistical independence of level sequences supported by different regular and irregular regions in classical phase space is not strictly satisfied. More precisely, this approximation becomes particularly poor if the measure of the classically chaotic regions is so small that the corresponding irregular levels become widely spaced. This is in disagreement with the quantum theory which predicts that irregular levels occur in pairs, because it is the interaction between them which makes them irregular (see below).

Other suggestions for the description of P(S) are the ensembles of banded matrices of Seligman *et al* (1985), the well known Brody distribution (Brody *et al* 1981), and the theoretical considerations of Yukawa (1985) which extend the results of Pechukas (1983).

It is clear that a universal one-parameter family of distributions P(S) for the transition region does not exist. One reason is that there is no universality in the large scale of nearly integrable systems. For example, the geometry of regular and chaotic regions in the classical phase space of a nearly integrable system is certainly not universal. The *approach* to the integrable case for arbitrary generic perturbations can be universal, however, and this is the essential point of the present work.

Let us thus study the statistics of the energy levels of a perturbed Hamiltonian

$$H = H_0 + \varepsilon H_1 \tag{1}$$

where H_0 is an integrable Hamiltonian with N freedoms, $N \ge 2$, H_1 is the perturbation and ε is the perturbation parameter. The level spacings distribution P(S) is a function of ε and H_1 . For $\varepsilon = 0$ P(S) is the Poisson distribution $\exp(-S)$, and P(0) does not vanish. By switching on the perturbation this changes abruptly and we shall find that

$$P(S) = \text{constant} \times S/\varepsilon$$

(2)

where the constant is independent of ε . The linear regime is valid for $S \leq \varepsilon$.

One naive idea of studying P(S) for small ε might be to resort to the first-order quantum perturbation theory (degenerate theory for pairs of degenerate levels of H_0 , and non-degenerate theory for other levels). All levels are split and shifted linearly with ε , then nothing happens! Indeed, the first-order perturbation theory is unable to describe the interaction between the levels and represents merely simple kinematics of spectra such that all spectral statistics are invariant. Therefore the first-order perturbation theory would predict Poisson statistics for the KAM systems, which is certainly wrong. To reach any conclusions along this line of argument one really has to study the motion of levels as described by the complete set of the equations as given by Pechukas (1983) and Yukawa (1985), or one has to take into account at least the second-order (differential) corrections. In order to explain the behaviour of P(S) for small S it is sufficient to resort to the perturbational analysis of pairs of levels.

I now present two random matrix models. The first is as follows. For the perturbation problem (1) we consider a diagonal matrix with elements E_{10} and E_{20} with Poisson statistics, which is continuously perturbed to a GOE or GUE matrix by a linear superposition. The secular determinant of the total random matrix is thus written as

$$\det \begin{vmatrix} E - E_{10} - \varepsilon H_{11} & -\varepsilon H_{12} \\ -\varepsilon H_{21} & E - E_{20} - \varepsilon H_{22} \end{vmatrix} = 0.$$
(3)

The two eigenvalues E_2 and E_1 , $E_2 \ge E_1$ are

$$E_{2,1} = \frac{1}{2} \{ E_{10} + E_{20} + \varepsilon (H_{11} + H_{22}) \pm [(E_{20} + E_{10} + \varepsilon (H_{11} - H_{22}))^2 + 4\varepsilon^2 |H_{12}|^2]^{1/2} \}.$$
(4)

We shall assume without loss of generality that the equilibrium point of the levels is stationary, i.e. $E_1 + E_2 = 0$, so that

$$E_{20} = -E_{10} = E_0/2 \qquad \qquad H_{11} = -H_{22} \tag{5}$$

and the eigenvalues simplify

$$E_{2,1} = \pm \frac{1}{2} [(E_0 + 2\varepsilon H_{11})^2 + 4\varepsilon^2 |H_{12}|^2]^{1/2}.$$
 (6)

The level spacing S depends on H as follows:

$$S = E_2 - E_1 = [(E_0 + 2\varepsilon H_{11})^2 + 4\varepsilon^2 |H_{12}|^2]^{1/2}.$$
(7)

As already explained we assume the following distributions:

$$P(E_0) dE_0 = a^{-1} \exp(-E_0/a) dE_0$$
(8)

$$P(H_{11}) dH_{11} = (\sigma \sqrt{\pi})^{-1} \exp(-H_{11}^2 / \sigma^2) dH_{11}$$
(9)

$$P(|H_{12}|) \mathbf{d}|H_{12}| = \begin{cases} (2/\sigma\sqrt{\pi}) \exp(-|H_{12}|^2/\sigma^2) \mathbf{d}|H_{12}| & \text{GOE} \\ (2/\sigma^2) \exp(-|H_{12}|^2/\sigma^2)|H_{12}| \mathbf{d}|H_{12}| & \text{GUE} \end{cases}$$
(10)

Now we seek the level spacings distribution

$$P(S) = \int \delta(S - [(E_0 + 2\varepsilon H_{11})^2 + 4\varepsilon^2 |H_{12}|^2]^{1/2}) \times P(E_0) dE_0 P(H_{11}) dH_{11} P(|H_{12}|) d|H_{12}|.$$
(11)

Here $\delta(s)$ is the Dirac delta function. The normalisation

$$\int_0^\infty P(S) \, \mathrm{d}S = 1 \tag{12}$$

is obviously satisfied. Integration over E_0 yields

$$P_{\pm}(S) = \int \frac{S \exp((2\varepsilon/a)H_{11} \mp a^{-1})(S^2 - 4\varepsilon^2|H_{12}|^2)^{1/2})}{a(S^2 - 4\varepsilon^2|H_{12}|^2)^{1/2}} \times P(H_{11}) \, \mathrm{d}H_{11} \, P(|H_{12}|) \, \mathrm{d}|H_{12}|$$
(13)

where both branches of $E_0 = -2\varepsilon H_{11} \pm (S^2 - 4\varepsilon^2 |H_{12}|^2)^{1/2}$ have been taken into account. Next we integrate over H_{11} and introduce the new parameter

$$\lambda = \sigma \varepsilon \tag{14}$$

which leads to

$$P_{\pm}(S) = \frac{S}{2a^{2}\sqrt{\pi}} \frac{e^{\lambda^{2}}}{\lambda} \int_{0}^{S/a} dx \frac{e^{-((S/a)^{2} - x^{2})^{1/2}}}{((S/a)^{2} - x^{2})^{1/2}} e^{-x^{2}/4\lambda^{2}} \\ \times \left[1 \pm \Phi\left(\frac{1}{2\lambda} \left((S/a)^{2} - x^{2}\right)^{1/2}\right) \mp \lambda\right) \right] \{x\sqrt{\pi}/2\lambda\}$$
(15)

where $\Phi(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-z^2} dz$ is the error function, and

$$P(S) = P_{+}(S) + P_{-}(S).$$
(16)

In case of GOE perturbation the curly bracket in the integrand of (15) must be unity. The mean level spacing a of the Poisson distribution (8) will be chosen so that the mean level spacing of P(S) is unity, i.e.

$$\int_0^\infty P(S)S\,\mathrm{d}S = 1. \tag{17}$$

We thus end up with a one-parameter family of distributions, the only parameter being $\lambda = \varepsilon \sigma$. The final result can be cast in the form

$$P(S,\lambda) = \frac{1}{a} f\left(\frac{S}{a},\lambda\right)$$
(18)

where

$$f(t,\lambda) = f_+(t,\lambda) + f_-(t,\lambda)$$
(19)

and

$$f_{\pm}(t,\lambda) = \frac{t e^{\lambda^2}}{2\lambda\sqrt{\pi}} \int_0^{\pi/2} d\varphi \ e^{\pm t \cos\varphi} \ e^{-(t^2/4\lambda^2) \sin^2\varphi} \\ \times \left[1 \pm \Phi \left(\mp \lambda + \frac{t}{2\lambda} \cos\varphi \right) \right] \{ (t\sqrt{\pi}/2\lambda) \sin\varphi \}$$
(20)

and a is determined by (17), i.e.

$$a = a(\lambda) = \left(\int_0^\infty \mathrm{d}t \, t f(t, \lambda)\right)^{-1}.$$
(21)

In case of GOE perturbation the curly bracket in the integrand of (20) must be taken equal to unity.

It is easy to obtain the slope dP/dS at S=0. We evaluate (15) in the limit $\lambda \to 0$, and $S \to 0$, assuming $S \ll \lambda$. Of course, $a \to 1$ as $\lambda \to 0$. Therefore

$$\frac{dP}{dS}\Big|_{S=0} = \frac{\sqrt{\pi}}{2\lambda} \qquad \text{as} \quad \lambda \to 0 \qquad (\text{for GOE perturbation}) \qquad (22)$$

and

$$\left. \frac{d^2 P}{dS^2} \right|_{s=0} = \frac{1}{2\lambda^2} \qquad \text{as} \quad \lambda \to 0 \qquad \text{(for GUE perturbation)}. \tag{23}$$

We see that the slope dP/dS at S = 0 scales inversely proportional to the perturbation parameter λ if the perturbation matrix H_{ij} is real symmetric Gaussian random, e.g. corresponding to the case that H_1 in (1) has time reversal symmetry. If H_{ij} is complex Hermitian Gaussian random matrix, then the level repulsion is quadratic and the second derivative obeys the scaling given in (23). There is of course no guarantee that this model for $P(S, \lambda)$, as given by (18)-(21), is accurate for arbitrarily large S. But there is every reason to expect that it is very good at small S. (Bohigas (1987) has an alternative two-dimensional model of random matrices.)

The second random matrix model is as follows. For most systems in the transition region there exists a one-parameter family of curves which gives a surprisingly good, although not exact, overall fit to the histograms for P(S). This empirical fact suggests that there is a strongly pronounced clustering of the actual P(S) near a most probable curve. Therefore I propose the idea to determine (i) the most probable level spacings distribution $P_m(S, \sigma)$ using the maximum entropy considerations under the constraint that the second moment is prescribed

$$\langle S^2 \rangle = \int_0^\infty S^2 P(S) \, \mathrm{d}S = 1 + \sigma^2. \tag{24}$$

(The second moment goes monotonically from 2 in the case of a Poisson to $4/\pi$ in the case of a Wigner distribution.) (ii) Next we would like to calculate the probability distribution for the deviations of the actual P(S) from the most probable curve $P_m(S, \sigma)$ with the same value of σ . To do this one must introduce a metric in the space of curves P(S), e.g. the uniform metric

$$d_{\infty}(f,g) = \sup_{x} |f(x) - g(x)|$$

for the positive definite functions defined on the semiaxis $[0, \infty)$, or the L^2 metric

$$d_2(f,g) = \left(\int_0^\infty dx (f(x) - g(s))^2\right)^{1/2}.$$

Secondly, and more importantly, we must introduce some metric in the space of Hamiltonians, which is more difficult to do, as the functions H(q, p) defined on the 2N-dimensional phase space (q, p) are neither integrable (normalisable) nor bounded. But we could proceed by considering first a finite-dimensional approximation to the infinitely dimensional space of Hamiltonians, e.g. by considering polynomial Hamiltonians up to a degree M. This is a Euclidean space of as many dimensions as there are general non-vanishing coefficients, and the measure is simply the Euclidean (Lebesgue) measure. With these tools we can now define the probabilities for a given Hamiltonian to have the level spacings distribution P(S) at a distance $d_2(P, P_m)$ from the most probable one, $P_m(S, \sigma)$, with the same value of σ .

Here I shall consider only the first problem (i) by using the two-dimensional random matrices. Let us assume that the Hermitian matrix H is such that the equilibrium point of the two levels does not move, i.e. Tr $H = H_{11} + H_{22} = 0$. We shall denote $x = H_{11}$ and $y = |H_{12}|$. P(x, y) dx dy is the probability that $H_{11} \in [x, x + dx] \subseteq \mathbb{R}$ and $|H_{12}| \in [y, y + dy] \subseteq [0, \infty)$. The requirement of maximum entropy (minimum information) is

$$I = -\int_{-\infty}^{\infty} dx \int_{0}^{\infty} dy P(x, y) \ln P(x, y) = \text{extremum}$$
(25)

with the constraints

$$\langle S^2 \rangle = \int_{-\infty}^{\infty} dx \int_{0}^{\infty} dy (x^2 + y^2) P(x, y) = 1 + \sigma^2$$
 (26)

and

$$\langle S \rangle = \int_{-\infty}^{\infty} dx \int_{0}^{\infty} dy \, (x^2 + y^2)^{1/2} P(x, y) = 1$$
 (27)

and

$$\int_{-\infty}^{\infty} \mathrm{d}x \int_{0}^{\infty} \mathrm{d}y \, P(x, y) = 1.$$
⁽²⁸⁾

Using the method of Lagrange multipliers we have the functional

$$\Phi = -\int P \ln P \, dx \, dy + \lambda \left[\int P \, dx \, dy - 1 \right] + \mu \left[\int P(x^2 + y^2)^{1/2} \, dx \, dy - 1 \right] + \nu \left[\int dx \, dy \, P(x^2 + y^2) - 1 - \sigma^2 \right].$$
(29)

The first variation of Φ must vanish

$$\delta \Phi = -\int \delta P(\ln P + 1) \, dx \, dy + \lambda \int \delta P \, dx \, dy + \mu \int dx \, dy \, \delta P(x^2 + y^2)^{1/2} + \nu \int dx \, dy \, \delta P(x^2 + y^2) = 0.$$
(30)

We obtain the distribution function P(x, y),

$$P(x, y) = \exp(\lambda - 1 + \mu (x^2 + y^2)^{1/2} + \nu (x^2 + y^2)).$$
(31)

Recalling that the level spacings distribution is

$$P(S) = \int \delta(S - (x^2 + y^2)^{1/2}) P(x, y) \, dx \, dy$$
(32)

we obtain for the real symmetric case

$$P_m(S,\sigma) = 2\pi S \exp(-1 + \lambda + \mu S + \nu S^2)$$
(33)

and for the complex Hermitian case

$$P_m(S, \sigma) = 4\pi S^2 \exp(-1 + \lambda + \mu S + \nu S^2).$$
(34)

The parameters λ , μ , ν are determined by the constraints (26)-(28) and are thus functions of σ . We have obtained the most probable level spacings distribution

 $P_m(S, \sigma)$, which is functionally simply a product of Poisson and Wigner distributions, but of course with accommodated coefficients.

One can expect this distribution to give a good overall fit to the numerical histograms. The agreement is expected to be better than in the case of Brody distribution, especially as the linear level repulsion is now correctly described.

It is very difficult to get statistically reliable data for small level spacings for Hamiltonian dynamical systems (Robnik 1984, Meyer *et al* 1984, Seligman *et al* 1984, 1985, Terasaka and Matsushita 1984, Ishikawa and Yukawa 1985). Recently Wintgen and Friedrich (1987) have given high-quality numerical level spacings histograms for the hydrogen atom in strong magnetic field, which is a classically chaotic system above a certain critical energy (Robnik 1981, 1982). (Similar but independent results have been obtained by Delande (1986).) There seems to be general agreement that the observed depression of numerical P(S) at small S as compared with the semiclassical formulae of Berry and Robnik (1984) is statistically reliable, and the present work offers a quantitative theoretical explanation. It is remarkable that the Brody distribution, which behaves as a general power law at small S, provides a good overall fit to the histograms. But the power law behaviour at small S is tested only qualitatively so far in the sense that $P(S) \rightarrow 0$ as $S \rightarrow 0$, and with the improvement of data I expect confirmation of the linear level repulsion, with the universal scaling of the slope $dP/dS|_{S=0} \sim 1/\varepsilon$ as $\varepsilon \rightarrow 0$ (see equation (22)).

Another suggestion to obtain more accurate numerical data with great ease concerns the statistics of zeros of random functions. After all the energy levels of a matrix H are given by the zeros of the determinant

$$\Delta(E) = \det(H - EI) \tag{35}$$

which is a function of the real variable E. The idea is to consider a random function with Poisson distributed zeros, such as a product of trigonometric functions with randomly distributed frequencies and phases, and perturb it. (The perturbation must satisfy the condition that levels are neither destroyed nor created in pairs.) A preliminary numerical study of this model (Robnik 1987) confirms linear level repulsion and the scaling property (22) at small S. However, there still remain questions concerning the correspondence between the classes of random functions and the classes of random matrices.

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