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Quantum chaos and fluctuation properties of regular and irregular spectra

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Abstract. Fluctuation properties of the regular and irregular energy levels for the Hénon-Heiles Hamiltonian are examined. The spacing distributions and the calculated values of the Δ_3-statistic show that there is no difference in the short range correlation properties of these spectra. Remarkably, the Δ_3 values agree with the results of random matrix theory.

Keywords. Quantum chaos; fluctuation properties; regular spectra; irregular spectra; spectral signature; spacing distribution.

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1. Introduction

During the last few decades much progress has been made in understanding the (time) evolution of classical dynamical systems in phase space. In particular the studies have provided a classification scheme for dynamical systems based on how "regular" or "erratic" the motion is in phase space. As a result with increasing "irregularity" of motion, the systems are in turn labelled periodic, quasi-periodic, ergodic, mixing and chaotic (*K*-systems). An account of the earlier work on dynamical systems has been given by Khinchin (1949) and the more recent formal developments are described by Arnold and Avez (1968), Ornstein (1974), Arnold (1978) and Krylov (1978). Ford (1973) reviewed these developments in a more physical and intuitive way.

In this paper our interest is in "regular" and chaotic motion. It is therefore worth recalling that, for regular (periodic and quasi-periodic) motion the system remains confined to a restricted region (in general invariant tori) of the total available phase space. Also recall that for a chaotic system the motion is over the entire available phase space; it is extremely "erratic" and it shows random behaviour. This occurs in spite of the fact that the system is fully (all degrees of freedom) described and the equations of motion governing its evolution are completely deterministic. Although many aspects of "regular" and chaotic motion in classical systems are fairly well understood, the way in which they are expressed in the corresponding quantum systems are not always equally clear. (For reviews on "quantum chaos" see Zaslavsky 1981 and Bohigas and Giannoni 1984).

The purpose of this paper is to discuss one aspect of the "quantum chaos" problem that has been extensively studied in recent years. More precisely, we describe how "regular" and chaotic motion in a *bound* classical Hamiltonian system will be reflected in the discrete energy spectrum of the corresponding quantum system. The suggestions in this respect have included (i) examining properties of individual energy levels (Percival 1973) and, (ii) examining statistical (fluctuation) properties (Zaslavsky *et al* 1974; Zaslavsky 1977) of a whole set of levels.

In view of these suggestions, we summarize in § 2 results of earlier studies on spectral signatures which characterize quantum "regular" levels and quantum "irregular" (chaotic) levels. We also point out (what in our view is) an omission in all studies involving fluctuation properties. It turns out that this has a bearing on signatures which are a consequence of statistical properties of energy levels.

Section 3 contains a brief description of our calculations and results for the Hénon-Heiles (Hénon and Heiles 1964) model Hamiltonian. A summary and concluding remarks are presented in § 4.

2. Spectral signatures of regular and irregular levels

Following Percival's work (Percival 1973) there are several studies proposing signatures in the energy spectrum that will distinguish between the "regular" levels (classically quasi-periodic motion in phase space) and the "irregular" levels (classically chaotic motion). The basic conclusion is that "irregular" levels correspond to large second differences (Pomphrey 1974) or "avoided" crossings (Noid *et al* 1980) in energy. This is not the case for "regular" levels. Further, it appears (Pullen and Edmonds 1981) that large second differences correspond to "avoided" crossings.

Another suggestion (Zaslavsky *et al* 1974; Zaslavsky 1977) has been to study the distribution of energy spacings between neighbouring levels. It has been shown that, for the "regular" spectrum, this distribution (Berry and Tabor 1977) is of the Poisson form, and for the "irregular" spectrum (McDonald *et al* 1979; Casati *et al* 1980; Pechukas 1983; Bohigas *et al* 1984; Haller *et al* 1984; Seligman *et al* 1984) it is essentially of the Wigner form due to repulsion between neighbouring levels belonging to the same (exact) symmetry.

It should be stressed however that for any interacting system neighbouring levels belonging to the same exact symmetry will repel each other. Since for "irregular" levels there are no other quantum numbers (constants of motion) except energy, level repulsion is to be expected in their spacing distribution. For "regular" motion if the system (having f degrees of freedom) is integrable there are $(f-1)$ other constants of motion besides energy. Even if the system is not integrable, for regular motion it follows from Kolmogorov-Arnold-Moser (KAM) theorem (see *e.g.* Arnold and Avez 1968) that the phase space trajectory will be on a deformed torus. This suggests that in this case also there ought to be in addition to energy $(f-1)$ other constants of motion. It is not clear at all how to determine these additional constants of motion for a non-integrable system. All the same it is crucial that they (actually the corresponding quantum numbers) be considered when obtaining the fluctuation properties of "regular" levels. If this is not done, the resulting properties would very likely be a consequence of a superposition of uncorrelated level sequences. We believe that the Poisson spacing distribution for the "regular" levels is an artefact arising from just such a superposition of uncorrelated energy levels. This is because no other quantum numbers except energy are taken account of in the earlier studies.

3. Fluctuation properties of Hénon-Heiles Hamiltonian

Keeping in view these considerations, we determine in this section the fluctuation properties of the energy eigenvalues of the modified Hénon-Heiles (Hénon and Heiles 1964; Pullen and Edmonds 1981) Hamiltonian. The reason for choosing this Hamiltonian is that it has only two degrees of freedom, but more important has been the fact that in our knowledge it is the Hamiltonian which has been most extensively studied in connection with classical and quantum chaotic behaviour.

For this Hamiltonian, we have obtained the nearest neighbour spacing distribution and the Δ_3-statistic of Dyson and Mehta (1963). For evaluating these properties we have very closely followed the approach of Haq *et al* (1982). We would like to determine (i) if there is a difference between the fluctuation properties of the "regular" and the "irregular" spectrum, and (ii) how these properties compare with the prediction of random matrix theory.

As we shall see, we are able to provide unambiguous answers using both the spacing distribution and the Δ_3-statistic.

We briefly describe our calculations next. The model Hamiltonian (Pullen and Edmonds 1981) is

$$H = \tfrac{1}{2}\,(p_x^2 + p_y^2 + x^2 + y^2) + \alpha(x^2 y - 1/3\, y^3), \tag{1}$$

where α is the strength parameter. Note that the anharmonic term has a 3-fold symmetry (C_{3v} point group) (Pullen and Edmonds 1981). We have separately calculated the eigenvalues for each of the 3-irreducible representations (labelled A_1, A_2, E) for $\alpha = 0{\cdot}088$. This particular value was used by Pomphrey (1974) and Pullen and Edmonds (1981). The diagonalization procedure used (reducing to tridiagonal form followed by bisection) was the same that Pullen and Edmonds followed. The number of eigenvalues we obtain for each symmetry below the escape energy ($1/6\alpha^2 = 21{\cdot}52$) is shown in table 1. The convergence of the eigenvalues was good to four significant places when enlarging the basis space. For each symmetry we identified the "regular" and the "irregular" levels by considering table 2 of Pullen and Edmonds. It turns out then that most of the levels below $E = E_c$ ($E_c = 14{\cdot}5$–$17{\cdot}5$) belong to the "regular" spectrum and those with $E > E_c$ belong to the "irregular" spectrum. E_c is different for the three symmetries. We then find that out a total of 171 levels, 87 belong to the regular part. The remaining 84 levels characterize irregular levels.

The fluctuations (Porter 1965; Mehta 1967; Brody *et al* 1981) in levels are (by definition) departures from a smooth uniform spectrum. Since for our model H the

Table 1. Number of eigenvalues for $\alpha = 0{\cdot}088$ for each symmetry below the escape energy ($= 21{\cdot}52$).

Symmetry type	Number of eigenvalues
$A1$	50
$A2$	37
E	84
Total	171

level density is not a constant, it is essential to "unfold" (Brody *et al* 1981) the spectrum and map it to one with constant density. The mapping we have chosen is

$$F(E) = a + bE + cE^2. \tag{2}$$

This is a natural choice because the quadratic term is the distribution function (continuous approximation) for the unperturbed oscillator. The parameters a, b, c were determined separately for each symmetry by a best fit to the calculated energy levels.

We very briefly discuss next the basic definition and physical meaning of the spacing distribution $p(x)$ and the Δ_3-statistic. $p(x)\,dx$ is the probability for the spacing between two levels, with no levels lying between them, to take a value between x and dx. Note that x is measured in units of constant mean spacing and $\int_0^\infty p(x)\,dx = 1$. As described in detail elsewhere (Bohigas and Giannoni 1975) the expressions for Δ_3 can be reduced (for purposes of calculations) to

$$\Delta_3(\bar{n}) = \frac{N^2}{16} - \frac{1}{\bar{n}^2}\left(\sum_{i=1}^{N} E_i\right)^2 + \frac{3N}{2\bar{n}^2}\left(\sum_{i=1}^{N} E_i^2\right) - \frac{3}{\bar{n}^4}\left(\sum_{i=1}^{N} E_i^2\right)^2 + \frac{1}{\bar{n}}\sum_{i=1}^{N}(N-2i+1)\,E_i. \tag{3}$$

In (3) $\bar{n}$ denotes a fixed energy interval in units of (constant) mean spacing and N is the actual number of energy levels in this interval. The N levels have energies E_i ($i = 1, \ldots N$). Physically, $\Delta_3(\bar{n})$ provides a measure of departure of the exact eigenvalue distribution function (staircase curve) from a straight line. It should be recalled that (Dyson and Mehta 1963) for the gaussian orthogonal ensemble (GOE) of real symmetric matrices, the mean $\Delta_3(\bar{n})$ over the ensemble is known for $\bar{n} \to \infty$. For finite values of $\bar{n}$ it has been obtained by Bohigas *et al* (1983) using Monte-Carlo calculations.

The results of our calculations for $p(x)$ and Δ_3 are discussed next.

3.1 *Spacing distributions*

When $\alpha = 0$, the system (equation (1)) is integrable and one has only a "regular" spectrum. The energy levels (two-dimensional harmonic oscillator) are labelled by the total number of quanta n and "angular momentum" l, where $n = 0, 1, 2, \ldots$, and for a fixed n, $l = -n, -n+2, \ldots n-2, n$. Note that all levels for a fixed n are degenerate. Clearly, the spacing distribution of levels with a fixed l is a δ-function, which shows extreme level repulsion and rigidity. One would obtain a Poisson distribution if one superimposes many uncorrelated l-sequences.

When $\alpha \neq 0$, the system is not integrable and classically one has either regular motion (KAM regime) or chaotic motion in phase space. In the former case, the motion in phase space is confined to a two-dimensional surface (deformed torus). Hence, there ought to be another "local" constant of motion (quantum number) besides energy for the "regular" levels. This quantum number should be included in the analysis of fluctuation properties of the "regular" levels. If this is done, then since the system (in C_{3v} oscillator basis) is an interacting system, one would expect level repulsion for both "regular" and "irregular" levels. Our results (without the additional quantum number for "regular" levels) are shown in figure 1. They show level repulsion for both "regular" and "irregular" levels. These results are different from those of Haller *et al* (1984) and Seligman *et al* (1984) for the "regular" levels. One possibility for the difference is that

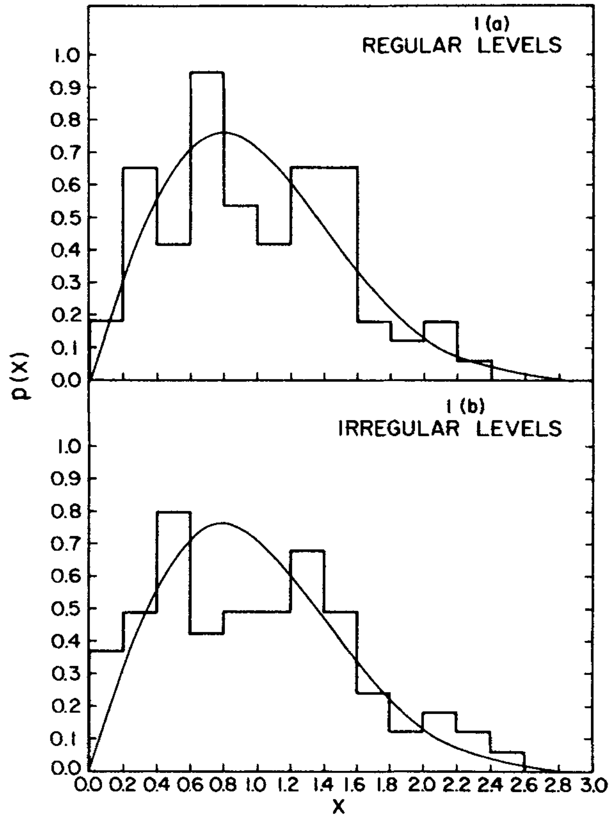

Figure 1. Spacing distributions for regular levels (figure 1a) and irregular levels (figure 1b). Histograms denote the calculated distributions for the Hénon-Heiles potential. Smooth curves denote the theoretical (Wigner) distribution $p(x) = \frac{\pi}{2} x \exp\left(-\frac{\pi}{4} x^2\right)$.

compared to our case, they may have a much larger number of uncorrelated sequences in their calculations.

3.2 Δ_3-*statistic*

We have evaluated $\bar{\Delta}_3(\bar{n})$ for $0 < \bar{n} \leqslant 10$ by separately taking the spectral average over the "regular" and the "irregular" levels belonging to each symmetry, and then taking the mean ("ensemble" average) over the three symmetry subspaces. The results are shown in table 2.

The result of $\bar{\Delta}_3(\bar{n})$ for $\bar{n} \leqslant 5$ clearly shows no discernible difference between the values for the "regular" and "irregular" spectrum. For values of $\bar{n} > 5$ the difference is $\approx 10\%$ but then the statistics are not as good as those for $\bar{n} < 5$. The agreement with the theoretical prediction of GOE is also very good for small $\bar{n}$ and deteriorates to 15–20% difference for larger $\bar{n}$. There is however no agreement between the calculated $\bar{\Delta}_3(\bar{n})$ and the Poisson distribution values.

In view of the numerical results, for $\bar{\Delta}_3$, it seems reasonable to conclude that whenever we have been able to carry out sharpest (best statistics) comparisons, there is

Table 2. Values of $\bar{\Delta}_3(\bar{n})$ for regular, irregular, GOE (from Bohigas *et al* 1983) and Poisson spectra ($\bar{\Delta}_3(\bar{n}) = \bar{n}/15$).

$\bar{n}$	$\Delta_3(\bar{n})$			
	regular	irregular	GOE	Poisson
0·25	0·0169	0·0169	0·0165	0·0167
0·50	0·0326	0·0334	0·0325	0·0333
0·75	0·0475	0·0489	0·0471	0·0500
1·0	0·0611	0·0630	0·0605	0·0667
2·0	0·1127	0·1147	0·1023	0·1333
3·0	0·1535	0·1506	0·1320	0·2000
4·0	0·1807	0·1770	0·1549	0·2667
5·0	0·1927	0·1953	0·1735	0·3333
6·0	0·1977	0·2100	0·1893	0·4000
7·0	0·2025	0·2204	0·2028	0·4667
8·0	0·2077	0·2267	0·2148	0·5333
9·0	0·2120	0·2340	0·2255	0·6000
10·0	0·2140	0·2379	0·2356	0·6667

no difference between the fluctuation properties of regular, irregular, and GOE spectra. Thus such fluctuation measures (statistic) are not likely to provide a signature for distinguishing between the "regular" and the "irregular" spectra. It is also remarkable that a system with just two degrees of freedom leads to fluctuation properties that are identical to GOE—essentially a parameter-free theory originally proposed for a system with a larger number of degrees of freedom.

4. Summary and concluding remarks

Our results show no significant difference in the fluctuation properties of regular, irregular and GOE spectra. As stated before, it is not clear why our results for "regular" spectra do not agree with those of Haller *et al* (1984) and Seligman *et al* (1984). While our statistics are small compared to theirs, it seems unlikely that our conclusions would be altered in a significant manner with improved statistics. For this purpose further calculations are currently in progress. The agreement between the results for "irregular" spectra and GOE is consistent with earlier results and seems to suggest (Bohigas *et al* 1984) universality in the behaviour of fluctuation properties—independent of the number of degrees of freedom.

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