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Fluctuations of quantum spectra and their semiclassical limit in the transition between order and chaos

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Abstract. We compare semiclassical and quantum mechanical (numerical) results for spectral statistics in the transition from order to chaos in the corresponding classical system. Scale invariant two-dimensional Hamiltonians are discussed and significant discrepancies are found only for level spacings smaller than one average spacing. For the semiclassical limit we use the result of Berry and Robnik for the nearest-neighbour spacing distribution and the extension of it to the Δ_3 statistic.

1. Introduction

During the last few years the implication of classical chaotic behaviour for the fluctuations of quantum spectra have been investigated from several points of view. Starting from early work (Berry and Tabor 1977, Berry 1983) there is increasing numerical evidence that strongly chaotic behaviour of the classical motion implies the spectral statistics of the Gaussian orthogonal ensemble (GOE) (Bohigas *et al* 1984, Seligman *et al* 1984), while ordered behaviour is associated with a random sequence of levels (the Poisson limit). The interpretation of the latter case is not completely unambiguous and requires further investigation (Seligman, Verbaarschot and Zirnbauer 1985 (henceforth referred to as SVZ), Casati and Chirikov 1984). Lately the transition between the two regions has received a considerable amount of attention. The numerical analysis of spectra in the transition region between order and chaos has been carried out by several groups (Haller *et al* 1984, Hirooka *et al* 1984, SVZ). Berry and Robnik (1984) have argued that in the semiclassical limit the eigenfunctions are localised in the ordered region of phase space or in one of the chaotic regions. In this limit they derived a closed formula for the nearest-neighbour spacing distribution.

In this paper we first review the argument of Berry and Robnik (1984) and show that the semiclassical limit of other spectral statistics such as the number variance and the Δ_3 statistic (Brody *et al* 1982) can readily be obtained following the same line of reasoning. Some problems of both a conceptual and a practical nature that may appear in this approach are discussed. We compare the semiclassical formulae with numerical results obtained elsewhere (SVZ). A discrepancy shows up for small level spacings. This was anticipated in previous work by Meyer *et al* (1984).

2. The semiclassical limit

We consider a two-dimensional chaotic system whose trajectories in phase space are characterised by ordered regions of total volume μ_1 and k disconnected chaotic regions of volumes μ_i, $i=2,\ldots,k$. Berry and Robnik (1984) argued that in the semiclassical limit the eigenstates of the system are localised within one of these regions. (In talking about phase space we may visualise these states in terms of their Wigner functions). When this assumption holds the spectra for different chaotic regions have to be superposed independently. For the ordered regions we expect a random spectrum and for the chaotic regions we expect a spectrum with GOE fluctuations. The average level density of each sequence is taken to be a constant proportional to the corresponding phase space fraction. Based on these assumptions Berry and Robnik (1984) evaluated the nearest-neighbour spacing distribution $P(S)$ and obtained

$$P(S)=\frac{\mathrm{d}^2}{\mathrm{d}S^2}\left[\exp(-\mu_1 S)\prod_{i=2}^{k}\operatorname{erfc}\left(\frac{\pi^{1/2}}{2}\mu_i S\right)\right] \tag{2.1}$$

where μ_i is the fraction of phase space volume corresponding to region i and S is the level spacing in units of the average spacing. Under the same assumptions we can obtain similar results for other quantities. For example the number variance $\Sigma^2(L)$ (i.e. the average variance of the number of states in an interval containing on average L levels) is additive (see also Pandey 1979). As a consequence we find

$$\Sigma^2(L)=\Sigma^2_{\mathrm{P}}(\mu_1 L)+\sum_{i=2}^{k}\Sigma^2_{\mathrm{GOE}}(\mu_i L), \tag{2.2}$$

where Σ^2_{P} and Σ^2_{GOE} are the Poisson and the GOE values for the number variance, respectively (see Brody *et al* 1982). Another statistic that essentially measures the stiffness of the spectrum is the Δ_3 statistic. In order to obtain it we have to normalise the spectrum by the local average level spacing $d(E)$ (i.e. the sequence $\{E_i\}$ is transformed in the sequence $\{E'_i\}$ by $E'_{i+1}=E'_i+[(E_{i+1}-E_i)/d(E_i)]$. For the levels E'_i in the interval $[\alpha,\alpha+L]$ Δ_3 is defined by

$$\Delta_3(\alpha,L)=L^{-1}\min_{A,B}\int_{\alpha}^{\alpha+L}\mathrm{d}x(N(x)-(Ax-B))^2 \tag{2.3}$$

where $N(x)$ is the integrated level density. ($N(x)$ is a staircase function jumping by one at each of the levels E'_i.) The minimalisation is over the parameters A and B. In this paper we use the ensemble average of $\Delta_3(\alpha,L)$ and denote it by $\bar{\Delta}_3(L)$. The argument α is omitted in $\bar{\Delta}_3(\mathrm{L})$ because this average does not depend on α. In the numerical calculations we do not have a statistical ensemble at our disposition and average instead the $\Delta_3(\alpha,L)$ over the spectrum. Also this quantity is denoted by $\bar{\Delta}_3(L)$. It has the advantage over the number variance that its variance is highly suppressed. This follows from the fact that it can be expressed as an average over the product of the number variance and a smooth function (Bohigas and Giannoni 1984)

$$\bar{\Delta}_3(L)=\frac{2}{L^4}\int_0^L\mathrm{d}r(L^3-2L^2r+r^3)\Sigma^2(r). \tag{2.4}$$

Therefore $\bar{\Delta}_3$ is also additive and we have

$$\bar{\Delta}_3(L)=\bar{\Delta}_{3\mathrm{P}}(\mu_1 L)+\sum_{i=2}^{k}\bar{\Delta}_{3\mathrm{GOE}}(\mu_i L), \tag{2.5}$$

where the subscripts have to be interpreted as in (2.2). Note that the argument L of $\bar{\Delta}_3(L)$ is equal to the *average* number of levels in a given interval, whereas the argument S of $P(S)$ is the spacing between two *neighbouring* levels measured in units of the average level spacing. As a consequence S and L have a different physical meaning (L is an average quantity whereas S is a 'stochastic variable').

In practice the evaluation of (2.1) and (2.5) has the problem that in two dimensions there may be many (usually infinitely many) different chaotic regions each of them occupying only a very small fraction μ_i of phase space. It may be very difficult to discriminate them from the regular orbits. Since the level density of each sequence of levels is proportional to μ_i, the semiclassical result for $\bar{\Delta}_3(L)$ will not change when we add the chaotic regions with $\mu_i < 1/L$ to the regular region μ_1. A similar result for the nearest-neighbour spacing distribution was found by Berry and Robnik (1984). They concluded that one has to distinguish the small chaotic regions from the regular ones only for large values of the level spacing. As an illustration of the aforementioned discussion and as a check of the consistency of (2.5) we consider the limit of an infinite number of chaotic regions with equal volumes. The value of $\bar{\Delta}_3(L)$ is given by

$$\bar{\Delta}_3(L) = \lim_{P\to\infty} P\bar{\Delta}_{3\mathrm{GOE}}\left(\frac{L}{P}\right) = \frac{L}{15} \tag{2.6}$$

thereby reproducing the Poisson limit. Here, and in the calculations of § 3 we have used the exact result for $\bar{\Delta}_{3\mathrm{GOE}}$ (see Bohigas and Giannoni 1984).

3. Comparison of numerical results and semiclassical formulae

In this section we discuss to what extent the semiclassical formulae agree with the numerical results available for the low lying part of the spectrum. As the semiclassical formulae depend sensitively on details of the structure of the classical orbits Berry and Robnik (1984) stressed the importance of using scale invariant systems. Otherwise the energy dependence of the classical motion will not allow a significant comparison.

The particular Hamiltonian we investigate is given by

$$H = \tfrac{1}{2}P_1^2 + \tfrac{1}{2}P_2^2 + a_1x_1^4 + a_2x^4 - a_{12}(x_1 - x_2)^4, \tag{3.1}$$

with $a_1 = 50/(0.8)^4$, $a_2 = 50/(1.2)^4$ and $a_{12} = 1.5$ or $a_{12} = 2.0$. The computation of the fractions of phase space covered by each of the chaotic regions is generally quite tedious. We use a Monte Carlo method. One hundred initial conditions are generated randomly according to the measure $\delta(E-H)\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}p_1\,\mathrm{d}p_2$. For each of these we compute the Lyapunov exponent following a method given by Benettin and Strelcyn (1974). In figure 1 we show a histogram of 100 exponents for the potential with $a_{12} = 1.5$. In this way we obtain a rough idea of which initial conditions belong to the same chaotic region. Two problems make this estimate insufficient. In the first place, several chaotic regions may have the same exponent and in the second place the computer time required for an accurate determination of the exponents is extremely long. Aside from the ordered region in figure 1 we can distinguish two disordered regions associated with the two peaks. The corresponding fractions of phase space are $\mu_1^a = 0.16$ (4), $\mu_2^a = 0.46$ (7) and $\mu_3^a = 0.38$ (6), respectively (we have given the error in the last digit in brackets). We use the upper index x of μ_i^x ($x = a, b, c$) to distinguish between the different ways the volumes have been obtained. In order to deal with the

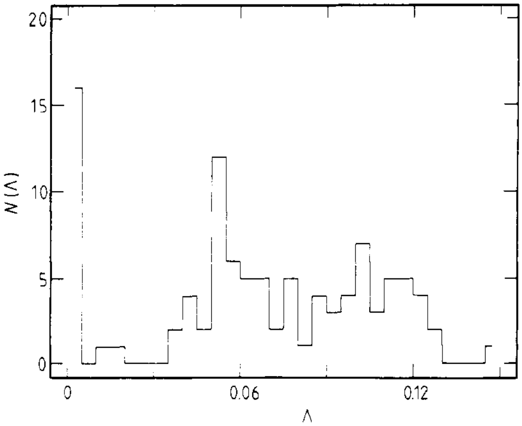

Figure 1. A histogram of the Lyapunov exponents Λ for the Hamiltonian given in (3.1) with $a_{12} = 1.5$. The bin size is equal to 0.005. From the figure we can derive an ordered region of phase space with volume fraction equal to 0.16 and two chaotic regions with fractions equal to 0.46 and 0.38.

problems mentioned above we have also made a Poincaré section for each of the initial conditions generated randomly. Using running times for the integration of the Hamilton equations that are large enough to give rise to several hundreds of section points we find in addition to the ordered region with volume $\mu_1^b = \mu_1^a = 0.16\ (4)$ three different chaotic regions. Their volumes have the values: $\mu_2^b = 0.48\ (7)$, $\mu_3^b = 0.14\ (4)$ and $\mu_4^b = 0.22\ (5)$. Increasing the running time for the Poincaré section by a factor of ten we find diffusion between the regions 2 and 3 but no diffusion to region 4 so that regions 2 and 3 merge into a new region 2. Now the fractions read as $\mu_1^c = 0.16\ (4)$, $\mu_2^c = 0.62\ (8)$ and $\mu_3^c = 0.22\ (5)$. We feel confident that this slow diffusion is not an artefact due to numerical inaccuracy.

Clearly the first method for calculating the chaotic volumes is less reliable but much more convenient because it does not involve any inspection of Poincaré sections.

In the last part of this section we compare the statistics obtained from an exact quantum mechanical calculation and their semiclassical limits with parameters as given above. The first 500 eigenvalues of the Schrödinger equation corresponding to the Hamiltonian equation (3.1) with $a_{12} = 1.5$ have been calculated using methods described in SVZ. The results for the nearest-neighbour spacing distribution $P(S)$ (histogram) and the $\bar{\Delta}_3(L)$ (dots) are plotted in figure 2. The dotted, full and broken curves respectively show the results of using the semiclassical formulae with the fractions μ_i^a, μ_i^b and μ_i^c, respectively. We first discuss the nearest-neighbour spacing distribution. At small S we find that none of the fractions gives adequate agreement. At larger values of S μ_i^b gives the best agreement but μ_i^a and μ_i^c are still fairly close. For the $\bar{\Delta}_3$ which mainly measures correlations for $L > 1$ the agreement obtained with μ_i^b for $L < 10$ is excellent but also μ_i^a and μ_i^c do not deviate much. The deviations at large L are already present in the integrable case. As we do not include them in the Poisson part of $\bar{\Delta}_3$ they can not be adjusted here. Treating all chaotic regions as a single one results in much larger deviations. Similar results have been found for $a_{12} = 2.0$. The naive method of using Lyapunov exponents yields for the chaotic volumina $\mu_2 = 0.46\ (7)$ and $\mu_3 = 0.45\ (7)$, while the volume of the ordered regions is found to be equal to

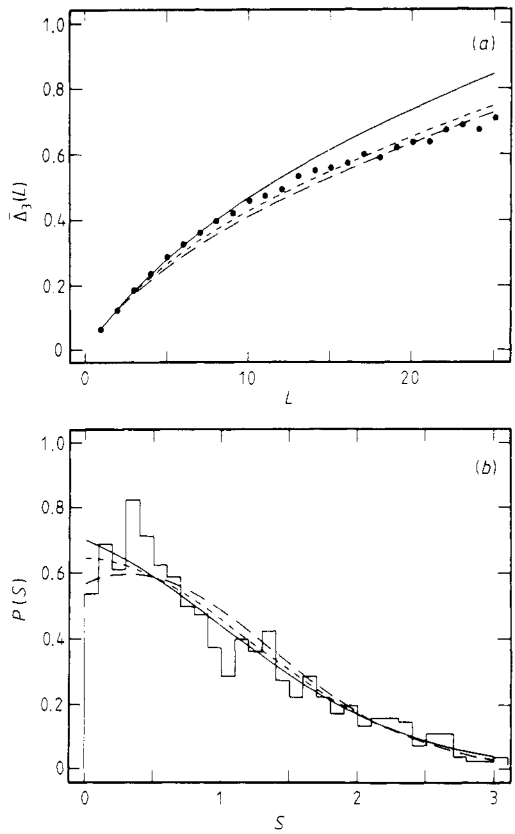

Figure 2. The $\bar{\Delta}_3$ statistic (a) and the nearest-neighbour spacing distribution $P(S)$ (b) for the Hamiltonian given in (3.1) with $a_{12} = 1.5$. The dots and the histogram have been obtained from an exact quantum mechanical calculation. The semiclassical results are depicted by the full curves, the dotted curves and the broken curves. They correspond to the partitionings of phase space (0.16, 0.48, 0.14, 0.22), (0.16, 0.46, 0.38) and (0.16, 0.62, 0.22), respectively. The first number in each sequence is the ordered fraction.

0.09 (3). Except for small values of S in the nearest-neighbour spacing distribution we find good agreement as is shown in figure 3.

Incidentally we want to remark that for $L < 50$ the $\bar{\Delta}_3(L)$ functions given by (2.5) can very well be fitted by the $\bar{\Delta}_3$ obtained from the random matrix model proposed in SVZ. This is not true for the short range part of the nearest-neighbour spacing distribution given by (2.1).

We can conclude that the agreement between the semiclassical formula for the nearest-neighbour spacing distribution and the quantum mechanical results for low-lying states deteriorates as S decreases. While this is not surprising, the good agreement for spacings greater than one mean level spacing is more of a surprise. Another unexpected result is that the agreement for the $\Delta_3(L)$ for $L < 10.0$ obtained with the fractioning μ_i^c is slightly worse than the agreement obtained with μ_i^b. (As already remarked above for larger values of L we cannot expect the semiclassical results to be correct.) However, this can easily be understood by realising that there is a big difference in time scales. At low energies the coupling between the regions that show

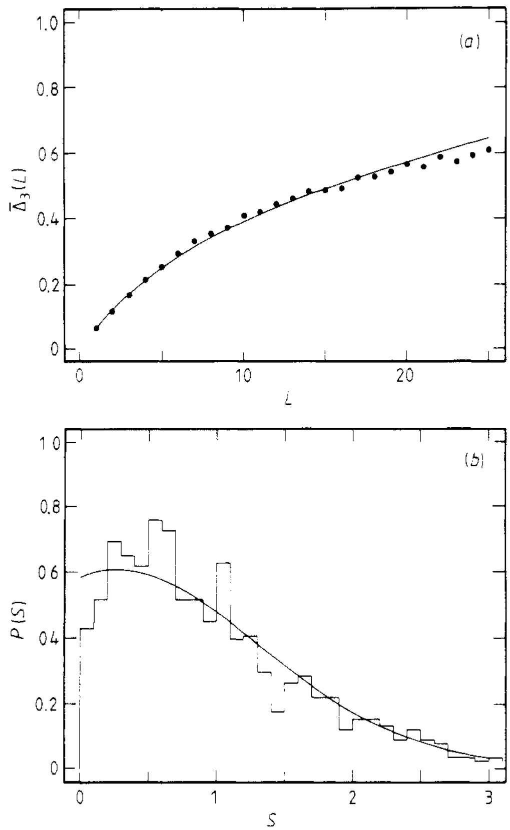

Figure 3. The $\bar{\Delta}_3$ statistic (a) and the nearest-neighbour spacing distribution (b) for the Hamiltonian given in (3.1) with $a_{12} = 2.0$. The dots and the histogram correspond to the exact quantum mechanical calculation. The semiclassical results given by the full line have been calculated with the partitioning (0.09, 0.45, 0.46) that has been obtained from an analysis of the distribution of the Lyapunov exponents. The first number in the sequence is the ordered volume fraction of phase space.

a long time diffusion becomes small and levels corresponding to the two different parts of the chaotic region will show only a weak level repulsion. This is not true at larger energies. Thus setting small diffusion coefficients equal to zero will give us a better approximation at low energies. Another improvement for the $\bar{\Delta}_3$ might be obtained by including the 'kink' (i.e. the additional stiffness at large L seen in the integrable system (SVZ and Casati and Chirkov 1984) in the ordered part of $\bar{\Delta}_3$.

Our present results complete those of Meyer *et al* (1984) who investigated a different two-dimensional system. These authors find that the parameters obtained by fitting the semiclassical formula for the nearest-neighbour spacing distribution (equation (2.1)) to the exact quantum mechanical results are in good agreement with those obtained from the classical equations of motion. Concerning their conclusions we want to make the following remarks.

(1) The bin size of 0.33 they choose to construct the histogram that displays their numerical results is too large to notice the discrepancies we found. This is particularly obvious once it is realised that quantum effects are most likely to show up for small values of the arguments of the spectral statistics.

(2) The system is not scaling and the classical properties are likely to change in the energy interval considered.

(3) The bin size may affect the values of the parameters which are obtained by fitting (2.1) to the exact quantum mechanical results. Indeed, the good agreement for large values of S is lost and no satisfactory agreement for small values of S is achieved for a smaller bin size.

To illustrate remarks (1) and (3) we tried to fit the results for $P(S)$ by one chaotic region of varying size. The quantum mechanical results and the semiclassical formula are shown in figure 4 for chaotic fractions $\mu_2=0.5$, $\mu_2=0.7$ and $\mu_2=0.9$. For a value of $\mu_2=0.7$ we would obtain a fit that looks acceptable at a bin size of 0.33. Yet at the present bin size it clearly shows insufficient repulsion for small values of S. Incidentally, the real value of the chaotic volume is 0.9. Note that fractioning of the chaotic region will always reduce the repulsion. At this point we want to mention the problem of comparing histograms to continuous curves. To improve the statistics one can increase the bin size but a point of diminishing returns will be reached soon because one only studies the average of a continuous function over an interval equal to the bin size.

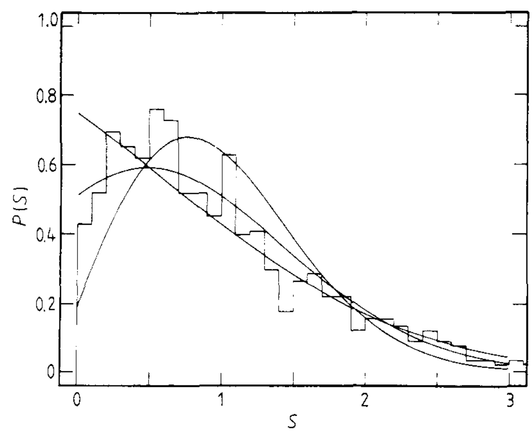

Figure 4. The exact quantum mechanical nearest-neighbour spacing distribution (histogram) for the Hamiltonian given in (3.1) with $a_{12}=2.0$. The full curves have been obtained from the semiclassical formula of Berry and Robnik (1984) with only one chaotic region. These curves which reach the value 0.75, 0.51 and 0.19 for $S=0.0$ correspond to the chaotic volume fractions 0.5, 0.7 and 0.9, respectively. The last number has been obtained from an analysis of the classical equations of motion.

4. Conclusions

The semiclassical result of Berry and Robnik (1984) for the nearest-neighbour spacing distribution can readily be extended to other quantities such as the number variance or the Δ_3 statistic. The question of these authors about how well the semiclassical formula represents the spectral statistics of the low-lying levels was investigated. Although we realise that our numerical evidence is limited we want to draw the following conclusions. At spacings less than one average level spacing the quantum effects produce quite a different nearest-neighbour spacing distribution. For larger values of S this distribution is well represented. The agreement improves if weakly connected chaotic regions are treated separately. The $\bar{\Delta}_3(L)$ statistic is an insensitive quantity for small values of its argument and therefore does not feel the aforementioned quantum effects. For not too large values of L it is very well described by the semiclassical formula. The deviations occurring at large values of L are generic to the low-lying levels of two-dimensional systems and might be eliminated by including them in the $\bar{\Delta}_3$ of the ordered part. The agreement between the quantum result and the semiclassical formula found by Meyer *et al* (1984) was shown to be insufficient to substantiate the validity of the semiclassical limit of the statistics for low-lying states. The results we found are in keeping with the fact that for low-lying states the transition from Poisson to GOE spectral statistics can be described by a one-parameter family of curves. In two dimensions the semiclassical laws generically depend on more than one parameter, so that extension of these to the low-lying part of the spectrum was not to be expected. On the other hand the agreement at intermediate spacings allows us to fix the free parameter in the universal transition. This could for example be the parameter of the random matrix model proposed by Zirnbauer and ourselves (Seligman *et al* 1984 and SVZ). Finally the observation that different regions connected with very small coupling act as if they were separate in the quantum limit, is of great interest for higher dimensions. In the presence of Arnold diffusion we expect only one chaotic region. On the other hand the diffusion coefficients between certain regions may be very small and the effect on the fluctuations of the low-lying part of the spectra is not immediately clear. However, the basic argument tells us that in this case only one chaotic region exists. Therefore, in the semiclassical limit the eigenvalue fluctuations during the transition between order and chaos depend only on the fraction of the total volume of phase space that is chaotic. As a function of this parameter we obtain a universal transition law given by the semiclassical formulae.

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