Quantum Chaos: Spectra and States

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I: Introduction

The most interesting thing about quantum chaos is that it does not exist. The second most interesting point is the question, why people are interested in this subject anyway. The last question is why I was invited to talk about this subject at a group theory meeting. Let me start with the last point: symmetry and groups enter the modeling of our problem in a crucial but well-known way. Actually excess of symmetry is indeed a problem when studying states,due to the basis dependence encountered. So I shall dwell a little more than usual on these questions. Nevertheless I believe that any important role of group theory in this field lies in the future.

The second point will be the center of this talk and we shall return to it at the end of this introduction.

Let us thus dwell briefly on the first point: in the present context we shall associate chaos with the properties of a Kolmogorov (K-) system, i.e. ergodicity and exponential divergence of trajectories. We also wish the quantization of our problem to be unique. Thus we focus on bounded hamiltonian systems with no ordering problem affecting quantisation. Two such systems are known analytically to be K-systems: Sinai's billiard and the stadion. In both cases we consider motion of a point particle in two dimensions. In the first case the particle is scattered by a disc and moves on a torus or equivalently with periodic boundary conditions in a rectangle. In the second case, external walls given by two semi-circles conected by parallel straight lines limit the domain. In both cases the corresponding problem in quantum mechanics may be set up straightforwardly by a hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) + V(q_1, q_2) \tag{1}$$

where $V = \infty$ inside the disc or outside the walls respectively. All problems asociated with such Hamiltonians , where the potential goes to infinity for large distances from the origin or with periodic boundary conditions have discrete spectra. This implies a countable number of frequencies and thus a quasi-periodic behaviour. This is not surprising as clearly the Schrödinger equation asociated to such Hamiltonians is linear.

How can then classical mechanics result as a limit of quantum mechanics for chaotic systems that have continuous spectra? Actually it cannot in any straightforward way! On one hand we have Ehrenfest's theorem about the classical behaviour of the center of mass of a wave packet. This certainly still holds, but it is not enough to define the behaviour of a point particle. For this we need the additional observation of Max Born that a macroscopic packet will be stable for a time of the order of the age of the universe. Yet it is well-known that this is not true for systems near classically unstable orbits such as bifurcation points.

For example a sequence of ideal (frictionless) billiard balls that are touching along a straight line will lead to a rapidly decaying packet for the last ball under impact on the first one. (W. Känzig, private communication). Similarly a stiff pendulum of massless suport and macroscopic length and point mass will produce a rapidly dispersing wave packet if released at the unstable eqilibrium point at the top with zero speed (E. Heller, private comunication).

Thus the transition from quantum to classical mechanics is quite non-triuial in the case of chaotic systems. The solution of the physical problem implied must be referred to the "measurement crowd"; personally I like the idea of coupling to an infinite number of degrees of freedom.

The problem we really want to deal with is a conceptually simpler one: what signs do we find in quantum mechanics if the corresponding classical systems undergoes a transition from order to chaos? Most sucessful work including our own was concentrated on spectra; these are basis invariant and thus very adequate for general studies. Some work has also been done on functions among wich Heller's is the most prominent[1]. We shall briefly review some of this work in the next section, in order to proceed then to a search of some invariant characteristics of functions.

In order to be basis independent we shall analyze random vectors; unfortunately a random choice implies the same orthogonal (or unitary) invariance that characterizes the eigenfunctions for the gaussian orthogonal (or gaussian unitary) ensemble, which turn out to be characteristic for the universal properties of chaotic systems. This "excess of symmetry" complicates the matter but we shall find that we can obtain non-trivial results by studying correlations in first order in $1/N$.

II: Spectral statistics

As mentioned above, the most successful work concerns spectra and in particular the field of spectral statistics. Clearly the density of levels is irrelevant as it is very well represented bei Weyl's formula,i.e. by the corresponding volume of phase space plus some surface and curvature correction terms that are principally important in billiards. Berry[2] conjectured early a close relation between the spectral statistics well-known in nuclear physics and the fluctuations of spectra in chaotic billiards. This connection was later confirmed by Bohigas *et al.*[3] To understand this clearly let me briefly define the Gaussian Orthogonal Ensemble (GOE). It is the ensemble of all real symmetric matrices, such that the entire ensemble is invariant under orthogonal transformations. We add the condition that each element be gaussian distributed around zero. We then find that the width for the distributions of all off-diagonal elements must be equal and differ from the ones for diagonal elements by a factor of two[4]. Balian[5] has shown that this definition may actually be derived from a minimum entropy requirement. Spectral statistics of these ensembles have been studied extensively, and we show in Fig. 1 the two most common statistics of fluctuations for the GOE, for nuclei, for the Sinai billiard and for random sequences[6]. These are obtained after unfolding the spectra with respect to spectral density, and normalizing the average spacing between levels to one. The nearest neighbour spacing distribution gives a histogram of the number of spacings $P(s)$ encountered around s in an interval usually chosen as $1/10$ of the average level spacing and then divided by the number of spacings. The variance $\Sigma_2(L)$ of the number of levels in an interval of length L, is a common measure,that depends only on the two-point function. $\Delta_3(L)$ is a smoothed version thereof.

Note that this applies under the hypothesis that the Hamiltonian can always be taken to be a real matrix. This property is connected to invariance under time-reversal. Indeed, if this invariance is broken, say by means of a sufficiently strong magnetic field, the spectral statistics are significantly modified. This is shown in Fig. 2, where the nearest-neighbour spacing distribution as well as the $\Delta_3(L)$ statistic are shown for an anharmonic oscillator with a potential of order six in an appropriate magnetic field[7]. It is seen that they differ from the GOE predictions, but are in good agreement with the GUE (Gaussian Unitary Ensemble) which is the counterpart of the GOE for hermitian matrices.

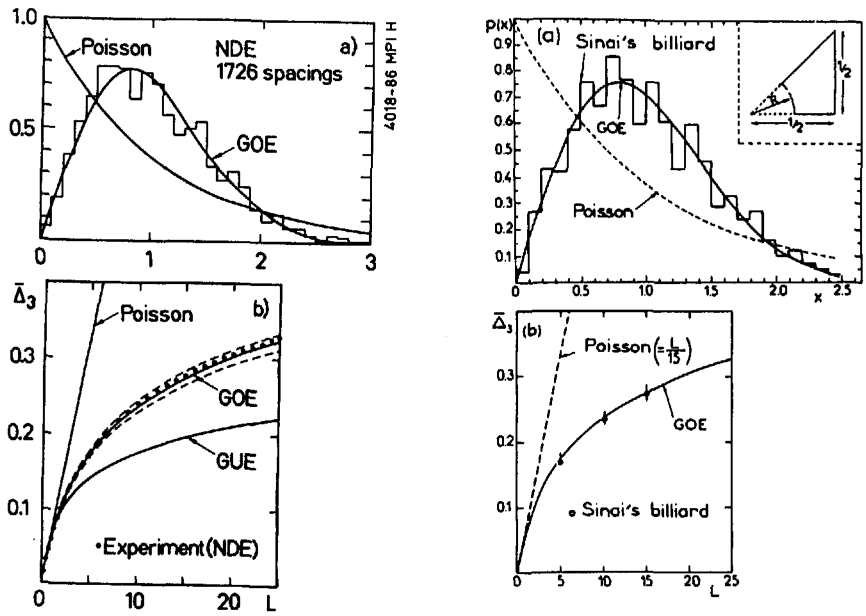

Fig. 1: $\Delta_3(L)$ and the nearest-neighbour spacing distribution $P(S)$ for the GOE, for the Sinai billiard, for nuclei and for random seqences

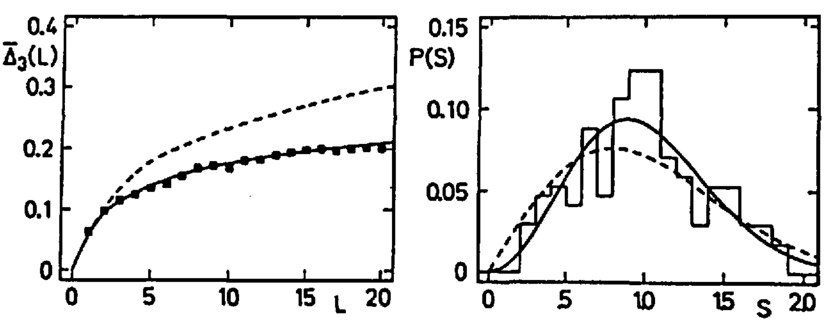

Fig. 2: $\Delta_3(L)$ and the nearest-neighbour spacing distribution for the eigenvalues of an anharmonic oscillator of degree six in a strong inhomogeneous magnetic field. Due to the breaking of time-reversal symmetry there is a clear disagreement with the predictions of the GOE, whereas there is good agreement with the GUE.

Other ensembles of symmetric hamiltonians have been treated numerically. Among them we will mention band matrices[8] as we shall use them in the next section. Results for a sharp or smooth cutoff have been found equivalent as long as the cutoff was faster then an exponential. We shall use a gaussian cutoff and we define the matrixelements of a band ensemble by

$$m_{ij} = g_{ij} \exp\left(-\left(\frac{i-j}{\sigma}\right)^2\right) \tag{2}$$

where g_{ij} are elements of a GOE matrix. To describe the transition from a Poisson to a GOE spectrum, one can either use these matrices or an ensemble of random diagonal matrices perturbed by a GOE (Porter–Rosenzweig model[9]). This last is formally defined as follows:

$$m_{ij} = g_{ij}(1 + \alpha\delta_{ij}) \tag{3}$$

Fig. 3 shows such a transition for a quartic oscillator and band matrices. The band width σ was fixed such as to fit the low end of Δ_3 [8]. The deviation of $\Delta_3(L)$ for large L is a saturation effect related to the existence of a shortest periodic orbit, and this "kink" will move to ever larger distances as we increase the energy and/or the dimensionality of the system[10]. An interpretation of the results in terms of classically chaotic and ordered regions seems to be adequate in the classical limit[11]. Deviations will always occur at short distances in the spectrum, and therefore models based on these interpretations give good results at long range in the spectrum[8]. Recent calculations by Bohigas *et al.*[12] show very nicely to what extent this picture is valid.

III: States—What we Know and What we Don't

It is clear that the situation must be more complicated if we want to consider states. The problem is that they depend on the basis one choses. For semi-classical consideration a phase space representation is desirable. Wigner functions are the logical choice, but they to chaos as well as for a sequence of band matrices with increasing band width.

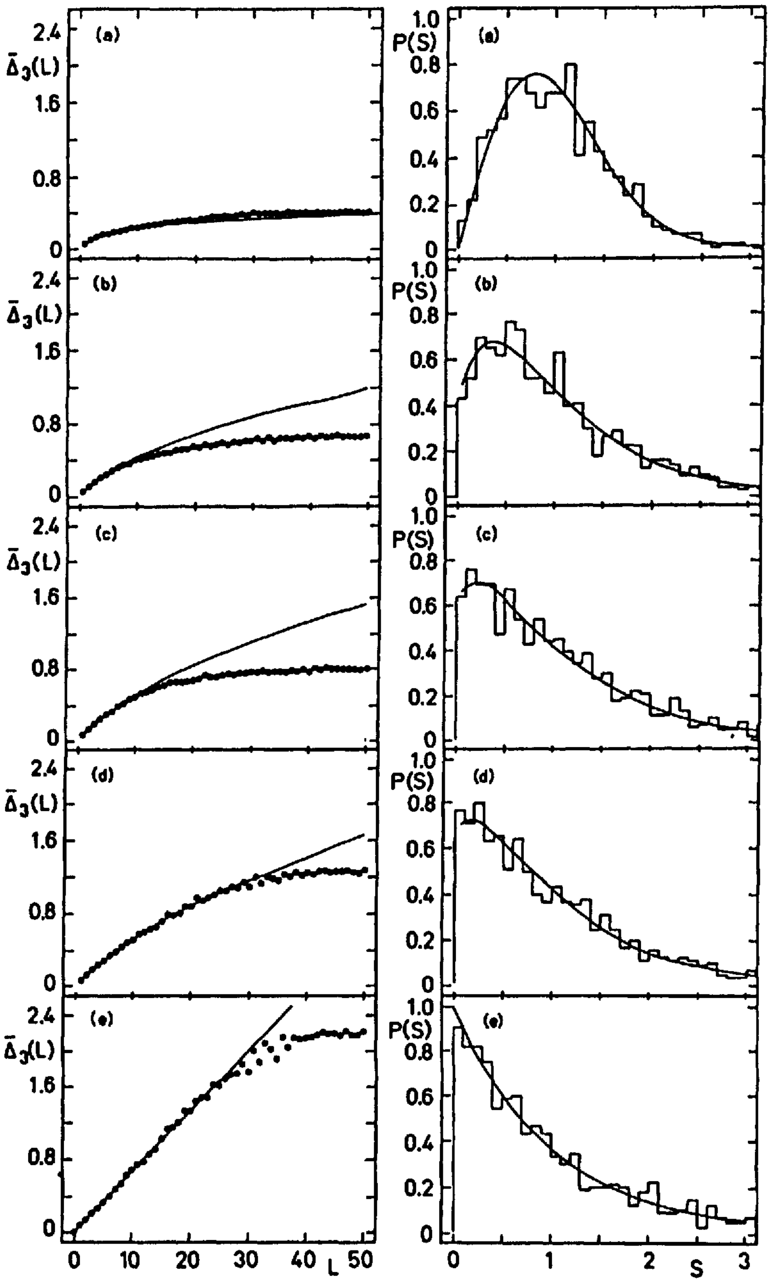

Fig. 3: $\Delta_3(L)$ for a sequence of quartic oscillators displaying a transition from order

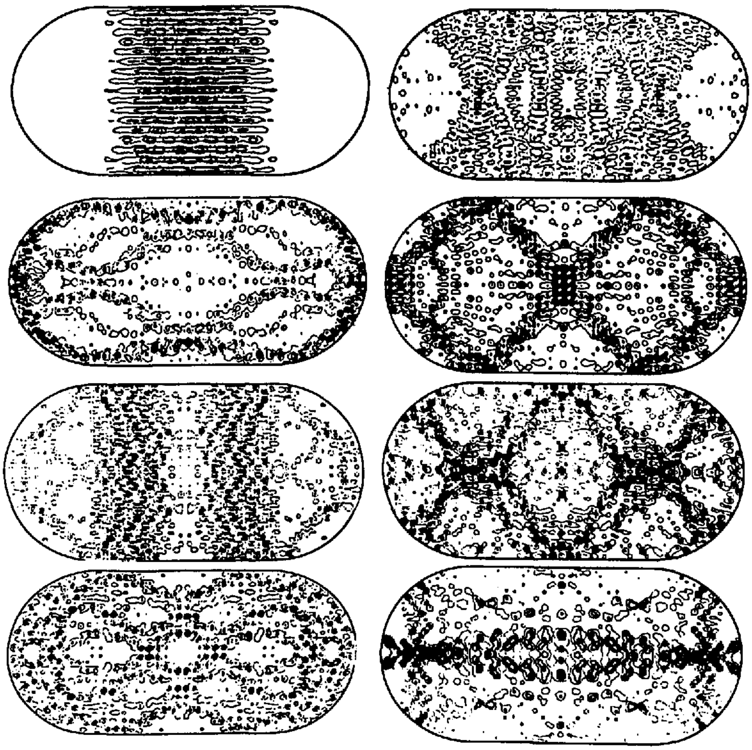

Fig. 4: Eigenstates of the stadium billiard. Note the concentration of the wave function along unstable periodic orbits.

are not always simple to handle or to interpret. Husimi functions are an often chosen alternative, but their interpretation is at best difficult and more likely wrong if the viewer is not very acustumed to their use. For two-dimensional billiards the problem is less serious because a representation in configuration space may readily be interpreted in phase space, as the absolute value of the momentum is fixed and only its angle is free. Berry originally conjectured gaussian noise as the result of chaos, but Heller showed the existence of scars, i.e. of concentrations of certain functions along one or several unstable periodic orbits[1]. In Fig. 4 we show Heller's results for the stadion. Semiclassical theory explains these facts partially[1] but it remains unclear why some orbits show scars while others do not.

Thus the states are not likely to be random but it is not easy in general to see the effect if we don't know the classical solutions; furthermore we lack a simple and basis-independent way to measure departures from randomness that may result from scars or unbroken tori or even other reasons as yet unknown.

We first of all shall try to see whatever may be the relevant properties in the framework of random matrix models. These are not expected to display scars and thus hopefully give the universal part of the transitional behaviour between order and chaos.

For this purpose we shall study the time evolution of states. We choose two random states $|a>$ and $|b>$ and consider the time evolution $|a(t)>= \exp(iHt)|a>$. Now we consider the quotient

$$Q = \frac{|<a|a(t)>|^2}{|<b|a(t)>|^2} \tag{4}$$

For short times Q will depend sensitively on the energies E_i. But, as $t \to \infty$, we find

$$Q_\infty = \frac{\sum_i |a_i|^4}{\sum_i |a_i|^2 |b_i|^2} \tag{5}$$

where a_i and b_i are the amplitudes of the expansion of $|a>$ and $|b>$ in terms of the eigenfunctions of the hamiltonian H. Q_∞ clearly depends only on the functions and it is thus interesting to see what averages over ensembles of hamiltonians we can obtain. The ensemble average of the numerator and of the denominator have been calculated separately by Ullah and Porter[13] for the GOE and for $<a|b>= 0$. The components a_i and b_i are then matrix elements of the orthogonal transformation between some arbitrary basis in which $|a>$ and $|b>$ are basis vectors and the basis in which H is diagonal. For a GOE the ensemble average will be an integration over the orthogonal group. This gives the same result for each term in the numerator and in the denominator. When forming the quotient the dependence on the size of the matrices cancels and we find for the quotient of the averages $Q'_\infty = 3$. For infinite dimensions it can also be shown that the expectation value of the quotient $\overline{Q}_\infty$ for a GOE is 3 but in this case corrections for finite dimensions exist and are known numerically to first order in $1/N$. If we omit the condition $< a|b >= 0$, they are of order $1/N^2$.

Things thus look fine. This quotient seems to carry a clear signature to show whether we have a GOE or not. Unfortunately this is not true because we have not yet specified how we plan to choose our arbitrary orthogonal pair $|a>$, $|b>$ and the only consistent way to choose this pair is to assume equal population on an N-sphere of states. Thus if we perform an ensemble average over all randomly chosen pairs $|a>$, $|b>$ we again find an integration over the orthogonal group and thus exactly the same result for any nondegenerate hamiltonian as for a GOE with a fixed pair of states.

We may decide to choose a fixed pair of vectors. Obviously there is no such thing as a random vector, but we can try to choose a typical one from a given ensemble. At least for large N that should make some sense. We must then take into account the ergodic properties of the ensemble[4], i.e. that an ensemble average will agree with a spectral average for almost all states. This means that we can choose the components a_i and b_i as random sequences subject only to the constraint of normalization and drawn from a gaussian distribution that becomes narrower as the dimension increases. The normalization is then a $1/N$ effect and we see that even for a fixed but typical pair $|a>$, $|b>$ we will find $Q_\infty = 3$ because the summation in the numerator and denominator simulate an ensemble average. In other words, we may say that a central limit theorem is responsible for this value of Q_∞. Indeed this quotient of three appears repeatedly in numerical studies (e.g. Heller, private communication) and thus seems to have no very relevant meaning. Excess of symmetry kills our goose.

Yet not all is lost. The arguments we gave depend crucially on the dimension of our space going to infinity. For the total Hilbert space this will generally be correct, but we may do our sampling on some restricted subspace. Actually this is more likely for any experimental situation. Typically we may be sampling only a given energy region, i.e. our sampling could be random on some subspace. We shall return to practical implications of

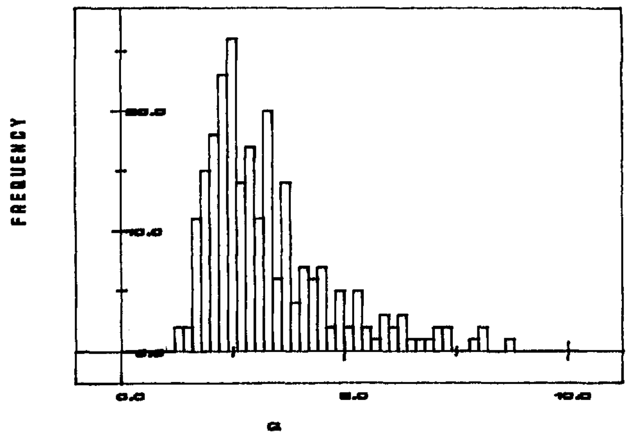

Fig. 5: The distribution of values of Q_∞ for a GOE for a given vector pair. The dimension N of the Hilbert space is equal to forty.

this approach in the conclusions. As far as modeling is concerned, it implies the use of ensembles of finite matrices.

To investigate the potential of such an approach we used the ensemble of band matrices and the Porter–Rosenzweig model both described above. Due to the central limit theorem mentioned above, it is clear that the width of the distribution of the quotient Q_∞ goes to zero as the dimension of the matrices goes to infinity, but for finite dimensions we obtain a finite width that decreases as $1/\sqrt{N}$. We shall now study how the individual values of Q_∞ behave if for a fixed pair of vectors we consider the ensemble of hamiltonians. We study the distribution of the quotients and the variance of this distribution.

Clearly for a diagonal ensemble of Hamiltonians this variance is zero for any N. For a GOE it is asymptotically zero, but it goes to zero rather slowly, namely as $const. \cdot N^{-1/2}$; the value of the constant is not available, as quotients are difficult to handle. We could have considered numerator and denominator separately, but for the transition models analytic results are not available in any case and thus we preferred to go all the way numerically.

Some figures will illustrate the points we have made. In Fig. 5 and Fig. 6 we show probability distribution functions of Q_∞ as the Hamiltonian is varied, for various choices of

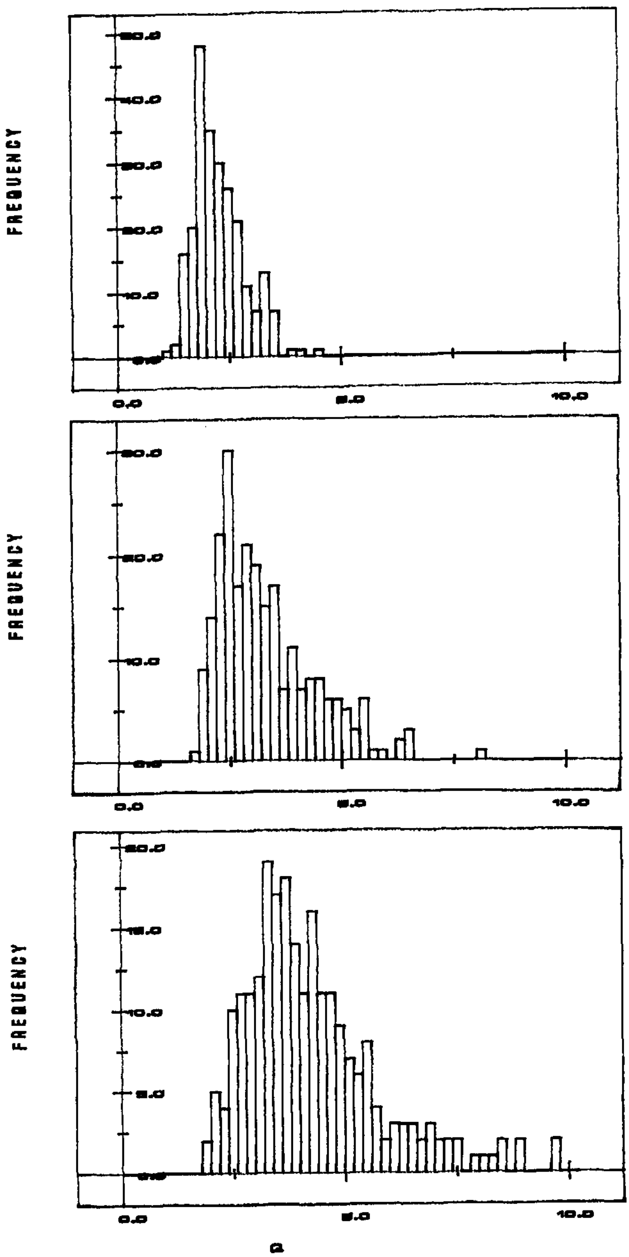

Fig. 6: Distribution of Q_∞ for three distinct vector pairs in a band matrix model with σ equal to one. Note that the distribution varies significantly depending upon the vector pair. The dimension N of the space is equal to forty.

vectors $|a>$ and $|b>$. In Fig. (5), we are showing the case of a GOE. In this case it is clearly a matter of indifference which vectors we choose. The data are for dimension N equal to 40. It is seen that the variance is still quite significant, i.e. the constant mentioned above is fairly large. Note that its average is three, as expected. On the other hand, Fig. (6a,b,c) show the case of a band matrix with $\sigma = 1$ and $N = 40$. The distributions are shown for three different choices of the vectors $|a>$ and $|b>$. These depend quite strongly on the pair of vectors chosen. The variance of the distribution function for a given pair is empirically found to be well correlated with the mean of the distribution function. In tables 1 and 2, this connection is indicated for the case of the band matrix model and of the Porter–Rosenzweig model respectively. Fig. (6a,b) show cases where the variance is smaller than in the GOE. This need not always be the case, however. In particular, the variance of distributions with exceptionally high mean may be larger than the GOE counterpart. Nevertheless, there is no possibility of confusion, since the average and the shape will be altogether different from the GOE case. Such a case is shown in Fig. (6c). For yet smaller values of σ, the variance would show a tendency to decrease and the average would vary over a broader range. These findings have indeed been confirmed, both for the band matrix and the Porter–Rosenzweig models.

IV: Conclusions

The spectral properties of quantum systems the classical analoga of which are in a transition from order to chaos are quite well understood. The surprising conclusion that classical order is associated to random spectra, while chaos implies small fluctuations is almost universally accepted. The two deviations, namely the harmonic oscillator and the saturatioun effect leading to long-range stiffness are both well understood. On the other hand, the discussion of the properties of wave functions is still in its beginnings. The subject of scars

Table 1

N	σ	Average	Variance
80	2	2.466	0.183
		2.561	0.210
		3.005	0.273
		3.620	0.440
		3.743	0.573
		4.154	0.581
40	1.	2.187	0.172
		2.692	0.455
		3.175	0.756
		3.758	0.609
		4.415	1.660
		5.027	1.510

Table 1: This gives the average and the variance of the distribution of Q_∞ for various choices of vectors for the band matrix model with width σ. The correlation between average and variance is apparent.

has called considerable attention in the last years, and we have seen some outstanding features of this kind. In the last section we presented a new approach to describe differences between functions associated with Poisson, GOE and intermediate ensembles.

We have seen that for finite matrix ensembles the wave functions show very clear and basis independent signature of order and chaos i.e. for the transition from Poisson to GOE-like behaviour. This behaviour does not depend on the transition model we choose and can thus be assumed to be universal, i.e. valid for a wide class of transition models.

Table 2

N	α	Average	Variance
40	.01	2.258	0.206
		2.497	0.243
		3.211	0.491
		3.620	0.741
		4.499	0.759

Table 2: This gives the average and the variance of the distribution of Q_∞ for various choices of vectors for the Porter–Rosenzweig model with parameter α.

The problem is how to apply this in the analysis of numerical or actual experiments. In the classical limit the method is useless as we would have large numbers of states involved. This does not imply—fortunately—that it may not be used way up in the spectrum as long as we restrict ourselves to a small number of states. The logical way seems to be to form a wave packet or some other superposition of eigenstates that cover a limited range of energy and to shift it over the energy range we have experimentally or numerically available. This sounds quite satisfactory if we consider the assumed ergodicity of our problems but we must keep in mind that we really change our state as we move up in energy; thus we are not doing exactly the same thing as in the ensemble treated in section III. Nevertheless we believe it should be tried, but we need scale invariant systems or at least systems that do not significantly change over the energy range under consideration.

As far as the connection to group theory is concerned, we have seen that the invariance properties of the ensemble we wish to analyze and of the space in which we perform our numerical experiments are closely related and thus make the detection of the former very difficult. A deeper group-theoretical background of the transition from order to chaos resides in the structure of phase space in the two cases. For chaotic systems time evolution for almost all points is given by the translation group along the infinite chaotic orbit, while for integrable systems a direct product of $O(2)$ groups characterizes the motion. An appropriate deformation might shed some light into the problem.

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