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# Selected topics on "Quantum Chaos"

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This talk will be a brief survey of a new ( 10 years old), inter-disciplinary area of research. Our review will be by necessity simplified and incomplete, but we shall give reference to many recent review articles (a very recent one being [17]).

By "quantum chaos" we mean the *problem* of understanding how the well understood features of complexity in a *classical* dynamical system (ergodicity, mixing, hyperbolicity, chaotic or stochastic behaviour of trajectories) manifest themselves when the same system is governed by *quantum mechanics*, e.g. because it has atomic size. - We have been studying this problem in collaboration with N.L. BALAZS (Stony Brook, USA) -.

Most realistic systems on the atomic scale ( nuclei, atoms, molecules) are indeed complex as classical systems, and their quantal equations of motion are also intractable. The potential of applications of research in this field is therefore enormous in all areas of quantum physics and chemistry, and for mathematical analysis as well.

Given that our theoretical understanding of the subject is still rather limited, such realistic systems are too difficult to study, because they exhibit complexity already at the *kinematical* level, due to their large number of coupled degrees of freedom. It is remarkable however, that *simple* classical systems with *very few* degrees of freedom can be found where the *dynamics* imposes a chaotic behaviour upon the *trajectories*.

Although such sytems are more abstract constructions seemingly unrelated to physics, they are likely to be better models to unravel the basic relations between classical chaos and quantum mechanics, and they are now under intensive study. Among these simple systems there is one class of *physical* systems on which actual experiments are performed, the Rydberg atoms in an external magnetic field [0].

Preliminary separate discussions of chaotic classical behaviour and of quantization are needed before we can describe the problems in handling both questions simultaneously. We shall then present some data on an especially simple model, the quantized baker's map, and conclude with suggestions for further research.

## 1. – *Classical motion : chaotic vs. regular* [1-2]

Classical mechanics means here the motion of point particles in a potential, as described by Newton's (or Hamilton's) equations of motion. This is *conservative* mechanics ; much of the literature on chaos in dynamical systems concerns *dissipative* aspects (attractors etc...) hence is not relevant here.

A most interesting example for our purposes is the case of a *planetary system*, because it is realized in Nature at two very different scales : the Solar system, governed by classical laws, and the hydrogen atom, governed by quantum laws. By a fluke, it is the same central attractive force law in $1/r^2$ which operates in both cases.

The motion of a planet around the Sun is the *most regular* possible. It is precisely *periodic* and accurately predictable for centuries. Its *stability* against both small external perturbations and uncertainties in the initial data, is an essential feature to ensure reliable predictions. Thus, planetary motion is an illustration of the *deterministic principle* according to which the equations of motion completely specify the future evolution if the initial state (i.e. positions + velocities) of the system is known at a given time.

By contrast, one can imagine other simple force laws which give rise to extremely *unstable* motions, in which the slightest uncertainty or perturbations upon (almost) any state of the system is *exponentially amplified* in the course of time, by $e^{\omega t}$ where $\omega > 0$ is called the Liapunov exponent. If moreover the trajectories are confined to a *bounded region* (often the effect of *nonlinear* couplings), then any uncertainty rapidly becomes comparable to the characteristic scale of the system, meaning that the future evolution is *unpredictable in pratice*. Indeed, systems with a positive Liapunov exponent and compact phase space have extremely *irregular*, *random-like* trajectories ; they are called *chaotic*.

It is not the form of the equations of motion which distinguishes regular and irregular systems (those equations can look equally *simple*), but the *number of constants of the motion*, besides the total energy $E = \frac{1}{2} mv^2 + V(q)$ which is always conserved.

In one degree of freedom, the fact that $E$ is constant allows to *integrate* the equations of motion, giving *stable periodic* trajectories. In N degrees of freedom, if the system is *separable* then each degree of freedom has *its* constant of the motion, and *its* own periodic evolution ;overall one has N constants of the motion giving rise to a *stable*, *quasi-periodic* trajectory. The natural coordinate-invariant generalization of separability gives a picture where N constants of the motion are still present, satisfying certain conditions of *complete integrability* which guarantee that all trajectories are quasi-periodic and stable, i.e., *regular*.

The basic perturbative result of classical mechanics, the KAM theorem shows that the constants of motion are *destroyed* under a generic perturbation of a completely integrable system. As soon as the coupling is introduced, *unstable regions* appear in the space of states ; still, the total volume occupied by regular, quasi-periodic trajectories does not immediately collapse but only at some finite value of the coupling. Nevertheless, *fully regular* motion is a privilege of the *completely integrable* case.

Such KAM systems present a very *intricate* mixture of regular and irregular behaviour ("soft chaos" [3]). In spite of their complexity, they are very popular because 1) they are generic, and often encountered in applications, 2) they seem amenable to perturbative treatments. However, the latter consistently seem to *break down* at the frontier of chaotic behaviour, which may result in a convenient signature for chaos but not in an investigation tool !

It may then be interesting to turn to *maximally chaotic systems*, where *any* constant of the motion (besides the energy) is excluded by virtue of the fact that a typical trajectory densely visits the *whole* energy surface. Such a system is called *ergodic* ; if it has a positive Liapunov exponent, it will then have extremely irregular trajectories ("hard chaos" [3]), yet it may be *simpler* to study than a system of the KAM type in the sense that its behaviour will be more homogeneous and have better *statistical* (e.g. ergodic, mixing...) properties.

No realistic physical system with potential forces has been *proved* to be ergodic ; the *anisotropic Kepler problem* seems ergodic and has been intensively studied [4]. The hard sphere gas in a box is ergodic [2], but to have really simple examples with very few degrees of freedom one must turn to more abstract models, which have certain simplifying features :

- the minimal number of degrees of freedom, *two* ;
- a motion confined to a bounded region by *external boundary conditions*, i.e.
  1) reflecting walls ( *billiard* problems), and/or
  2) periodic boundary conditions (e.g., motion on a Euclidean torus, which is a plane square with opposite edges pairwise identified).
- in the interior region, dynamics is essentially given by *free motion.*

Billiards giving a chaotic motion are (Fig. 1) the *stadium* (a) and the Sinai billiard on a torus (b). Chaotic models on periodic spaces are the free (= geodesic) motion on a compact surface of constant negative curvature (Fig. 2) [5-6], and the motion under several attractive Coulomb potentials on a torus [7].

A further simplifying abstraction replaces continuous motion by motion in *discrete time steps* given by a canonical, 1-1 mapping of the phase space onto itself. Such sytems may now be chaotic in *one* degree of freedom since there is no energy to be conserved in general. Two examples of chaotic maps (Fig. 3) on the *torus as phase space* are (a) Arnold's "cat maps" (linear matrix transformations with integer coefficients) and (b) the *baker's map.*

An important feature of all models listed above is that they have *quantal equivalents.* We now discuss the problem of their quantization.

2) *Equations of motion :quantal vs. classical* [8].

A point particle in a potential V (q) on the "atomic scale" is no longer described by classical mechanics but by a *wave mechanics* specified by Schrödinger's equation $i\hbar\partial\psi/\partial t = H\psi$ where $H$ is the linear *self-adjoint* operator $-\hbar^2\Delta + V(q)$ ; $|\psi(q)|^2$ is the probability density of the particle at the point $q$, and $\psi(q)$ has a rapidly varying phase with wavelengths on the scale of Planck's constant $\hbar$, which is very small in macroscopic units ($\simeq 10^{-27} erg \times cm$). The classical behaviour is to be recovered in the limit $\hbar \to 0$, the same way as wave optics restores geometrical optics in the short wavelength limit.

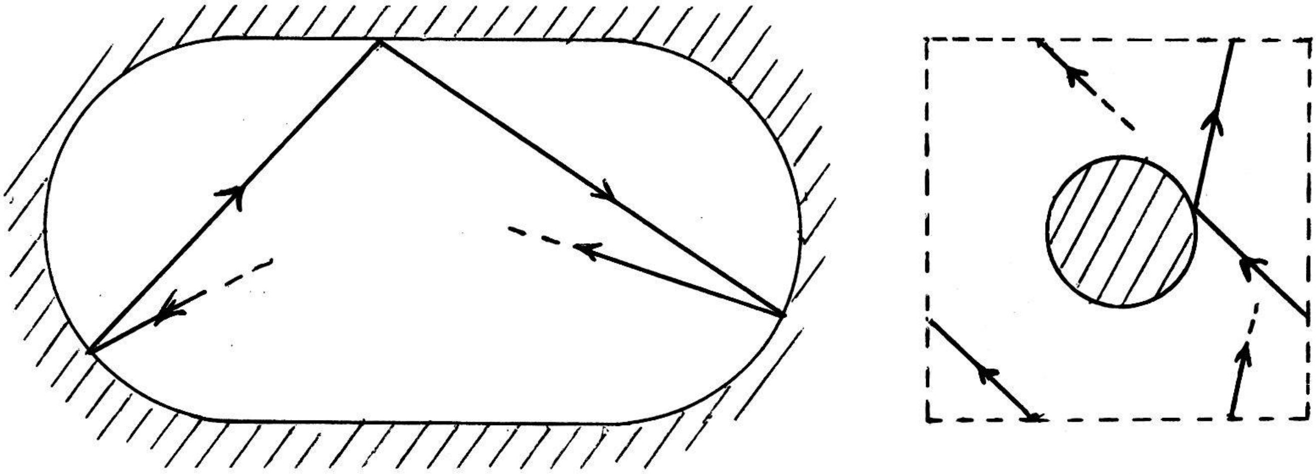

Fig. 1: a) the stadium billiard; b) the Sinai billiard.

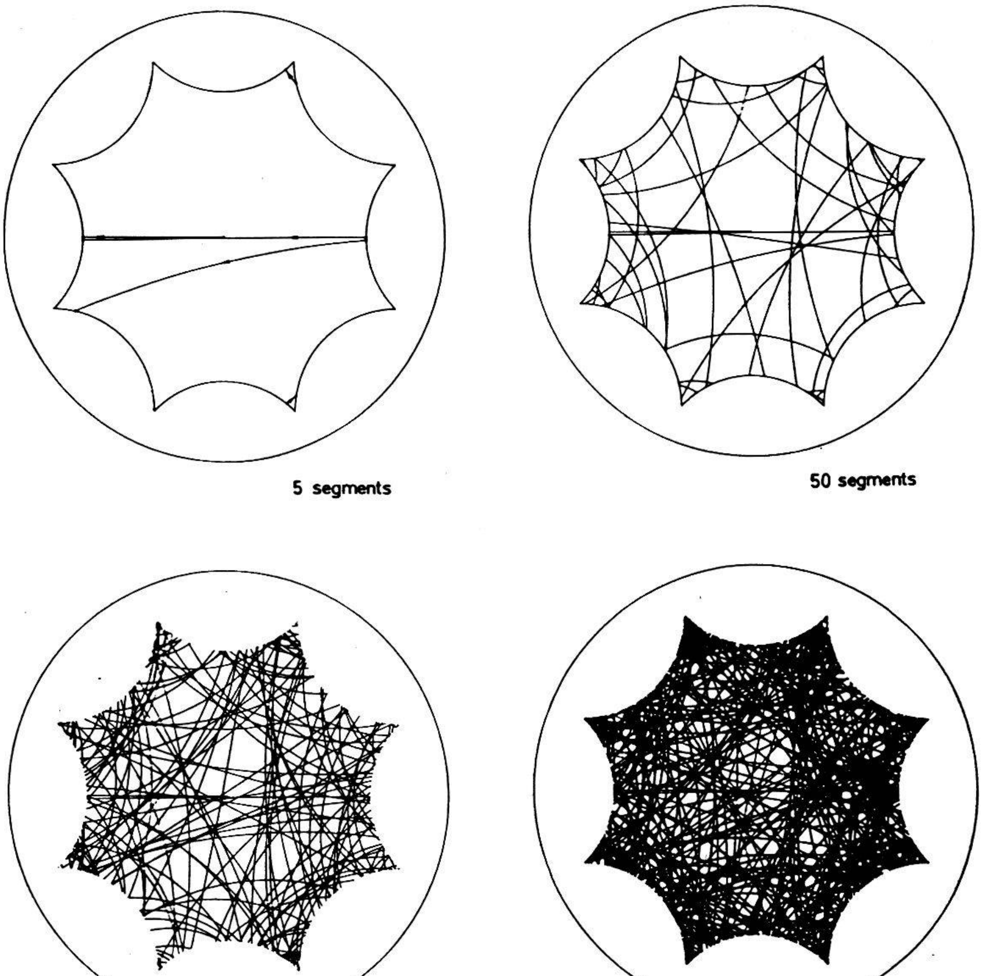


Fig . 2: a typical trajectory (unstable and ergodic) on a compact surface of constant negative curvature; this surface is represented by an octagon whose opposite edges must be identified (from [6]).

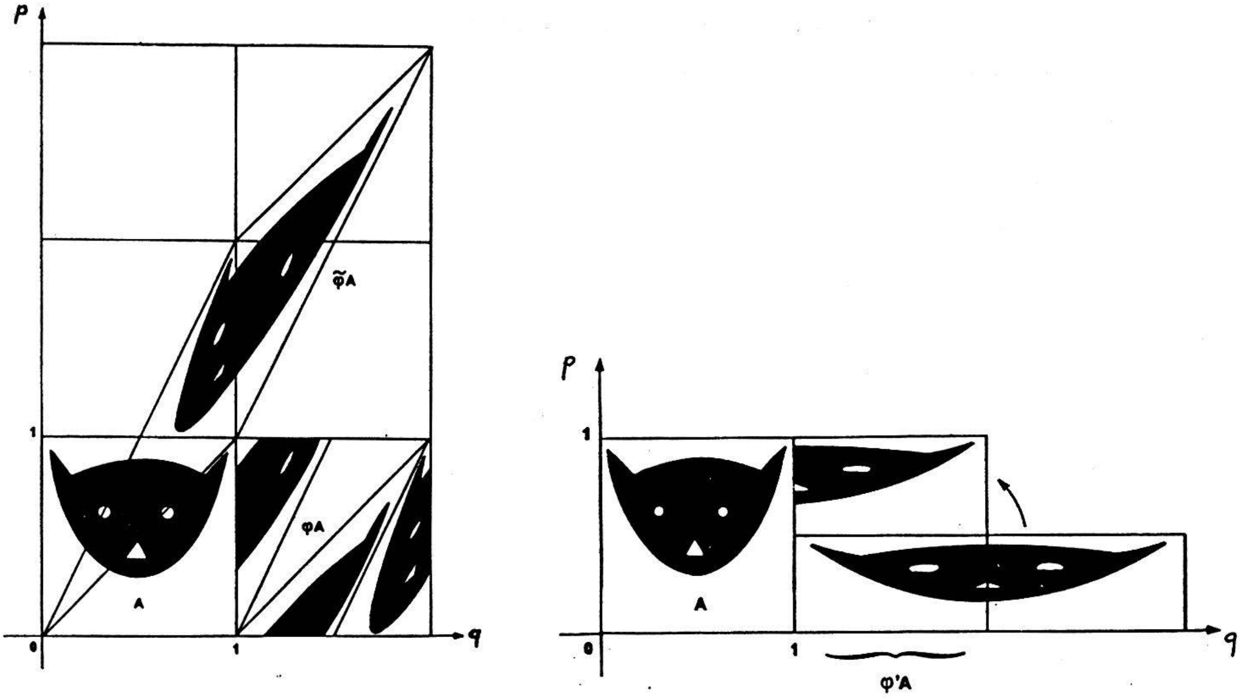


Fig.3: a) "cat map" b) baker's map (taken from [1]).

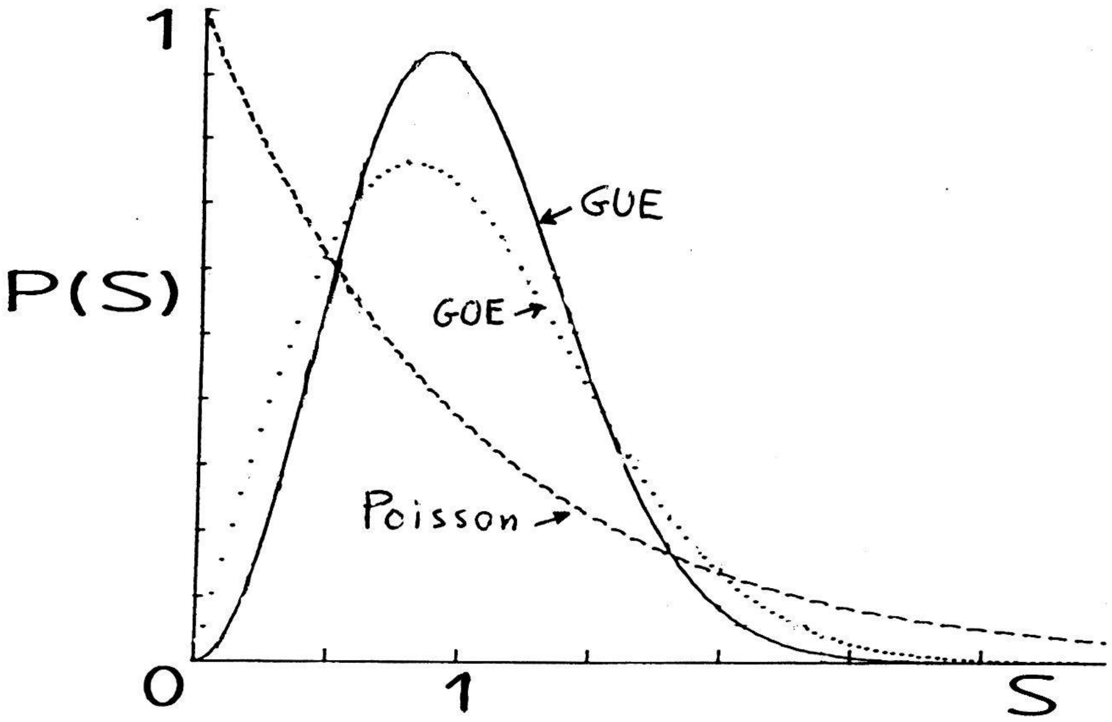


Fig. 4: nearest-neighbour spacing distributions for standard level statistics (see [21]).

For the various dynamical systems which we have considered and which are not described by potentials, we have to face the problem of *quantization*, to invent the "correct wave equation" corresponding to the given classical dynamics. While this is not a well-posed problem with an automatic and unique answer, satisfactory solutions are available for the cases we have listed.

Free motion on a surface is quantized by taking for $H$ the linear operator $-\hbar^2\Delta$ ($\Delta$ being the Laplace-Beltrami operator in case of a curved surface). Reflection of the waves upon a billiard wall is enforced by Dirichlet (or, at will, Neumann) *boundary conditions* at the wall, while periodic boundary conditions can be imposed directly on the wave function $\psi(q)$ itself.

It is not immediate to adapt these quantization recipes to the case of discrete time dynamics. Here, quantization must replace the classical area-preserving map with a linear *unitary operator* acting upon the wave function $\psi(q)$ (a *quantum map* [9]).This has been realized for a handful of models, notably the kicked pendulum map [10], the cat map [11], certain maps on a sphere [12], and the baker's map (see below) [13].

We conclude that the quantization of the *equations of motion*, while being a necessary and sometimes non trivial step, does not constitute an essential problem. This operation is actually insensitive to the regular or irregular nature of the classical solutions, and can be achieved for many chaotic systems of interest.

## 3. - *Chaos and quantum mechanics : the problems* [8, 14-17].

Classical chaoticity creates problems in quantum mechanics insofar as the behaviour of the *solutions* (of the quantized equations of motion) is considered ; those problems are basically *unsolved*, although some were recognized as early as 1917, by Einstein [18].

Classical chaos appears in *bounded* systems, for which the quantal Hamiltonian operator $H$ usually has a *discrete eigenvalue spectrum*. The diagonalization of $H$ then amounts to a decompostion of the quantal motion in a countable sum of normal modes (linear oscillators). Such a motion is linear, quasi-periodic, stable. Considered as an abstract dynamical system, quantal motion is thus *not chaotic* at all, but perfectly regular, and in fact completely integrable (albeit infinite-dimensional).

However, if one wishes to solve a particular Schrödinger equation, it is not the *abstract* possibility of diagonalizing $H$ which matters, but the possibility of finding *explicit formulas* (be they exact or approximate) for that purpose. All standard solvable quantum systems are very special separable systems, and no perturbative scheme based on them can bring us close to any strongly chaotic system. This then allows the quantized version of a chaotic system to differ by *fine analytical properties*, perhaps, from a quantized regular system. The problem of "quantum chaoticity" is for us to isolate those properties. We can split this problem into several overlapping questions [13]:

a) where and how is each chaotic feature of the classical motion encoded into the quantized motion through quantization?

b) how does the classical limit of quantum *solutions* take place?

c) can the quantum solutions be analytically described in terms of classical trajectories, and how?

d) how is classical chaoticity restored in the classical limit?

We shall see in the next section that considerable information has been gathered about this problem, thanks to the selection and (mostly numerical) study of more and more models, but that at the same time analytical tools are still lacking to provide sufficiently explicit answers to any of the questions.

Remark : two quantized chaotic problems are actually *exactly solvable in some sense* : the cat maps [11] and the motions on compact surfaces of constant negative curvature [5-6], the solutions of which are related to the Selberg trace formula. This property makes these models of paramount importance, but at the same time it may profoundly alter the relationships between quantization and classical chaoticity from what they are in generic problems.

## 4. - *A brief status report.*

We shall present a selection of data about the quantal manifestations of classical stochasticity. We shall exclusively deal with strongly chaotic, time-independent systems and observe chaotic manifestations on a) the eigenvalues, b) the eigenfunctions, c) the time evolution.

All approaches tend to conform to the following, rather disappointing, pattern.

1) A general formula or property, valid irrespectively of the classical regularity or chaoticity, is taken as a starting point.

2) If the system is completely integrable, the formula can be made more precise and explicit, producing a well defined analytical behaviour of the quantity under consideration (typically, a reliable semi-classical approximation, often known beforehand).

3) If the system is chaotic, the absence of that behaviour is definitely observed on the numerical data, but no substitute analytical behaviour can be inferred or deduced from the initial general formula, nor by any other means.

4) The failing analytical study tends to be replaced by the search for statistical properties, which is empirically more successful but often remains based on conjectures.

We now specialize the discussion to the various types of solutions.

a) *Eigenvalues* [19]

A general relationship between eigenvalues and classical motion is provided by the periodic orbit sum [8],

$$\#\{E_k < E\} \simeq (2\pi\hbar)^{-N} \int_{E(p,q)< E} dp\, dq + \sum_{\gamma} A_\gamma\, e^{iS_\gamma/\hbar}$$

where $E(p,q) = \dfrac{p^2}{2m} + V(q)$ is the classical energy function, the index $\gamma$ runs over all classical *periodic* orbits at the energy $E$, and $S_\gamma$ is the corresponding action $\oint_\gamma p\, dq$.

For an integrable system, the sum can be evaluated, resulting in a semi-classical eigenvalue formula which is just the EBK quantization rule :

$E = H\{\vec{I}_\nu\}$,

where $H\{\vec{I}\}$ is the classical energy function of the action coordinates of the system, and $H\left\{\vec{I}_\nu\right\}$ is that same function restricted to the *quantized actions*, which are the integer multiples of $\hbar$ (up to a shift).

For a chaotic system, on the other hand, the number of orbits with action $\leqslant S$ proliferates *exponentially* with $S$, and this causes the periodic orbit sum to be badly *divergent* in a complex region of the $E$ plane *enclosing the* *quantal spectrum* [20]. This method is now totally useless to predict *individual* eigenvalues, and the problem of their evaluation remains open. Now, the leading non-oscillatory term in the periodic orbit sum can be viewed as a smoothed or averaged level density, while the remainder can be treated as *fluctuations*, and studied *statistically*. For an integrable system, this can be done explicitly using the EBK formula, and a *Poissonian* level distribution is derived. For chaotic systems the level distributions appear rather to follow the GOE (or GUE) distributions of *random matrix theory* [21].

The distribution of *nearest neighbour spacings*, measured in units of the local average spacing, are shown on Fig. 4 for the Poissonian, GOE and GUE level distributions.The latter two exhibit *level repulsion* (statistical suppression of small spacings). All this means that the level density for a chaotic system shows *milder fluctuations* around its average then for a regular system.

Thus, statistical properties of the level fluctuations seem to be clear manifestations of classical chaotic behaviour. There are some problems, however. All arguments trying to *show* that classical chaoticity implies GOE or GUE behaviour of the quantal levels have to rely on *ad hoc* assumptions. In fact, while there is considerable numerical evidence supporting this statement, there are also important exceptions, such as the spectrum of the quantized motion on a compact surface of constant negative curvature [6]. It seems to us that random matrix behaviour would rather describe a *generic* feature of the system, like its having *no discrete or continuous symmetry whatsoever*. While classical chaotic behaviour is strongly correlated with this property, it definitely does *not* coincide with it.

b) *Eigenfunctions* [22 - 25 ]

The eigenfunctions of $H$, solutions of $H\psi = E\psi$, describe the stationary quantum states and the eigenvalues give their corresponding energies. It is natural to search for links between the eigenfunctions and the *classical invariant states*, especially in the semi-classical limit $\hbar \to 0$.

If the position space is N-dimensional Euclidean space, then it is expected on general grounds that such a limiting behaviour will most pregnantly manifest itself upon the *Wigner function* [22 -23]

$$W(q,p,\hbar) = (2\pi\hbar)^{-N} \int_{\mathbb{R}^N} \psi(q-r/2)\ \psi^*(q+r/2)\ e^{ipr/\hbar}\ ,$$

which should tend to a phase distribution of classical particles as $\hbar \to 0$.

For a completely integrable system, with N constants of the motion $H_1 \cdots, H_N$, we have effectively shown that the Wigner function associated with a *joint eigenfunction* (of all the quantized constants of the motion) has the limiting form [22]

$$W\ (q,\ p,\ \hbar) \sim \delta\ (H_1 - h_1) \cdots \delta\ (H_N - h_N),$$

which is a reduced *microcanonical* distribution obtained by freezing all the classical constants of the motion. This limiting form is in fact equivalent to the *WKB* expression of the eigenfunction $\psi$ itself, which can be written as a *finite sum* of travelling waves each of the form $ae^{is/\hbar}$ (such a wave has a regular shape closely controlled by a bundle of classical orbits, see Fig. 5 and [25]).

By analogy, we have conjectured that for an ergodic system, which has no constant of motion besides the energy, the limiting form of the Wigner function ( for an eigenstate of energy E) should be the *unrestricted microcanonical* distribution [22]

$$W\ (q,\ p,\ \hbar) \sim \delta\ (E(q,\ p) - E)\ .$$

This conjecture has recently been *proved* to be true in a certain weak sense [26].

However, contrary to the integrable case, we have no idea of *any* analytical wave form for $\psi$ itself which would produce a Wigner function having the microcanonical form. It is true that $|\psi(q)|^2 = \int_{\mathbb{R}^N} W\ (q,\ p)dp$, but the approximation

$|\psi(q)|^2 \sim \int_{\mathbb{R}^N} \delta(E(q,p) - E)dp$ seems only to specify the *locally averaged* modulus of $\psi(q)$; we cannot describe analytically the fine behaviour of $\psi$, which looks highly *irregular* ; it has been conjectured in fact that this eigenfunction behaves like a *Gaussian random function* [24]. (Any attempt to express $\psi$ more accurately as a sum of travelling waves is expected to *diverge* due to the exponential proliferation of terms induced by classical

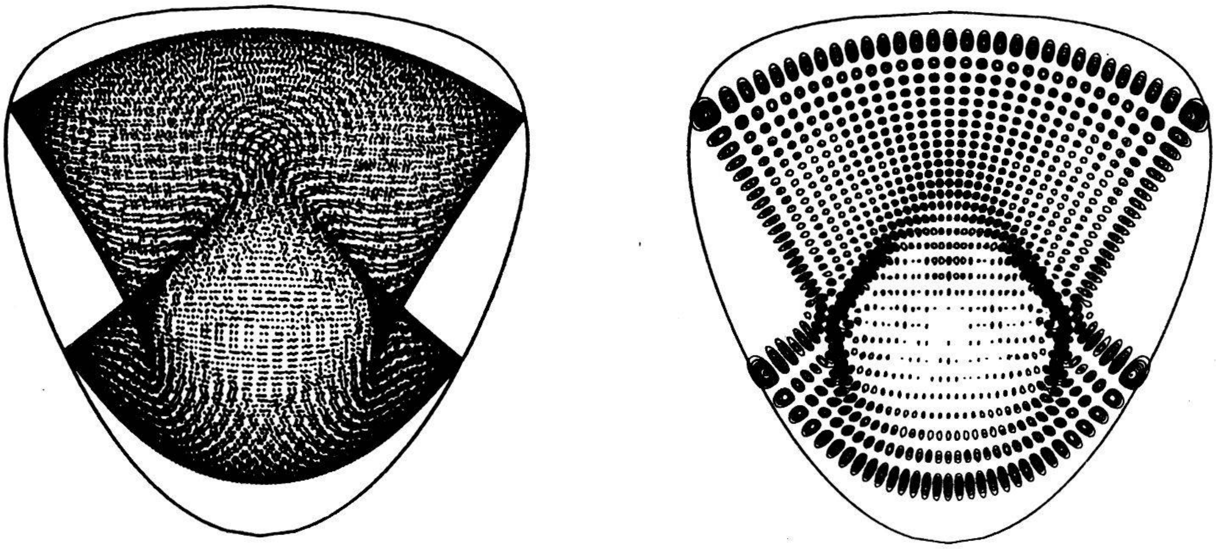

Fig. 5: an example of regular motion in 2 degrees of freedom: a regular trajectory (left) and a regular quantal eigenstate associated with it (right) (taken from [25]).

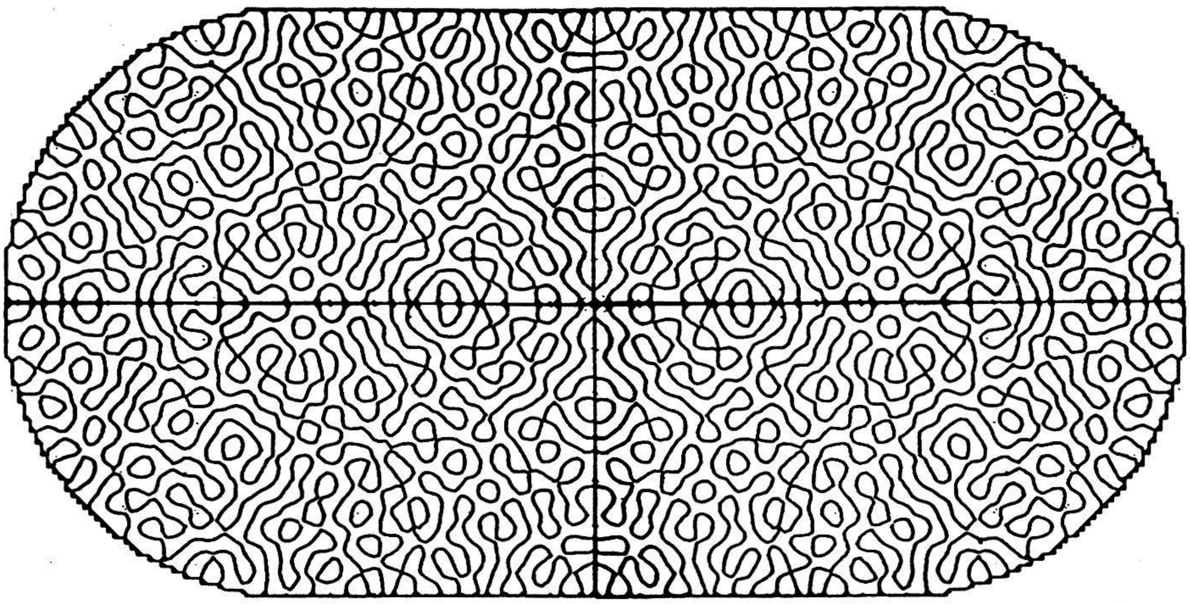

Fig. 6: an irregular eigenfunction in the stadium (taken from [27]). (shown are the nodal lines)

chaoticity).

Thus, a chaotic eigenfunction should look smoothly spread out on large scales (according to the microcanonical distribution) but very irregular on fine scales. However, numerical studies on the stadium ([25, 27] and Fig. 6) and the baker's map not only show that many eigenfunctions have this appearance, but also that not a few exhibit *strong regular patterns* which seem to be controlled by special families of classical trajectories (e.g. "scars" above periodic orbits [25]). There is no fully satisfying theory to explain those regular features at the quantal level.

c) *Time-evolution.*

The short-time evolution of any quantum system is accurately controlled by classical evolution according to the Van Vleck semi-classical propagator formula,

$$\psi\,(q,t) \sim (2\pi i\hbar)^{-N/2} \int \left[\sum_{\gamma} \left| det\, \frac{\partial^2 S_\gamma}{\partial q \partial q'} \right|^{\frac{1}{2}} \chi_\gamma e^{iS_\gamma(q,q')/\hbar}\right] \psi\,(q',0)\, dq',$$

where $\gamma$ labels the classical orbits going from $q'$ to $q$ in time $t$, and $S_\gamma$ is the action along $\gamma$ ($\chi_\gamma$ is the Maslov phase correction).

It can be expected that such a semi-classical formula will fail at later times when the classical evolution generates fine details in phase space of area $\lesssim \hbar$ [9, 28]. For a chaotic system with Liapunov exponent $\omega$ the break-up time is extremely short, $t_c \simeq \omega^{-1} |log\, \hbar|$, and for $t \gtrsim t_c$ the nature of the relationship between the quantal and classical evolutions becomes a total mystery. Our present semi-classical knowledge only applies for $t \lesssim \omega^{-1} |log\, \hbar|$, preventing us from *interchanging the order of limits* $\hbar \to 0$ and $t \to \infty$. This lack of uniformity of the classical limit with respect to time confirms how difficult it is to analyze the stationary, time-independent properties of quantized chaotic systems.

## 5. – *A model : the quantized baker's map* [13]

The classical baker's map is a precewise continuous, area-preserving, 1- 1 map of a rectangular phase space into itself (Fig. 3b). Quantum mechanics on such a phase space of finite area A is inconsistent unless

$(2\pi\hbar)^{-1}$ $A = N$ is an *integer*, which specifies the *finite* dimension of the quantal Hilbert space. If the area is kept fixed, the classical limit $\hbar \to 0$ requires $N \to \infty$ [11, 13].

It is possible to construct a quantal analogue of the baker's map in the form of a unitary $N \times N$ matrix, B, which acts on the Hilbert space of quantum state vectors, and reduces in a suitable way to the classical baker's map as $N \to \infty$. We find

$$B = F_N^{-1} \left( \begin{array}{c|c} F_{N/2} & 0 \\ \hline 0 & F_{N/2} \end{array} \right),$$

where $F_M$ is the finite Fourier transformation on M sites, with matrix elements $(F_M)_{mn} = M^{-1/2}\, e^{2\pi i mn/M}$.

In spite of its formal simplicity, this matrix shows a highly *complex* and challenging behaviour as $N \to \infty$. In particular, we cannot describe analytically the fine details of its eigenvalue distribution, while its eigenfunctions show a puzzling variety of regular and irregular patterns (Fig. 7). We think that this model and its generalizations offer new opportunities to understand some of the basic relationships between classical chaos and quantum mechanics.

## 6. – *Conclusion*

The study of "quantum chaos" is, from the point of view of theoretical understanding, in a stage of active development in many different directions. (An up to date and complete review is [17]).

Simple models, exhibiting all the essential chaotic features with minimal ancillary technical or numerical complications, are still in rather short supply. A greater variety of them is needed because quantal manifestations of classical chaos have multiple facets.

Among all possible avenues of research, the *morphology of eigenfunctions* raises the greatest variety of questions and is likely to exhibit effects of classical chaos in the most visible way.

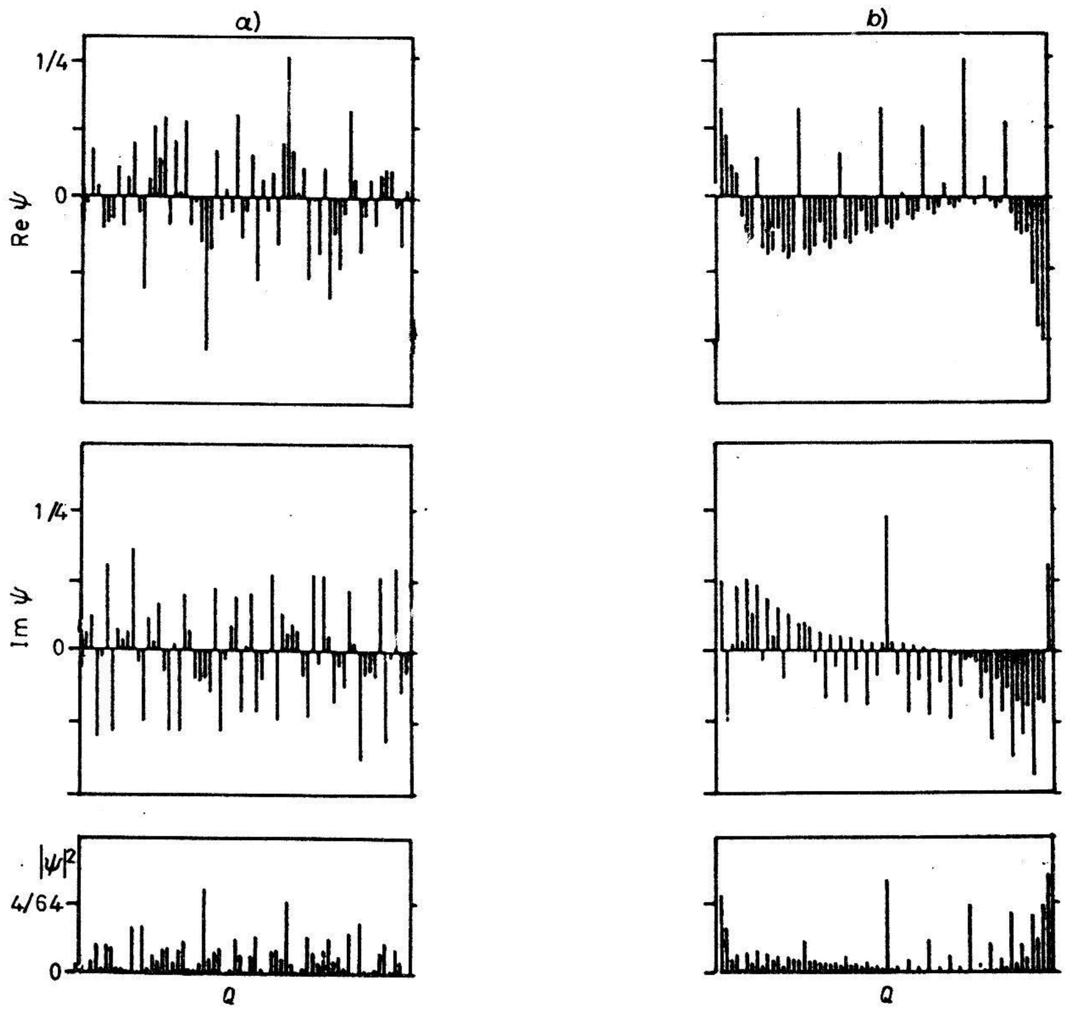


Fig. 7: two eigenfunctions of the quantized baker's map for N=64 (left: irregular, right: regular) (taken from [13]).

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