ASPECTS OF CHAOS IN CONSERVATIVE DYNAMICAL SYSTEMS

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ABSTRACT

The occurrence of chaotic motions in classical dynamical systems and its relevance to physical situations is discussed. The question of whether this classical phenomenon has a meaningful quantum parallel is current; some approaches are reviewed.

INTRODUCTION

A NEW cross-disciplinary area of basic research—the study of chaotic phenomena—has emerged in recent years[1-5]. This has in part, been due to the recognition of the essential nonlinearity of real physical systems (as opposed to idealized models which are almost always linear approximations), and has brought about the realization that there can be novel, unintuitive and unpredictable behaviours associated with even the simplest nonlinear systems.

Chaos is most conveniently thought of, as a dynamical phenomenon, the situation being such that complete knowledge of a system at one time *still* renders impossible the task of predicting the future (or past) history of the system. This unpredictability is not due to any 'uncertainty' or 'fluctuations'—the chaotic behaviour that is discussed in this article is a product of strictly deterministic equations[6].

A dynamical system D is simply defined as the collection of an independent variable, t (which can either be continuous or discrete) dependent variables, $\mathbf{x}$, and the equations of motion for $\mathbf{x}$ given by some prescription $P(\mathbf{x})$,

$$D = \{t; \mathbf{x}; P(\mathbf{x})\} \tag{1}$$

Apart from the most obvious case of systems in classical mechanics—where t is the time, $\mathbf{x}$ refers to position and momentum variables, and $P(\mathbf{x})$ represent the classical equations of motion—a variety of physical situations can be viewed as dynamical systems. Examples can be drawn from several areas—*e.g.* chemical reactions,

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C$$

then t is again the time, $\mathbf{x}$ refers to the concentration of the species A, B, C and $P(\mathbf{x})$ is defined *via* the equations

$$dx_A/dt = -k_1 x_A x_B + k_2 x_C$$

$$dx_B/dt = -k_1 x_A x_B + k_2 x_C$$

$$dx_C/dt = k_1 x_A x_B - k_2 x_C$$

Discrete dynamical systems obtain in some problems in population biology[7]. The normalized population of some species at generation t is related to the population at generation $(t+1)$ by a recursive relation; one example is the logistic equation,

$$x_{t+1} = a x_t (1 - x_t)$$

The detailed knowledge of $\mathbf{x}$ as a function of t defines a trajectory or orbit in the configuration space of dimension n (where n is the number of dependent variables). When the equations of motion are nonlinear, some properties of these orbits can be as random as the outcome of coin-toss experiments. (In the literature, the words 'chaotic', 'stochastic', 'erratic', 'irregular', 'random' have at one time or the other been used synonymously. The preferred nomenclature at present[4] is *self-generated* or *deterministic* chaos). Figure 1 shows two orbits of a nonlinear system, in order to visually contrast the possible complexity of chaotic orbits with the simplicity of non-chaotic or regular behaviour; the dynamical system is a "*billiard*", a generalization of the familiar particle-in-a-box problem to enclosures with reflecting boundaries and arbitrary shapes.

Dynamical systems are further classified as conservative and dissipative. These are distin-

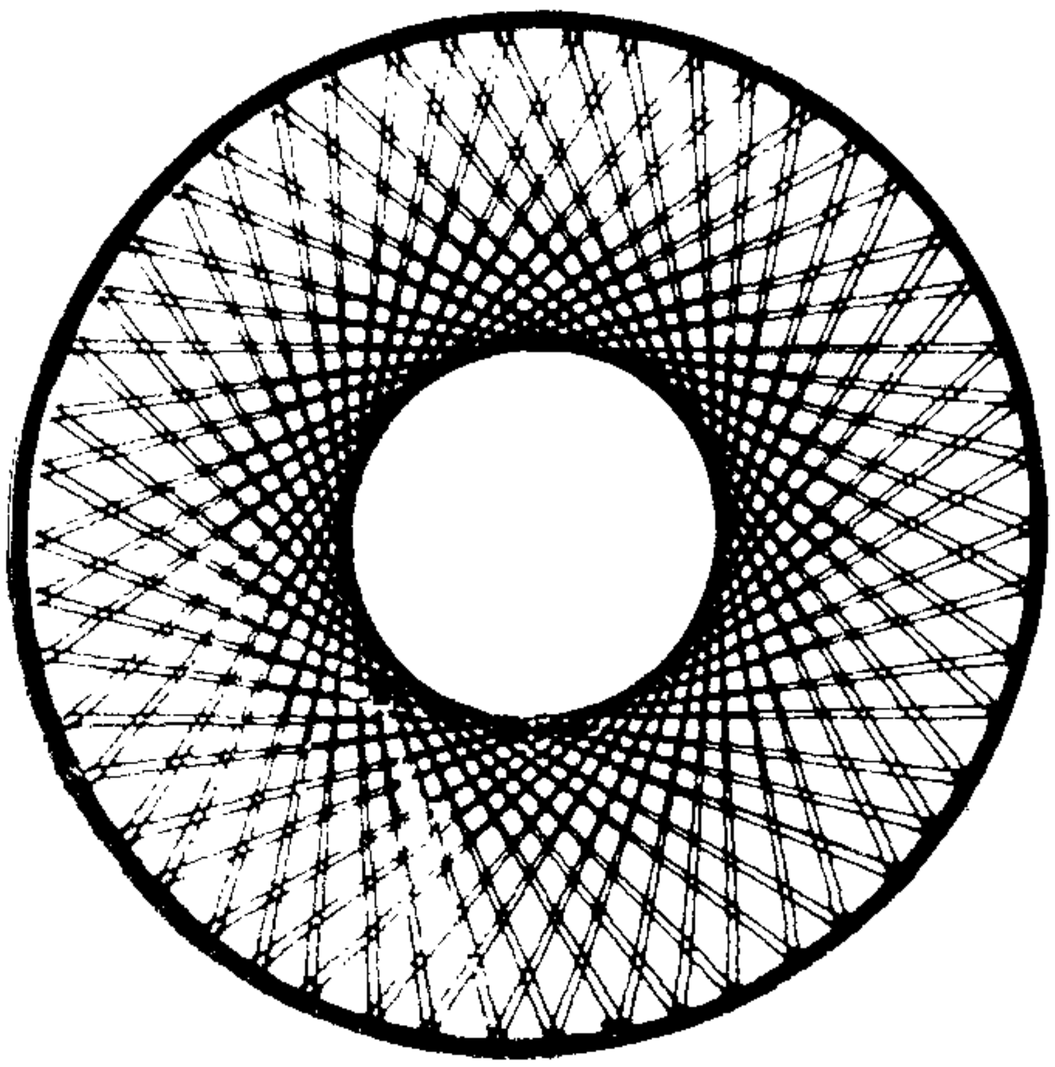

Figure 1a. A typical orbit in a circular billiard. Within the billiard, the potential $V = 0$; at the boundary, $V = \infty$. Thus there is only specular scattering at the edges. All orbits in this system are of this type: note the inner caustic curve formed by the orbit.

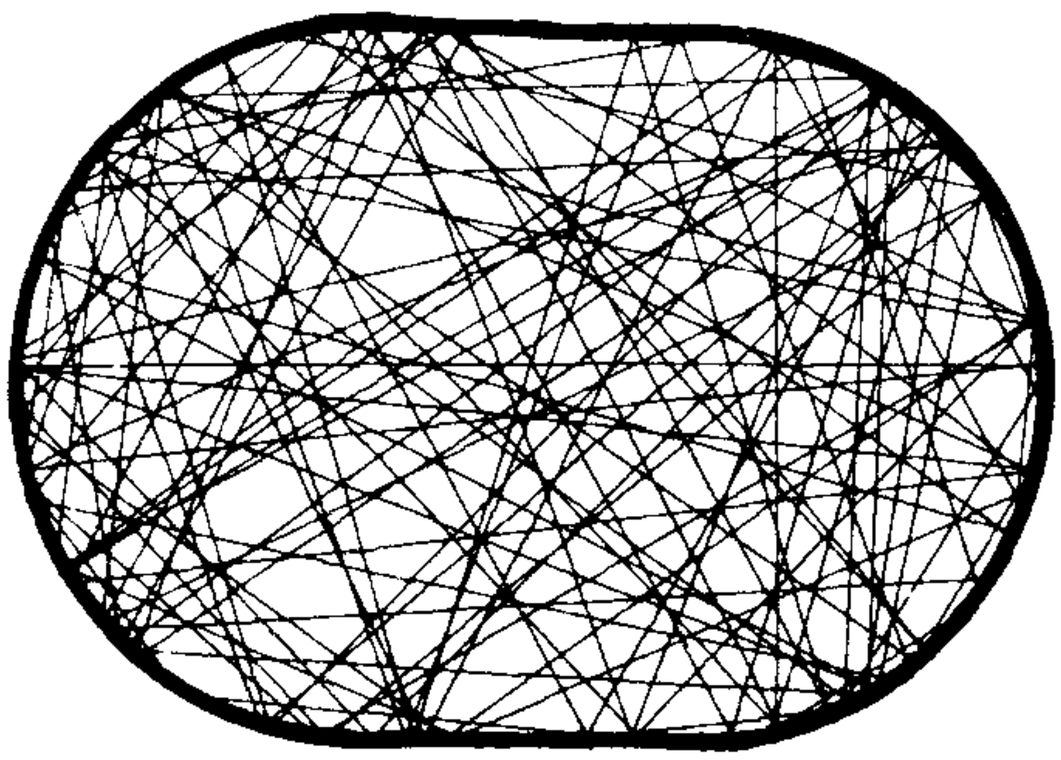

Figure 1b. A typical orbit in a "stadium" billiard. Unlike figure 1a, there is no caustic curve. All regions of the enclosure are visited by the orbit, unlike the excluded inner area in the previous figure.

guished by the fact that volumes in the configuration space are conserved under the evolution in the former case, while for the latter, any volume shrinks asymptotically. An important class of conservative systems are those described by a Hamiltonian. The phenomenology of chaos in these two kinds of systems is somewhat different. In this article we restrict attention to the latter class[8].

CONSERVATIVE SYSTEMS: HAMILTONIAN MECHANICS

The equations of motion for Hamiltonian systems are the Hamilton's equations; **x** denotes position, **q**, momentum, **p**, variables, and the configuration space is termed the phase space. This space is of dimension $2n$ where n is the number of degrees of freedom. Thus

$$D = \{t; \mathbf{q}, \mathbf{p}; \mathrm{d}\mathbf{q}/\mathrm{d}t = \partial H/\partial \mathbf{p}, \quad \mathrm{d}\mathbf{p}/\mathrm{d}t = -\partial H/\partial \mathbf{q}\} \quad (2)$$

Furthermore, there is at least one constant of the motion, the Hamiltonian function $H(\mathbf{p}, \mathbf{q})$ itself, since $\mathrm{d}H/\mathrm{d}t = 0$. (With no loss of generality, we have taken H to be autonomous). As is well known[9-11], one can often find a generating function for a canonical transformation to new variables such that the transformed Hamiltonian is a function of the new momentum variables alone (this is the usual transformation to action-angle variables):

$$(\mathbf{p}, \mathbf{q}) \rightarrow (\mathbf{I}, \theta) \quad (3)$$

$$H(\mathbf{p}, \mathbf{q}) \rightarrow H'(\mathbf{I})$$

$$\mathrm{d}\mathbf{I}/\mathrm{d}t = -\partial H'/\partial \theta = \mathbf{0}$$

and thus the **I**'s are constants of the motion. Systems for which this is possible are termed *integrable*. The hallmarks of integrable systems are (i) there are n constants of the motion (the n **I** variables), (ii) the equations of motion can be explicitly solved—these systems are *regular* (predictable), and (iii), if the constants are in involution, *i.e.* if the Poisson bracket $\{I_j, I_k\} = 0$ for all j, k, then the orbits are *constrained* to lie on n-dimensional tori in the phase space[11,12]. (Note that this is a severe restriction the dimension of the phase space is $2n$, while that of the motion is only n). A special class of integrable systems are those that can be reduced to n uncoupled 1-dimensional problems—these are termed separ-

able (and in fact constitute the most familiar examples of integrable systems).

However, integrable systems are rare—most Hamiltonian systems are nonintegrable, *i.e.* no transformation to action—angle variables exists in the (generic) typical case. Further, there is no simple way by which a system can be shown to be integrable other than by explicitly constructing the integrals of motion. Recently[13–15], it has been seen that many integrable systems can be identified by the fact that the equations of motion have the Painlevé property—that their general solution in the complex time plane has no movable singularities other than poles. The connexion between integrability and the Painlevé property is not completely understood and forms the basis of much current research interest[14,15].

It might be thought that in nonintegrable systems, since the restriction of the motion to n-dimensional tori is removed, the orbits are free to wander over the entire energy hypersurface (the Hamiltonian is always a constant of the motion). If true, the ergodic hypothesis of Boltzmann – that time and space averages of dynamical variables are equal – would be valid. In reality, however, this conjecture is false, as was shown by the Kolmogorov–Arnold–Moser (KAM) theorem[11,12]. The KAM theorem states that in a nonintegrable system that is perturbed from an integrable one, when the perturbation is sufficiently small, then most of the motion remains on n-dimensional tori. Further, the KAM theory provides a convergent perturbation scheme through which the toroidal motion in a nonintegrable system can be constructed. The phenomenology of the orbit motion in such systems is best discussed via an example, the most notable being the study by Hénon and Heiles[16] of stellar motion in an axisymmetric galaxy. The relevant Hamiltonian

$$H = (p_x^2 + p_y^2 + x^2 + y^2)/2 + x^2 y - y^3/3 \quad (4)$$

is identical to that for two coupled mechanical oscillators. The phase space is of dimension 4, the constant energy hypersurface is of dimension 3, and if integrable, the motion would lie on 2-dimensional tori (figure 2). The orbits can be

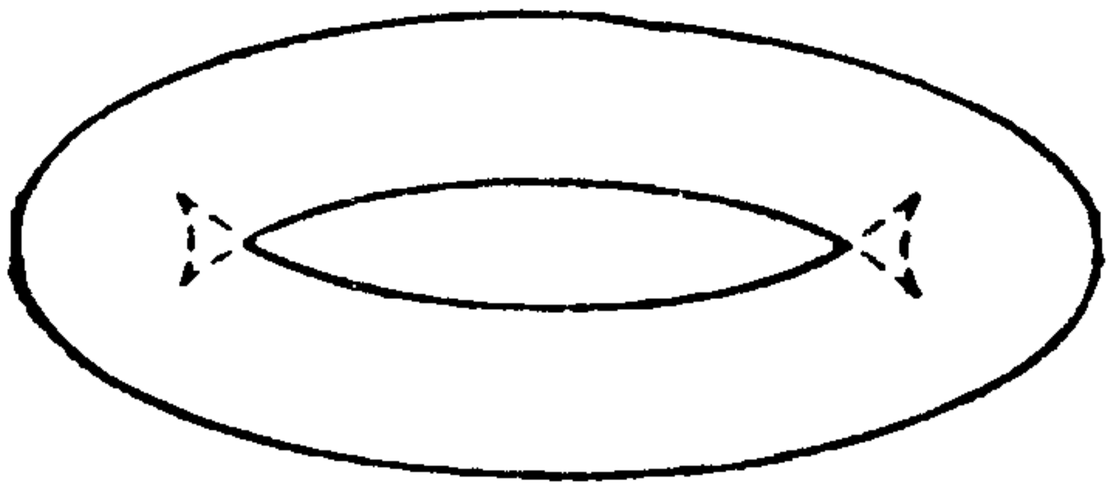

Figure 2. Example of a 2-dimensional torus.

visualized by slicing through the 3-d energy shell with a 2-d plane. The intersection of a torus with this plane would be a closed curve. Such a representation is known as a Poincaré surface-of-section. [To obtain this, the equations of motion are integrated for some set of initial conditions at a fixed value of H, and the values of y and p_y are noted when $x = 0$, and for a given direction of p_x, either $p_x < 0$ or $p_x > 0$]. At low energies, when H is small, the nonintegrable term x^2y is also small; in figure 3a the successive points seem to lie on smooth curves in the y, p_y plane. Note that these tori are quite distorted from the tori of the integrable system. As the energy is increased, a new type of motion becomes apparent, typified by the points in Fig. 3b which have no discernible pattern. This latter type of motion is termed chaos. Finally, as the energy is increased further, almost all tori disappear (figure 3c) and the motion is largely chaotic. However, it must be noted that in any nonintegrable system there is always some chaotic motion regardless of the size of the perturbation term—if figure 3a were redrawn on a sufficiently large scale, microscopic regions of chaotic motions would be seen[4,5] interspersed among the tori, similar to figure 3b.

Considerable effort[17] has been devoted to a determination of the so-called chaotic transition, when the motion in a given nonintegrable system changes from being largely toroidal to largely chaotic. (For the Hénon-Heiles system[4], this happens around $H = E = 1/10$). The most successful of these methods are based on an examination of the interaction of internal resonances that can occur[18] in coupled oscillator systems.

Although nonlinearity is a necessary condition for nonintegrability, it is not sufficient. Extremely

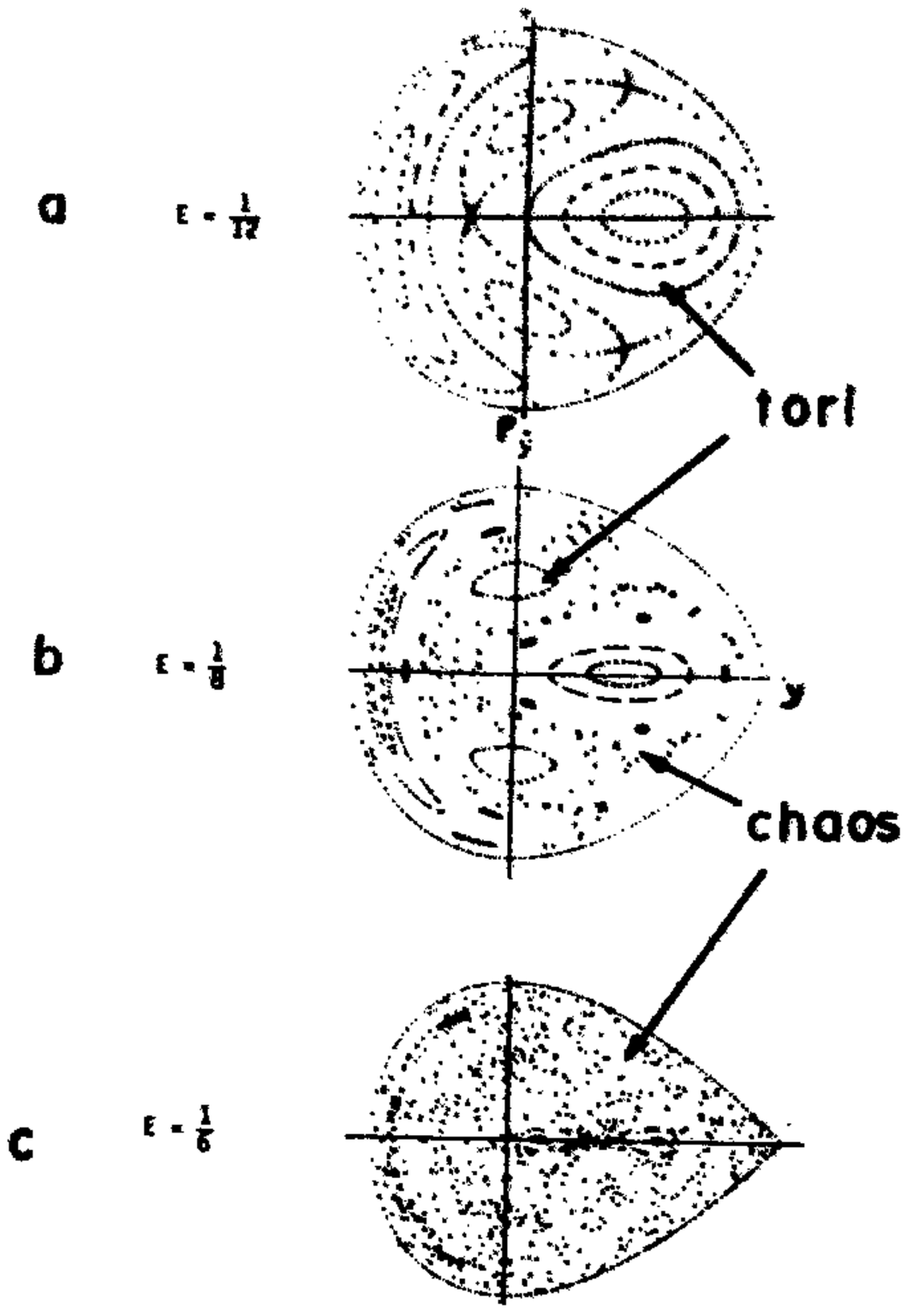

Figure 3. Surfaces of section in the p_y, y plane at $x = 0$ for the Hénon-Heiles system. Smooth curves can be drawn through some sequences of points; this is the hallmark of toroidal motion. A single chaotic orbit is responsible for the random sequences of points in each of figures 3b & c.

nonlinear systems can be integrable—a famous example is the "Toda lattice" of particles interacting *via* an exponential potential. For the case of three particles, the Hamiltonian,

$$H = (p_x^2 + p_y^2)/2 + \{\exp(2y + 2\sqrt{3}x) + \exp(2y - 2\sqrt{3}x) + \exp(-4y)\}/24 - 1/8$$

permits the (very non-obvious) second constant of the motion, in addition to H,

$$F = 8p_x(p_x^2 - 3p_y^2) + (p_x + \sqrt{3}p_y) \exp(2y - 2\sqrt{3}x) + (p_x - \sqrt{3}p_y) \times \exp(2y + 2\sqrt{3}x) - 2p_x \exp(-4y)$$

One can check that $\{F, H\} = -\mathrm{d}F/\mathrm{d}t = 0$, and thus all motion in this extremely nonlinear system lies on 2-tori.

Several qualitative differences exist between toroidal and chaotic motions—the most striking being the dimensionality of the orbit: n in the former case, and usually $2n-1$ in the latter (although in some cases of intermediate, fractal dimension have also been seen). Furthermore, regular motion is stable in the sense that nearby regular orbits separate only *linearly* in time, whereas nearby chaotic orbits separate at an *exponentially* fast rate. This latter property is an example of the extreme sensitivity of chaotic motions to initial conditions, and allows for a quantitative characterization of the degree of chaos in terms of the Liapunov exponent, the rate of separation of orbits. Another quantifiable difference between these kinds of motion is the range of frequencies present. Toroidal motion is periodic or quasiperiodic, and hence there can be at most, a finite set of frequencies present. Chaotic motion is aperiodic—the frequency spectrum is virtually continuous. The fourier transform of $x(t)$ or $y(t)$, the *power spectrum* thus offers a convenient characterization of the different types of motion in nonintegrable systems.

Since Hamiltonians such as (4) arise in a variety of contexts—*e.g.* astronomy, plasma physics, electronic circuits, atomic physics, molecular vibrations—several aspects of the nonintegrable dynamics are of interest[19]. In the next section we discuss one such aspect, the quantum mechanics of nonintegrable systems[5, 20, 21].

QUANTIZATION OF NONINTEGRABLE SYSTEMS

Since the early days of quantum theory, it has been recognized that nonintegrable systems pose a special problem *vis-a-vis* quantization. Recall that the Bohr–Sommerfeld (B-S) principle (in one dimension, *e.g.* for a simple harmonic oscillator) relies on computing the action integral along a closed classical orbit (figure 4),

$$I = \frac{1}{2\pi} \oint p \, \mathrm{d}q \qquad (5)$$

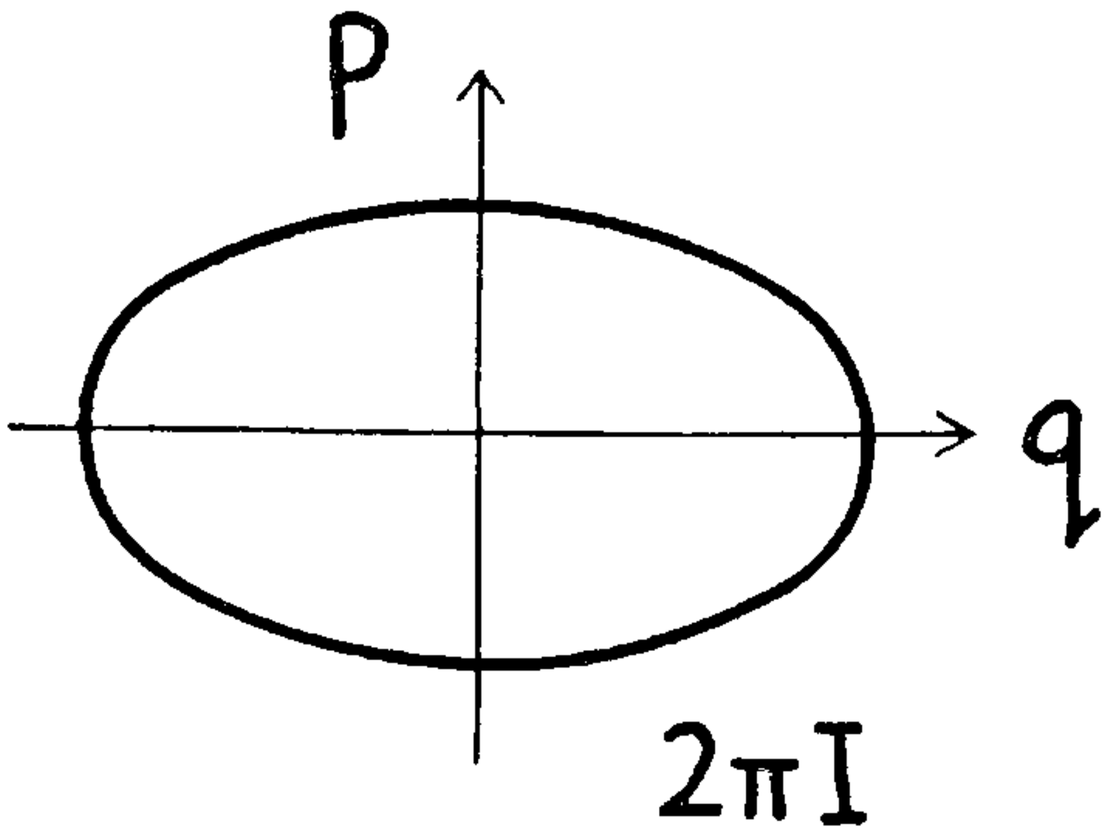

Figure 4. An orbit in a 1-dimensional potential. The action is the area enclosed within the curve.

and obtaining the quantum levels by the condition $I = m\hbar$ with m as an integer. When a multidimensional system is separable, the generalization of the B-S rule is obvious; however, when the system is nonseparable, (whether it is integrable or not), a modification of the B-S principle is necessary. This was suggested by Einstein[22], by requiring that the action integrals be computed along independent paths C_i on tori, and individually quantizing these,

$$I_i = \oint_{C_i} \mathbf{p}\cdot \mathrm{d}\mathbf{q} \quad i = 1, 2 \ldots . n \tag{6}$$

$$I_k = m_k h \quad k = 1, 2, \ldots . n \tag{7}$$

Note that there are n independent paths on a n-torus (figure 5). Along with refinements introduced by Brillouin, Keller and Maslov, this principle (EBKM) forms the basis[20,21] for the semiclassical quantization of nonseparable systems. Since the only requirement is that the appropriate tori must be found such that the condition (7) is satisfied (it is necessary to replace m_k in (7) by $(m_k + \alpha_k/4)$ where α_k an integer, depends on the nature of the classical orbit), the EBKM quantization rule can be applied to integrable as well as nonintegrable systems. In recent times, many different practical methods of

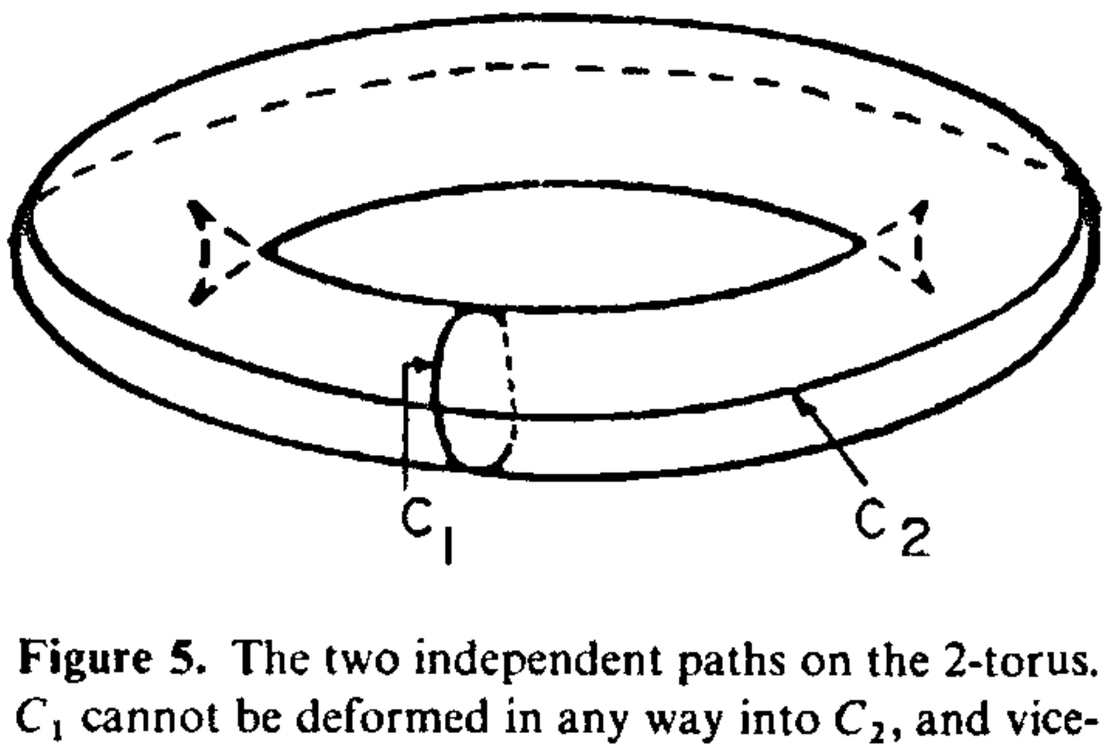

Figure 5. The two independent paths on the 2-torus. C_1 cannot be deformed in any way into C_2, and vice-versa.

implementing such a rule have been developed[20,21].

However, torus based semiclassical methods run into problems in nonintegrable systems when chaotic motions occur—the integral in (6) is no longer properly defined since the path C_i cannot be specified. For a Hamiltonian system such as the Hénon-Heiles, this means that the higher lying states cannot be quantized by a semiclassical technique—chaotic motions occur mainly at the higher energies in such systems.

There are alternate, non-semiclassical methods by which the quantum mechanics of systems such as (4) can be studied. The Hamiltonian operator corresponding to the classical system is

$$\hat{H} = \underbrace{-\frac{h^2}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{1}{2}(x^2+y^2)}+\underline{x^2y - y^3/3} \tag{8}$$

$$= \qquad \hat{H}_0 \qquad + \quad \hat{H}_1 \tag{9}$$

The standard technique of diagonalizing $\hat{H}$ in the basis of $\hat{H}_0$ can be employed to give 'exact' eigenfunctions and eigenvalues. When these results are compared with the semiclassical ones it is seen that the agreement is quite good for the low-lying states; eigenvalues are correct to within a few per cent, and the quantum eigenfunctions occupy the same general region of coordinate $(x - y)$ space as the semiclassical tori.

In the energy range where the semiclassical method fails due to the lack of toroidal motion,

there are several quantum levels that can be determined by the latter 'exact' procedure. A natural question that arises is whether there is any essential difference between the two types of quantum states—those that have a semiclassical parallel, and those that do not.

Based on the classical-quantum correspondence principle, Percival[20] conjectured the existence of two different classes of quantum eigenstates in systems that reduce to nonintegrable classical systems in the limit. Termed, Regular and Irregular eigenvalue spectra, these levels have distinctly different properties, analogous to the difference in properties of toroidal and chaotic orbit motions. For regular states,

1) it is possible to identify n 'good' quantum numbers (on a torus, it is possible to define n 'good' actions),
2) the eigenvalues are stable under perturbations
3) 'strong' selection rules operate—a given state is strongly coupled to a small set of other states, leading to a simple absorption spectrum of a few lines.

For irregular states, on the other hand,

1) it is not possible to identify any quantum numbers (action variables are undefined for chaotic motions),
2) eigenvalues are unstable and show large variations under small perturbations,
3) the absorption spectrum shows broad lines—a given irregular state is weakly coupled to several other states of similar energy.

Other distinctions can also be made, that deal with the statistics of level spacings in the two types of levels, with correlation functions, the nodal patterns of the wavefunctions, behaviour under collision conditions, the statistical properties of the Wigner phase-space distributions associated with the two kinds of states, etc.

Several specific systems have been theoretically examined and have shown this kind of distinction to exist. Much of the concern in this area has come from studies in intramolecular problems, primarily since molecules are small quantum dynamical systems and thus offer a possibility of experimental verification. It must however be mentioned that so far there have been no *unambiguous* experimental studies (in molecular spectroscopy, for example) that have been able to unequivocally identify the presence of these two contrasting types of quantum states.

A case in point is the recent experiment of Klemperer[23] on the high overtone spectroscopy of the HCN molecule. While the classical dynamics on the best available potential surfaces shows extensive regions of chaotic trajectories, the quantum energy levels, as measured by accurate spectroscopic means show no irregularities, or any of the properties associated with the irregular spectrum. The relevance of classical studies to an inherently quantum problem is not entirely clear, but it suggests that other factors, such as the role of the relative size of h, the Planck's constant, needs to be taken into account as well, in applying the correspondence principle.

Marcus and co-workers[21,24,25] have noted that several of the properties of the irregular spectrum could be ascribed to the existence of several near-degeneracies in the eigenvalue spectrum. Specifically, it was seen that the eigenvalue *vs* perturbation parameter plots for systems such as

$$H = (p_x^2 + p_y^2 + x^2 + y^2)/2 + \lambda(x^2 y - y^3/3) \qquad (10)$$

(which is the Hénon-Heiles system rewritten in terms of a perturbation parameter, λ) showed "avoided crossings" or "anti-crossings" rather than actual crossings. When two or more states are almost degenerate—when they undergo such avoided crossings, then it is to be expected that the irregular spectrum will ensue; the individual states lose their quantal identity as typified by the quantum numbers or the specific nodal patterns. This, however, is a heuristic picture of quantum chaos, although it has been seen to be true of most reported studies of quantum irregular behaviour (figure 6).

More recently, it has been suggested[26] that a better candidate for observing quantum chaos may be the system of a single electron bound to the surface of liquid helium by its (weak) electrostatic image charge. The removal of the electron from the surface by microwave radiation proceeds via chaotic classical mechanics, and thus

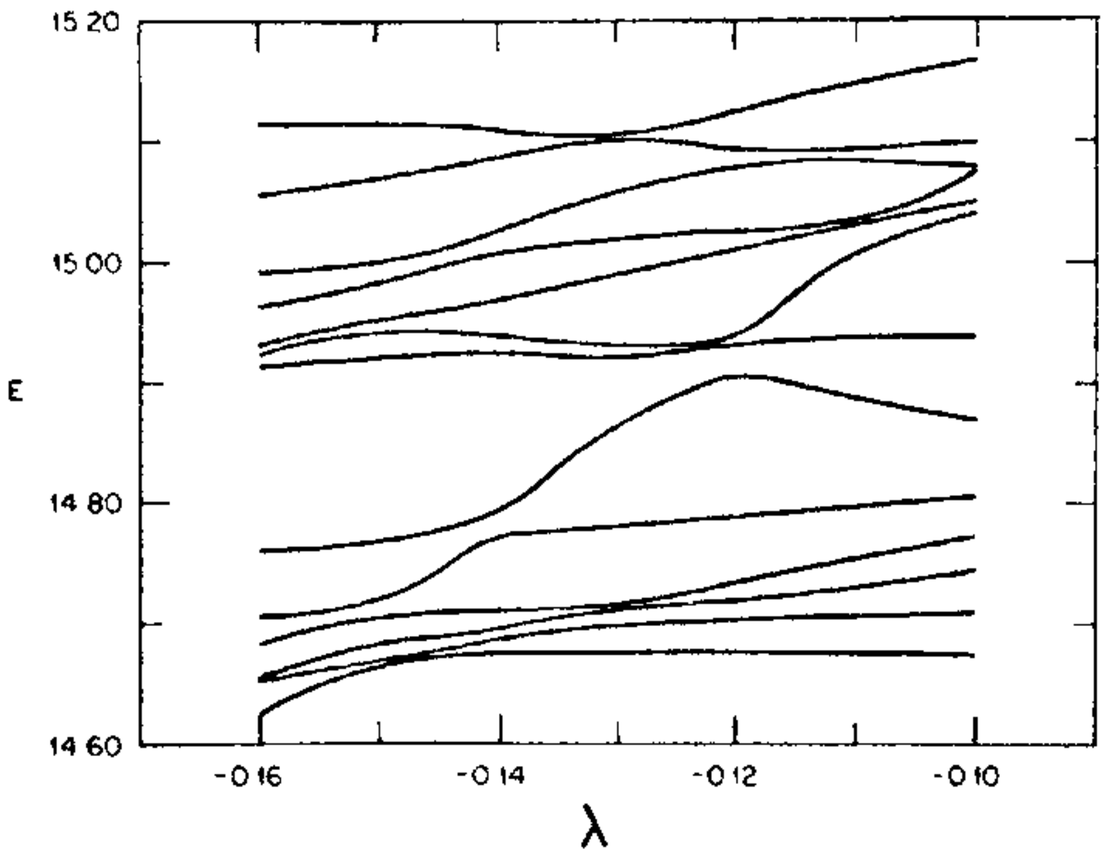

Figure 6. Plot of energy levels (eigenvalues) *vs.* perturbation parameter in a system similar to (10). Note the erratic variation of the eigenvalues with λ introduced by the existence of avoided crossings.

the actual (quantum) experiment could help to determine whether classical chaos does in fact have a well defined quantum parallel.

It should be clarified that in quantum mechanics indeterminacy is abundant—*viz* position-momentum uncertainty. This kind of indeterminacy, which is quite distinct from the quantum chaos discussed in this section, is intrinsic to the quantum nature of things. In the purely classical case, systems of arbitrary complexity can be constructed, such that the outcome of strictly deterministic equations of motion is apparently as random as may be desired. Whether a deterministic basis can in fact be provided for quantum uncertainty is not clear[6,27].

CONCLUSION

In this article a survey of some features of classical chaos in conservative dynamical systems, and one particular aspect of current research interest—quantum chaos—has been given. Necessarily, there are omissions since the scope of the general field of chaos is vast. Dissipative dynamical systems which find a wider range of applications have not been treated here. For these the classical theory, which is distinct from the conservative case, is well substantiated by a variety of experiments.

Nonlinearity, as has been illustrated above, often gives rise to complicated and unexpected behaviour. At the same time, nonlinearity is quite common, and by and large, a nonlinear system is also nonintegrable. The very ubiquity of non-integrable systems, and indeed that of chaos, therefore makes a detailed study of such phenomena imperative.

3 April 1984

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NEWS

ENVIRONMENTAL BIOINORGANIC CHEMISTRY

A tripartite US-Italy-China conference on environmental bioinorganic chemistry, took place in San Miniato in June 1983. In addition, UK, Swiss and Swedish delegates were also present.

Major topics of the conference included pollution caused by heavy metals, in particular, by toxic and carcinogenic metals such as mercury, cadmium, lead and arsenic; environmental damage caused by radioactivity from nuclear plants or from the recycling of nuclear materials; environmental damage in the Mediterranean sea and other marine environments; and the problem of acid rain. The scientific bases of the toxicity of heavy metals in living organisms were also considered.

The main priorities of the conference were to correlate the directions of research, and encourage international cooperation between Italy, the US, China and other countries, since there is a great deal of concern for the protection of the environment and for the possible damage which can be caused by heavy metals. Within this context, it is necessary still to learn a great deal about the chemical basis of toxicity, *i.e.* the chemical reactions that lead to inflammation, cell degeneration and irreversible damage to the nervous system. Such problems are aggravated by the fact that different animals respond in different ways to toxic stress. For example, the mouse eliminates arsenic in a different way from the rabbit. This is because the mouse has a blood protein that can coordinate directly with arsenic and can then eliminate it through normal blood exchange.

Genetically manipulated algae and bacteria can be designed to remove copper, nickel, silver and uranium very efficiently. Progress is being made in increasing the selectivity of particular metals. Work at Berkeley has resulted in complexing agents that can selectively remove extraneous metals from living organisms and radioactive metals from blood.

Another objective in environmental management is the control of salinity which, for example, has been studied both in Padua and Sheffield. Such environmental problems have major economic repercussions. It has been argued for example, that if international industry could invest 2 per cent of its turnover in the recuperation and recycling of dangerous substances, the final benefit to society would be at least 10 times greater than the initial investment.

The Conference was sponsored by the Italian National Council for Research, and the National Science Foundation of Washington. One of its main aims was to correlate directions of research between the three main countries involved so that the wastage of the scarce manpower and funding way be avoided in the future. (*Chemistry in Britain, December 1983, p. 1016*).