Kolmogorov Pathways from Integrability to Chaos and Beyond

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Abstract. Two limits of Newtonian mechanics were worked out by Kolmogorov. On one side it was shown that in a generic integrable Hamiltonian system, regular quasi-periodic motion persists when a small perturbation is applied. This result, known as Kolmogorov-Arnold-Moser (KAM) theorem, gives mathematical bounds for integrability and perturbations. On the other side it was proven that almost all numbers on the interval between zero and one are uncomputable, have positive Kolmogorov complexity and, therefore, can be considered as random. In the case of nonlinear dynamics with exponential (i.e. Lyapunov) instability this randomnesss, hidden in the initial conditions, rapidly explodes with time, leading to unpredictable chaotic dynamics in a perfectly deterministic system. Fundamental mathematical theorems were obtained in these two limits, but the generic situation corresponds to the intermediate regime between them. This intermediate regime, which still lacks a rigorous description, has been mainly investigated by physicists with the help of theoretical estimates and numerical simulations. In this contribution we outline the main achievements in this area with reference to specific examples of both low-dimensional and high-dimensional dynamical systems. We shall also discuss the successes and limitations of numerical methods and the modern trends in physical applications, including quantum computations.

1 A General Perspective

At the end of the 19^{th} century H. Poincaré rigorously showed that a generic Hamiltonian system with few degrees of freedom described by Newton's equations is not integrable [1]. It was the first indication that dynamical motion can be much more complicated than simple regular quasi–periodic behavior. This result puzzled the scientific community, because it is difficult to reconcile it with Laplace determinism, which guarantees that the solution of dynamical equations is uniquely determined by the initial conditions. The main developments in this direction came from mathematicians; they were worked out only in the middle of 20^{th} century by A.N. Kolmogorov and his school. In the limiting case of regular integrable motion they showed that a generic nonlinear pertubation does not destroy integrability. This result is nowadays

R. Livi, S, Ruffo, and D. Shepelyansky, Kolmogorov Pathways from Integrability to Chaos and Beyond, Lect. Notes Phys. **636**, 3–32 (2003)
http://www.springerlink.com/

formulated in the well–known Kolmogorov–Arnold–Moser (KAM) theorem [2]. This theorem states that invariant surfaces in phase space, called tori, are only slightly deformed by the perturbation and the regular nature of the motion is preserved. The rigorous formulation and proof of this outstanding theorem contain technical difficulties that would require the introduction of refined mathematical tools. We cannot enter in such details here. In the next we shall provide the reader a sketch of this subject by a simple physical illustration. More or less at the same time, Kolmogorov analyzed another highly nontrivial limit, in which the dynamics becomes unpredictable, irregular or, as we say nowadays, *chaotic* [3]. This was a conceptual breakthrough, which showed how unexpectedly complicated the solution of simple deterministic equations can be. The origin of chaotic dynamics is actually hidden in the initial conditions. Indeed, according to Kolmogorov and Martin-Löf [3,4], almost all numbers in the interval $[0, 1]$ are uncomputable. This means that the length of the best possible numerical code aiming at computing n digits of such a number increases proportionally to n, so that the number of code lines becomes infinite in the limit of arbitrary precision. For a given n, we can define the number of lines l of the program that is able to generate the bit string. If the limit of the ratio l/n as $n \to \infty$ is positive, then the bit string has positive Kolmogorov complexity. In fact, in real (computer) life we work only with computable numbers, which have zero Kolmogorov complexity and zero–measure on the [0,1] interval. On the other hand, Kolmogorov numbers contain infinite information and their digits have been shown to satisfy all tests on randomness. However, if the motion is stable and regular, then this randomness remains confined in the tails of less significant digits and it has no practical effect on the dynamics. Conversely, there are systems where the dynamics is unstable, so that close trajectories separate exponentially fast in time. In this case the randomness contained in the far digits of the initial conditions becomes relevant, since it extends to the more significant digits, thus determining a chaotic and unpredictable dynamics. Such chaotic motion is robust with respect to generic smooth perturbations [5]. A well known example of such a chaotic dynamics is given by the Arnold "cat" map

$$\begin{aligned} x_{t+1} &= x_t + y_t \mod 1 \\ y_{t+1} &= x_t + 2y_t \mod 1 \ , \end{aligned} \tag{1}$$

where x and y are real numbers in the $[0, 1]$ interval, and the subscript $t = 0, 1, \ldots$ indicates discrete time. The transformation of the cat's image after six iterations is shown in Fig. 1. It clearly shows that the cat is chopped in small pieces, that become more and more homogeneously distributed on the unit square. Rigorous mathematical results for this map ensure that the dynamics is ergodic and mixing [6,7]. Moreover, it belongs to the class of K-systems, which exhibit the K-property, i.e. they have positive Kolmogorov-Sinai entropy [8–10]. The origin of chaotic behavior in this map is related to the exponential instability of the motion, due to which the distance $\delta r(t)$

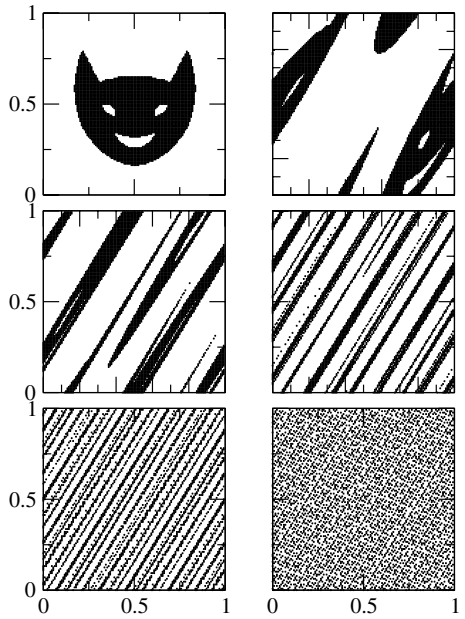

Fig. 1. Arnold "cat" map: six iterations of map (1) from left to right and from top to bottom

between two initially close trajectories grows exponentially with the number of iterations t as

$$\delta r(t) \sim \exp(ht)\ \delta r(0). \tag{2}$$

Here, h is the Kolmogorov-Sinai (KS) entropy (the extension of these concepts to dynamical systems with many degrees of freedom will be discussed in Sect. 5). For map (1) one proves that $h = \ln[(3+\sqrt{5})/2] \approx 0.96$ so that for $\delta r(0) \sim O(10^{-16})$, approximately at $t = 40$, $\delta r(40) \sim O(1)$. Hence, an orbit iterated on a Pentium IV computer in double precision will be completely different from the ideal orbit generated by an infinite string of digits defining the initial conditions with infinite precision. This implies that different computers will simulate different chaotic trajectories even if the initial conditions are the same. The notion of sensitive dependence on initial conditions, expressed in (2), is due to Poincaré [11] and was first emphasized in numerical experiments in the seminal papers by Lorenz [12], Zaslavsky and Chirikov [13] and Henon-Heiles [14]. However, the statistical, i.e. average, properties associated with such a dynamics are robust with respect to small perturbations [5]. It is worth stressing that this rigorous result does not apply to non–analytic perturbations in computer simulations due to round–off errors. Nonetheless, all experiences in numerical simulations of dynamical chaos confirm the stability of statistical properties in this case as well, even if no mathematical rigorous proof exists. Physically, the appearance of statistical properties is related to

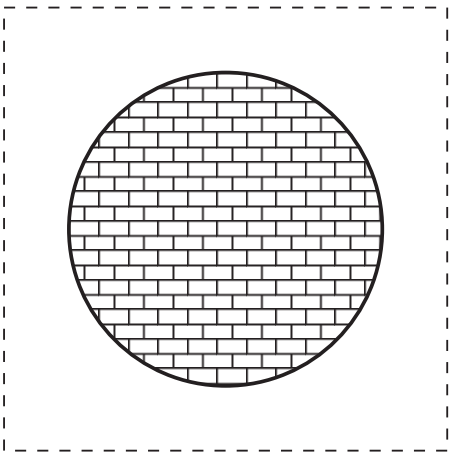

Fig. 2. Sinai billiard: the disc is an elastic scatterer for a point mass particle which freely moves between collisions with the disc. The dashed contour lines indicate periodic boundary conditions: a particle that crosses them on the right (*top*) reappears with the same velocity on the left (*bottom*) (the motion develops topologically into a torus)

the decay in time of correlation functions of the dynamical variables, which for map (1) is exponential.

These results are the cornerstones of the origin of statistical behavior in deterministic motion, even for low–dimensional dynamical systems. However, a K-system (like Arnold cat map (1)) is not generic. Significant progress towards the description of generic physical systems was made by Sinai [15], who proved the K-property for the billiard shown in Fig. 2. It was also proved by Bunimovich [16] that the K-property persists also for "focusing" billiards, like the stadium (see Fig. 3). However, physics happens to be much richer than basic mathematical models. As we will discuss in the following sections, the phase space of generic dynamical systems (including those with many degrees of freedom) contains intricately interlaced chaotic and regular components. The lack of rigorous mathematical results in this regime left a broad possibility for physical approaches, involving analytical estimates and numerical simulations.

2 Two Degrees of Freedom: Chirikov's Standard Map

A generic example of such a chaotic Hamiltonian system with divided phase-space is given by the Chirikov standard map [17,18]:

$$I_{t+1} = I_t + K\sin(\theta_t)\ ;\ \ \theta_{t+1} = \theta_t + I_{t+1}\ \ (\mathrm{mod}\ \ 2\pi)\ . \tag{3}$$

In this area-preserving map the conjugated variables (I, θ) represent the action I and the phase θ. The subscript t indicates time and takes non-negative

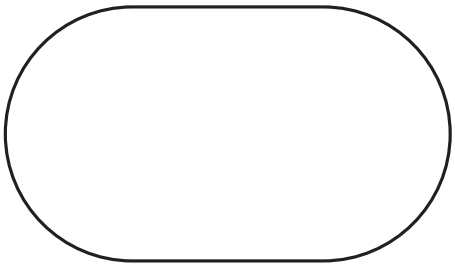

Fig. 3. Bunimovich or "stadium" billiard: the boundary acts as an elastic wall for colliding point mass particles, which otherwise move freely

integer values $t = 0, 1, 2, \ldots$. This mapping can be derived from the motion of a mechanical system made of a planar rotor of inertia M and length l that is periodically kicked (with period τ) with an instantaneous force of strength K/l. Angular momentum I will then vary only at the kick, the variation being given by $\Delta I = (K/l)l \sin\theta$, where θ is the in-plane angle formed by the rotor with a fixed direction when the kick is given. Solving the equations of motion, one obtains map (3) by relating the motion after the kick to the one before (having put $\tau/M = 1$). Since this is a forced system, its energy could increase with time, but this typically happens only if the perturbation parameter K is big enough. Map (3) displays all the standard behaviors of the motion of both one-degree-of-freedom Hamiltonians perturbed by an explicit time-dependence (so-called 1.5 degree of freedom systems) and two-degree-of-freedom Hamiltonians. The extended phase-space has dimension three in the former case and four in the latter. The phase-space of map (3) is topologically the surface of a cylinder, whose axial direction is along I and extends to infinity, and whose orthogonal direction, running along circumferences of unit radius, displays the angle θ. For $K = 0$ the motion is integrable, meaning that all trajectories are explicitly calculable and given by $I_t = I_0, \theta_t = \theta_0 + tI_0 (mod\ \ 2\pi)$. If $I_0/2\pi$ is the rational p/q (with p and q integers), every initial point closes onto itself at the q-th iteration of the map, i.e. it generates a periodic orbit of period q. A special case is $I_0 = 0$, which is a line made of an infinity of fixed points, a very degenerate situation indeed. All irrationals $I_0/(2\pi)$, which densely fill the I axis, generate quasi-periodic orbits: As the map is iterated, the points progressively fill the line $I = const.$ Hence, at $K = 0$ the motion is periodic or quasi-periodic. What happens if a small perturbation is switched on, i.e. $K \neq 0$, but small? This is described by two important results: the Poincaré-Birkhoff fixed point theorem (see Chap. 3.2b of [19]) and the Kolmogorov-Arnold-Moser (KAM) theorem [2](see also the contribution by A. Celletti et al. in this volume).

The Poincaré-Birkhoff theorem states that the infinity of periodic orbits issuing from rational $I_0/(2\pi)$ values collapse onto two orbits of period q, one stable (elliptic) and the other unstable (hyperbolic). Around the stable orbits,

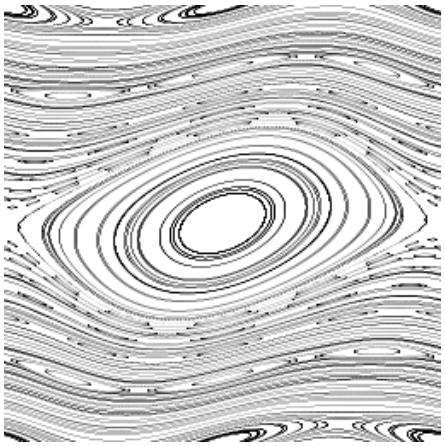

Fig. 4. Phase-space of the Chirikov standard map (3) in the square $(2\pi \times 2\pi)$ for $K = 0.5$

"islands" of stability form, where the motion is quasi-periodic. The biggest of such islands is clearly visible in Fig. 4 and has at the center the elliptic fixed point $(I = 0, \theta = \pi)$ which originates from the degenerate line of fixed points $I = 0$ as soon as $K \neq 0$.

The KAM theorem states that most of the irrational $I_0/2\pi$ initial values generate, at small K, slightly deformed quasi-periodic orbits called KAM-tori. Traces of the integrability of the motion survive the finite perturbations. Since irrationals are dense on a line, this is the most generic situation when K is small. This result has been transformed into a sort of paradigm: slight perturbations of an integrable generic Hamiltonian do not destroy the main features of integrability, which are represented by periodic or quasi-periodic motion. This is also why the KAM result was useful to Chirikov and coworkers to interpret the outcome of the numerical experiment by Fermi, Pasta and Ulam, as we discuss in Sects. 3 and 4.

There is still the complement to the periodic and quasi-periodic KAM motion to be considered! Even at very small K, a tiny but non vanishing fraction of initial conditions performs neither a periodic nor a quasi-periodic motion. This is the motion that has been called "chaotic", because, although deterministic, it has the feature of being sensible to the smallest perturbations of the initial condition [11–14,18].

Let us summarize all of these features by discussing the phase-space structure of map (3), as shown for three different values of K: $K = 0.5$ (Fig. 4), $K = K_g = 0.971635\ldots$ (Fig. 5) and $K = 2.0$ (Fig. 6).

For $K = 0.5$, successive iterates of an initial point θ_0, I_0 trace lines on the plane. The invariant curves $I = \text{const}$, that fill the phase-space when $K = 0$, are only slightly deformed, in agreement with the KAM theorem. A region foliated by quasi-periodic orbits rotating around the fixed point

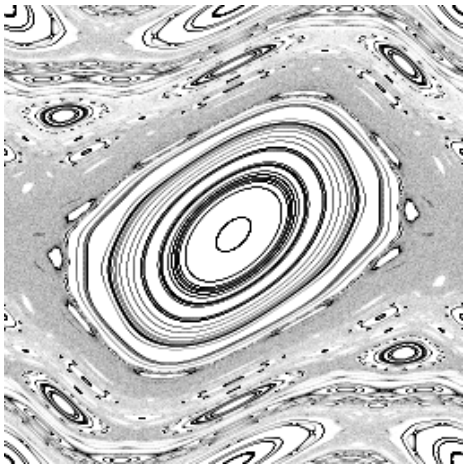

Fig. 5. Same as Fig. 4 for $K = K_g = 0.971635...$

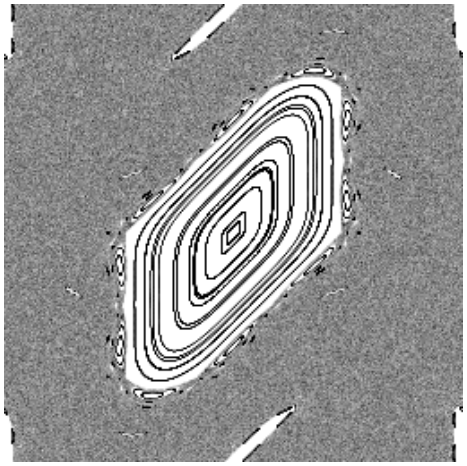

Fig. 6. Same as Fig. 4 for $K = 2$

$(I = 0, \theta = \pi)$ appears; it is called "resonance". Resonances of higher order appear around periodic orbits of longer periods. Their size in phase-space is smaller, but increases with K. Chaos is bounded in very tiny layers. Due to the presence of so many invariant curves, the dynamics in I remains bounded. Physically, it means that although work is done on the rotor, its energy does not increase. A distinctive quantity characterizing a KAM torus is its rotation number, defined as

$$r = \lim_{t\to\infty} \frac{\theta_t - \theta_0}{2\pi t} \ . \tag{4}$$

One can readily see that it equals the time averaged action $< I_t/(2\pi) >_t$ of the orbit, and its number theoretic properties, namely its "irrationality", are central to the dynamical behavior of the orbit. Numerical simulations indicate that for model (3) the most robust KAM torus corresponds to the "golden mean" irrational rotation number $r = r_g = (\sqrt{5}-1)/2$. Let us recall some number theoretic properties. Let a_i be positive integers and denote by

$$\cfrac{1}{a_1 + \cfrac{1}{a_2 + \cdots}} \equiv [a_1, a_2, \dots] \tag{5}$$

the continued fraction representation of any real number smaller than one. It turns out that r_g contains the minimal positive integers in the continued fraction, $r_g = [1, 1, 1, \dots]$. Indeed, this continued fraction can be resummed by solving the algebraic equation $r_g^{-1} = 1 + r_g$, which clearly has two solutions that correspond to two maximally robust KAM tori. The "golden mean" rotation number r_g corresponds to the "most irrational" number; in some nontrivial sense, it is located as far as possible from rationals. Rational winding numbers correspond to "resonances", and are the major source of perturbation of KAM curves. It is possible to study numerically the stability of periodic orbits with the Fibonacci approximation to the golden mean value $r_n = p_n/q_n \to r_g$ with $q_n = 1, 2, 3, 5, 8, 13 \dots$ and $p_n = q_{n-1}$. This approach has been used by Greene and MacKay and it has allowed them to determine the critical value of the perturbation parameter $K_g = 0.971635...$ at which the last invariant golden curve is destroyed [20,21]. The phase-space of map (3) at $K = K_g$ is shown in Fig. 5. It is characterized by a hierarchical structure of islands of regular quasi-periodic motion centered around periodic orbits with Fibonacci winding number surrounded by a chaotic sea. Such a hierarchy has been fully characterized by MacKay [21] for the Chirikov standard map using renormalization group ideas. A similar study had been conducted by Escande and Doveil [22] for a "paradigm" 1.5-degrees of freedom Hamiltonian describing the motion of a charged particle in two longitudinal waves. Recently, these results have been made rigorous[23], by implementing methods very close to the Wilson renormalization group [24].

For $K > K_g$ the last KAM curve is destroyed and unbounded diffusion in I takes place. With the increase of K, the size of stable islands decreases (see Fig. 6) and for $K \gg 1$, the measure of integrable components becomes very small. In this regime of strong chaos the values of the phases between different map iterations become uncorrelated and the distribution function $f(I)$ of trajectories in I can be approximately described by a Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \frac{D}{2}\frac{\partial^2 f}{\partial I^2} \ , \tag{6}$$

where $D =< (I_{t+1} - I_t)^2 >_t$ is the diffusion constant. For $K \gg 1$, $D \approx K^2/2$ (so-called quasi-linear theory). Thus, due to chaos, deterministic motion can

be described by a statistical diffusive process. As a result, the average square action grows linearly with the number of iterations $< I_t^2 >= I_0^2 + Dt$ for large t.

From the analytical viewpoint the onset of chaos described above has been first obtained by Chirikov on the basis of the resonance-overlap criterion [25]. Let us come back to the representation of the Chirikov standard map in terms of the equations of motion of the Hamiltonian of the kicked rotor

$$H(I,\theta,t) = I^2/2 + K\cos\theta \sum_m \delta(t-m) = I^2/2 + K\sum_m \cos(\theta - 2\pi m t) \ , \tag{7}$$

where $\delta(t)$ is the Dirac δ-function and the sum represents the action of the periodic kicks. The expansion of the periodic δ-function in Fourier series leads to the second expression for the Hamiltonian (7), where the sum runs over all positive/negative integers m. This second form of the Hamiltonian clearly shows the importance of resonances, where the derivative of the phase θ is equal to the external driving frequency $\dot{\theta} = I_m = 2\pi m$. Assuming that the perturbation is weak ($K \ll 1$), we obtain that, in the vicinity of the resonant value of the action, the dynamics is approximately described by the Hamiltonian of a pendulum $H_p = (I-I_m)^2/2 + K\cos\phi$ where $\phi = \theta - 2\pi m t$ is the resonant phase (with respect to the usual pendulum, this one has gravity pointing upward). Indeed, in the first approximation, all non-resonant terms can be averaged out so that the slow motion in the vicinity of I_m becomes similar to the dynamics of a pendulum, given by the term with $m = 0$. The pendulum has two qualitatively different types of motion: phase rotations for an energy $H_p > K$ and phase oscillations for an energy $H_p < K$. In the phase-space (I,θ) these two motions are separated from each other by the separatrix curve $I - I_m = \pm 2\sqrt{K}\sin(\phi/2)$ which at $H_p = K$ starts from the unstable equilibrium point at $\phi = 0$. Thus, the size of the separatrix is, $\Delta\omega_r = \Delta I = 4\sqrt{K}$, while the distance between the resonances $\dot{\phi} = \Omega_m = 2\pi m$ is $\Omega_d = \Omega_{m+1} - \Omega_m = 2\pi$. Two close unperturbed nonlinear resonances overlap when the size of the resonance becomes larger than the distance between them, $\Delta\omega_r > \Omega_d$. Above this resonance-overlap border, a trajectory can move from one resonance to another and the motion becomes chaotic on large scale (as we have commented above, chaos is present even for the smaller K values, but it is restricted to thin layers). In the case of the map (3) this simple criterion gives the critical parameter $K_c = \pi^2/4 \approx 2.5$,larger than the real value $K_g = 0.971635...$ determined by the Greene method. In fact, this simple criterion does not take into account the effects of secondary order resonances and of the finite size of chaotic layers appearing around the separatrix. Considering both effects reduces the border approximately by a factor 2.5 [18]. Thus, in the final form, the Chirikov resonance-overlap criterion can be written as

$$K_c \approx 2.5(\Delta\omega_r/\Omega_d)^2 > 1 \ . \tag{8}$$

Invented by Chirikov in 1959, this physical criterion remains the main analytical tool for determining the chaos border in deterministic Hamiltonian systems. When Chirikov presented his criterion to Kolmogorov, the latter said: "one should be a very brave young man to claim such things!". Indeed, a mathematical proof of the criterion is still lacking and there are even known counterexamples of nonlinear systems with a hidden symmetry, such as the Toda lattice (see Chap. 1.3c of [19]), where the dynamics remains integrable for $K \gg K_c$. However, such systems with a hidden symmetry are quite rare and specific, while for generic Hamiltonian systems the criterion works nicely and determines very well the border for the onset of chaos. An extension and a deep understanding of Chirikov criterion in the renormalization group approach has allowed an improvement and its extensive application to systems with many degrees of freedom [26]. Chirikov resonance overlap criterion finds also applications in such diverse physical systems as particles in magnetic traps [25,18,27], accelerator physics [28], highly excited hydrogen atoms in a microwave field [29], mesoscopic resonance tunneling diodes in a tilted magnetic field [30].

In fact, the Chirikov standard map gives a local description of interacting resonances, assuming that resonance amplitudes slowly change with action I. This is the main reason why this map finds such diverse applications. For example, a modest modification of the kick function $f(\theta) = \sin\theta$ and the dispersion relation $\theta_{t+1} = \theta_t + {I_t}^{-3/2}$ in (3) is sufficient to give a description of the dynamics of the Halley's comet in the solar system [31].

For small perturbations, chaos initially appears in a chaotic layer around the separatrix of a nonlinear resonance. Some basic questions about the effects of nonlinear perturbations in the vicinity of the separatrix were first addressed by Poincaré [1], who estimated the angle of separatrix splitting. The width of the chaotic layer was determined by Chirikov on the basis of the overlap criterion (8) in [17,18]. In fact, for small perturbations, *e.g.* K in map(3), the external frequency ω is much larger than the resonance oscillation frequency ω_0. In such a case, the relative energy w of a trajectory randomly fluctuates inside the chaotic separatrix layer whose width is exponentially small, *e.g.* for the map (3) $|w| < w_s \approx 8\pi\lambda^3 \exp(-\pi\lambda/2)$, where $\lambda = \omega/\omega_0 = 2\pi/\sqrt{K} \gg 1$. Even for $K = 0.5$ the width of the layer is very small and it is hardly visible in Fig. 4 ($w_s \approx 0.015$). It is interesting to note that the dynamics inside the chaotic layer is described by a simple separatrix map, which is similar to the map (3): $y_{t+1} = y_t + \sin x_t, x_{t+1} = x_t - \lambda \ln|y_{t+1}|$ where $y = \lambda w/w_s$ and x is the phase of the rotation [18]. The width of the separatrix layer increases with K as well as the size of primary and secondary resonances. At some critical value K_c the last invariant curve becomes critical. For map (3) $K_c = K_g = 0.971635....$ For $K > K_g$ the golden invariant curve is destroyed and it is replaced by an invariant Cantor set ("cantorus") which allows trajectories to propagate diffusively in action I. Rigorous mathematical results prove the existence of the cantori [32–34]. However, in spite of fundamental advances

in ergodic theory [6,7], a rigorous proof of the existence of a finite measure set of chaotic orbits for map (3) is still missing, even for specific values of K.

The absence of diffusion for small perturbations is typical of 1.5 and 2 degrees of freedom systems. For three or more degrees of freedom, resonances are no longer separated by invariant KAM curves and form a connected web that is dense in action space. Hence, chaotic motion along resonances can carry the orbit arbitrarily close to any region of the phase space compatible with energy conservation. This mechanism is called Arnold diffusion, since Arnold [35] first described its existence. Arnold diffusion is present also for negligible perturbations, but its rate becomes vanishingly small. A theoretical calculation of this rate was first performed by Chirikov[18] and later refined by several authors (see chapter 6 of [19] for a review). Beautiful illustrations of the Arnold web have been obtained by Laskar through the use of frequency analysis [36].

While the local structure of divided phase space is now well understood, the statistical properties of the dynamics remain unclear, in spite of the simplicity of these systems. Among the most important statistical characteristics is the decay of the time correlation function $C(\tau)$ in time and the statistics of Poincaré recurrences $P(\tau)$. The latter is defined as $P(\tau) = N_\tau/N$, where N_τ is the number of recurrences in a given region with recurrence time $t > \tau$ and N is the total number of recurrences. According to the Poincaré theorem (for an easy illustration see Chap. 7.1.3 of [37]), an orbit of a Hamiltonian system always returns sufficiently close to its initial position. However, the statistics of these recurrences depends on the dynamics and is different for integrable and chaotic motion. In the case of strong chaos without any stability islands (e.g. the Arnold cat map (1)), the probability $P(\tau)$ decays exponentially with τ. This case is similar to the coin flipping, where the probability to stay head for more than τ flips decays exponentially. The situation turns out to be different for the more general case of the dynamics inside the chaotic component of an area-preserving map with divided phase space. Studies of $P(\tau)$ for such a case showed that, at a large times, recurrences decay with a power law $P(\tau) \propto 1/\tau^p$ with an exponent $p \approx 1.5$ (see [38] and Fig. 7). Investigations of different maps also indicated approximately the same value of p, even if it was remarked that p can vary from map to map, and that the decay of $P(\tau)$ can even oscillate with $\ln \tau$. This result is of general importance. It can also be shown that it determines the correlation function decay $C(\tau)$ via the relation $C(\tau) \propto \tau P(\tau)$. The statistics of $P(\tau)$ is also well suited for numerical simulations, due to the natural property $P(\tau) > 0$ and to its statistical stability. Such a slow decay of Poincaré recurrences is related to the sticking of a trajectory near a critical KAM curve, which restricts the chaotic motion in phase space [38]. Indeed, when approaching the critical curve with the border rotation number r_g , the local diffusion rate D_n goes to zero as $D_n \sim |r_g - r_n|^{\alpha/2} \sim 1/q_n^\alpha$ with $\alpha = 5$, where $r_n = p_n/q_n$ are the rational convergents for r_g as determined by the continued fraction expansion. The theoretical value $\alpha = 5$ follows from a resonant theory of critical

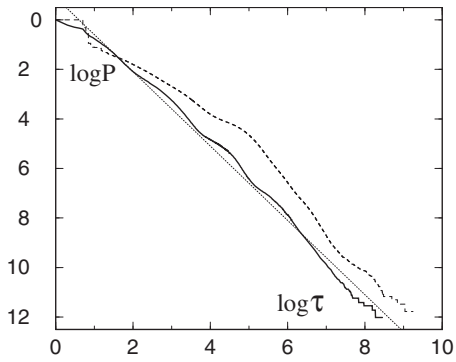

Fig. 7. Poincaré recurrences $P(\tau)$ in the Chirikov standard map (3) at $K = K_g$ (*dashed curve*) and in the separatrix map (see text) with the critical golden boundary curve at $\lambda = 3.1819316$ (*full curve*). The return line is $I = y = 0$. The *dotted straight line* shows the power-law decay $P(\tau) \propto 1/\tau^p$ with $p = 1.5$. [From [38]]

invariant curves [21,38] and is confirmed by numerical measurements of the local diffusion rate in the vicinity of the critical golden curve in the Chirikov standard map [39]. Such a decrease of the diffusion rate near the chaos border would give the exponent $p = 3$, if everything was determined by the local properties of principal resonances p_n/q_n. However, the value $p = 3$ is significantly different from the numerically found value $p \approx 1.5$ (see [38,40] and Fig. 7). At the same time, the similarity of the decay of $P(\tau)$ in two very different maps with critical golden curves is in favor of the universal decay of Poincaré recurrences; it is possible that the expected value $p = 3$ will be reached at very large τ.

3 Many Degrees of Freedom: The Numerical Experiment of Fermi, Pasta, and Ulam

At the beginning of the 50's one of the first digital computers, MANIAC 1, was available at Los Alamos National Laboratories in the US. It had been designed by the mathematician J. von Neumann for supporting investigations in several research fields, where difficult mathematical problems could not be tackled by rigorous proofs[1]. Very soon, Enrico Fermi realized the great potential of this revolutionary computational tool for approaching some basic physical questions, that had remained open for decades. In particular, MANIAC 1 appeared to be suitable for analyzing the many aspects of nonlinear problems, that could not be accessible to standard perturbative methods. Thanks to his deep physical intuition, Fermi pointed out a crucial problem,

[1] It should be mentioned that MANIAC 1 was mainly designed for supporting research in nuclear physics, which yielded the production of the first atomic bomb.

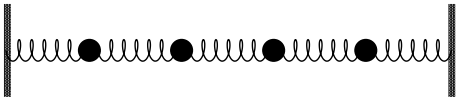

Fig. 8. The FPU chain of oscillators coupled by nonlinear springs

that had been raised already in 1914 by the dutch physicist P. Debye. He had suggested that the finiteness of thermal conductivity in crystals should be due to the nonlinearities inherent in the interaction forces acting among the constituent atoms. Although experimental results seemed to support such a conjecture, a convincing explanation based on a microscopic theory was still lacking fourty years later[2]. In collaboration with the mathematician S. Ulam and the physicist J. Pasta, Fermi proposed to integrate, on the MANIAC 1 the dynamical equations of the simplest mathematical model of an anharmonic crystal: a chain of harmonic oscillators coupled by nonlinear forces (see Fig. 8). In practice, this is described by a classical Hamiltonian of the form

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{\omega^2}{2}(q_{i+1} - q_i)^2 + \frac{\nu}{n}(q_{i+1} - q_i)^n, \tag{9}$$

where the integer space index i labels the oscillators, whose displacements with respect to equilibrium positions and momenta are q_i and p_i, respectively. The integer exponent $n > 2$ identifies the nonlinear potential, whose strength is determined by the coupling parameter ν. For the sake of simplicity, Fermi, Pasta and Ulam considered the cases $n = 3, 4$, with ν denoted as α and β, respectively (from which the names "α" and "β" models).

The complex interactions among the constituent atoms or molecules of a real solid are reduced to harmonic and nonlinear springs, acting between nearest-neighbor equal–mass particles. Nonlinear springs apply restoring forces proportional to the cubic or quartic power of the elongation of particles from their equilibrium positions[3]. Despite such simplifications, the basic ingredients that one can reasonably conjecture to be responsible for the main physical effect (i.e. the finiteness of thermal conductivity) had been taken into account in the model.

In this form the problem was translated into a program containing an integration algorithm that MANIAC 1 could efficiently compute. It should be stressed that further basic conceptual implications of this numerical experiment were known from the very beginning to Fermi and his collaborators.

[2] Only recently further progress has been made in the understanding of the role of nonlinearity and disorder, together with spatial constraints, in determining transport properties in models of solids and fluids; for a review see [41].

[3] These simplifications can be easily justified by considering that any interaction between atoms in a crystal can be well approximated by such terms, for amplitudes of atomic oscillations much smaller than the interatomic distance: this is the typical situation for real solids at room temperature and pressure.

In fact, they also expected to verify a common belief that had never been amened to a rigorous mathematical proof: In an isolated mechanical system with many degrees of freedom (i.e. made of a large number of atoms or molecules), a generic nonlinear interaction among them should eventually yield equilibrium through "thermalization" of the energy. On the basis of physical intuition, nobody would object to this expectation if the mechanical system starts its evolution from an initial state very close to thermodynamic equilibrium. Nonetheless, the same should also be observed for an initial state where the energy is supplied to a small subset of oscillatory modes of the crystal; nonlinearities should make the energy flow towards all oscillatory modes, until thermal equilibrium is eventually reached. Thermalization corresponds to energy equipartition among all the modes[4]. In physical terms, this can be considered as a formulation of the "ergodic problem". This was introduced by the austrian physicist L. Boltzmann at the end of the 19^{th} century to provide a theoretical explanation of the apparently paradoxical fact, namely that

the time–reversible microscopic dynamics of a gas of hard spheres should naturally evolve on a macroscopic scale towards thermodynamic equilibrium, thus yielding the "irreversible" evolution compatible with the second principle of thermodynamics.

In this perspective, the FPU[5] numerical experiment was intended to test also if and how equilibrium is approached by a relatively large number of nonlinearly coupled oscillators, obeying the classical laws of Newtonian mechanics. Furthermore, the measurement of the time interval needed for approaching the equilibrium state, i.e. the "relaxation time" of the chain of oscillators, would have provided an indirect determination of thermal conductivity[6].

In their numerical experiment FPU considered relatively short chains, up to 64 oscillators[7], with fixed boundary conditions.[8] The energy was initially stored in one of the low, i.e. long–wavelength, oscillatory modes.

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[4] The "statistical" quality of this statement should be stressed. The concept of energy equipartition implies that the time average of the energy contained in each mode is constant. In fact, fluctuations prevent the possibility that this might exactly occur at any instant of time.

[5] In the following we shall use the usual acronym for Fermi-Pasta-Ulam.

[6] More precisely, according to Boltzmann's kinetic theory, the relaxation time τ_r represents an estimate of the time scale of energy exchanges inside the crystal: Debye's argument predicts that thermal conductivity κ is proportional to the specific heat at constant volume of the crystal, C_v, and inversely proportional to τ_r, in formulae $\kappa \propto C_v/\tau_r$.

[7] Such sizes were already at the limit of computational performances of MANIAC 1, whose execution speed was much smaller than a modern home pc.

[8] The particles at the chain boundaries are constrained to interact with infinite mass walls, see Fig. 8.

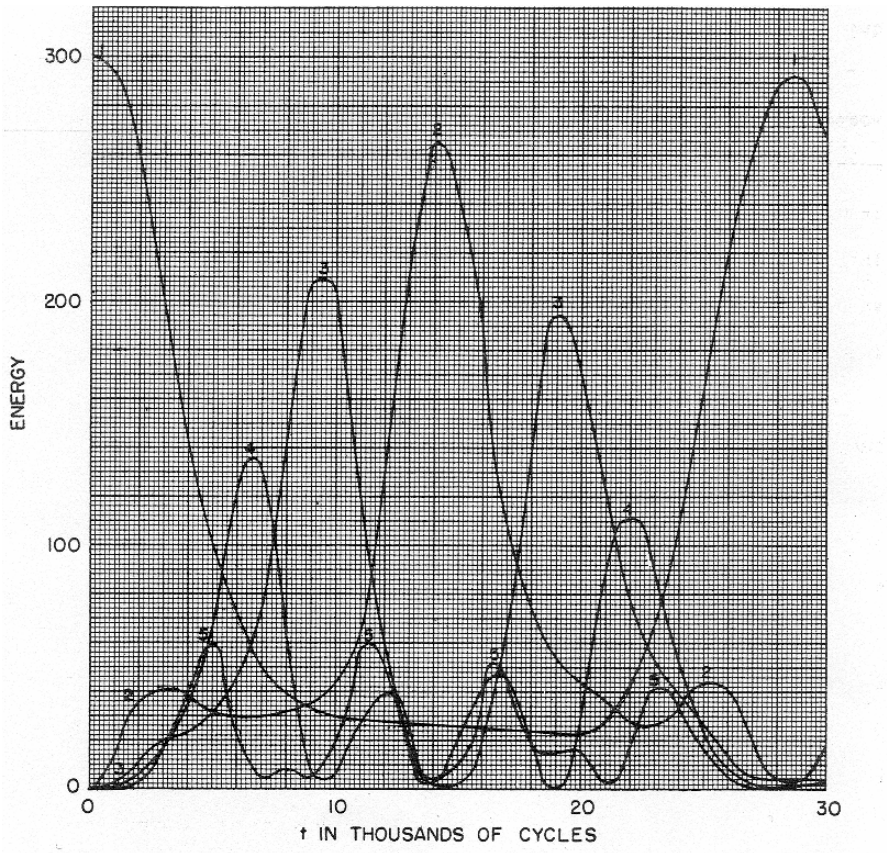

Fig. 1. The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. N = 32; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

Fig. 9. Energy recurrence in the first 5 Fourier modes in the FPU α model. The figure is taken from [44]

Surprisingly enough, the expected scenario did not appear. Contrary to any intuition the energy did not flow to the higher modes, but was exchanged only among a small number of low modes, before flowing back almost exactly to the initial state, yielding the recurrent behavior shown in Fig. 9.

Even though nonlinearities were at work neither a tendency towards thermalization, nor a mixing rate of the energy could be identified. The dynamics exhibited regular features very close to those of an integrable system.

Almost at the same time as this numerical experiment, A.N. Kolmogorov outlined the first formulation of the KAM theorem (see Sect. 2). FPU

certainly were not aware of his achievement, that indicated that all regular features of the dynamics are kept by integrable hamiltonian systems subject to a small enough perturbation. This could have guided the authors to realize that the nonlinear effects were too small a perturbation of the integrable harmonic chain to prevent regular motion. A deeper understanding of the implications of the FPU experiment on ergodicity and KAM theorem had to wait for more than one decade, for the numerical experiment of Izrailev and Chirikov [42] and Chirikov's overlap criterion [43] (see also Sect. 5).

It should be mentioned that Fermi was quite disappointed by the difficulties in finding a convincing explanation, thus deciding not to publish the results. They were finally published in 1965, one decade after his death, in a volume containing his Collected Papers [44]. The FPU report is probably the most striking example of a crucial achievement which never appeared as a regular paper in a scientific journal, but which, nonetheless, has been a major source of inspiration for future developments in science. Actually, while the understanding of the mechanisms of relaxation to equilibrium and ergodicity mainly concerned the later efforts of european scientists, some american researchers concentrated their attention in trying to interpret the regular motion of the FPU chain in a different way. The first contribution came from a seminal paper by the M.D. Kruskal, a physicist at Princeton, and N.J. Zabusky, a mathematician at Bell Laboratories, in 1965 [45]. This was the starting point for the large physical literature on nonlinear lattice vibrations, that are nowadays called "solitons". In fact, Kruskal and Zabusky were interested in studying the continuum limit of the FPU chain. In particular, Zabusky later conjectured that the dynamical conditions investigated by FPU in their numerical experiment could be explained by an appropriate equation in the continuum limit [46]. This idea is quite natural, since the FPU experiment showed that when a long–wavelength, i.e. low–frequency, mode was initially excited, the energy did not flow towards the small–wavelength, i.e. high–frequency, modes. Since discreteness effects are associated with the latter modes, one can reduce the set of ordinary differential equations describing the chain to an effective partial differential equation that should provide a confident description of long–wavelength excitations. Actually, the continuum limit of the FPU chain was found to correspond to a Korteweg-deVries like equation[9]

$$u_t + \epsilon u^{n-2} u_x + \mu u_{xxx} = 0 \ , \tag{10}$$

where u is the spatial derivative of the displacement field once the right-going wave is selected, and n is the order of the nonlinearity in 9. Exact solutions of such equations can be explicitly found in the form of propagating nonlinear waves. The reader should take into account that the coefficients ϵ

[9] It should be mentioned that performing continuum limits of lattice equations is quite a delicate mathematical problem, as discussed in [47] and also, more recently, in [48]

and μ depend on crucial parameters of the model: the energy of the initial excitation, or, equivalently, the strength of the nonlinear force. For large strength or high energy, the "dispersive" term μu_{xxx} becomes negligible with respect to the nonlinear term $\epsilon u^{n-2} u_x$ and (10) reduces to the first two terms on the left hand side. This reduced partial differential equation has running wave solutions that become unstable after a specific time scale, so-called "shocks". This time scale can be estimated on the basis of the parameters appearing in the equation. Without entering into mathematical details, one can say that the reduced equation describes excitations similar to sea waves, which break their shape because the top of the wave propagates more rapidly than the bottom[10]. This analysis provides a convincing explantion for the FPU experiment. In fact, one can easily conclude that FPU performed their numerical simulations in conditions where the chain was well represented by (10), with a sufficiently large dispersion coefficient μ. Accordingly, the typical instabilities due to discreteness effects might have become manifest only after exceedingly long times, eventually yielding destruction of the regular motion. Moreover, this analysis is consistent with the (almost) contemporary findings of the numerical experiment by Izrailev and Chirikov [42], which show that at high energies or high nonlinearities, the regular motion is rapidly lost.

4 Energy Thresholds

An alternative explanation for the localization of the energy in a small portion of long–wavelength Fourier modes in the FPU chain can be obtained using the resonance–overlap criterion discussed in Sect. 2. It is worth pointing out that the same criterion provides a quantitative estimate of the value of the energy density above which regular motion is definitely lost.

In order to illustrate this interesting issue, we have to introduce some simple mathematical tools. Let us first recall that the Hamiltonian of the Fermi-Pasta-Ulam model (9) can be rewritten in linear normal Fourier coordinates (Q_k, P_k) (phonons)

$$H = \frac{1}{2} \sum_k \left(P_k^2 + \omega_k^2 Q_k^2 \right) + \beta V(\mathbf{Q}) \ , \tag{11}$$

where the nonlinear potential $V(\mathbf{Q})$, whose strength is determined by the coupling constant β[11], controls the energy exchange among the normal modes and ω_k is the the k-th phonon frequency (e.g. $\omega_k = 2\sin(\pi k/N)$ for periodic boundary conditions). The harmonic energy of the k-th normal mode is defined as $E_k = (P_k^2 + \omega_k^2 Q_k^2)/2$. If the energy H is small enough the time–averaged phonon energies $\bar{E}_k(T) = T^{-1} \int_0^T E_k(t) dt$ show an extremely

[10] A clear survey on this class of partial differential equations can be found in [50], Sects. 7 and 8. See also [49]

[11] We restrict ourselves to the quartic nonlinearity $n = 4$ in (9), hence $\nu \equiv \beta$

slow relaxation towards the equipartition state (defined by $E_k = const$) as T increases. On the contrary, at higher energies, the equipartition state is reached in a relatively short time. The presence of these qualitatively different behaviors when the energy is varied was in fact predicted by Chirikov and Izrailev [42] using the "resonance overlap" criterion. Let us give here just a brief sketch of the application of this criterion to the FPU β model. The corresponding Hamiltonian can be written in action-angle variables and, as an approximation, one can consider just one Fourier mode. In fact, this is justified at the beginning of the evolution, when most of the energy is still kept by the initially excited mode.

$$H = H_0 + \beta H_1 \approx \omega_k J_k + \frac{\beta}{2N} \left(\omega_k J_k\right)^2 \ , \tag{12}$$

where $J_k = \omega_k Q_k^2$ is the action variable. In practice, only the nonlinear self-energy of a mode is considered in this approximation. H_0 and H_1 are the unperturbed (integrable) Hamiltonian and the perturbation, respectively. Indeed $\omega_k J_k \approx H_0 \approx E$ if the energy is initially put in mode k. It is then easy to compute the nonlinear correction to the linear frequency ω_k, giving the renormalized frequency ω_k^r

$$\omega_k^r = \frac{\partial H}{\partial J_k} = \omega_k + \frac{\beta}{N}\omega_k^2 J_k = \omega_k + \Omega_k. \tag{13}$$

When $N \gg k$, then

$$\Omega_k \approx \frac{\beta H_0 k}{N^2}. \tag{14}$$

The "resonance overlap" criterion consists of verifying whether the frequency shift is on the order of the distance between two resonances:

$$\Delta\omega_k = \omega_{k+1} - \omega_k \approx N^{-1} \ , \tag{15}$$

(the last approximation being again valid only when $N \gg k$), i.e.

$$\Omega_k \approx \Delta\omega_k \ . \tag{16}$$

One obtains from this equation an estimate of ϵ_c, the "critical" energy density multiplied by β, above which sizeable chaotic regions develop and a fast diffusion takes place in phase space while favouring relaxation to equipartition. the form of ϵ_c is

$$\epsilon_c = \left(\frac{\beta H_0}{N}\right)_c \approx k^{-1} \ , \tag{17}$$

with $k = O(1) \ll N$. Summarizing, primary resonances are weakly coupled below ϵ_c and this in turn induces a slow relaxation process to equipartition.

Conversely, above ϵ_c, fast relaxation to equipartition is present, due to "primary resonance" overlap.

The presence of an energy threshold in the FPU–model separating different dynamical regimes was first identified numerically by Bocchieri et al. [51]. A numerical confirmation of the predictions of the resonance overlap criterion was obtained by Chirikov and coworkers [52]. Further confirmations came for more refined numerical experiments [53,54], showing that, for sufficiently high energies, regular behaviors disappear, while equipartition among the Fourier modes sets in rapidly. Later on [55], the presence of the energy threshold was characterized in full detail by introducing an appropriate Shannon entropy, which counts the number of effective Fourier modes involved in the dynamics (at equipartition this entropy is maximal). Around ϵ_c, the scaling with energy of the maximal Lyapunov exponent (see Sect. 5) also changes, revealing what has been called the "strong stochasticity threshold" [56]. Below ϵ_c, although primary resonances do not overlap, higher order resonances may, yielding a slower evolution towards equipartition [57,58]. The time scale for such an evolution has been found to be inversely proportional to a power of the energy density [59].

After having illustrated the main developments along the lines suggested by the resonance–overlap criterion, it is worth adding some further comments about the existence of an energy threshold, which separates the regular dynamics observed by FPU at low energies from the highly chaotic dynamical phase observed at higher energies.

In their pioneering contribution, Bocchieri and coworkers [51] were mainly concerned by the implications for ergodic theory of the presence of an energy threshold. In fact, the dynamics at low energies seems to violate ergodicity, although the FPU system is known to be chaotic. This is quite a delicate and widely debated issue for its statistical implications. Actually, one expects that a chaotic dynamical system made of a large number of degrees of freedom should naturally evolve towards equilibrium. We briefly summarize here the state of the art on this problem. The approach to equipartition below and above the energy threshold is just a matter of time scales, that actually turn out to be very different from each other. An analytical estimate of the maximum Lyapunov exponent λ (see Sect. 5) of the FPU problem [60] has pointed out that there is a threshold value, ϵ_T, of the energy density, $\epsilon = \beta H/N$, at which the scaling of λ with ϵ changes drastically:

$$\lambda(\epsilon) \sim \begin{cases} \epsilon^{1/4} & \text{if } \epsilon > \epsilon_T; \\ \epsilon^2 & \text{if } \epsilon < \epsilon_T. \end{cases} \tag{18}$$

This implies that the typical *relaxation time*, i.e. the inverse of λ, may become exceedingly large for very small values of ϵ below ϵ_T. It is worth stressing that this result holds in the thermodynamic limit, indicating that the different relaxation regimes represent a statistically relevant effect. To a high degree of confidence, it is found that ϵ_T in (18) coincides with ϵ_c in (17). A more controversial scenario has been obtained by thoroughly investigating

the relaxation dynamics for specific classes of initial conditions. When a few long–wavelength modes are initially excited, regular motion may persist over times much longer than $1/\lambda$ [57]. On the other hand, numerical simulations and analytic estimates indicate that any threshold effect should vanish in the thermodynamic limit [58,59,61]. An even more complex scenario is obtained when a few short-wavelength modes are excited: solitary wave dynamics is observed, followed by slow relaxation to equipartition [62]. It is worth mentioning that some regular features of the dynamics have been found to persist even at high energies (e.g., see [63]), irrespectively of the initial conditions. While such regularities can still play a crucial role in determining energy transport mechanisms [41], they do not significantly affect the robustness of the statistical properties of the FPU model in equilibrium at high energies. In this regime, the model exhibits highly chaotic dynamics, which can be quantified by the spectrum of characteristic Lyapunov exponents. A general description of these chaoticity indicators and their relation with the concept of "metric entropy", introduced by Kolmogorov, is the subject of the following section.

5 Lyapunov Spectra and Characterization of Chaotic Dynamics

The possibility that unpredictable evolution may emerge from deterministic equations of motion is a relatively recent discovery in science. In fact, a Laplacian view of the laws of mechanics had not taken into account such a possibility: the universality of these laws guaranteed that cosmic order should extend its influence down to human scale. The metaphore of divinity as a "clockmaker" was suggested by the regularity of planetary orbits and by the periodic appearance of celestial phenomena, described by the elegant mathematical language of analytical mechanics. Only at the end of the 19^{th} century did the french mathematician H. Poincaré realize that unpredictability is in order as a manifestation of the dynamical instability typical of mechanical systems described by a sufficiently large number of variables[12]. His studies on the stability of the three–body problem with gravitational interaction led him to introduce the concept of "sensitivity with respect to the initial conditions" (see also the contribution by A. Celletti et al. in this volume). He meant that two trajectories, whose initial conditions were separated by an infinitesimal difference, could yield completely different evolution after a suitable lapse of time. This finding is at the basis of what we nowadays call "deterministic chaos", which has been identified as a generic feature of a host of dynamical models of major interest in science and its applications. Here we do not aim at providing the reader a full account of the fascinating history of deterministic chaos. Many interesting books and articles for specialists and newcomers

[12] In fact, such a number is not that large: three independent dynamical variables are enough to allow for unpredictable evolution.

in science are available (for instance, an introductory survey to the subject can be found in [50,37]). We rather want to focus our attention on the crucial contribution of A.N. Kolmogorov in this field.

In order to fully appreciate Kolmogorov's achievements it is useful to discuss certain concepts, introduced for quantifying deterministic chaos. In a chaotic dynamical system two infinitesimally close trajectories, say at distance $\delta(0)$ at time $t = 0$, evolve in time by amplifying exponentially their distance, i.e. $\delta(t) \sim \delta(0) \exp \lambda t$. The exponential rate of divergence $\lambda > 0$ measures the degree of chaoticity of the dynamics. In an isolated dynamical system described by a finite number of variables, such an exponential increase cannot last forever, due to the finiteness of the available phase space. Nonetheless, Oseledec's multiplicative theorem [64] guarantees that, under quite general conditions, the following limit exists

$$\lambda = \lim_{t\to\infty} \lim_{\delta r(0)\to 0} \frac{1}{t} \ln \frac{\delta r(t)}{\delta r(0)} \ . \tag{19}$$

Accordingly λ can be interpreted as the "average" exponential rate of divergence of nearby trajectories, where the average is made over the portion of phase space accessible to the trajectory (see also (2)). It is worth stressing that this quantity is independent of the choice of the initial conditions, provided they belong to the same chaotic component of the phase space. More generally, in a deterministic system described by N dynamical variables or, as one should say, "degrees–of–freedom", it is possible to define a *spectrum of Lyapunov exponents*, λ_i with $i = 1, \cdots, N$, i.e. one for each degree–of–freedom. Conventionally, the integer i labels the exponents from the highest to the smallest one. The stability of a generic trajectory in a multi–dimensional space is, in principle, subject to the contribution of as many components as there are degrees of freedom. This is quite a difficult concept that requires a rigorous mathematical treatment, to be fully appreciated[13]. Intuitively, one can say that the sum $S_n = \sum_{i=1}^{n} \lambda_i$ measures the average exponential rates of expansion, or contraction, of a volume of geometric dimension n in phase space. Accordingly, $S_1 = \lambda_1 \equiv \lambda$ is equivalent to the definition (19), since a "1–dimensional volume" is a generic trajectory in phase space; $S_2 = \lambda_1 + \lambda_2$ gives the divergence rate of a surface; $S_N = \sum_{i=1}^{N} \lambda_i$ is the average divergence rate of the whole phase space. In dissipative dynamical systems, S_N is negative, so that the phase space volume is subject to a global contraction. Nonetheless, the presence of at least one positive Lyapunov exponent, $\lambda_1 > 0$, is enough for making the evolution chaotic: in this case, the trajectory approaches a *chaotic (strange) attractor*. For Hamiltonian systems, according to Liouville's theorem, any volume in phase space is conserved and $S_N = 0$; moreover, for each $\lambda_i > 0$ there exists $\lambda_{N-i} = -\lambda_i$[14]. In summary,

[13] For this purpose we refer the reader to [65].

[14] For each conserved quantity like energy, momentum etc., there is a pair of conjugated exponents that are zero. Stated differently, each conservation law amounts

chaotic evolution implies that a small region in phase space (for instance, the volume identifying the uncertainity region around an initial condition) is expanded and contracted with exponential rates along different directions in phase space. After a time on the order of $1/\lambda$ the distance between two infinitesimally close initial conditions will take the size of the accessible phase space: accordingly, we have no means of predicting where the image of an initial point will be in phase space, by simply knowing the image of an initially closeby point. An infinite precision in the determination of the initial conditions would be required in order to cope with this task. From a mathematical point of view, the determinism of the equations of motion remains unaffected by a chaotic evolution; from a physical point of view, determinism is lost, since the possibility of "predicting" is guaranteed only in the presence of a stable deterministic evolution. In fact, in contrast with mathematics, physics has to deal with precision and errors: in a chaotic dynamics we cannot control the propagation of an initial, arbitrarily small uncertainty.

At this point the very meaning of physics as a predictive science can become questionable, since chaotic dynamics seems to be present in the great majority of natural phenomena. On the other hand, the impossibility of an exact determination of the trajectories does not exclude the possibility of having statistical knowlodge about a chaotic system. The theory of Statistical Mechanics by Boltzmann is the first example where deterministic dynamical rules were replaced by statistical concepts. Actually, the practical impossibility of following the evolution equations of a large number of particles in a diluted gas interacting by elastic collisions led Boltzmann to encompass the problem by introducing an evolution equation for a distribution function $f(\mathbf{r}, \mathbf{v}, t)$. This function tells us about the probability of finding, at time t, a particle of the gas in a given position $\mathbf{r}$ and with velocity $\mathbf{v}$. This probably depends on some global properties of the gas, like the temperature and the occupied volume, rather than on the fine details of the collision dynamics. Boltzmann showed that the evolution equation for $f(\mathbf{r}, \mathbf{v}, t)$ is irreversible and consistent with the second principle of thermodynamics: entropy tends naturally to increase while approaching the equilibrium state, which corresponds to maximal entropy. The great intuition of A.N. Kolmogorov was that a similar, thermodynamic like, description could be adapted to chaotic dynamics. It is important to point out also the main conceptual difference of Kolmogorov's approach with respect to Boltzmann. There is no need for replacing chaotic equations with something else. The crucial observation is that unpredictable dynamical systems can depend on some global feature, i.e. an internal time, like $1/\lambda$, and on the geometric structure of the phase space

to a geometrical constraint that limits the access of the trajectory to a submanifold of phase space. Integrability can be a consequence of all λ_i's being zero, i.e. there can be as many conservation laws as the number of degrees of freedom. However, it can happen that the system is not necessarily integrable and the rate of divergence is weaker than exponential.

(possibly including different kinds of attractors). As a substitute for thermodynamic entropy, Kolmogorov introduced the concept of *metric entropy*. The conceptual breakthrough is that a mechanical description is replaced by a statistical description in terms of a measure: more precisely, we study the evolution of regions of the phase space rather than single trajectories. On this basis, one can easily notice that the concept of "metric entropy" was taken by Kolmogorov directly from information theory. Let us sketch his approach: some mathematics is necessary even if we shall not enter into the technical details[15]. Consider a set of n possible events, that in an experiment can be observed with probabilities $p_1, p_2, \cdots, p_n$, respectively ($\sum_i p_i = 1$). Information theory attributes the information content $-\ln p_j$ to the observation of the j-th event. Accordingly, the average information content associated with an experiment with n possible outcomes is $H = -\sum_{j=1}^{n} p_j \ln p_j$. As a first step towards extending this definition to chaotic dynamics, Kolmogorov introduced a partition of the phase space A into n disjoint subsets $A_1, A_2, \cdots, A_n$, with $A_i \cap A_j = 0$ if $i \neq j$: finding, at some instant of time, the trajectory in one of these subsets is the "event" for chaotic dynamics. By identifying the probability p_j with the measure $\mu(A_j)$ of the subset A_j, one can define the "entropy" associated with the partition A as

$$H(A) = -\sum_{j=1}^{n} \mu(A_j) \ln \mu(A_j). \tag{20}$$

Let us indicate with the symbol ϕ^{-t} the backward in time evolution operator (or "flux") over a time span $-t$, so that $\phi^{-t}A$ represents the partition generated by ϕ^{-t} from A, by taking the intersection of all the back iterates of each initial subset A_i. After n iterations, the application ϕ^{-t} generates a partition

$$A^{(n)} = A \cap (\phi^{-t}A) \cap (\phi^{-2t}A) \cap \cdots \cap (\phi^{-nt}A) \ , \tag{21}$$

where the symbol $\cap$ also denotes the intersection of two partitions. One can say that the proliferation with n of the elements of the partition (21) provides us with a measure of how fast the dynamics divides the original partition A, making it finer and finer. The main idea of Kolmogorov is to obtain a quantitative measure of the degree of chaoticity, or *mixing*, by the average information produced between two iterations

$$H(A, \phi^{-t}) = \lim_{n\to\infty} [H(A^{(n+1)}) - H(A^{(n)})] \tag{22}$$

Finally, since one aims to obtain an upper estimate of the information produced by the dynamics, the definition of *metric Kolmogorov-Sinai entropy* amounts to

$$h(\phi^{-t}) = \sup_{A} H(A, \phi^{-t}). \tag{23}$$

[15] We refer the reader aiming at a rigorous approach to [66]

This quantity is a dynamical indicator, which depends only on the nature of the dynamics. The *internal time* of the system is then given by $1/h$. Three different situations may then appear: $h = 0$ for regular motion (e.g., periodic dynamics), $h = \infty$ for a fully non–deterministic evolution (e.g., a dynamics subject to the influence of external noise), and $0 < h < \infty$ for a deterministic chaotic system. The russian mathematician Ya. B. Pesin [67] proved a remarkable relation between Kolmogorov's metric entropy and the positive component of the Lyapunov spectrum

$$h = \sum_{j=1}^{m} \lambda_j \quad , \quad \lambda_m > 0 > \lambda_{m+1}. \tag{24}$$

It is now evident that for systems with one degree of freedom, $h = \lambda$. The russian mathematician Ya.G. Sinai was the first to propose a simple dynamical model exhibiting mixing properties [15]. He considered a billiard with convex reflecting walls (see Fig. 2) and he proved that the flux associated with the dynamics of a bouncing ball has positive metric entopy. Later, another russian mathematician L.A. Bunimovich showed that the same result is obtained for the stadium billiard [16], where there is no convexity (see Fig. 3), thus indicating that the presence of mixing requires weaker conditions. These contributions also shed some light on the possibility that metric entropy could be at the basis of a statistical description of more physical models, like a gas of hard spheres (the mathematical model of a diluted gas as introduced by Boltzmann) or the FPU chain discussed in Sect. 3. Nonetheless, we should at least point out that the relation between mixing and statistical measure necessarily has to deal with the introduction of the so-called thermodynamic limit, i.e. the limit in which the number of degrees of freedom goes to infinity. In general, this limit does not commute with the limit $t \to \infty$ in (19) and (22). In other words, the results of the measurement of λ and h may depend on the order according to which these limits are performed. Stimulated by a discussion with D. Ruelle at IHES in Paris in 1984, two of the authors and their colleague A. Politi numerically investigated this problem for the FPU chain and other similar dynamical models. They obtained evidence for the existence of a limit curve for the spectrum of Lyapunov exponents in the thermodynamic limit [68] (see Fig. 10). Further numerical indications for the existence of such a limit for a variety of physical systems have been obtained afterwards, but a rigorous mathematical proof is still lacking, although some attempts in this direction have been made [69–71]. The existence of a Lyapunov spectrum in the thermodynamic limit is also used as an hypothesis in the proof of the Gallavotti-Cohen fluctuation-dissipation relation for forced reversible systems [72].

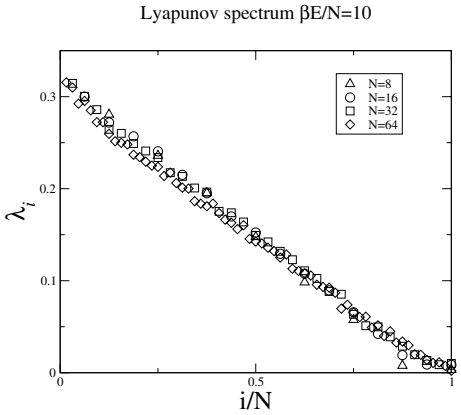

Fig. 10. The spectrum of positive Lyapunov exponents of the FPU *beta* model for different chain lengths, from 8 up to 64 oscillators

6 Quantum Computers and Quantum Chaos

In spite of the fundamental contributions by mathematicians and physicists in the understanding of chaotic dynamics, the role on numerical simulations of chaos can hardly be overestimated. Indeed, computer simulations made possible the investigation of the richness of chaos in all of its details and made the image of chaos familiar to the public. At present, the new technological developments related to quantum information and computation open new horizons to the simulations of chaos.

Indeed, a great deal of attention has been devoted in the last years to the possibility of performing numerical simulations on a quantum computer. As it was already stressed long time ago by Feynman [73], the massive parallelism allowed by quantum mechanics enables us to operate on an exponential number of states using a single quantum transformation. The recent development of quantum information processing has shown that computers designed on the basis of the laws of quantum mechanics can perform some tasks exponentially faster than any known classical computational algorithm (see *e.g.* [74]). The best known example of such a task is the integer factorization algorithm proposed by Shor. The quantum computer can be viewed as a system of qubits (two-level systems), on which "one-qubit" rotations and "two-qubit" transformations allow one to realize any unitary transformation in the exponentially large Hilbert space [74]. At present simple algorithms with up to seven qubits have been realized with nuclear spins in a molecule (NMR) and cold trapped ions.

Quantum computation sheds a new light on chaotic dynamics. Indeed, due to quantum parallelism, a quantum computer can iterate the Liouville density distribution for $O(2^{2n_q})$ classical trajectories in the Arnold cat map (1) in $O(n_q)$ quantum operations (e.g. "one-qubit" rotations and control-NOT

"two-qubit" gates), while a classical simulation requires $O(2^{2n_q})$ operations [75]. For these simulations the phase-space of (1) is discretized in N^2 cells with coordinates (x_i, y_j), $x_i = i/N$ and $y_j = j/N$, $i, j = 0, \ldots, N-1$, $N = 2^{n_q}$. The quantum algorithm simulates this discretized dynamics with the help of 3 quantum registers. The first two registers describe the position x_i and the momentum y_j of N^2 points in the discretized phase-space, where each register contains n_q qubits. The remaining $n_q - 1$ qubits in the third register are used as a work space. An initial classical Liouville distribution can then be represented by a quantum state proportional to $\sum_{i,j} a_{ij}|x_i > |y_j > |0 >$ where the coefficients $a_{i,j}$ are 0 or 1, corresponding to the classical density. The classical dynamics of map (1) is performed with the help of modular additions on the basis of the quantum algorithm described in [76]. The third register holds the curries of the addition and the result is taken modulo N by eliminating the last curry. One map iteration is done in two additions performed in parallel for all classical trajectories in $O(n_q)$ quantum gates.

An example of classical dynamics on a 128×128 lattice is shown in Fig. 11 (left). After $t = 10$ iterations the cat image becomes completely chaotic. Even if the exact dynamics is time reversible the minimal random errors in the last bit (round-off errors) make it effectively irreversible due to dynamical chaos and exponential growth of errors.

Hence, the initial image is not recovered after 10 (or 200) iterations forward/backward (see Fig. 11), even if these minimal errors are done only once at the moment of time inversion. On the contrary the quantum computation remains stable to 1% random errors in the phase of unitary rotation performed by each quantum gate: accordingly, the time reversibility of motion is preserved (see Fig. 11 (right)). In fact the precision of quantum computation remains sufficiently good during a time scale $t_f \propto 1/(\epsilon^2 n_q)$ where ϵ is the error amplitude in quantum gate rotations [75]. The physical origin of this result is related to the fact that the imperfection at each gate rotation transfers probability of the order ϵ^2 from the exact state to all the other states. At the same time the classical error propagates exponentially, due to chaotic deterministic dynamics. This result demonstrates a qualitative difference in the nature of classical and quantum errors. Indeed, quantum perturbation theory guarantees that small quantum errors weakly perturb the evolution. Conversely, from the viewpoint of quantum mechanics (spin flip) a classical error is large even in the last bit and this is the reason why it propagates exponentially in the case of simulations of chaotic dynamics. Thus, despite the common lore that quantum computers are very vulnerable to noise, the study of the Arnold cat map dynamics shows that classical unstable motion, for which classical computers display exponential sensibility to errors, can be simulated accurately with exponential efficiency by a realistic quantum computer [75].

There are also other quantum algorithms which allow the simulations of complex quantum dynamics in a polynomial number of gates for an exponentially large Hilbert space. For example, the quantum dynamics of map

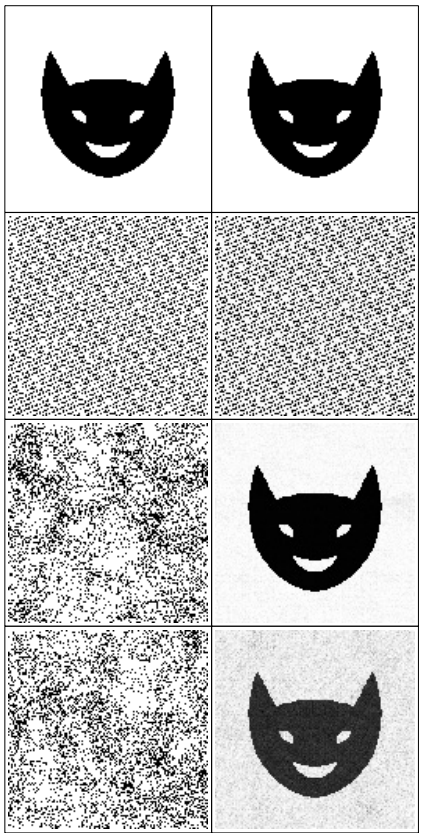

Fig. 11. Dynamics of the Arnold cat map (obtained by interchanging x and y in (1)) simulated on a classical computer (left) and quantum computer (right), on a 128×128 lattice. *Upper row:* initial distribution; *second row:* distributions after $t = 10$ iterations; *third row:* $t = 20$, with time inversion made after 10 iterations; *bottom row:* distributions at $t = 400$, with time inversion made at $t = 200$. Left: the classical error of one cell size ($\epsilon = 1/128$) is done only at the moment of time inversion; right: all quantum gates operate with quantum errors of amplitude $\epsilon = 0.01$; grayness is proportional to the probability $|a_{i,j}|^2$, $n_q = 7$, 20 qubits in total. [From [75]]

(3) can be simulated in $O(n_q^3)$ gates for the vector size $N = 2^{n_q}$ [77]. This opens new links between quantum computation and the field of quantum chaos, which investigates the properties of quantum systems with a chaotic classical limit. The field of quantum chaos has become an independent area of research, closely related to mesoscopic physics, Anderson localization in disordered potential, random matrix theory and periodic orbit quantization in the regime of chaos. due to space constraints, we cannot describe in any

detail this novel and fertile research field. We can only address the reader to reviews and books that can provide her/him with an exhaustive overview on this subject [29,78–81].

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