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Role of Chaos for the Validity of Statistical Mechanics Laws: Diffusion and Conduction

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Abstract. Several years after the pioneering work by Fermi, Pasta and Ulam, fundamental questions about the link between dynamical and statistical properties remain still open in modern statistical mechanics. Particularly controversial is the role of deterministic chaos for the validity and consistency of statistical approaches. This contribution reexamines such a debated issue taking inspiration from the problem of diffusion and heat conduction in deterministic systems. Is microscopic chaos a necessary ingredient to observe such macroscopic phenomena?

3.1 Introduction

Statistical mechanics, founded by Maxwell, Boltzmann and Gibbs, aims to explain the macroscopic properties of systems with a huge number of degrees of freedom without specific assumptions on the microscopic dynamics, a part from ergodicity [1, 2]. The discovery of deterministic chaos [3], beyond its undoubted important implications on many natural phenomena, enforced us to reconsider some basic problems standing at the foundations of statistical mechanics such as, for instance, the applicability of a statistical description to low-dimensional systems. However, even after many years, the experts do not agree yet on the basic conditions which should ensure the validity of statistical mechanics.

The spectrum of viewpoints found in literature is rather wide, ranging from the Landau (and Khinchin [4]) earlier belief on the key role of the many degrees of freedom and the (almost) complete irrelevance of ergodicity, to the opinion of those who, as Prigogine and his school [5] consider chaos as the crucial requirement to develop consistent statistical approaches. Recently some authors (e.g. Lebowitz [6] and Bricmont [7]) have given new life to the

debate [10, 5], renewing the intuition of Boltzmann [8] and Maxwell [9] on the relevance of the huge number of particles in macroscopic systems.

This volume offers the opportunity to celebrate the 100th and 50th anniversaries of two of the most influential works in statistical physics: Einstein's work on Brownian motion (1905) [11] and Fermi's one (1955) on the non-linear chain of oscillators (*al secolo* the FPU work, from the authors Fermi, Pasta and Ulam [12]). We shall discuss some aspects related to diffusion problems and heat conduction focusing on the role of (microscopic) chaos for the occurrence and robustness of these (macroscopic) phenomena. Transport phenomena, despite their ubiquity in everyday life, are still subject of debate among theoretic physicists.

Because of the variety of specific interactions and technical difficulties in realistic systems, simplified microscopic models are unavoidable tools for the study of transport mechanism. Several simulations and theoretical works have shown that, in systems with very strong chaos (namely hyperbolic systems), there exists a close relationship between transport coefficients (e.g. viscosity, diffusivity, thermal and electrical conductivity) and indicators of chaos (Lyapunov exponents, KS entropy, escape rates) [13, 14]. At a first glance, the existence of such relations would support the point of view of who considers chaos as the basic ingredient for the applicability of statistical mechanics. However, it is not possible to extend those results to generic systems. In fact, we shall see that many counterexamples prove that chaos is not a necessary condition for the emergence of robust statistical behaviors [15, 16]. In particular, we shall see that phenomena such as diffusion [17] and heat conduction [18] may take place also in non-chaotic systems. These and many other examples provide indication that microscopic chaos is not the unique possible origin of macroscopic transport in dynamical systems.

The material is organized into two, almost self-contained, parts. In the first, after a brief historical introduction to the different microscopic models proposed to explain macroscopic diffusion, we discuss a recent experiment (and the consequent debate it stimulated) aimed to prove that microscopic chaos is at the origin of Brownian motion. This gives us the possibility to introduce and discuss the problem of diffusion in non-chaotic deterministic systems, and to point out the necessary microscopic conditions to observe diffusion. The second part is mostly devoted to a discussion of the celebrated FPU numerical experiments and its consequences for the ergodic problem and heat conduction. We shall see that there are non-chaotic models displaying (macroscopic) heat conduction, confirming the non-essential role of chaos on transport.

3.2 On the Microscopic Origin of Macroscopic Diffusion

At the beginning of the twentieth century, the atomistic theory of matter was not yet fully accepted by the scientific community. While searching for phe-

nomena that would prove, beyond any doubt, the existence of atoms, Einstein realized that "...according to the molecular-kinetic theory of heat, bodies of microscopically-visible size suspended in a liquid will perform movements of such magnitude that they can be easily observed in a microscope...," as he wrote in his celebrated paper in 1905 [11]. In this work, devoted to compare the different predictions that classical thermodynamics and molecular-kinetic theory of heat make about those small bodies, Einstein argued that their motion has a diffusive character. Moreover, he discovered an important relation among the diffusion coefficient D, the fluid viscosity η, the particles radius a (having assumed spherical particles), Avogadro's number N_A, the temperature T and the gas constant R:

$$D = \frac{1}{N_A} \frac{RT}{6\pi\eta a} \ . \tag{3.1}$$

Einstein relation (3.1), which may be seen as the first example of the fluctuation–dissipation theorem [19], allowed for the determination of Avogadro's number [20] and gave one of the ultimate evidences of the existence of atoms.

Einstein's work on Brownian motion (BM) is based on statistical mechanics and thermodynamical considerations applied to suspended particles, with the assumption of velocity decorrelation.

One of the first successful attempts to develop a purely dynamical theory of BM dates back to Langevin [21] that, as himself wrote, gave "... a demonstration [of Einstein results] that is infinitely more simple by means of a method that is entirely different." Langevin considered the Newton equation for a small spherical particle in a fluid, taking into account that the Stokes viscous force it experiences is only a mean force. In one direction, e.g. the x-direction, one has

$$m\ \frac{d^2x}{dt^2} = -6\pi\eta a\ \frac{dx}{dt} + F \ , \tag{3.2}$$

where m is the mass of the particle. The first term of the r.h.s. is the Stokes viscous force. The second one $F(t)$ is a fluctuating random force, independent of $v = dx/dt$, modeling the effects of the huge number of impacts with the surrounding fluid molecules, which is taken as a zero-mean, Gaussian process with covariance $\langle F(t)F(t')\rangle = c\delta(t - t')$. The constant c is determined by the equipartition condition $\langle (dx/dt)^2 \rangle = RT/(mN_A)$, i.e. $c = 12\pi\eta aRT/N_A$.

Langevin's work along with that of Ornstein and Uhlenbeck [22] are at the foundation of the theory of stochastic differential equations. The stochastic approach is however unsatisfactory being a phenomenological description.

The next theoretical challenge toward the building of a dynamical theory of Brownian motion is to understand its microscopic origin from first principles. Almost contemporarily to Einstein's efforts, Smoluchowski tried to derive the large-scale diffusion of Brownian particles from the similar physical assumptions about their collisions with the fluid molecules [23].

A renewed interest on the subject appeared some years later, when it was realized that even purely deterministic systems composed of a large number of particles give rise to macroscopic diffusion, at least on finite time scales. These models had an important impact in justifying Brownian motion theory and, more in general, in deriving a consistent microscopic theory of irreversibility.

Some of these works considered chains of harmonic oscillators of equal masses [24, 25, 26, 27], while others [28, 29] analyzed the motion of a heavy impurity linearly coupled to a chain of equal mass oscillators. When the number of oscillators goes to infinity, the momentum of the heavy particle was proved to behave as a genuine stochastic process described by the Langevin equation (3.2). When their number is finite, diffusion remains an effective phenomenon lasting for a (long but) finite time.

Soon after the discovery of dynamical chaos [30], it was realized that simple low-dimensional deterministic systems may also exhibit a diffusive behavior. In this framework, the two-dimensional Lorentz gas [31], describing the motion of a free particle through a lattice of hard round obstacles, provided the most valuable example. As a consequence of the obstacle convexity, particle trajectories are chaotic, i.e. aside from a set initial conditions of zero measure, exhibit a positive and finite Lyapunov exponent,. At long times, for the case of billiards, the mean squared displacement from the particle initial position grows linearly in time. A Lorentz system with periodically arranged scatterers is closely related to the Sinai billiard [32, 33], which can be obtained from the former by folding the trajectories into the unitary lattice cell. The extensive study on billiards has shown that chaotic behavior might usually be associated with diffusion in simple low-dimensional models, supporting the idea that chaos was at the very origin of diffusion. However, more recently (see, e.g. [17]) it has been shown that even non-chaotic deterministic systems, such as a bouncing particle in a two-dimensional billiard with polygonal but randomly distributed obstacles (wind-tree Ehrenfest model), may exhibit a diffusion-like properties. This example can lead to think that the external source of randomness may play a role similar to chaos (for a more detailed discussion about this point see Sect. 3.2.2).

Deterministic diffusion is a generic phenomenon present also in simple chaotic maps on the line. Among the many contributions we mention the work by Fujisaka, Grossmann [34, 35] and Geisel [36, 37]. A typical example is the one-dimensional discrete-time dynamical system:

$$x(t+1) = [x(t)] + F(x(t) - [x(t)]) , \qquad (3.3)$$

where $x(t)$ (the position of a point-like particle) performs diffusion in the real axis. The bracket $[\cdot]$ denotes the integer part of the argument. $F(u)$ is a map defined on the interval $[0, 1]$ that fulfills the following requirements:

(i) The map, $u(t+1) = F(u(t))$ (mod 1) is chaotic.

(ii) $F(u)$ must be larger than 1 and smaller than 0 for some values of u, so to have a non-vanishing probability to escape from each unit cell (a unit cell of real axis is every interval $C_\ell \equiv [\ell, \ell + 1]$, with $\ell \in \mathbb{Z}$).

(iii) $F_r(u) = 1 - F_l(1 - u)$, where F_l and F_r define the map in $u \in [0, 1/2[$ and $u \in [1/2, 1]$ respectively. This anti-symmetry condition with respect to $u = 1/2$ is introduced to avoid a net drift.

A very simple and much studied example of F is

$$F(u) = \begin{cases} 2(1+a)u & \text{if } u \in [0, 1/2[\\ 2(1+a)(u-1)+1 & \text{if } u \in [1/2, 1] \end{cases}, \tag{3.4}$$

where $a > 0$ is the control parameter. It is useful to remind the link between diffusion and velocity correlation, i.e. the Taylor–Kubo formula, that helps to unravel how diffusion can be realized in different ways. The velocity correlation function is defined as $C(\tau) = \langle v(\tau)v(0)\rangle$, where $v(t)$ is the velocity of the particle at time t. It is easy to see that for continuous time systems [e.g. (3.2)]

$$\langle (x(t) - x(0))^2 \rangle \simeq 2\, t \int_0^t d\tau\, C(\tau). \tag{3.5}$$

Standard diffusion, with $D = \int_0^\infty d\tau\, C(\tau)$, is always obtained whenever the hypotheses for the validity of the central limit theorem are verified:

(i) finite variance of the velocity: $\langle v^2 \rangle < \infty$;
(ii) faster than τ^{-1} decay of the velocity correlation function $C(\tau)$.[1]

The first condition, independently of the microscopic dynamics under consideration (stochastic, deterministic chaotic or regular), excludes unphysical models, i.e. with infinite variance for the velocity. The second requirement corresponds to a rapid memory loss of initial conditions. It is surely verified for the Langevin dynamics where the presence of the stochastic force entails a rapid decay of $C(\tau)$. In deterministic regular systems, such as the model of many oscillators, the velocity decorrelation (i.e. the small fluctuations of $C(\tau)$ around zero, for almost all the time) is the result of the huge number of degrees of freedom that act as a heat bath on a single oscillator. In the (non-chaotic) Ehrenfest wind-tree model decorrelation originates from the disorder in the obstacle positions. Deterministic chaotic systems, in spite of the fact that non-linear instabilities generically lead to a memory loss, are more subtle. Indeed, there are many examples, namely intermittent systems [38], characterized by a slow decay of the velocity correlation function.

We end this section by asking whether it is possible to determine, by the analysis of a Brownian particle, if the microscopic dynamics underlying the observed macroscopic diffusion is stochastic, deterministic chaotic or regular.

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[1] In discrete-time systems, the velocity $v(t)$ and the integral $\int d\tau C(\tau)$ are replaced by the finite difference $x(t+1) - x(t)$ and by the quantity $\langle v(0)^2\rangle/2 + \sum_{\tau \geq 1} C(\tau)$, respectively.

3.2.1 Chaos or Noise? A Difficult Dilemma

Inferring the microscopic deterministic character of Brownian motion on an experimental basis would be attractive from a fundamental viewpoint. Moreover it could provide further evidence to some recent theoretical and numerical studies [39, 40]. Before discussing a recent experiment [41] in this direction, we must open the "Pandora box" of the longstanding and controversial problem of distinguishing chaos from noise in signal analysis [42] (see also [45, 46, 47, 48, 49, 50]). For the sake of clearness on the terminology used here, we specify that "chaos" refers to the motions originating from a deterministic system with at least one positive but finite Lyapunov exponent, and therefore a positive and finite Kolmogorov–Sinai entropy; "noise" instead denotes the outcomes of a continuous valued stochastic process with infinite value of Kolmogorov–Sinai entropy.

The first observation concerning the chaos/noise distinction is that, very often in the analysis of experimental time series, there is not a unique model of the "system" that produced the data. Moreover, even the knowledge of the "true" model might not be an adequate answer about the character of the signal. From this point of view, BM is a paradigmatic example: in fact it can be modeled by a stochastic as well as by a deterministic chaotic or regular process.

In principle, a definite answer exists. If we were able to determine the maximum Lyapunov exponent (λ) or the Kolmogorov–Sinai entropy (h_{KS}) of a data sequence, we would know without uncertainty whether the sequence was generated by a deterministic law ($\lambda, h_{\mathrm{KS}} < \infty$) or by a stochastic one ($h_{\mathrm{KS}} \to \infty$). Nevertheless, there are unavoidable practical limitations in computing such quantities. They are indeed defined as infinite time averages taken in the limit of arbitrary fine resolution. But, in experiments, we have access only to a finite, and often very limited, range of scales and times.

However, there are measurable quantities that are appropriate for extracting meaningful information from the signal. In particular, we shall consider the (ϵ, τ)-entropy per unit time [51, 52, 53] $h(\epsilon, \tau)$ that generalizes the Kolmogorov–Sinai entropy (for details see next section (3.8)). In a nutshell, while for evaluating h_{KS} one has to detect the properties of a system with infinite resolution, for $h(\epsilon, \tau)$ a finite scale (resolution) ϵ is involved. The Kolmogorov–Sinai entropy is recovered in the limit $\epsilon \to 0$, i.e. $h(\epsilon, \tau) \to h_{\mathrm{KS}}$. This means that if we had access to arbitrarily small scales, we could answer the original question about the character of the law that generated the recorded signal. Even if this limit is unattainable, still the behavior of $h(\epsilon, \tau)$ provides a very useful scale-dependent description of the signal character [42, 54].

For instance, chaotic systems ($0 < h_{\mathrm{KS}} < \infty$) are typically characterized by $h(\epsilon, \tau)$ attaining a plateau $\approx h_{\mathrm{KS}}$, below a resolution threshold, ϵ_{c}, associated with the smallest characteristic length scale of the system. Instead, for $\epsilon > \epsilon_{\mathrm{c}}$ $h(\epsilon, \tau) < h_{\mathrm{KS}}$, and in this range the details of the ϵ-dependence may be

informative on the large scale (slow) dynamics of the system (see, e.g. [42, 54]). Indeed, at large scales typically chaotic systems give rise to behaviors rather similar to stochastic processes (e.g. the diffusive behavior discussed in the previous subsection) with characteristic ϵ-entropy. In stochastic signals, although $h_{KS} = \infty$, for any $\epsilon > 0$, $h(\epsilon, \tau)$ is a finite function of ϵ and τ. The dependence of $h(\epsilon, \tau)$ on ϵ and τ, when known, provides a characterization of the underlying stochastic process (see [51, 53]). For instance, stationary Gaussian processes with a power spectrum[2] $S(\omega) \propto \omega^{-(2\alpha+1)}$ (being $0 < \alpha < 1$) are characterized by a power-law ϵ-entropy [51]:

$$\lim_{\tau \to 0} h(\epsilon, \tau) \sim \epsilon^{-1/\alpha} \; . \tag{3.6}$$

The case $\alpha = 1/2$, corresponding to the power spectrum of a Brownian signal, would give $h(\epsilon) \sim \epsilon^{-2}$. Other stochastic processes, such as time uncorrelated and bounded ones, are characterized by a logarithmic divergence below a critical scale, ϵ_c, which may depend on τ.

Definition and Computation of the ϵ-Entropy

For the sake of self-consistency in this subsection we provide some basic information on the definition and measurement (from experimental data) of the ϵ-entropy, which was originally introduced in the context of information theory by Shannon [52] and, later, by Kolmogorov [51] in the theory of stochastic processes. The interested reader may find more details in [53] and [55].

An operative definition of $h(\epsilon, \tau)$ is as follows. Given the time evolution of a continuous variable $\mathbf{x}(t) \in \Re^d$, that represents the state of a d-dimensional system, one introduces the vector in $\Re^{md}$

$$\mathbf{X}^{(m)}(t) = (\mathbf{x}(t), \ldots, \mathbf{x}(t + m\tau - \tau)) \; , \tag{3.7}$$

which represents a portion of the trajectory, sampled at a discrete time interval τ. After partitioning the phase space $\Re^d$ using hyper-cubic cells of side ϵ, $\mathbf{X}^{(m)}(t)$ is coded into an m-word: $W^m(\epsilon, t) = [i(\epsilon, t), \ldots, i(\epsilon, t + m\tau - \tau)]$, where $i(\epsilon, t+j\tau)$ labels the cell in $\Re^d$ containing $\mathbf{x}(t+j\tau)$. For bounded motions, the number of available cells (i.e. the alphabet) is finite. Under the hypothesis of stationarity, the probabilities $P(W^m(\epsilon))$ of the admissible words $\{W^m(\epsilon)\}$ are obtained from the time evolution of $\mathbf{X}^{(m)}(t)$. Then one introduces the m-block entropy, $H_m(\epsilon, \tau) = -\sum_{\{W^m(\epsilon)\}} P(W^m(\epsilon)) \ln P(W^m(\epsilon))$, and the quantity $h_m(\epsilon, \tau) = [H_{m+1}(\epsilon, \tau) - H_m(\epsilon, \tau)]/\tau$. The (ϵ, τ)-entropy per unit time, $h(\epsilon, \tau)$ is defined by [52]

$$h(\epsilon, \tau) = \lim_{m \to \infty} h_m(\epsilon, \tau) \; . \tag{3.8}$$

The Kolmogorov–Sinai entropy is obtained in the limit of small ϵ:

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[2] The power spectrum $S(\omega)$ is the Fourier transform of $\langle (x(t) - x(0))^2 \rangle$.

$$h_{\mathrm{KS}} = \lim_{\epsilon \to 0} h(\epsilon, \tau) \ . \tag{3.9}$$

In principle, in deterministic systems $h(\epsilon)$, and henceforth h_{KS}, depend neither on the sampling time τ [3] nor on the chosen partition because its rigorous definition[53] would require the infimum to be taken over all possible partitions with elements of size smaller than ϵ. However, in practical computations, the specific value of τ is important, and the impossibility to take the infimum over all the partitions implies that, at finite ϵ, $h(\epsilon)$ may depend on the chosen partition. Nevertheless, for small ϵ, the correct value of the Kolmogorov–Sinai entropy is usually recovered independently of the partition [3].

Let us stress that partitioning the phase space does not mean a discretization of the states of the dynamical system, which still evolves on a continuum. The partitioning procedure corresponds to a coarse-grained description (due, for instance, to measurements performed with a finite resolution), that does not change the dynamics. On the contrary, discretizing the states would change the dynamics, implying periodic motions in any deterministic systems. This happens, for instance, in any floating point computer simulations; however such periods are, apart from trivial cases, very long and practically undetectable.

In experimental signals, usually, only a scalar variable $u(t)$ can be measured, and moreover the dimensionality of the phase space is not known a priori. In these cases, one uses delay-embedding techniques [45, 46], where the vector $\mathbf{X}^{(m)}(t)$ is build as $(u(t), u(t+\tau), \ldots, u(t+m\tau-\tau))$, now in $\Re^m$. This is a special instance of (3.7). Then to determine the entropies $H_m(\epsilon)$, very efficient numerical methods are available (the reader may find an exhaustive review in [45]). The delay-embedding procedure can be applied to compute the ϵ-entropy of deterministic and stochastic signals as well. The dependence of the ϵ-entropy on the observation scale ϵ can be used to characterize the process underlying the signal [53].

In the following, we exemplify the typical difficulties by analyzing the map:

$$x(t+1) = f(x(t)) = x(t) + p \ \sin(2\pi x(t)) \ . \tag{3.10}$$

As soon as $p > 0.7326\ldots$, $f(x)$ is such that $f(x) > 1$ and $f(x) < 0$ for some $x \in]0, 1[$. This implies that the trajectory can travel across different unitary cells giving rise to large-scale diffusion, i.e. asymptotically:

$$\langle [x(t) - x(0)]^2 \rangle \simeq 2Dt \ , \tag{3.11}$$

where D is the diffusion coefficient. We note that $p = \mathrm{O}(1)$ sets the intrinsic scale of the displacements to be $\mathrm{O}(1)$. Therefore, as far as the ϵ-entropy is concerned, for $\epsilon \ll 1$ (small-scale observations) one should be able to recognize that the system is chaotic, i.e. $h(\epsilon)$ displays a plateau at $h_{\mathrm{KS}} = \lambda$. For $\epsilon \gg 1$ (large scale observations), due to the diffusive behavior, $h(\epsilon)$ is characterized by the scaling (3.6) with $\alpha = 1/2$, therefore
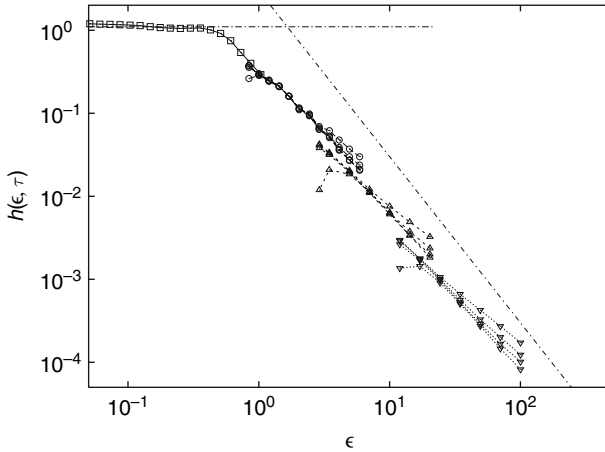
Fig. 3.1. Numerically evaluated (ϵ, τ)-entropy for the map (3.10) with $p = 0.8$ computed by the standard techniques [45] at $\tau = 1$ (∘), $\tau = 10$ (△) and $\tau = 100$ (▽) and different *block length* ($m = 4, 8, 12, 20$). The *boxes* refer to the entropy computed with $\tau = 1$ but by using periodic boundary condition over 40 cells. The use of periodic boundary conditions is necessary to probe scales small enough to recover the Lyapunov exponent. The *straight lines* correspond to the two asymptotic behaviors, $h(\epsilon) = h_{\mathrm{KS}} \simeq 1.15$ and $h(\epsilon) \sim \epsilon^{-2}$

$$h(\epsilon) \simeq \begin{cases} \lambda & \text{for } \epsilon \ll 1 \\ D/\epsilon^2 & \text{for } \epsilon \gg 1 \end{cases}, \tag{3.12}$$

where λ is the Lyapunov exponent and D is the diffusion coefficient. The typical problems encountered in numerically computing $h(\epsilon)$ can be appreciated in Fig. 3.1. First notice that the deterministic character (i.e. $h(\epsilon, \tau) \approx h_{\mathrm{KS}}$) appears only at $\epsilon < \epsilon_c \approx 1$. However, the finiteness of the data set imposes a lower cut-off scale ϵ_d below which no information can be extracted from the data (see [56]). As for the importance of the choice of τ note that if τ is much larger or much shorter than the characteristic time-scale of the system at the scale ϵ, then the correct behavior of the ϵ-entropy [42] cannot be properly recovered. Indeed the diffusive behavior $h(\epsilon) \sim \epsilon^{-2}$ is roughly obtained only by considering the envelope of $h_m(\epsilon, \tau)$ evaluated at different values of τ. The reason for this is that the characteristic time of the system is determined by its diffusive behavior $T_\epsilon \approx \epsilon^2/D$. On the other hand, the plateau at the value h_{KS} can be recovered only for $\tau \approx 1$, even if, in principle, any value of τ could be used.

We also mention that if the system is deterministic, to have a meaningful measure of the entropy, the embedding dimension m has to be larger than information dimension of the attractor [3].

Experiments on the Microscopic Origin of Brownian Motion

We are now ready to discuss the experiment and its analysis reported in [41]. In this experiment, a long-time record (about 1.5×10^5 data points) of the motion of a small colloidal particle in water was sampled at regular time intervals ($\Delta t = 1/60$ s) with a remarkable high spatial resolution (25 nm). To our knowledge, this is the most accurate measurement of a BM. The data were then processed by means of standard methods of non-linear time-series analysis [45] to compute the ϵ-entropy.[3] This computation shows a power-law dependence $h(\epsilon) \sim \epsilon^{-2}$. Actually, similarly to what is displayed in Fig. 3.1, this behavior is recovered only by considering the envelope of the $h(\epsilon, \tau)$-curves, for different τs. However, unlike to Fig. 3.1, no saturation $h(\epsilon, \tau) \approx$ const. is observed for small ϵ. Nevertheless, the authors *assume* from the outset that the system dynamics is deterministic and, since in deterministic systems $h(\epsilon, \tau) \leq h_{\mathrm{KS}} \leq \sum_i^+ \lambda_i$, deduce from the positivity of $h(\epsilon)$ the existence of positive Lyapunov exponents. Their conclusion is thus that microscopic chaos is at the origin of the macroscopic diffusive behavior.

However, as several works pointed out (see [57, 58]), the huge amount of involved degrees of freedom (Brownian particle and the fluid molecules), the impossibility to reach a (spatial and temporal) resolution high enough, and the limited amount of data points do not allow for such optimistic conclusions. Avoiding a technical discussion on these three points we simply notice that the limitation induced by the finite resolution is particularly relevant to the experiment. For example, if the analysis of Fig. 3.1 would be restricted to the region with $\epsilon > 1$ only, then discerning whether the data were originated by a chaotic system or by a stochastic process would be impossible.

Particularly interesting is the fact that, as shown by Dettman et al. [17, 57], the finite amount of data severely limits our ability to distinguish not only if the signal is deterministic, chaotic or stochastic but also if it is deterministic regular, i.e. of zero entropy. The following example serves as a clue to better understand the way in which a deterministic non-chaotic systems may give rise (at least on certain temporal and spatial scales) to a stochastic behavior.

Let us consider two signals, the first generated by a continuous random walk:

$$\dot{x}(t) = \sqrt{2D}\eta(t) \,, \tag{3.13}$$

where η is a zero mean Gaussian variable with $\langle \eta(t)\eta(t') \rangle = \delta(t - t')$, and the second obtained as a superpositions of Fourier modes:

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[3] Of course in data analysis, only scalar time series are available and the dimensionality of the space of state vectors is a priori unknown. However, one can use the delay embedding technique to reconstruct the phase-space. In this way, the ϵ-entropy can be evaluated as discussed in the previous section. It is worth stressing that this procedure can be applied even though the equations of motion of the system, which generated the signal, are unknown. Moreover, this approach is meaningful independently of the stochastic or deterministic nature of the considered signal.
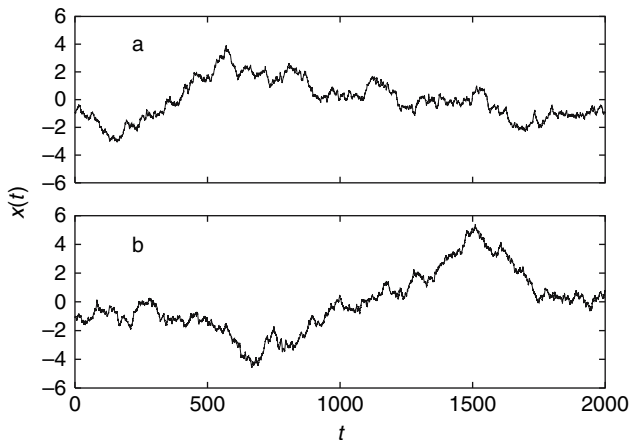
Fig. 3.2. a Signals obtained from (3.14) with $M = 10^4$ and random phases uniformly distributed in $[0, 2\pi]$. The numerically computed diffusion constant is $D \approx 0.007$. **b** Time record obtained with a continuous random walk (3.13) with the same value of the diffusion constant as in **a**. In both cases, data are sampled with $\tau = 0.02$, i.e. 10^5 data points

$$x(t) = \sum_{i=1}^{M} X_{0i} \sin\left(\Omega_i t + \phi_i\right) \ . \tag{3.14}$$

The coordinate $x(t)$ in (3.14), upon properly choosing the frequencies [29, 42] and the amplitudes (e.g. $X_{0i} \propto \Omega_i^{-1}$), describes the motion of a heavy impurity in a chain of M linearly coupled harmonic oscillators. We know [29] that $x(t)$ performs a genuine BM in the limit $M \to \infty$. For $M < \infty$ the motion is quasi-periodic and regular, nevertheless for large but finite times it is impossible to distinguish signals obtained by (3.13) and (3.14) (see Fig. 3.2). This is even more striking looking at the computed ϵ-entropy of both signals (see Fig. 3.3).

The results of Fig. 3.3 along with those by Dettman et al. [57] suggest that, by assuming also the deterministic character of the system, we are in the practical impossibility of discerning chaotic from regular motion.

It is worth mentioning that recently some interesting works [43, 44] applied the entropy analysis to the motion of a heavy impurity embedded in an FPU-chain (see Sect. 3.3.1), which is a chaotic variant of the above example. The purpose was again to infer the chaotic character of the whole FPU-chain by observations on the impurity motion only. It was found that the impurity does not alter the behavior of the FPU-chain so it can be considered as a true probe of the dynamics. The impurity performs a motion that, when observed at small but finite resolutions, closely resembles a Brownian motion. Time series (ϵ, τ)-entropy analysis both in momentum and position allows for detecting the chaotic nature of the FPU unperturbed system, and clearly locating the stochasticity threshold.
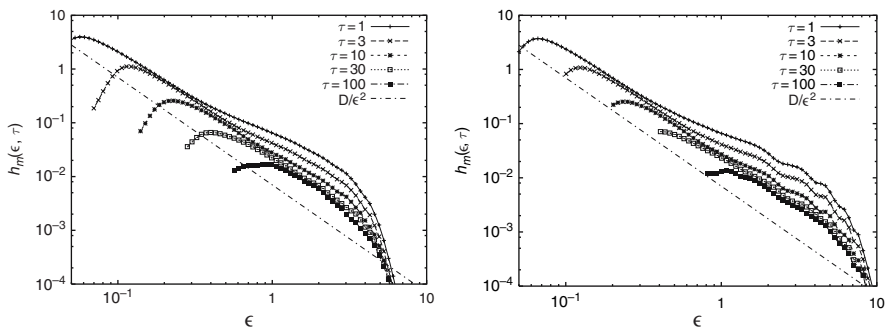
Fig. 3.3. Numerically evaluated (ϵ, τ)-entropy using using 10^5 points from the time series of Fig. 3.2. We show the results for embedding dimension $m = 50$. The *straight lines* show the D/ϵ^2 behavior

From the above discussion, one reaches a pessimistic view on the possibility to detect the "true" nature of a signal by means of data analysis only. However, the situation is not so bad if the question about the character of a signal is asked only relatively to a certain interval of scales. In this case, in fact, it is possible to give an unambiguous classification of the signal character based solely on the entropy analysis and free from any prior knowledge of the system/model that generated the data. Moreover the behavior of $h(\epsilon, \tau)$ as a function of (ϵ, τ) provides a very useful "dynamical" classification of stochastic processes [53, 59]. One has then a practical tool to classify the character of a signal as deterministic or stochastic, on a given scale, without referring to a specific model, and is no longer obliged to answer the metaphysical question, whether the system that produced the data was a deterministic or a stochastic [42, 60] one.

3.2.2 Diffusion in Deterministic Non-chaotic Systems

With all the proviso on its interpretation, Gaspard et al. [41] experiment had a very positive role not only in stimulating the discussion about the chaos/noise distinction but also in focusing the attention on deep conceptual aspects of diffusion. From a theoretical point of view, the study of chaotic models exhibiting diffusion and their non-chaotic counterpart is indeed important to better understand the role of microscopic chaos on macroscopic diffusion.

In Lorentz gases, the diffusion coefficient is related, by means of periodic orbits expansion methods [13, 14, 61], to chaotic indicators such as the Lyapunov exponents. This suggested that chaos was or might have been the basic ingredient for diffusion. However, as argued by Dettman and Cohen [17], even an accurate numerical analysis based on the ϵ-entropy, being limited by the finiteness of the data points, has no chance to detect differences in the diffusive behavior between a chaotic Lorentz gas and its non-chaotic counterpart,

such as the wind-tree Ehrenfest's model. In the latter model, particles (wind) scatter against square obstacles (trees) randomly distributed in the plane but with fixed orientation. Since the reflection by the flat edges of the obstacles cannot produce exponential separation of trajectories, the maximal Lyapunov exponent is zero. The result of [17] implies thus that chaos may be not indispensable for having deterministic diffusion. The question may be now posed on what are the necessary microscopic ingredients to observe deterministic diffusion at large scales.

We would like to remark that, in the wind-tree Ehrenfest's model, the external randomness amounting to the disordered distribution of the obstacles is crucial. Hence, one may conjecture that a finite spatial entropy density h_S is necessary for observing diffusion. In this case, deterministic diffusion might be a consequence either of a non-zero "dynamical" entropy ($h_{KS} > 0$) in chaotic systems or of a non-zero "static" entropy ($h_S > 0$) in non-chaotic systems. This is a key-point, because someone can argue that a deterministic infinite system with spatial randomness can be interpreted as an effective stochastic system.[4]

With the aim of clarifying this point, we consider here a spatially disordered non-chaotic model [62], which is the one-dimensional analog of a two-dimensional non-chaotic Lorentz system with polygonal obstacles. Let us start with the map defined by (3.3) and (3.4), and introduce some modifications to make it non-chaotic. One can proceed as exemplified in Fig. 3.4, that is by replacing the function (3.4) on each unit cell by its step-wise approximation generated as follows. The first-half of C_ℓ is partitioned in N micro-intervals
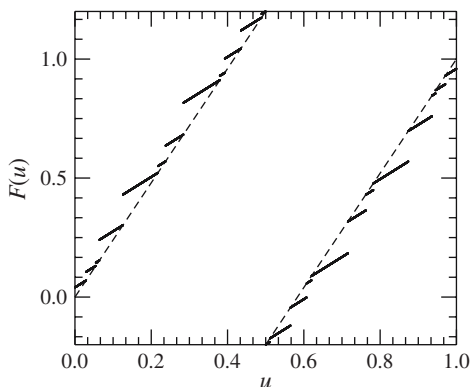

Fig. 3.4. Sketch of the random staircase map in the unitary cell. The parameter a defining the macroscopic slope is set to 0.23. Half domain $[0, 1/2]$ is divided into $N = 12$ micro-intervals of random size. The map on $[1/2, 1]$ is obtained by applying the antisymmetric transformation with respect to the center of the cell $(1/2, 1/2)$

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[4] This is probably a "matter of taste."

$[\ell + \xi_{n-1}, \ell + \xi_n[$, $n = 1, \ldots, N$, with $\xi_0 = 0 < \xi_1 < \xi_2 < \cdots < \xi_{N-1} < \xi_N = 1/2$. In each interval, the map is defined by its linear approximation

$$F_\Delta(u) = u - \xi_n + F(\xi_n) \qquad \text{if } u \in [\xi_{n-1}, \xi_n[\ , \qquad (3.15)$$

where $F(\xi_n)$ is (3.4) evaluated at ξ_n. The map in the second half of the unit cell is then determined by the anti-symmetry condition with respect to the middle of the cell. The quenched random variables $\{\xi_k\}_{k=1}^{N-1}$ are uniformly distributed in the interval $[0, 1/2]$, i.e. the micro-intervals have a *random* extension. Further they are chosen independently in each cell C_ℓ (so one should properly write $\xi_n^{(\ell)}$). All cells are partitioned into the same number N of randomly chosen micro-intervals (of mean size $\Delta = 1/N$). This modification of the continuous chaotic system is conceptually equivalent to replacing circular by polygonal obstacles in the Lorentz system [17].

Since F_Δ has slope 1 almost everywhere, the map is no longer chaotic, violating the condition *i)* (see Sect. 3.2). For $\Delta \to 0$ (i.e. $N \to \infty$) the continuous chaotic map (3.3) is recovered. However, this limit is singular and as soon as the number of intervals is finite, even if extremely large, chaos is absent. It has been found [62] that this model still exhibits diffusion in the presence of both quenched disorder and a quasi-periodic external perturbation

$$x(t+1) = [x(t)] + F_\Delta(x(t) - [x(t)]) + \gamma \cos(\alpha t) \ . \qquad (3.16)$$

The strength of the external forcing is controlled by γ and α defines its frequency, while Δ indicates a specific quenched disorder realization. The sign of γ is irrelevant; without lack of generality we study the case $\gamma > 0$.

The diffusion coefficient D is then numerically computed from the linear asymptotic behavior of the mean quadratic displacement, see (3.11). The results, summarized in Fig. 3.5, show that D is significantly different from zero only for values $\gamma > \gamma_c$. For $\gamma > \gamma_c$, D exhibits a saturation close to the value of the chaotic system (horizontal line) defined by (3.3) and (3.4). The existence of a threshold γ_c is not surprising. Due to the staircase nature of the system, the perturbation has to exceed the typical discontinuity of F_Δ to activate the "macroscopic" instability which is the first step toward the diffusion. Data collapsing, obtained by plotting D versus γN, in Fig. 3.5 confirms this argument. These findings are robust and do not depend on the details of forcing. Therefore, we have an example of a non-chaotic model in the Lyapunov sense by construction, which performs diffusion.

Now the question concerns the possibility that the diffusive behavior arises from the presence of a quenched randomness with non-zero spatial entropy per unit length. To clarify this point, similarly to [17], the model can be modified in such a way that the spatial entropy per unit cell is forced to be zero, and see if the diffusion still persists.

Zero spatial entropy per unit length may be obtained by repeating the same disorder configuration every M cells (i.e. $\xi_n^{(\ell)} = \xi_n^{(\ell+M)}$). Looking at the diffusion of an ensemble of walkers it was observed that diffusion is still present
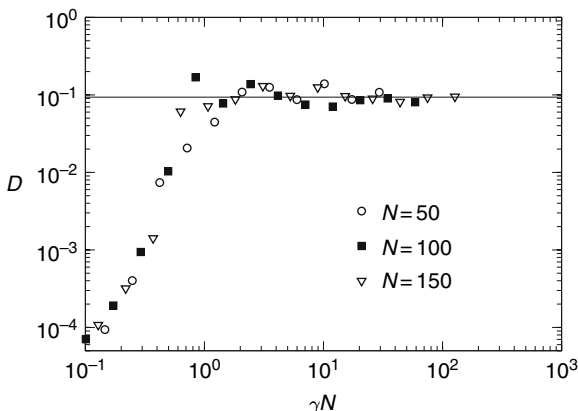
Fig. 3.5. Log–Log plot of the dependence of the diffusion coefficient D on the external forcing strength γ. Different data relative to a number of cell micro-intervals $N = 50$, 100 and 150 are plotted vs the natural scaling variable γN to obtain a collapse of the curves. Horizontal line represents the result for chaotic system (3.3, 3.4)

with D very close to the expected value (as in Fig. 3.5). A careful analysis (see [62] for details) showed that the system displays genuine diffusion for a very long times even with a vanishing (spatial) entropy density, at least for sufficiently large M.

These results along with those by Dettman and Cohen [17] allow us to draw some conclusions on the fundamental ingredients for observing deterministic diffusion (both in chaotic and non-chaotic systems).

- An instability mechanism is necessary to ensure particle dispersion at small scales (here small means inside the cells). In chaotic systems, this is realized by the sensitivity to the initial condition. In non-chaotic systems, this may be induced by a finite size instability mechanisms. Also, with zero maximal Lyapunov exponent one can have a fast increase of the distance between two trajectories initially close [63]. In the wind-tree Ehrenfest model this stems from the edges of the obstacles, in the "stepwise" system of Fig. 3.4 from the jumps.
- A mechanisms able to suppress periodic orbits and therefore to allow for a diffusion at large scale.

It is clear that the first requirement is not very strong while the second is more subtle. In systems with "strong chaos," all periodic orbits are unstable and, so, it is automatically fulfilled. In non-chaotic systems, such as the non-chaotic billiards studied by Dettman and Cohen and the map (3.16), the stable periodic orbits seem to be suppressed or, at least, strongly depressed, by the quenched randomness (also in the limit of zero spatial entropy). However, unlike the two-dimensional non-chaotic billiards, in the one-dimensional system (3.4,3.15,3.16), the periodic orbits may survive to the presence of disorder,

so we need the aid of a quasi-periodic perturbation to obtain their destruction and the consequent diffusion.

3.3 The Heritage of the Fermi–Pasta–Ulam Problem for the Statistical Mechanics

The ergodic theory begun with Boltzmann's effort to justify the determination of average values in kinetic theory. Ergodic hypothesis states that time averages of observables of an isolated system at the equilibrium can be computed as phase averages over the constant-energy hyper-surface. This statement can be regarded as the first attempt to establish a link between statistical mechanics and the dynamics of the underlying system. One can say that proving the validity of ergodic hypothesis provides a "dynamical justification" of statistical ensembles.

The ergodic problem, at an abstract level, had been attacked by Birkhoff and von Neumann who proved their fundamental theorems on the existence of time averages and established a necessary and sufficient condition for the ergodicity. In spite of their mathematical importance, on a practical ground such theorems do not help very much to really solve the ergodic problem in statistical physics.

There exists a point of view according to which the effectiveness of a statistical mechanics approach resides mainly on the presence of many degrees of freedom rather than on the underlying (chaotic or regular) dynamics. Khinchin in his celebrated book *Mathematical Foundation of the Statistical Mechanics* [4] presents some important results on the ergodic problem that need no metrical transitivity. The main point of his approach relies on the concept of relevant physical observables in systems with a huge number of degrees of freedom. Since physical observables are non-generic functions (in mathematical sense), the equivalence between time and ensemble averages should be proved only for a restricted class of relevant observables. Moreover for physical purposes, it is "fair" to accept the failure of ergodicity for few (in the sense of sets of small measure) initial conditions.

In plain words, Khinchin's formulation, coinciding with Boltzmann's point of view (see, e.g., Chap. 1 of [2]), asserts that statistical mechanics works, independently of ergodicity, because the (most meaningful) physical observables are practically constant, a part in regions of very small measure, on the constant energy surface. Within this approach, dynamics have a marginal role, and the existence of "good statistical properties" is granted by the large number of degrees of freedom. However, the validity of Khinchin's statement restricts to a special class of observables not covering all the physically interesting possibilities. Therefore for each case, a detailed study of the specific dynamics is generally needed to assess the statistical properties of a given system.

The issue of ergodicity is naturally entangled with the problem of the existence of non-trivial conserved quantities (first integrals) in Hamiltonian systems. Consider a system governed by the Hamiltonian

$$H(\mathrm{I}, \phi) = H_0(\mathrm{I}) + \epsilon H_1(\mathrm{I}, \phi) , \qquad (3.17)$$

where $\mathrm{I} = (I_1, \ldots, I_M)$ are the action variables and $\phi = (\phi_1, \ldots, \phi_M)$ are the phase variables. If $\epsilon = 0$ the system is integrable, there are M independent first integrals (the actions I_i) and the motion evolves on M-dimensional tori. Two questions arise naturally. Do the trajectories of the system (3.17) remain "close" to those of the integrable one? Do some conserved quantity, besides energy, survive in the presence of a generic (small) perturbation $\epsilon H_1(\mathrm{I}, \phi)$? Of course whenever other first integrals exist the system cannot be ergodic.

In a seminal work, H. Poincaré [64] showed that generally a system like (3.17) with $\epsilon \neq 0$ does not possess analytic first integrals other than energy. This result sounds rather positive for the statistical mechanics approach. In 1923, Fermi [65], generalizing Poincaré's result, proved that for generic perturbations H_1 and $M > 2$, there cannot exist, on the $2M - 1$ dimensional constant-energy surface, even a single smooth[5] surface of dimension $2M - 2$ that is analytical in the variables (I, ϕ) and ϵ. From this result, Fermi argued that generic (non-integrable) Hamiltonian systems are ergodic.

At least in the physicists' community, this conclusion was generally accepted and, even in the absence of a rigorous demonstration, there was a vast consensus that the non-existence theorems of regular first integrals implied ergodicity.

3.3.1 FPU: Relaxation to Equilibrium and Ergodicity Violation

Thirty-two years later Fermi itself, together with Pasta and Ulam, with one of the first numerical experiments, in the celebrated paper *Studies of Nonlinear Problems* [12] (often referred with the acronym FPU) showed that the ergodic problem was still far from being solved. The FPU model studies the time evolution of a chain of N particles, interacting by means of non-linear springs:

$$H = \sum_{n=0}^{N} \left[\frac{p_n^2}{2m} + \frac{K}{2}(q_{n+1} - q_n)^2 + \frac{\epsilon}{\alpha}(q_{n+1} - q_n)^\alpha \right] , \qquad (3.18)$$

with boundary conditions $q_0 = q_{N+1} = p_0 = p_{N+1} = 0$, $\alpha = 3$ or 4 and $K > 0$. The Hamiltonian is of the form (3.17) with a harmonic (integrable) part and a non-integrable (anharmonic) term $\mathrm{O}(\epsilon)$. For $\epsilon = 0$, one has a collection of N non-interacting harmonic modes of energies E_ks, which remain constant. What happens if an initial condition is chosen in such a way that all the energy is concentrated in a few normal modes, for instance $E_1(0) \neq 0$ and $E_k(0) = 0$ for $k = 2, \ldots, N$? Before the FPU work, the general expectation would have

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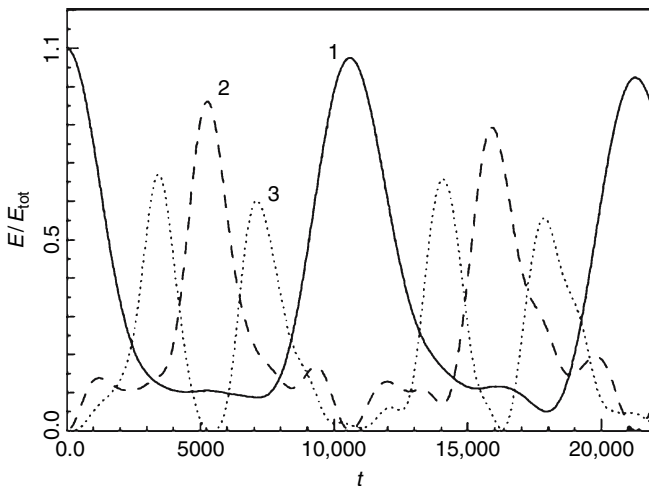[5] For instance, analytic or differentiable enough.

Fig. 3.6. $E_1(t)/E_{\text{tot}}$, $E_2(t)/E_{\text{tot}}$, $E_3(t)/E_{\text{tot}}$ for the FPU system, with $N = 32$, $\alpha = 3$, $\epsilon = 0.1$ and energy density $\mathcal{E} = E_{\text{tot}}/N = 0.07$. (Courtesy of G. Benettin [66])

been that the first normal mode would have progressively transferred energy to the others and that, after some relaxation time, every $E_k(t)$ would fluctuate around the common value. Therefore, it came as a surprise the fact that no tendency toward equipartition was observed, even for long times. In other words, a violation of ergodicity and mixing was found. Figure 3.6 shows the time evolution of the fraction of energy contained in three modes ($k = 1, 2, 3$), in a system with $N = 32$.

At the beginning all the energy is contained in mode 1. Instead of a distribution of the energy among all the available modes, with a loss of memory of the initial state, the system exhibits a close to periodic behavior. The absence of equipartition can be well appreciated looking at Fig. 3.7, where the quantities

$$E_{(\text{av})k}(T) = \frac{1}{T} \int_0^T E_k(t) \mathrm{d}t, \qquad \text{with} \quad k = 1, \ldots, N, \qquad (3.19)$$

i.e. the energies in the modes, averaged along the observation time T, are displayed. As one can see, almost all of the energy remains confined in the first four modes.

The existence of non-ergodic behavior in non-integrable Hamiltonian systems is actually a consequence of the so-called KAM theorem [67, 68, 69], whose first formulation, due to A. N. Kolmogorov, dates back to the year before the FPU paper. This was surely unbeknown to Fermi and his colleagues. The FPU result can be seen (a posteriori) as a numerical "verification" of the KAM theorem and, above all, of its physical relevance, i.e. the tori survival for physically significant values of the non-linearity. After Kolmogorov and

FPU, it is now well established that ergodicity is a non-generic property of mechanical systems.

Concerning the FPU problem, in terms of the KAM theorem, the following scenario, at least for large but finite times, can be outlined [70, 71, 72]. For N particles and for a given energy density $\mathcal{E} = E/N$ there is a threshold ϵ_c for the strength of the perturbation such that

(a) if $\epsilon < \epsilon_c$ the KAM tori are dominant and the system is essentially regular;
(b) if $\epsilon > \epsilon_c$ the KAM tori are negligible and the system is essentially chaotic.

However, the long-time evolution of very large chains with small ϵ is hindered by the presence of metastable states. To probe such an asymptotics by numerical simulations is extremely hard, for a discussion on the subject see the contributions by Benettin et al. and Lichtenberg et al. in this volume.

In most of the physical situations where the strength of the perturbation (i.e. the Hamiltonian) is fixed, the control parameter is $\mathcal{E}$. There exists a critical energy density, separating regular from chaotic behaviors. This is evident by comparing Fig. 3.8 with Fig. 3.7. In Fig. 3.8 the same quantities of Fig. 3.7 are plotted, but now they refer to a system where the energy density is much greater than before: $\mathcal{E} = 1.2$; the system has entered the chaotic region and equipartition is established.

However, also when most KAM tori are destroyed, and the system turns out to be chaotic, the validity of ordinary statistical mechanics is not automatically granted. Indeed the relaxation time for reaching equipartition may
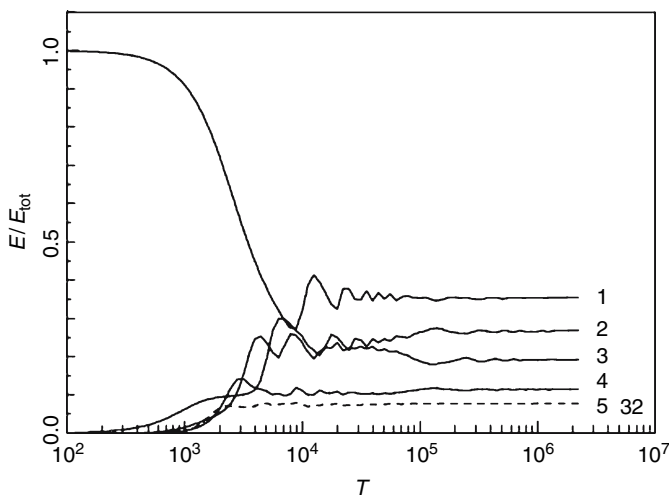

Fig. 3.7. Time averaged fraction of energy, in modes $k = 1, 2, 3, 4$ (*bold lines*, from top to below) and $\sum_{k=5}^{32} E_{(av)k}(T)/E_{tot}$ (*dashed line*). The parameters of the system are the same as in Fig. 3.6 (Courtesy of G. Benettin [66].)
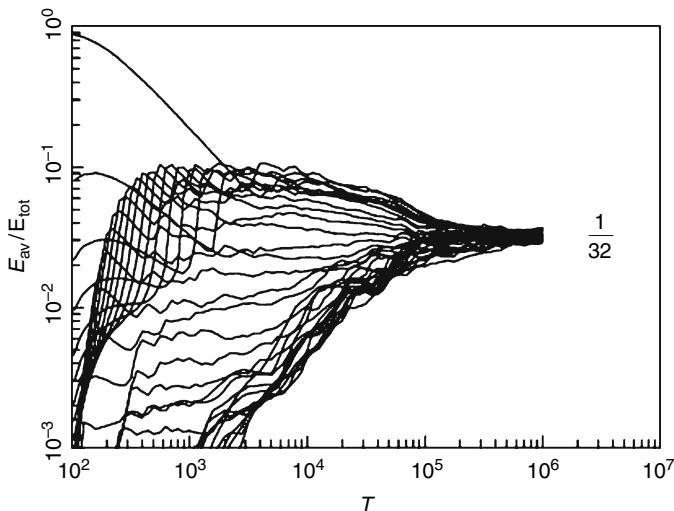
Fig. 3.8. Time-averaged fraction of energy, in all the modes $k = 1, \ldots, 32$. The parameters of the system are $N = 32$, $\alpha = 3$, $\epsilon = 0.1$ and energy density $\mathcal{E} = E_{tot}/N = 1.2$ (Courtesy of G. Benettin [66])

become very large (see [73, 74, 75, 76, 77, 78, 79] for a detailed discussion about this point).

The problem of slow relaxation is rather common in high-dimensional Hamiltonian systems, where [80, 81] though the phase-space volume occupied by KAM tori decreases exponentially with the number of degrees of freedom (which sounds like a good news for statistical mechanics) nonetheless very long time-scales are involved. This means that it takes an extremely long time for the individual trajectories to forget their initial conditions and to invade a non-negligible part of the phase space. Indeed, even for very large systems, Arnol'd diffusion is very weak and different trajectories, although with a high value of the Lyapunov exponent, maintain some of their own features for a very long time.

We conclude this part emphasizing that also in high-dimensional systems the actual role of chaos is not yet well understood. For instance, in [82] detailed numerical computations on the FPU system show that both the internal energy and the specific heat, computed with a time average, as functions of the temperature are rather close to the prediction of the canonical ensemble. This is true also in the low-energy region (i.e. low temperature) where the system behaves in a regular way (the KAM tori are dominant). This supports Khinchin approach (though the observables are not in the class of the sum functions[6]) on the poor role of dynamics. Indeed strong chaos seems to be

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[6] Khinchin defines sum functions as any function of the form $\sum_{n=1}^{N} f_n(q_n, p_n)$, f_n assuming order 1 values. Such observables, in the large N limit, are self-averaging,

unnecessary for the prediction of the statistical mechanics to hold. However, this is not the end of the story because in other non-linear systems (such as a chain of coupled rotators) the situation is different: even in the presence of strong chaos one can observe disagreement between time average and ensemble average [82].

In the following, we discuss the problem of heat transport that allows us to discuss the role of chaos for the validity of transport properties.

3.3.2 Heat Transport in Chaotic and Non-chaotic Systems

As stated in the introduction, a part of the statistical mechanics community accepts the picture according to which the instabilities of microscopic particle dynamics are the basic requirement for the onset of macroscopic transport. In this framework, several works [13, 14] have shown that, in some systems, there exists a relationship between transport coefficients (thermal or electrical conductivity, viscosity, diffusivity, etc.) and Lyapunov exponents. Such a link is of remarkable importance because it establishes a straightforward connection between the microscopic dynamical properties of a system and its macroscopic behavior, which is the main goal of statistical mechanics. However, as exemplified in the previous sections, chaotic dynamics does not seem to be a necessary condition to both equilibrium and out-of-equilibrium statistical mechanics approaches. In fact, we have seen that transport may occur even in the absence of deterministic chaos. These counterexamples pose some doubts on the generality and so on the conceptual relevance of the links found between chaotic indicators and macroscopic transport coefficients.

Heat conduction is a typical phenomenon that needs a microscopic mechanism leading to normal diffusion that distributes particles and their energy across the whole system. Since a chaotic motion has the same statistical properties of a "random walk," when observed at finite resolution, this mechanism can be found in the presence of either exponential instability in deterministic dynamics or intrinsic disorder and non-linearities.

In the context of the conduction problem, FPU chains have recently played an important role in further clarifying the transport properties of low spatial dimension systems. FPU models represent simple but non-trivial candidates to study heat transport by phonons in solids whenever their boundaries are kept at different temperatures. This issue becomes even more interesting at low spatial dimensions where the constraints set by the geometry may induce anomalous transport properties characterized by the presence of divergent transport coefficients in the thermodynamic limit [83]. Thermal conductivity χ, defined via the Fourier's Law

$$J = -\chi \nabla T \;,$$

i.e. they are practically constant on the constant-energy surface, aside a region of small measure.

relates the heat (energy) flux J to a temperature gradient. When a small temperature difference $\delta T = T_1 - T_2$ is applied to the ends of a system of linear size L, the heat current across the system is expected to be

$$J = -\frac{\chi \delta T}{L} \ .$$

For some one- and even two-dimensional systems, theoretical arguments, confirmed by several simulations, predict a scaling behavior $J \sim L^{\alpha-1}$ implying a size dependent conductivity

$$\chi(L) = L^\alpha \ . \tag{3.20}$$

As a consequence, χ diverges in the limit $L \to \infty$ with a power law whose exponent $\alpha > 0$ depends on the specific system considered. The presence of this divergence is referred to as *anomalous heat conduction* in contrast with normal conduction which, according to dimensional analysis of Fourier's Law, prescribes a finite limit for χ. FPU chains are systems where the anomaly in the heat transport is clearly observed. Its origin can be traced back to the existence of low-energy modes which survive long enough to propagate freely before scattering with other modes. Such modes can carry much energy and since their motion is mainly ballistic rather than diffusive, the overall heat transport results to be anomalous. Models other than FPU indeed presents this peculiar conduction, as widely shown in the literature [18, 84, 85]. Then the issue is the general understanding of the conditions leading to this phenomenon and more specifically the role of microscopic dynamical instabilities. A well-known chaotic system, such as the Lorentz Gas in a channel [86] configuration, provides an example of a system with normal heat conduction. This model consists of a series of semicircular obstacles with radius R arranged in a lattice along a slab of size $L \times h$ ($h \ll L$) see Fig. 3.9. As in a Lorentz system, particles scatter against obstacles but do not interact with each other.
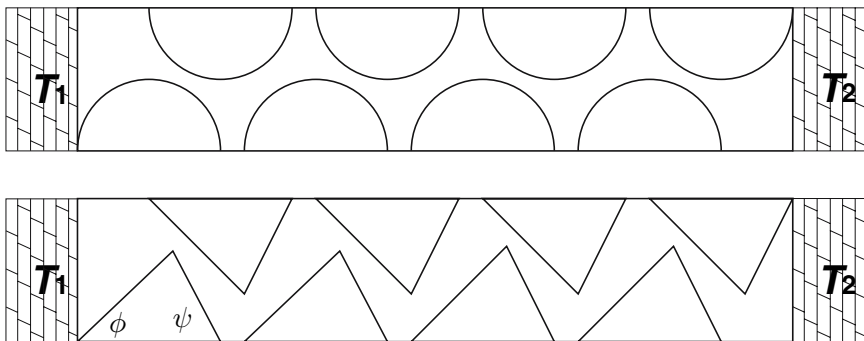

Fig. 3.9. Example of channel geometry used in [84, 86] to study heat transport in low-dimensional chaotic (*upper panel*) and non chaotic billiards (*lower panel*)

Two thermostats at temperatures T_1 and T_2 respectively are placed at each end of the slab to induce transport. They reinject into the system those particles reaching the ends with a velocity drawn from a Gaussian velocity distribution with variance proportional to the temperatures T_1 and T_2. In the case of semicircular obstacles, the system is chaotic and one observes a standard Fourier's Law [86].

In [18] and [84], some non-chaotic variants of the Lorentz channel have been proposed in order to unravel the role of exponential instabilities in the heat conduction. In those models, called the Ehrenfest Channel, the semicircular obstacles were replaced with triangular ones, so that the system is trivially non-chaotic since collisions with flat edges of the obstacles cannot separate trajectories more than algebraically. The results show that when two angles (e.g. ϕ and ψ) of the triangles are irrational multiple of π, the system exhibits a normal heat conduction. On the contrary, for rational ratio, such as isosceles right triangles, the conduction becomes anomalous. The single particle heat flux across N cells $J_1(N)$ scales as $J_1(N) \sim N^\alpha$, while the temperature gradient behaves as $1/N$ implying that $\chi(N)$ diverges as $N \to \infty$. The explanation of such a divergence can be found in the single-particle diffusivity along the channel direction which occurs in a non-standard way. Indeed, the evolution of a large set of particles has a mean squared displacements from initial conditions which grows in time with a power-law behavior

$$\langle [x(t) - x(0)]^2 \rangle \sim t^b$$

with an exponent $1 < b < 2$. This super-diffusion is the unique responsible for a divergent thermal conductivity independently of Lyapunov instabilities, since the model has a zero Lyapunov exponents.

When an Ehrenfest Channel with anomalous thermal conductivity is disordered, for instance, by randomly modulating the height of triangular obstacles or their positions along the channel, the conduction follows Fourier's law, becoming normal [18]. This scenario is rather similar to that one discussed in Sect. 3.2.2 for diffusion on non chaotic maps.

The works in [83, 87, 88] suggest that the anomalous conduction is associated with the presence of a mean free path of energy carriers that can behave abnormally in the thermodynamic limit. For FPU the long mean free path is due to soliton-like ballistic modes. In the channels, the long free flights, between consecutive particle collisions, become relevant. The above considerations suggest a very week role of chaos for heat transport, and for transport in general, since also systems without exponential instability may show transport, even anomalous.

3.4 Concluding Remarks

The problem of distinguishing chaos from noise cannot receive an absolute answer in the framework of time series analysis. This is due to the finiteness

of the observational data set and the impossibility to reach an arbitrary fine resolution and high embedding dimension. However, we can classify the signal behavior, without referring to any specific model, as stochastic or deterministic on a certain range of scales.

Diffusion may be realized in both stochastic and deterministic systems. In particular, as the analysis of polygonal billiards and non-chaotic maps (see Sect. 3.2.2) shows, chaos is not a prerequisite for observing diffusion and, more in general, nontrivial statistical behaviors.

In a similar way, we have that for the validity of heat conduction chaos is not a necessary ingredient. Also in systems with zero maximal Lyapunov exponent (see [84, 85, 86]) the Fourier's law (or its anomalous version) can hold.

We conclude by noticing that the poor role of exponential instability for the validity of statistical laws does not seem to be limited to transport problems. For instance it is worth mentioning the interesting results of Lepri et al. [89] showing that the Gallavotti–Cohen formula [90], originally proposed for chaotic systems, holds also in some non-chaotic model.

Acknowledgments

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