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Initial growth of Boltzmann entropy and chaos in a large assembly of weakly interacting systems

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Abstract

We introduce a high-dimensional symplectic map, modeling a large system, to analyze the interplay between single-particle chaotic dynamics and particles interactions in thermodynamic systems. We study the initial growth of the Boltzmann entropy, S_B, as a function of the coarse-graining resolution (the late stage of the evolution is trivial, as the system is subjected to no external drivings). We show that a characteristic scale emerges, and that the behavior of S_B vs t, at variance with the Gibbs entropy, does not depend on the resolution, as far as it is finer than this scale. The interaction among particles is crucial to achieve this result, while the rate of entropy growth, in its early stage, depends essentially on the single-particle chaotic dynamics. It is possible to interpret the basic features of the dynamics in terms of a suitable Markov approximation.

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1. Introduction

Statistical mechanics was founded by Maxwell, Boltzmann and Gibbs for the equilibrium description of systems with a very large number of particles. Boltzmann and Gibbs are often considered the champions of two different points of view about statistical mechanics: this *vulgata* takes Gibbs as the founder of the ensemble approach, and Boltzmann as the promoter of a dynamical theory based on the ergodic hypothesis. Consequently, modern textbooks [1] use Gibbs's terminology for the ensembles (i.e., microcanonical, canonical and grandcanonical), although both ergodicity and ensembles are Boltzmann's inventions (cf. Refs. [2–5]).

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There is an unanimous consensus on the statistical description of thermodynamic equilibrium states by means of a suitable ensemble, i.e., a probability density, $\rho_{eq}(\mathbf{X})$, in the Γ phase space. In particular, $S_G = -k_B \int \rho_{eq}(\mathbf{X}) \ln \rho_{eq}(\mathbf{X}) \, d\mathbf{X}$ is universally recognized as the equilibrium thermodynamic entropy, S_{eq}. On the contrary, a consistent definition of non-equilibrium entropy remains an open problem. In the following and in Section 2, we summarize well known facts about this subject, in order to introduce the perspective of the present paper, and to set our notation. Two main points of view can be identified in this context.

The "Gibbsian" one [6] considers as a fundamental object an ensemble of points in Γ, with density $\rho(\mathbf{X}, 0)$, representing the distribution of microstates compatible with the initial non-equilibrium macroscopic conditions. To overcome the effects of the Liouville theorem, one performs a coarse-graining of the phase space, introduces a coarse-grained version of the density, $\rho_{cg}(\mathbf{X}, 0)$, and obtains a coarse-grained entropy $S_{cg}(0) = -k_B \int \rho_{cg}(\mathbf{X}, 0) \ln \rho_{cg}(\mathbf{X}, 0) \, d\mathbf{X}$. The Hamiltonian evolution of the initial microstates can lead $\rho_{cg}(\mathbf{X}, t)$ to an equilibrium distribution whose entropy will be the evolved $S_{cg}(t)$.

The difficulties with the "phase space coarse-graining" recipe are as old as the recipe itself, and they may be well represented by a sentence adapted from Jaynes [7]: "Any really satisfactory demonstration of the second law must therefore be based on a different approach than coarse-graining", since the variation of S_{cg} "is due only to the artificial coarse-graining operation and it cannot therefore have any physical significance…" (note that this statement concerns the "artificial" phase space coarse-graining, not all forms of coarse-graining). Or else, as Mackey writes [8]: "Experimentally, if entropy increases to a maximum only because we have reversible mixing dynamics and coarse graining due to measurement imprecision, then the rate of convergence of the entropy (and all other thermodynamic variables) to equilibrium should become slower as measurement techniques improve. Such phenomena have not been observed."

In the "Boltzmannian" point of view [4], one defines the (Boltzmann) entropy, S_B, with reference to a single macroscopic system and to the values of the macroscopic variables, identifying its macrostate M. One takes $S_B = k_B \ln |M|$, where k_B is the Boltzmann' s constant and $|M|$ is the phase space volume occupied by the microstates with the same macrostate. Now one follows the dynamics of one allowed microstate and the evolution it induces on $\ln |M|$. One would like to obtain that, for "almost" all the initial microstates, the induced behavior of S_B conforms to the laws of thermodynamics. For instance, in the case of a dilute gas, a useful macroscopic variable to define the thermodynamic state of the system, is the one-particle distribution function $f(\mathbf{q}, \mathbf{p}, t)$, obtained by an appropriate coarse-graining in the μ-space. In this case (and only in this case) the logarithm of the volume occupied by the compatible microstates is well approximated by: $-N \int\int f(\mathbf{q}, \mathbf{p}, t) \ln f(\mathbf{q}, \mathbf{p}, t) \, d\mathbf{q} \, d\mathbf{p}$. So, for a dilute gas, the Boltzmann entropy takes the form:

$$S_B = -Nk_B \int f(\mathbf{q}, \mathbf{p}, t) \ln f(\mathbf{q}, \mathbf{p}, t) \, d\mathbf{q} \, d\mathbf{p} \tag{1}$$

and is expected to increase, according to the Boltzmann equation, as Lanford [9] demonstrated to be true, in a suitable limit.[1]

Differently from the phase space description, which requires one ensemble of many identical systems, in order to do the statistics, in the μ-space description the statistics concerns the particles of a single system. Therefore, while the Γ-space statistics can be built for systems of any number of particles, even just one, the μ-space statistics requires the single system under consideration to be made of a large number of particles.

One has to note that the two entropies are equivalent at equilibrium while in non-equilibrium situations, in principle, they test different features of a given system. The Gibbs entropy concerns the spreading in phase space of the initial ensemble of microstates, which is selected by the interesting macroscopic observables. In this picture, the time evolution of these observables plays no role. Differently, the Boltzmann entropy concerns the evolution of phase space volumes, as determined directly by the evolution of the interesting observables.

The debate on Boltzmann entropy, Gibbs entropy and irreversibility has been renewed by a paper of Lebowitz [4].

[1]One should observe that the system must be specified in terms of macroscopic variables, which implies that a different Boltzmann entropy could be defined, by considering different observables. The particles density is the most appropriate quantity in our case, and we concentrate only on that, since this is not expected to make any qualitative difference in our arguments.

The aim of our paper is to contribute to the understanding of the role of coarse-graining procedures, and of deterministic chaos, in non-equilibrium statistical mechanics. Specifically, we consider the problem of the onset of entropy growth; that is, we address the following question: for a non-equilibrium system, with given initial values of the Gibbs and Boltzmann entropies $S_G(0)$ and $S_B(0)$, at what times t do $S_G(t)$ and $S_B(t)$ begin to vary? How do the coarse-grainings in either Γ- or μ-spaces affect these events? In the recent years very interesting results in ensemble theory à *la* Gibbs have been obtained by means of Lorentz type models [10,11]. These results, in particular, show that, after the process of Gibbs entropy variation started, its asymptotic time behavior is not sensible to the performed coarse-graining. We underline that we are here interested in the very initial stage of the process, where these results do not apply. Moreover we discuss the entropy evolution in an isolated system, where there is no stationary entropy production.

For a system consisting of N non-interacting particles, a one-particle density, $f(\mathbf{q}, \mathbf{p}, t)$, can be seen as a phase space distribution, $\rho(\mathbf{q}, \mathbf{p}, t)$, of an ensemble of N single-particle systems. The coordinates and velocities of the N particles represent one state of a system, in a $6N$-dimensional Γ-space, by which one builds a distribution in a six-dimensional μ-space. However, they represent also N independent states in the six-dimensional Γ-space of single-particle systems. Although conceptually different, f and ρ are the same function in this case, evolve in the same way, hence the corresponding Boltzmann and Gibbs entropies also evolve in the same way, and there is no intrinsic evolution of $\eta_{ni}(t) = -k_B \int f(\mathbf{q}, \mathbf{p}, t) \ln f(\mathbf{q}, \mathbf{p}, t) \, d\mathbf{q} \, d\mathbf{p} = -k_B \int \rho(\mathbf{q}, \mathbf{p}, t) \ln \rho(\mathbf{q}, \mathbf{p}, t) \, d\mathbf{q} \, d\mathbf{p}$. Indeed, if a coarse-graining is performed either in μ- or Γ-space, the time evolution of the coarse-grained η_{ni} can be delayed further and further by taking finer and finer partitions. The fact is that, in this case, a non-arbitrary evolution of the entropy can only be produced by the integration away of the uninteresting variables (defined once the interesting ones are chosen) from the μ-density, i.e., by performing a "trivial partition" of the μ-space [8].

It is known [12,13] that a form of irreversibility may be found in chaotic systems of non-interacting particles. Indeed, free particles in a box homogenize their spatial coordinates; and in irregularly shaped boxes their velocity distribution can become isotropic; but a relaxation of velocities to a Maxwellian is impossible, in the absence of interactions. Thus, such systems may describe, for some aspects, highly rarefied gases, or Knudsen gases in an irregular container.[2]

When all the canonical variables in the μ-space are interesting, we can no more make entropy grow by hiding some variable: particles must interact to obtain a growth. With interactions, $f(\mathbf{q}, \mathbf{p}, t)$ recovers its meaning of one-particle density, and loses its similarity with a Gibbs ensemble. We show that a characteristic scale emerges in the μ-space of interacting chaotic particle systems, which can be interpreted as the scale at which the "diffusive" small scale behavior, due to the interactions, smoothes the fragmented structures created by the chaotic dynamics. This implies that the growth of S_B becomes independent of the resolution, as long as the observation scale is finer than the characteristic one. But to achieve this, it is of fundamental importance that the number of particles be large, i.e., that the one-particle distribution describes a macroscopic system.

We conclude that:

(a) the onset of entropy variation in the Gibbs case has no intrinsic meaning; indeed, it can be delayed at will in time, since it depends on an arbitrary choice (the size of the graining) that is external to the dynamics. This is the same both for interacting and non-interacting systems, as well as for large or small systems.
(b) The Boltzmann entropy (at least the particular case we consider) begins to change at an intrinsic time that is fixed by the dynamics. This requires a large system of interacting particles (otherwise one falls back in the Gibbs case).

Various of these ideas have been previously addressed. See, for instance, Ref. [16] for the graining in phase space induced by a graining in μ-space and the choice of macro-variables, and for the relation between the one-particle distribution function of interacting and of non-interacting particle systems. Here we express these ideas in a quantitative form, besides reporting the discovery of the characteristic scale in the μ-space of interacting systems.

[2]The lack of interactions imparts very interesting (cf. Refs. [14,15]) properties to such gases. Their behavior, like in Knudsen gases, is dominated by the collisions with the walls of the container.

In Section 2 we briefly summarize basic facts about Gibbs and Boltzmann entropies. In Section 3 we introduce a high-dimensional symplectic map simulating a large system, consisting of weakly interacting chaotic subsystems, and we show the behavior of the Boltzmann entropy S_B vs time. The main result is that, for interacting subsystems, S_B is independent of the details of the coarse-graining in μ-space, if the graining is sufficiently fine: an intrinsic graining scale is found in μ-space. The interactions are absolutely necessary for this result; however, it is remarkable that some numerical aspects of S_B (e.g. its slope not too far after the growth started) depend only on the chaotic properties of the single subsystem. In Section 4 we interpret our results through a mechanism similar to that of decoherence in the semiclassical limit of quantum mechanics. Conclusions and perspectives are given in Section 5.

2. On the Gibbs and Boltzmann entropy

Consider a Hamiltonian system of N particles, whose microscopic states are described by vectors $\mathbf{X}(t)$ in the phase space Γ. Denoting by $\rho(\mathbf{X})\,\mathrm{d}\mathbf{X}$ the probability for a state to be found in the phase space volume $\mathrm{d}\mathbf{X}$, one defines the Gibbs entropy as

$$S_G(\{\rho\}) = -k_B \int \rho(\mathbf{X}) \ln \rho(\mathbf{X})\,\mathrm{d}\mathbf{X}, \tag{2}$$

where k_B is the Boltzmann's constant. The time evolution $\mathbf{X}(0) \to \mathbf{X}(t)$ is ruled by Hamilton's equations, hence S_G is constant in time, by Liouville's theorem. Nevertheless, a coarse-graining by cells of size Δ in Γ leads to an increase of the coarse-grained Gibbs entropy[3]

$$S_G(t,\Delta) = -k_B \sum_i p_\Delta(i,t) \ln p_\Delta(i,t), \tag{3}$$

where the coarse-grained probability $p_\Delta(i,t)$ is given by

$$p_\Delta(i,t) = \int_{\Lambda_{i,\Delta}} \rho(\mathbf{X},t)\,\mathrm{d}\mathbf{X} \tag{4}$$

and $\Lambda_{i,\Delta}$ is the cell of linear size Δ, centered at $\mathbf{X}^{(i)}$. For chaotic systems with initial probability distribution supported on a small region of linear size σ, simple arguments (see Appendix A) suggest that, after a short transient time t_λ, for some time $S_G(t,\Delta)$ increases linearly:

$$S_G(t,\Delta) - S_G(0,\Delta) \simeq \begin{cases} 0, & t < t_\lambda, \\ h_{KS}(t - t_\lambda), & t_\lambda < t < t_e, \end{cases} \tag{5}$$

where h_{KS} is the Kolmogorov–Sinai entropy of the system,

$$t_\lambda \sim \frac{1}{\lambda_1} \ln\left(\frac{\sigma}{\Delta}\right), \tag{6}$$

λ_1 is the first Lyapunov exponent and t_e is the time when the linear regime ends. As pointed out, the prediction of Eq. (5) is limited to times which are not too long, so that the saturation regime is not involved; moreover it is not always correct: it holds only if intermittency effects are negligible (see Appendix A and Ref. [17] for more details on Eqs. (5) and (6)).

Consider now Boltzmann's viewpoint, for a system of N weakly interacting particles. A one-body probability distribution function $f(\mathbf{q},\mathbf{p},t)$ (the probability density of finding a particle in a given volume of the single-particle space μ) can be introduced without any reference to an ensemble of macroscopically identical systems, each represented by a different point in Γ-space. Indeed, let us consider one single system made of a large number N of identical particles, in a d-dimensional physical space, let us introduce a cell size Δ in the μ-space and let be $N \gg \Delta^{-2d}$, so that each cell contains a statistically relevant number of particles. Then, the

[3] $S_G(t,\Delta)$ is the discretization of S_G, by cells of size Δ, except for an additive term $k_B \ln \Delta$. At fixed Δ, this term is constant and not relevant for the entropy variations in time.

one-particle coarse-grained distribution is defined by

$$f_{\Delta}(\mathbf{q}^{(j)}, \mathbf{p}^{(k)}, t) = \frac{1}{N}\sum_{i=0}^{N} \Theta\left(1 - \frac{2|\mathbf{q}^{(j)} - \mathbf{q}_i(t)|}{\Delta}\right)\Theta\left(1 - \frac{2|\mathbf{p}^{(k)} - \mathbf{p}_i(t)|}{\Delta}\right), \tag{7}$$

where $\Theta(z)$ is the Heaviside step function and $\mathbf{q}^{(j)}$, $\mathbf{p}^{(k)}$ are the coordinates of the center of each cell C_{jk} having linear size Δ, and volume Δ^{2d}, in the appropriate units. This μ-space function suitably identifies a macrostate for a dilute gas whose volume $\Delta\Gamma$ in phase space is related to the Boltzmann entropy by

$$S_B = k_B \log \Delta\Gamma. \tag{8}$$

In the case at hand, S_B can be well approximated by

$$S_B = -Nk_B \sum_{j,k} f_{\Delta}(\mathbf{q}^{(j)}, \mathbf{p}^{(k)}) \ln f_{\Delta}(\mathbf{q}^{(j)}, \mathbf{p}^{(k)}), \tag{9}$$

where terms dependent on Δ and N have been disregarded. The Boltzmann entropy for these systems can also be written as

$$S_B(t) = -Nk_B \int f(\mathbf{q}, \mathbf{p}, t) \ln f(\mathbf{q}, \mathbf{p}, t)\, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{p}, \tag{10}$$

where f is the regular μ-space probability distribution, obtained in the $N \to \infty$, $\Delta \to 0$ limit of Eq. (7). For dilute systems under the hypothesis of molecular chaos, the celebrated Boltzmann's H-theorem holds:

$$\frac{\mathrm{d}S_B}{\mathrm{d}t} \geqslant 0. \tag{11}$$

The validity of the molecular chaos hypothesis has been demonstrated for the class of dilute systems in the Grad limit, where $N \to \infty$ and the interaction range goes to zero in order to keep the total cross-section constant [9,18].

Some textbooks connect Boltzmann's and Gibbs's approaches noticing that in dilute systems

$$\rho(\mathbf{X}, t) \simeq \prod_{j=1}^{N} f(\mathbf{q}_j, \mathbf{p}_j, t), \tag{12}$$

hence $S_G \simeq S_B$. But this is only partially justified. There are at least two important conceptual differences between the two approaches:

- Gibbs' point of view is based on the ensemble, i.e., on an abstract collection of identical systems, and does not depend on the number of particles of which each system is made. Differently, Boltzmann's approach does not require an ensemble of copies of the same system, but needs $N \gg 1$, in order to compute $f(\mathbf{q}, \mathbf{p}, t)$ for the single system.
- The Gibbs entropy deals with the Γ-space, and necessitates a coarse-graining procedure in order to avoid the consequences of the Liouville theorem and grow in an irreversible evolution. Boltzmann's graining of the μ-space is introduced to deal with a smooth empirical distribution and to define a macrostate, so the entropy can grow despite the Liouville theorem.

Thus, (12) must be interpreted *cum grano salis*, lest one is mislead by (11) into believing that the Gibbs entropy (2) grows. In the following, we show that, for long enough times and non-vanishing interactions, the growth of S_B does not depend on the cell size, while this is not so for non-interacting systems.

3. The Boltzmann entropy of a chaotic system

3.1. The discrete time model

Consider a system of $N \gg 1$ non-interacting particles moving in a periodic array of fixed convex scatterers, with which they collide elastically. The position of the scatterers should avoid the presence of collisionless

trajectories, i.e., the horizon should be finite. It is well established that such a system, known as the Lorentz gas,[4] is chaotic and displays asymptotic diffusion. The Gibbs entropy of such a system obeys $S_G(t) = S_G(0)$, while the coarse-grained entropy increases linearly with t, for $t > t_\lambda$ (before saturation). It is easy to see that $h_{KS} = Nh_1$, where h_1 is the Kolmogorov–Sinai entropy of a single particle, and $S_B = S_G = \text{constant}$, because the particles are independent, and the probability distribution in phase space factorizes in N identical terms.

Quite different is the case of interacting particles, as for the generalization of the Lorentz gas of Ref. [19], where particles are not point-like, but have a finite size and collide with the scatterers, as well as with each other. The study of such a system, for a large number of particles, is very expensive from a computational point of view. Therefore, we propose a system of coupled symplectic maps as a substitute for the particle system, which shares its main features, considering a two-dimensional map, with one "coordinate" and one "momentum", in place of each particle. We introduce a form of interaction among these "particles", requiring that:

- in the absence of interactions, the single-particle dynamics in the corresponding μ-space be chaotic and volume preserving;
- in the presence of interactions, the dynamics of the whole system, described by the vector $\mathbf{X} = (\mathbf{Q}, \mathbf{P})$, $\mathbf{Q} = (q_1, \ldots, q_n)$, $\mathbf{P} = (p_1, \ldots, p_n)$, be symplectic and volume preserving in the Γ-space.

The symplectic map is defined by

$$\begin{cases} q_i = \partial G(\mathbf{Q}', \mathbf{P})/\partial p_i \bmod 1, \\ p_i' = \partial G(\mathbf{Q}', \mathbf{P})/\partial q_i' \bmod 1 \end{cases} \tag{13}$$

where the generating function $G(\mathbf{Q}', \mathbf{P})$ is given by

$$G(\mathbf{Q}', \mathbf{P}) = \mathbf{Q}'\mathbf{P} - \frac{|\mathbf{P}|^2}{2} - \frac{k}{2\pi}\sum_{i=0}^{N}\sum_{j=0}^{N_S}\cos[2\pi(q_i' - Y_j)] - \frac{\varepsilon}{4\pi}\sum_{i=0}^{N}\sum_{n=-M/2}^{M/2}\cos[2\pi(q_i' - q_{i+n}')] \tag{14}$$

with $q_i, p_i \in [0, 1]$. To make the numerical simulations faster, we assume that each "particle" interacts with a limited number M of other "particles", N_S is the number of fixed "obstacles" having positions Y_j, which play the role of the convex scatterers in the Lorentz gas, and N is the number of "particles". The parameters k and ε represent the interaction strength between particles and obstacles and among particles, respectively. If $k = \varepsilon = 0$ the particles are free. The functional form of G is reminiscent of the standard map, which is a paradigm of symplectic dynamics. The boundary conditions on the variables are periodic, and the interactions do not present discontinuities at the boundaries. Substituting Eq. (14) into (13), one finds:

$$\begin{cases} q_i' = q_i + p_i \bmod 1, \\ p_i' = p_i + k\sum_{j=0}^{N_S}\sin[2\pi(q_i' - Y_j)] + \varepsilon\sum_{n=-(M/2)}^{M/2}\sin[2\pi(q_i' - q_{i+n}')] \bmod 1. \end{cases} \tag{15}$$

Since the system is symplectic, the dynamics described by the points $(\mathbf{Q}, \mathbf{P})$ will preserve volumes in phase space.

3.2. Numerical results

In the following, we calculate the one-particle distribution for a given cell size (cf. Eq. (7)), as a function of time. Then, we study the growth with time of the corresponding Boltzmann entropy per particle, defined by

$$\eta(t, \Delta) = -k_B\sum_{j,k} f_\Delta(q^{(j)}, p^{(k)}, t)\,\log f_\Delta(q^{(j)}, p^{(k)}, t) \tag{16}$$

[4]In Lorentz's original model, the moving particles were considered in thermal equilibrium with the scatterers, which is impossible to achieve without energy exchanges between scatterers and particles, as in the present model.

by varying the interaction strength ε and the cell size Δ. In our computations, where we set $k_B = 1$ for convenience, there are no *a priori* assumptions such as the hypothesis of molecular chaos; the quantity $f_\Delta(q,p,t)$ evolves according to the exact dynamics.

As discussed in the Introduction and in Section 2, (16) is correct (in the sense that it is linked to the interesting volume of phase space) only in the case of dilute systems. For systems, whose potential energy is not a tiny fraction of the total, it has been proposed [16,20] that a similar relation may still be used, with the prescription to count only microstates corresponding to a fixed total energy E. Even for non-interacting systems the quantity (16) characterizes the extension of the macrostate in phase space, provided that the empirical distribution f_Δ is a good approximation of a particle density $f(q,p,t)$. This requires $\Delta \gg N^{-1/2d}$, which allows (16) to be close to (8).

We choose N_S and k (both related to the single-particle chaotic behavior) in such a way that the Lyapunov exponent of the single-particle dynamics is not too large, and there are no KAM tori, which constitute barriers for the transport. In particular $N_S = 10^3$ and $k = 0.017$ realize this requirement. The obstacle positions are selected at random, with a uniform p.d.f. An example of a trajectory in the one-particle (q,p) space, for $N = 10^7$, is shown in Fig. 1. The result is that the Lyapunov exponent is $\lambda \approx 0.162$. We perform simulations with different values of ε and, for initial non-equilibrium condition, we take a cloud of points distributed according to a Gaussian of r.m.s.d $\sigma = 0.01$, having the point $(q,p) = (\frac{1}{4}, \frac{1}{2})$ as a center (we checked that this point is far enough from the regular islands, see Fig. 1). At each time, we compute the differences between the entropy per particle and its initial value at several resolutions Δ:

$$\delta S(t,\Delta) = \eta(t,\Delta) - \eta(0,\Delta). \tag{17}$$

We begin with $\varepsilon = 0$. The entropy growth shown in Fig. 2 is only due to the discretization procedure, since the equation ruling the evolution of $f(q,p,t)$ obeys the Liouville theorem. This means that the "true" Boltzmann entropy for $\Delta \to 0$ is constant in time. As shown in Fig. 2, the curves of the entropy differences as functions of time stay constant up to a time t_λ depending on Δ. After this transient, and for a certain time interval, the slope of $\delta S(t,\Delta)$ is practically the same for all curves and is approximately given by h_{KS} (see Eq. (5)). Looking at the curves of the entropy differences as functions of Δ, Fig. 3, it is possible to extrapolate the behavior for $\Delta \to 0$: far from the saturation (for small times) and for Δ not too large, these curves go correctly to zero when $\Delta \to 0$, and are well fitted by a power law:

$$\delta S(t,\Delta) \propto \Delta^2. \tag{18}$$

This suggests that the relevant parameter for understanding the finite resolution behavior of the entropy differences is the cell area Δ^2. For $t > t_\lambda$, one has

$$\delta S(t,\Delta) = a \log(\Delta) + b. \tag{19}$$

The behavior of Eqs. (18) and (19) is consistent with Eq. (5), taking into account that the rate of entropy growth after t_λ is generally different from the Lyapunov exponent, leading to $a \neq 1$ [17]. As noted in the

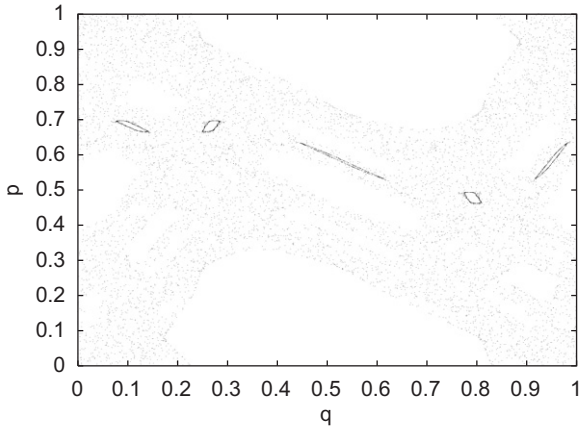

Fig. 1. A trajectory generated by 10^4 map iterations in the phase space of a single particle, with $N_S = 10^3$, $k = 0.017$, $\varepsilon = 0$.

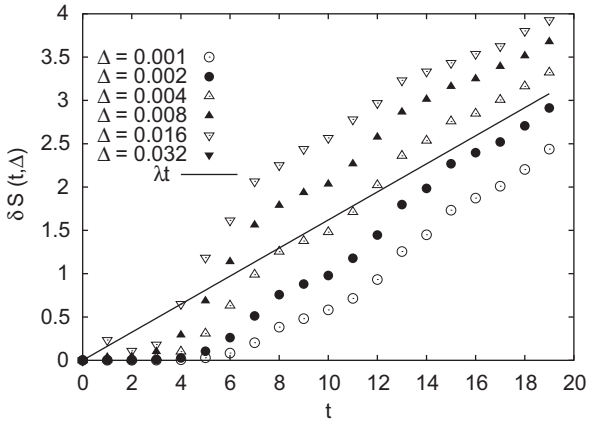

Fig. 2. $\delta S(t,\Delta)$ with $\varepsilon = 0$ (non-interacting particles) as a function of t for different values of Δ. The slope of the straight line equals Lyapunov exponent.

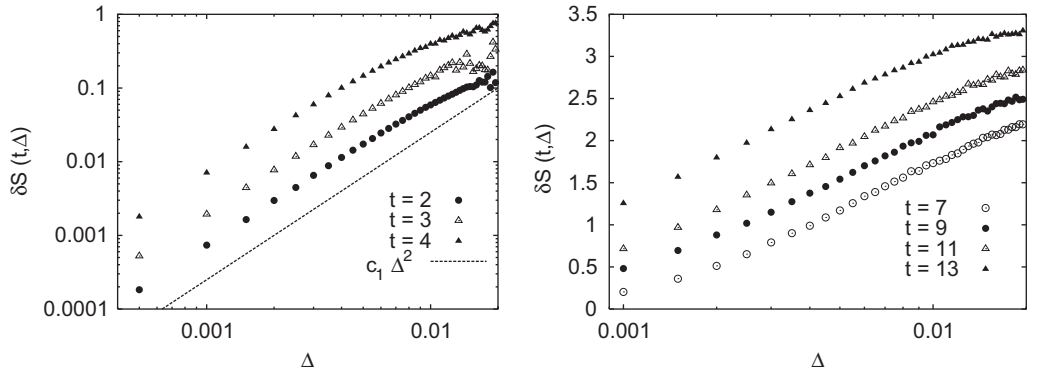

Fig. 3. $\delta S(t,\Delta)$ with $\varepsilon = 0$ (non-interacting particles) as a function of Δ, for small values of t (left) and large values of t (right). In the left panel, the dotted line shows the expected behavior $\delta S(t,\Delta) \propto \Delta^2$, while the logarithmic behavior is clearly visible in the right panel (notice the log-linear scale).

Introduction, when $\varepsilon = 0$ the behaviors of S_B and S_G are the same, because the given one-particle density, $f(q,p,t)$, obtained from N non-interacting particles, is nothing but the density, $\rho(q,p,t)$, describing a Gibbs ensemble of N single-particle systems.

Fig. 2 seems to imply that a suitable coarse-graining procedure allows the entropy to increase, after a certain time, in spite of Liouville's theorem. Such a growth would have been an intrinsic property of the dynamics if it had been associated with an intrinsic graining scale, but the only intrinsic scale of a non-interacting system is $l_c \sim N^{-1/2d}$ (in the present case $d = 1$). However, l_c cannot be used to define the coarse-grained Boltzmann entropy, because there is no statistics on that scale. The correct derivation of the Boltzmann entropy requires that $N \to \infty$ while $\Delta \to 0$, in such a way that Δ stays much larger than l_c. This is the extrapolation of Fig. 3, where one can see how the effect of Liouville's theorem on S_G is restored. That this picture is correct, is proved by Fig. 4 for the entropy growth as a function of Δ, with different values of N. Indeed, in Fig. 4, one observes that the curves for different N collapse to a unique curve which tends to zero, both at short and long times, if $\Delta \gg l_c$. In other words, if the cells are occupied by a statistically relevant number of particles, the behavior of the entropy is unique and shows no evolution in time. In the following, we fix $N = 10^7$, that is large enough for our range of Δ values.

Consider now the "interacting" case, i.e., $\varepsilon > 0$. Figs. 5 and 6 show that $\delta S(t,\Delta)$ does not extrapolate anymore to zero when $\Delta \to 0$, and for small (fixed) times, they are well fitted by

$$\delta S(t,\Delta) \approx c_0 + c_1 \Delta^2. \tag{20}$$

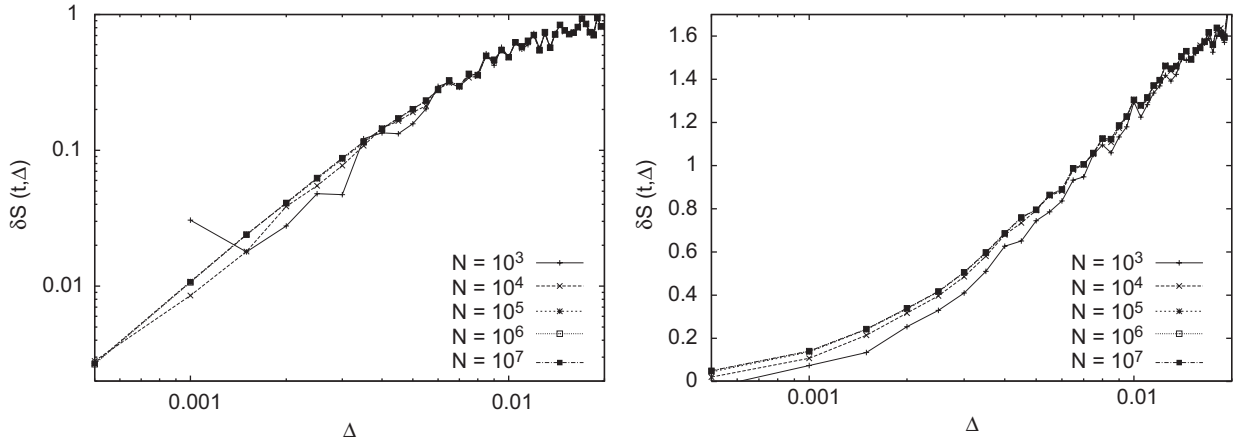

Fig. 4. Comparison of Boltzmann entropy growth as a function of Δ at fixed time, plotted for different values of N. Parameters are $k = 0.017$, $\varepsilon = 0$ and $N_S = 1000$; $t = 3$ in the left picture and $t = 9$ in the right one. Small numerical differences between these figures and Fig. 3 are due to a different realization of the obstacles positions.

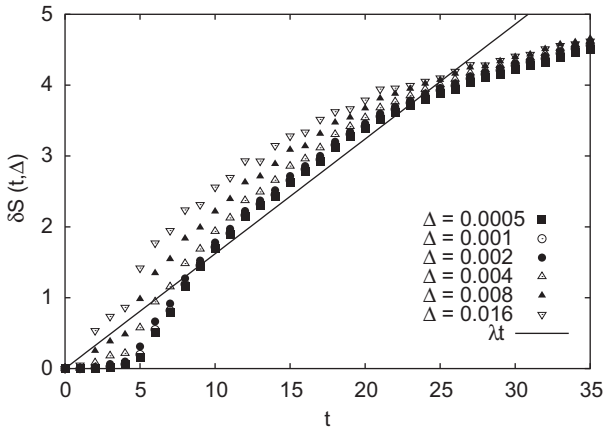

Fig. 5. $\delta S(t, \Delta)$ with $\varepsilon = 10^{-4}$ as a function of t for different values of Δ. The straight line slope equals the Lyapunov exponent.

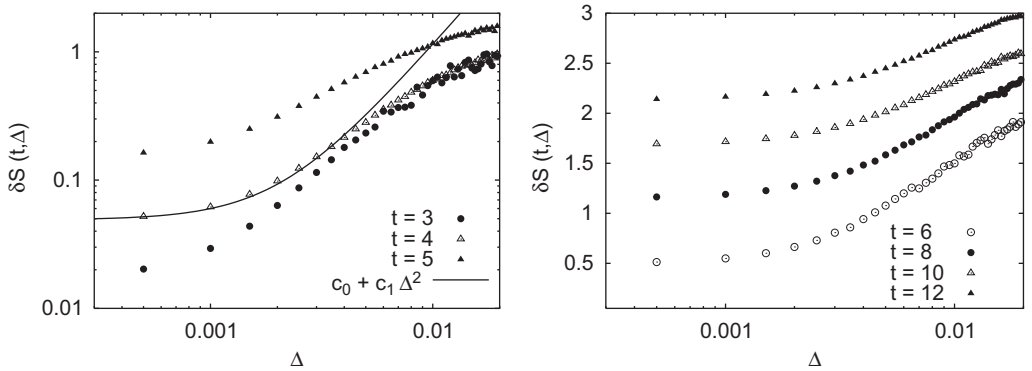

Fig. 6. $\delta S(t, \Delta)$ with $\varepsilon = 10^{-4}$ as a function of Δ for small values of t (left panel) and large values of t (right panel). In the left panel the line shows the behavior $c_0 + c_1\Delta^2$, while in the right panel $\delta S(t, \Delta)$ shows a weak dependence on Δ for $\Delta \to 0$.

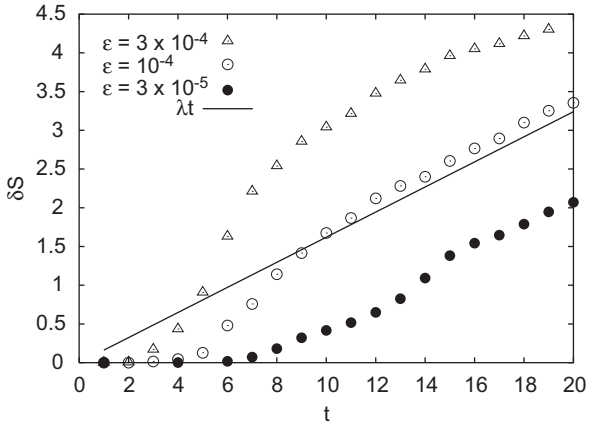

Fig. 7. Extrapolation for $\Delta \to 0$ of the curves $\delta S(t, \Delta)$ as a function of t for various values of ε.

After a characteristic time depending on ε, $t_*(\varepsilon)$, the entropy shows a weak (logarithmic) dependence on Δ and correctly extrapolates to a finite value for $\Delta \to 0$ (see Fig. 7).

Let us now summarize and comment on the previous results:

(a) For non-interacting systems ($\varepsilon = 0$), because of the absence of an intrinsic graining scale (except for l_c, which cannot be used), the growth of $\delta S(t, \Delta)$ reflects the properties of the observation tools, i.e., the statement that $\delta S \simeq 0$ for $t \lesssim t_\lambda(\Delta)$ and that $\delta S \simeq \lambda(t - t_\lambda(\Delta))$ for $t \gtrsim t_\lambda(\Delta)$, has a "subjective" character. Since t_λ increases as Δ decreases, not only does the value of the entropy depend on the coarse-graining, but the entropy growth depends (for "small" t) on the resolution scale, as noticed also in Ref. [21].

(b) For weakly interacting systems, there is an effective cell size $\Delta_*(\varepsilon, \lambda)$, such that $\delta S(t, \Delta)$ does not depend on Δ, if $\Delta < \Delta_*(\varepsilon, \lambda)$. Here, the entropy growth is objective, i.e., the limit for $\Delta \to 0$ of $\delta S(t, \Delta)$ exists, is finite, hence is an intrinsic property of the system (cf. Fig. 6).

(c) The role of chaos in the limit of vanishing coupling is relevant: the slope of $\delta S(t, \Delta)$, for intermediate values of t, is given by the Lyapunov exponent; but the existence of an effective cell size $\Delta_*(\varepsilon, \lambda)$ and the corresponding $t_*(\varepsilon, \lambda)$ depends on the coupling strength ε, and on λ.

(d) In the evaluation of Eqs. (7) and (16), no assumptions, such as the hypothesis of molecular chaos or of system's dilution, are made. Mathematically, we can define the entropy of a distribution as in Eq. (16) in full generality. However, we consider only the weakly interacting limit of small ε, for the physical reason that only in such a case does this entropy represent the Boltzmann entropy and does it afford a proper thermodynamic meaning.

(e) For small values of ε, the time evolution of $f(q, p, t)$ differs from the case $\varepsilon = 0$ only on very small scales; in other words, the coupling is necessary for the "genuine" growth of the entropy, but it does not have any dramatic effect on $f(q, p, t)$ at scales $\Delta \gtrsim \Delta_*$. Indeed, as shown in Fig. 8, the non-interacting and the weakly interacting cases do not appear to be so different, in terms of the one-particle phase space distribution.

4. Interpretation of the results

Because the number of particles is large in our simulations, one may expect the effect of the interaction on each particle to be described by a kind of thermal bath. The single-particle dynamics can then be mimicked by chaotic dynamics (corresponding to the symplectic map of Eq.(15) with $\varepsilon = 0$) coupled to a noise term whose strength is $O(\varepsilon)$:

$$\begin{cases} q_i(t+1) = q_i(t) + p_i(t) \bmod 1, \\ p_i(t+1) = p_i(t) + k \sum_j \sin[2\pi(q_i(t+1) - Y_j)] + \sqrt{2D}\xi_i(t) \bmod 1, \end{cases} \tag{21}$$

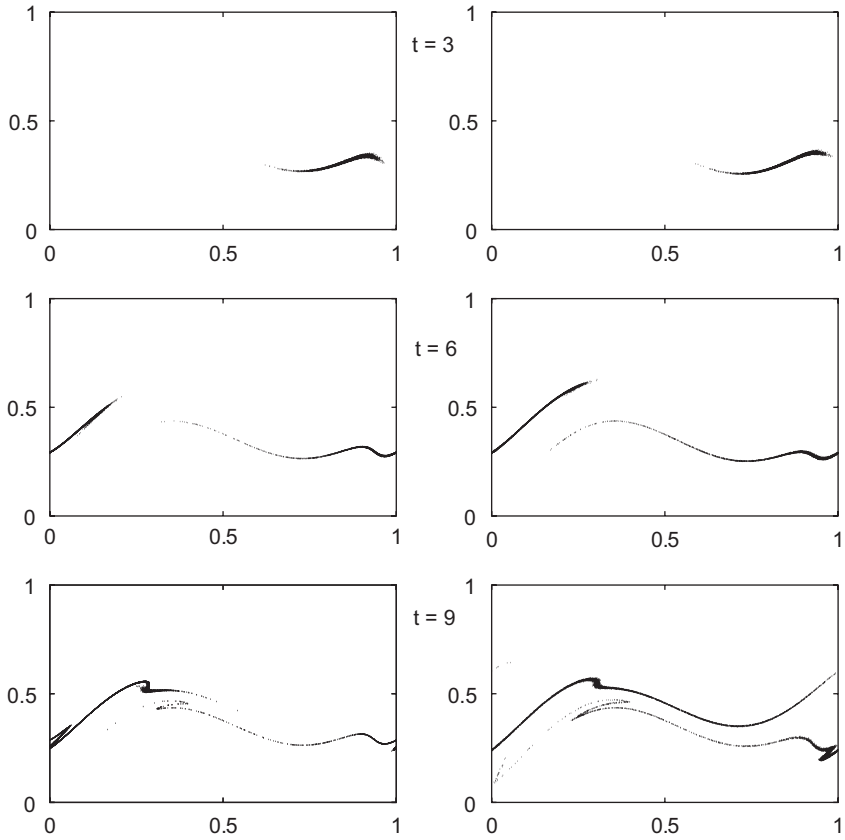

Fig. 8. Snapshots of the evolution in the single-particle projection of the phase space, in the non-interacting case (left) and in the interacting case with $\varepsilon = 10^{-4}$ (right), with $M = 100$. Times increase from top to bottom.

where the ξ_i are i.i.d. Gaussian variables with zero mean and unitary variance, i.e.,

$$\langle \xi_i(t) \rangle = 0, \quad \langle \xi_i(t) \xi_j(t') \rangle = \delta_{t,t'} \delta_{i,j}. \tag{22}$$

This amounts to assume that $f(q, p, t)$ evolves according to a discrete time Fokker–Planck equation. If each particle gives an uncorrelated contribution to the noise term, one can roughly estimate the diffusion coefficient D as $M\varepsilon^2/4$. This heuristic estimate is well supported by numerical simulations of (15): the quantity $\delta S(t, \Delta)$ practically does not change at varying M and ε, keeping $M\varepsilon^2$ constant.

In this framework, one can introduce a characteristic time t_c, defined as the time in which the scale of the noise induced diffusion reaches the smallest scale originated by the deterministic chaotic dynamics [22]. The so defined t_c would correspond to $t_*(\varepsilon, \lambda)$ introduced above. Consequently, noting that the characteristic lengths of noise and of chaos go as $\sqrt{M\varepsilon^2 t/2}$ and $\sigma \exp(-\lambda t)$, respectively, t_c may be estimated from the following transcendent equation:

$$\varepsilon \sqrt{M t_c/2} = \sigma \exp(-\lambda t_c). \tag{23}$$

This holds on the spatial scales already reached by the diffusion process:

$$\varepsilon \sqrt{M t/2} > \Delta, \tag{24}$$

beyond which the value of the entropy still depends on the size of Δ (i.e., the curves $S_B(\Delta)$ display the behavior $S_B(t, \Delta) \sim \Delta^2$). For example, in the case with $\varepsilon = 10^{-4}$, $\sigma = 0.01$, $M = 100$ and $\lambda = 0.162$, one obtains $t_c \simeq 9$, and, in agreement with our interpretation, for $t > 9$, all the curves in Fig. 7 present the same slope compatible with the Lyapunov exponent λ.

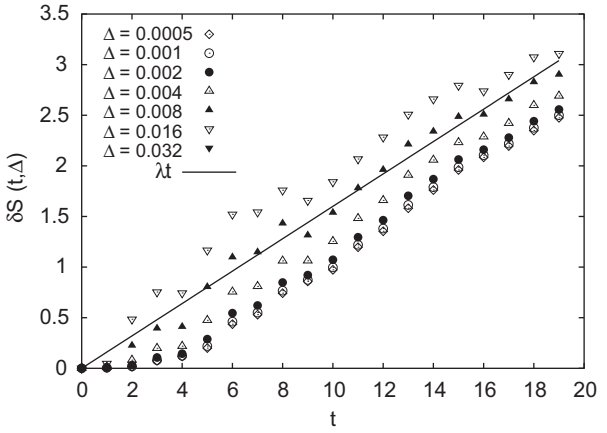

Fig. 9. Numerical simulation of $N = 10^7$ particles evolving according to (21) with $\varepsilon_{eq} = 10^{-4}$. Notice the similar qualitative behavior observed in Fig. 5.

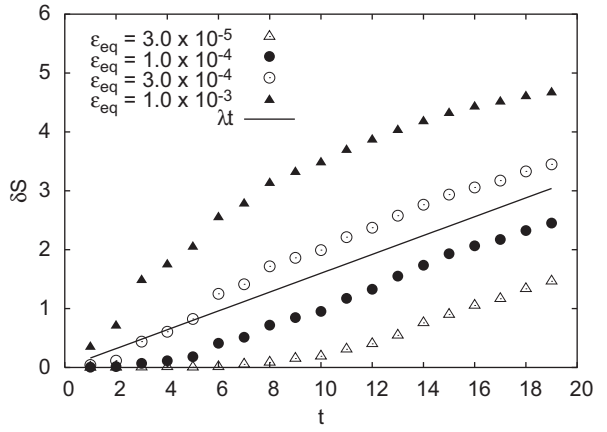

Fig. 10. Extrapolation for $\Delta \to 0$ of $\delta S(t, \Delta)$, for some values of ε_{eq}. Qualitatively, the extrapolated curves are similar to the interacting case (cf. Fig. 7).

As a numerical check of the consistency of this modelization, we studied system (21), and compared the results with a given D with those of the deterministic system of Eq. (15) with

$$\varepsilon = \varepsilon_{eq} \equiv 2\sqrt{\frac{D}{M}}. \tag{25}$$

The results, shown in Figs. 9 and 10, are qualitatively similar to the deterministic interacting case (15), confirming the validity of the approach.

A similar reasoning leads to the decoherence mechanism proposed by Zurek and Paz [23] for the semiclassical limit of quantum mechanics. We note that rather subtle conceptual points are present in the decoherence process for the semiclassical limit. This is so because two theories are involved (classical and quantum mechanics) with very different ontological status (deterministic and non-deterministic, respectively). In our case, roughly speaking, we mimic the first equation of the BBGKY hierarchy of a dilute system, consisting of weakly interacting chaotic particles, with a suitable Fokker–Planck equation.

5. Conclusions and perspectives

We have studied the initial stage of the entropy evolution in a system of weakly coupled chaotic subsystems, which can be considered as a model of weakly interacting particles in an environment with convex obstacles.

In the non-interacting limit the behavior of the Boltzmann entropy strongly depends on the coarse-graining resolution (the cell size Δ). Since the only characteristic length is l_c, which must be much smaller than Δ, the growth of $S(t, \Delta)$ cannot be considered an intrinsic property of the system. By contrast, in the weakly interacting case the short time behavior of the Boltzmann entropy becomes independent of the observation scale, assuming an intrinsic character: that is, for $\Delta < \Delta_*(\varepsilon, \lambda)$, one observes a well defined shape of $\delta S(t)$ vs t. Also, in the early stage of entropy variation for $t \gtrsim t_*(\varepsilon, \lambda)$, $\delta S(t)$ increases roughly linearly, with a slope given by the Kolmogorov–Sinai entropy of the single (non-interacting) chaotic system. Summarizing, the interaction is necessary for an effective cell size Δ_* and for the time evolution of the Boltzmann entropy to be "objective" instead of "subjective", while other numerical aspects, like the slope of $\delta S(t)$ for $t \gtrsim t_*$, are effectively determined only by the degree of chaos in the single subsystems. In addition, the effect of the weak coupling among the chaotic subsystems can be successfully modeled by a noise term, which allows us to estimate the value of $t_*(\varepsilon, \lambda)$.

Let us now comment on the relevance of these results for the case of point-like particles in an environment made of very heavy particles. If the "obstacles" were not infinitely massive, the independent particles would exchange energy with them, like photons in a black body cavity. The photons do not interact with each other, but interact with the walls, reach a thermal equilibrium with them, and acquire a temperature. A similar behavior has been obtained in the Lorentz-like model of Ref. [24]. In our framework, this would amount to set the interaction ε to zero, and to switch on an interaction between particles and obstacles which now are allowed to move. Denoting with Y_J and W_J the coordinate and the momentum of the Jth obstacle, one can generalize (13) introducing a suitable interaction among the "light" particles and the heavy obstacles. The Γ-space is now given by $(\mathbf{Q}, \mathbf{Y}; \mathbf{P}, \mathbf{W})$. Then, the "light" particles are indirectly coupled with each other, as in Ref. [24]; the heavy particles play the role of interaction carrier particles and essentially we fall back in the case considered in this paper. Clearly, an interaction carried by heavy particles will be very weak and will involve very small scales, which are difficult to observe in numerical simulations; nevertheless, there are no reasons to expect any conceptual difference from the scenario described in the present paper, which is consistent with that of Ref. [24].

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Appendix A. On the connection between chaos and Gibbs entropy

Consider a deterministic dynamical law

$$\mathbf{X} \to T^t \mathbf{X} \tag{A.1}$$

(where $\mathbf{X}$ is a D-dimensional vector) and a probability density $\rho(\mathbf{X}, t)$, that gives a distribution of states of the system throughout its phase space at a time t. The Gibbs entropy of ρ is given by

$$S_G(\rho_t) = -\int \rho(\mathbf{X}, t) \ln[\rho(\mathbf{X}, t)] \, \mathrm{d}\mathbf{X}. \tag{A.2}$$

If $J(\mathbf{x}, t)$ is the Jacobian of (A.1), a straightforward computation yields

$$S_G(\rho_t) = S_G(\rho_0) + \int \rho(\mathbf{X}, t) \ln |J(\mathbf{X}, t)| \, \mathrm{d}\mathbf{X}. \tag{A.3}$$

Of course, in the case of volume conserving evolutions, one has: $S_G(\rho_t) = S_G(\rho_0)$. Therefore in order to have an entropy variation one needs a coarse-graining.

Let us consider a hyper-cubic partition and let us define the probability $p_\Delta(i, t)$ to find the state of the system in the cell i at time t:

$$p_\Delta(i, t) = \int_{\Lambda_{i,\Delta}} \rho(\mathbf{X}, t) \, \mathrm{d}\mathbf{X}, \tag{A.4}$$

where $\Lambda_{i,\Delta}$ is the region singled out by the ith cell. The Δ-coarse-grained Gibbs entropy is

$$S_G(t,\Delta) = -\sum_i p_\Delta(i,t)\,\ln\, p_\Delta(i,t).$$

If one considers a distribution of initial conditions differing from zero only on a region of linear size σ, one can give an argument to suggest that, after a transient and for a time not too long,

$$S_G(t,\Delta) = S_G(0,\Delta) + h_{KS}t. \tag{A.5}$$

To obtain Eq. (A.5) one can argue as follows. Assume that the system has m positive Lyapunov exponents and that $\rho(\mathbf{X},0)$ is localized around $\mathbf{X}^c(0)$. In a suitable reference system (with the axes along the eigendirections of the Lyapunov exponents), if $\rho(\mathbf{X},0)$ has a Gaussian shape, $\rho(\mathbf{X},t)$, for some times, is still well approximated by a Gaussian with variances

$$\sigma_j^2(t) = \sigma_j^2(0)\,\exp\{2\lambda_j t\} \tag{A.6}$$

therefore:

$$\rho(\mathbf{X},t) \simeq \prod_{j=1}^{D} \frac{1}{\sqrt{2\pi\sigma_j^2(t)}}\mathrm{e}^{-(X_j - X_j^c(t))^2/2\sigma_j^2(t)}, \tag{A.7}$$

where $\mathbf{X}^c(t)$ is the state evolved from $\mathbf{X}^c(0)$. From this, in the fine-grained case, one gets

$$S(\rho_t) = S(\rho_0) + \sum_j \ln\frac{\sigma_j(t)}{\sigma_j(0)} = S(\rho_0) + \sum_{j=1}^{D}\lambda_j t.$$

It is clear that $S_G(\rho_t) = S_G(\rho_0)$ if the phase space volume is conserved. Considering now the coarse-grained probability (A.4), along the directions of the negative Lyapunov exponents $(m+1, m+2, \ldots)$, for a long enough t one has that

$$\sigma_k(t) \sim \sigma\mathrm{e}^{-|\lambda_k|t} \leqslant \Delta. \tag{A.8}$$

In a Hamiltonian system the Lyapunov exponents pair, i.e., $\lambda_D = -\lambda_1, \lambda_{D-1} = -\lambda_2, \ldots$; therefore the phase space volume conservation can be no more verified if

$$t \geqslant t_\lambda \sim \frac{1}{\lambda_1}\ln\frac{\sigma}{\Delta}. \tag{A.9}$$

This implies that

$$p_\Delta(i,t) \simeq \prod_{j=1}^{m}\frac{1}{\sqrt{2\pi\sigma_j^2(t)}}\mathrm{e}^{-(X_j^{(i)} - X_j^c(t))^2/2\sigma_j^2(t)}$$

if (A.9) holds. Therefore $S_G(t,\Delta) = S_G(0,\Delta)$ as long as $t \leqslant t_\lambda$ while for larger times one obtains

$$S_G(t,\Delta) = S_G(0,\Delta) + \sum_{j=1}^{m}\lambda_j t.$$

With the aid of the Pesin's formula

$$h_{KS} = \sum_{\lambda_i > 0}\lambda_i, \tag{A.10}$$

Eq. (A.5) follows.

Of course, the transition from (A.3) to (A.5) is allowed by the fact that, in the presence of a coarse-graining, the contracting eigendirections (corresponding to the negative values of the Lyapunov exponents) cannot balance the effects of the expanding ones.

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