

Kolmogorov-Sinai Entropy and Lyapunov Exponents Related to Information and Transport Processes

Milena Kheilova, Marian Strunc

Department of Physics, Faculty of Electrical Engineering and Computer Science,
Technical University Brno, Technicka 8, 616 00 Brno, Czech Republic,
++420-5-4114 3395, ++420-5-4114 3207, fax ++420-5—4114 3433,
kheilova@dphys.fee.vutbr.cz, strunc@dphys.fee.vutbr.cz,

Frantisek Solc

Department of Control, Faculty of Electrical Engineering and Computer Science,
Technical University Brno, Bozetechova 2, 612 66 Brno, Czech Republic,
++420-5-41141158, fax ++420-5—4114 1123,
solc@dame.fee.vutbr.cz.

Abstract

This paper deals with the connection between the Kolmogorov-Sinai entropy, and Lyapunov exponents describing the microscopic dynamics of particle systems, and the quantities characterizing the macroscopic properties of the systems. The problem of creation and destruction of information and the connection of these processes with Kolmogorov-Sinai entropy are analysed. The Lyapunov exponents which are also the measure of chaotic behaviour are related to the average loss or gain of information.

Keywords: Kolmogorov-Sinai entropy, Lyapunov exponents, information entropy, transport coefficients, entropy production

1 Introduction

Recently, a number of approaches have been developed to connect the microscopic dynamics of particle systems to the macroscopic properties of systems, in non-equilibrium stationary states (Rondoni, 2000; Gilbert, Dorfman 1999), based on the theory of dynamical systems. In this connection the question arises about the relation between the quantities used in the theory of dynamical systems, such as Kolmogorov-Sinai entropy (KSE), and Lyapunov exponents (LE) on the one hand, and the macroscopic quantities, such as transport coefficients or the quantities from the realm of irreversible thermodynamics, entropy production etc., on the other hand. In this context the notion of information and the quantity information entropy are commonly used. The use of the word „information” is connected with considerable confusion. Two apparently contradictory statements can be found in literature about the chaotic systems behaviour: i) chaotic systems create information, ii) chaotic systems destroy information

(Hilborn, 2000), or i) KSE is a measure of a loss of information (Schuster, 1999), ii) KSE is a measure of information gain (Dorfman, 1999; Parker, Chua 1987). The

purpose of this paper is: i) to clarify these notions and to explain the relations between corresponding quantities, ii) to show the connections between LE, KSE and the physical quantities from the domain of irreversible thermodynamics and statistical physics.

2 Creation and Destruction of Information

KSE and LEs are the basic theoretical tools used for quantifying chaotic behaviour. Before we introduce these quantities we first review the concept of information creation and destruction for the use in describing the behaviour of dissipative dynamical systems (Parker, Chua 1987; Shaw 1981; Eckmann, Ruelle 1985).

For simplicity, we consider an autonomous dynamical system with expanding flow Φ . We suppose that the state of the system can be measured within a resolution δ . We assume that there are two observers who measure the state of the system at two different times. Observer 1 observes the state of the system at time t_1 to be x_1 . Observer 2 measures the state at time $t_2 > t_1$ to be x_2 . Observer 1 knows that the state at t_1 lies somewhere inside $B_\delta(x_1)$ —the δ ball centred at x_1 and that the state at t_2 must lie inside $\Phi(B_\delta(x_1))$. Observer 2 knows that the state at t_2 lies somewhere inside $B_\delta(x_2)$; that is the later observer knows more about the state of the system because $B_\delta(x_2)$ is contained in $\Phi(B_\delta(x_1))$, see Fig.1.

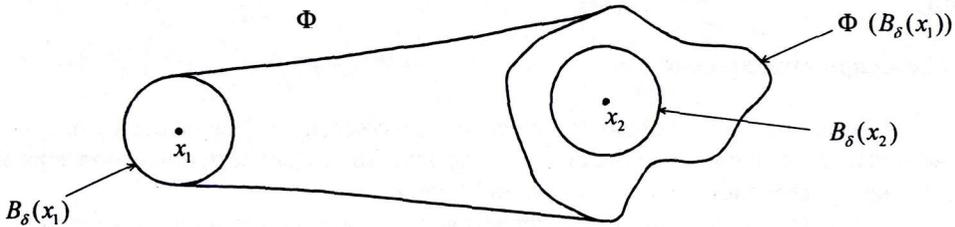


Fig.1: Observer 2 possesses more precise information about the state of the system

Thus an expanding flow is often viewed as creating information. In other words for an expanding system it is less accurate to use x_1 to anticipate the state at the time t_2 than to observe the state at t_2 . The ability to anticipate later states diminishes (due to lack of precision on initial condition). We note that from this point of view we could also speak about the loss of information. On the contrary the contracting flow is viewed as destroying information. Of course, a chaotic trajectories are bounded, thus a chaotic system must contract the state volume in some directions and expand in other directions.

Now we shall try to express these statements in a quantitative way. The amount of information is quantified by the Shannon entropy. Let us consider a system with discrete states numbered with $i = 1, \dots, s$, which are associated with the probabilities p_i . Then the Shannon entropy is defined as the mean uncertainty per state

$$I = -\sum_{i=1}^s p_i \ln p_i \quad (1)$$

with

$$\sum_{i=1}^s p_i = 1. \quad (2)$$

The Shannon entropy can be defined also for continuous systems (Haken, 1988). Now we consider a dynamical system with expanding flow. Observer 2 measures the state of the system at time t_2 and anticipates the state of the system at time t_1 (i.e. the retrospective question). Observer 1 observes the state of the system at time t_1 . He knows that the state of the system lies somewhere at $B_\delta(x_1)$. The information entropy corresponding to observer 1 has its maximum, because the probability density is uniform on $B_\delta(x_1)$. The information entropy corresponding to observer 2 at time t_2 has its maximum too but information entropy corresponding to observer 2 at time t_1 is smaller because the probability density is concentrated on a contracted part of $B_\delta(x_2)$. The fact that the information entropy (as a measure of the lack of knowledge about the state of the system in B_δ) has decreased can be interpreted as a gain of information, or increase of information.

Finally, we note that the loss of information is associated with prognostic question, the increase of information with retrospective question (for the systems with expanding flow).

3 The Lyapunov Exponents

LE may be used to obtain the measure of the sensitive dependence upon initial conditions that is characteristic of chaotic behaviour. LE are connected with concepts of predictability, especially with the predictability time.

In this section we give an interpretation to the LE in terms of the information concept.

Consider a differentiable (almost everywhere, except, possibly, for a set of measure zero) transformation F on the interval $[0,1]$. Let x_0 be one initial point and $x = x_0 + \varepsilon$ nearby initial point. We then apply the iterated map function n times to x_0 and x . The LE is given by the following equation (Schuster, 1984)

$$\lambda = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln |F'(x_i)|. \quad (3)$$

Now we shall show that the LE measures the average „loss of information“ or the „gain of information“ about the position of a point in $[0,1]$ after one iteration.

As an illustration we consider linear map, see fig. 2. We separate interval $[0,1]$ into m equal intervals and assume that a point x_0 can occur in each of them with equal probability $p=1/m$. The bit number missing an observer to know in which interval x_0 occurs is

$$b_0 = -\ln \frac{1}{m} = \ln m. \quad (4)$$

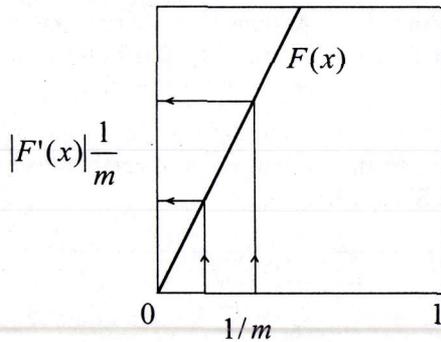


Fig.2: The map $F(x)$ changes the length of an interval

Linear map $F(x)$ changes the length of an interval by a factor $a = |F'(x)|$. The corresponding decrease of resolution leads to a loss of information after the mapping which equals the difference of the bit numbers before and after iteration step

$$\Delta b = \ln m - \left(-\ln \frac{a}{m}\right) = \ln |F'(x_0)|. \quad (5)$$

Averaging this expression over many iterations leads to the following expression for the mean loss of the information

$$\overline{\Delta b} = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \ln |F'(x_i)|. \quad (6)$$

Using eqs. 3, 6 we obtain the relation between the Lyapunov exponent and the mean loss of information

$$\lambda = \overline{\Delta b}. \quad (7)$$

The loss of information corresponds to a prognostic question. With respect to the retrospective question the right hand side of eq. 7 can be interpreted as a information gain (Beck, Schlögl, 1997).

4 The Kolmogorov-Sinai Entropy

4.1 Kolmogorov-Sinai Entropy and the Loss of Information

The concept of entropy in a dynamical system was formalized by Kolmogorov. In the literature on the nonlinear dynamics alternative definitions of the KSE are used.

In this section we shall discuss the KSE defined in the following way (Schuster, 1984; Grassberger, Procaccia, 1983):

Consider a dynamical system with f degrees of freedom. Suppose that the phase space is partitioned into boxes of size ϵ^f . Assume that there is an attractor in the phase space and that the trajectory $\mathbf{x}(t) = [x_1(t), x_2(t), \dots, x_f(t)]$ is in the basin of attraction. The state of the system is measured at intervals of time τ . Let $P_{i_0 i_1 \dots i_n}$ be the joint probability that $\mathbf{x}(t=0)$ is in box i_0 , $\mathbf{x}(t=\tau)$ is in box i_1, \dots , and $\mathbf{x}(t=n\tau)$ is in box i_n . The information needed to locate the system on a special trajectory $i_0^* \dots i_n^*$ with precision ϵ is quantified by the Shannon entropy

$$K_n = - \sum_{i_0 \dots i_n} P_{i_0 \dots i_n} \ln P_{i_0 \dots i_n} . \quad (8)$$

The differences $K_{n+1} - K_n$ can be interpreted as information needed to anticipate in which cell i_{n+1}^* the system will be if we know that it was previously in $i_0^* \dots i_n^*$. In other words $K_{n+1} - K_n$ measures our loss of information (or the missing information) about the system from time $n\tau$ to time $(n+1)\tau$. Then KSE is introduced as the average rate of information loss

$$h_{KS} = \lim_{\tau \rightarrow 0} \lim_{\epsilon \rightarrow 0} \lim_{N \rightarrow \infty} \frac{1}{N\tau} \sum_{n=0}^{N-1} (K_{n+1} - K_n) = - \lim_{\tau \rightarrow 0} \lim_{\epsilon \rightarrow 0} \lim_{N \rightarrow \infty} \frac{1}{N\tau} \sum_{i_0 \dots i_n} P_{i_0 \dots i_n} \ln P_{i_0 \dots i_n} . \quad (9)$$

For maps (transformations) with discrete time steps $\tau = 1$, the limit $\tau \rightarrow 0$ is omitted.

4.2 Kolmogorov-Sinai Entropy and the Gain of Information

To illustrate the mechanism of information increasing in discrete-time dynamical systems, consider the so called Arnold cat transformation:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = T \begin{pmatrix} x \\ y \end{pmatrix} \pmod{1} \quad (10)$$

with

$$T = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad (11)$$

where a, b, c, d are all integers, $\det T = 1$.

Dorfman (Dorfman 1995) assumed the initial configuration A for the Arnold cat map with

$$T = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \quad (12)$$

in the form of a small square in the lower left-hand corner, see Fig.3. He had stated that the original set after n iterations got stretched along the unstable manifold and compressed in the stable direction. The evolution of the initial configuration after three iterations is shown in Fig 4. Suppose that the characteristic dimension of the initial set A is of the order of resolution parameter δ . As a consequence, observer 1 who

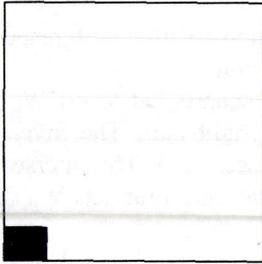


Fig.3: The initial set A for the Arnold cat map

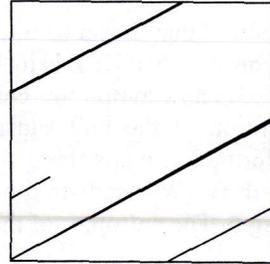


Fig.4: The initial set A after three iterations

measures the state of the system, cannot resolve two points in A . As time passes the initial set will be stretched along the unstable direction and observer 2 who measures the state of the system can easily resolve the images of points of the initial set.

The notion of creation (expanding flow) or destruction (contracting flow) of information can be quantified. The exponential rate at which information is obtained is determined by the KSE. The definition of KSE can be understood by first defining the partition W of the space X , and then defining the entropy of the partition W .

Now we look more carefully at the KSE definition. Let $W = (W_1, W_2, \dots, W_\alpha)$ be a finite partition of space X . For every piece W_j we write $B^{-k}W_j$ for the set of points mapped by B^k to W_j . We then denote by $B^{-k}W$ the partition $(B^{-k}W_1, \dots, B^{-k}W_\alpha)$. The partition $B^{-k}W$ is deduced from W by time evolution. Finally, $W^{(n)}$ is defined as

$$W^{(n)} = W \vee B^{-1}W \vee \dots \vee B^{-n+1}W. \quad (13)$$

The partition $W^{(n)}$ is the partition generated by W in a time interval of length n . Kolmogorov and Sinai defined the entropy of a partition in terms of a normalized invariant measure μ on the phase space, by the relation

$$H(W) = -\sum_{i=1}^{\alpha} \mu(W_i) \ln \mu(W_i) \quad (14)$$

with

$$\sum_{i=1}^{\alpha} \mu(W_i) = 1. \quad (15)$$

$H(W)$ is the information entropy of the partition W . In other words $H(W)$ is a measure of our uncertainty as to where the point $x \in X$ is relative to the partition W . The term $H(W^{(n)})$ expresses the information entropy over an interval of time of length n . To express how much information is obtained per step, we define the quantity

$$h = \lim_{n \rightarrow \infty} [H(W^{(n+1)}) - H(W^{(n)})] = \lim_{n \rightarrow \infty} \frac{1}{n} H(W^{(n)}). \quad (16)$$

We note that a lot of work goes into showing that this limit exists (Gutzwiller, 1991). The quantity h still depends on the choice of the partition. The KSE is defined as the supremum of the expression 16 over all possible finite partitions of the space at $t = 0$,

$$h_{KS} = \sup_{W_i} h. \quad (17)$$

We remind that h can be interpreted as a rate of information creation with respect to the partition W . Then KSE is its limit for finer and finer partition.

As an example we consider a partition of the unit square. Let $W = (W_0, W_1)$ be a partition of the unit square into its left half and its right half. The inverse baker transformation maps these two sets to $B^{-1}(W_i)$, $i = 0, 1$, see Fig.5. The intersections of W_i with $B^{-1}(W_j)$ leads to a new partition of the unit square into four sets $W_i \cap B^{-1}(W_j)$, see Fig.6. The entropies of the partitions are

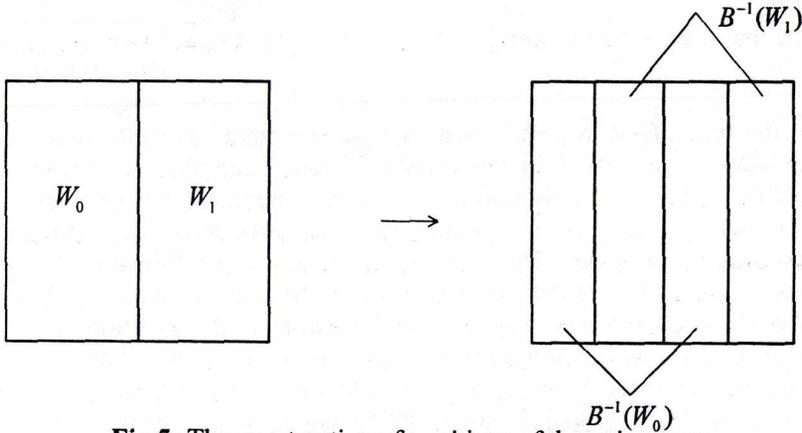


Fig.5: The construction of partitions of the unit square for the baker's transformation

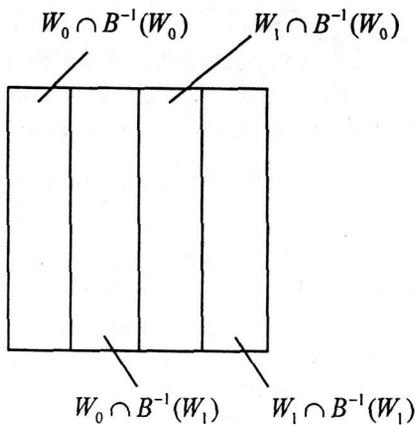


Fig.6: The partition of the unit square into sets

$$H(W^{(n+1)}) = \ln 2^{n+1}, \quad n = 0, 1, \dots \quad (18)$$

The KSE is then

$$h_{KS} = \ln 2. \quad (19)$$

5 Kolmogorov-Sinai Entropy and Lyapunov Exponents Related to Transport Coefficients

A new line of research in transport theory has been developed over the past few years, relating macroscopic properties of large systems to the properties of the underlying microscopic dynamics. There are two main approaches to transport theory which are based on the notions of chaos theory:

i) the escape rate or chaotic scattering theory formalism for computing transport coefficients,

ii) the Gaussian thermostat method for computing transport coefficients.

These methods allow to relate macroscopic transport quantities, such as transport coefficients, to microscopic dynamical quantities, like Lyapunov-exponents and Kolmogorov-Sinai entropy.

5.1 The Escape Rate Formalism

First we shall describe the escape-rate formalism (Dorfman, 1999; Gaspard, 1995; Cohen, 1995). The system under consideration is an open system with absorbing boundaries. Once a point passes a boundary, it can never return to the bounded system. As illustration we may imagine a Brownian particle diffusing in a fluid inside a container with absorbing boundaries. A standard, mesoscopic description of the system consists in the solution of the diffusion equation for the probability density of the Brownian particle inside the container. From the microscopic point of view the motion of the particle is described by some transformation in the phase space of the entire system. The escape-rate method relates the decay rate (the probability of finding the particle inside the container is an exponentially decreasing function of time with decay coefficient) to dynamical properties of the deterministic microscopic dynamics of the system.

This statement can be demonstrated with the following example. We take the discrete map:

$$x_{n+1} = \left\{ \begin{array}{ll} \frac{x_n}{p_0} & \text{for } 0 < x_n < \frac{1}{2} \\ \frac{x_n - 1}{p_1} + 1 & \frac{1}{2} < x_n < 1, \end{array} \right\} \quad (20)$$

where $p_0, p_1 < 1/2$, $0 < x_n < 1$.

After first step of the mapping, points between p_0 and $1-p_1$ leave the unit interval. Let the S_n be the number of survivors after n steps, i.e. the number of trajectories staying in the phase space. For large n one observes an exponential decay of S_n :

$$\frac{S_n}{S_0} = \exp(-\gamma_d n), \quad (21)$$

where γ_d is dynamical escape rate.

In our case it can be proved

$$\gamma_d = \ln \frac{1}{p_0 + p_1}. \quad (22)$$

The set of points that remain forever in the unit interval under the mapping 20, a repeller F_R , is a set of zero Lebesgue measure with an uncountable infinity of points (Cantor set). In (Gaspard, 1995) it is shown, that for Anosov systems the relation holds

$$\gamma_d = \sum_{\lambda_i > 0} \lambda_i(F_R) - h_{KS}(F_R), \quad (23)$$

where the sum is over all positive Lyapunov exponents on the repeller F_R , h_{KS} is the Kolmogorov-Sinai entropy on the repeller F_R .

We note that Pesin's theorem does not apply to the open systems.

Now we consider a system consisting of a particle of mass m and energy E , moving among a fixed set of scatterers which are in a region R of infinite extent in all directions except one, the x -direction. The scatterers are confined to the interval $0 \leq x \leq L$. Absorbing walls are placed at the planes at $x = 0$ and $x = L$. The set of the trajectories of the moving particle inside the region R which have started with all possible initial positions and velocities forms the repeller F_R . For the dynamical escape rate γ_d , eq. 23 holds.

On the other hand, the system under consideration may be described by the diffusion equation

$$\frac{\partial P(\vec{r}, t)}{\partial t} = D \nabla^2 P(\vec{r}, t). \quad (24)$$

For large L and for large times after some initial time the probability for the distribution of particles in the x -direction has the form

$$P(x, t) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L} \exp\left(-\left(\frac{n\pi}{L}\right)^2 Dt\right), \quad (25)$$

where D is the diffusion coefficient.

The slowest decaying mode $n = 1$ decays as $\exp\left(-\frac{\pi^2 Dt}{L^2}\right)$. Thus the escape rate (for large systems) is defined as

$$\gamma = \frac{\pi^2 D}{L^2}. \quad (26)$$

By identifying the escape rate γ given by eq. 26 with the dynamical escape rate γ_d given by eq. 23 we receive the relation for the diffusion coefficient D

$$D = \lim_{L \rightarrow \infty} \frac{L^2}{\pi^2} \left(\sum_{\lambda_i > 0} \lambda_i(F_R) - h_{KS}(F_R) \right). \quad (27)$$

The eq. 27 has been applied to Lorentz gases where the scatterers are disks or spheres placed at random in the plane or in the space.

5.2 The Gaussian Thermostat Method

In attempting to simulate transport processes in fluids on a computer (Gilbert, Dorfman, 1999; Cohen, 1995) it was noticed that external fields imposed to a system led to changes in the energy of a system. To deal with this problem it was used so called „internal thermostat“ - a fictitious frictional force, in fact, which maintained the energy at some constant value. The theoretical analyses has led to the connections between transport theory (transport coefficients such as coefficient of shear viscosity, coefficient of diffusion etc.), and chaotic dynamics (KSE and LEs) and the irreversible thermodynamics (entropy production, entropy).

As a simple illustration we consider a system of N identical charged particles. An external electric field \mathbf{E} is applied to this system. The particles will begin to drift and accelerate. To keep the kinetic energy of the particle constant we can add a friction term α ($\alpha > 0$) to the momentum equation

$$\dot{\mathbf{p}} = q\mathbf{E} - \alpha(\mathbf{p})\mathbf{p}, \quad (28)$$

where $\alpha(\mathbf{p})$ is fixed by the condition that the kinetic energy stays constant. As a consequence

$$\alpha(\mathbf{p}) = q \frac{\mathbf{E} \cdot \mathbf{p}}{p^2}. \quad (29)$$

The equations of motion are

$$\left. \begin{aligned} \dot{\mathbf{r}} &= \mathbf{p} \\ \dot{\mathbf{p}} &= q\mathbf{E} - q \frac{\mathbf{E} \cdot \mathbf{p}}{p^2} \mathbf{p} \end{aligned} \right\} \quad (30)$$

Because of a friction term the phase-space volumes are not preserved in time. The modified Liouville equation can be written in the following form

$$\frac{d\rho}{dt} = \alpha \rho. \quad (31)$$

Here ρ is a distribution function in Γ space.

The rate of change of a phase-space volume v can be obtained by using the modified Liouville equation. The result is

$$\frac{dv(t)}{dt} = -\alpha v. \quad (32)$$

The volume in phase-space will decrease ($\alpha > 0$). This change is associated with the sum of the LEs

$$v(t) = v(0) \exp \left[t \sum_j \lambda_j \right]. \quad (33)$$

The connection between transport coefficients and the sum of all the LEs of the system is established by incorporating the irreversible thermodynamics into the framework of dynamical systems theory. In this context two expressions for the irreversible entropy production are used. The first one is the usual relation between the irreversible entropy production P and the thermodynamic fluxes J_i and forces X_i

$$P = \sum_i J_i X_i. \quad (34)$$

From now on we suppose unit volume of physical system.

The other of these expressions for the entropy production is based on the Gibbs (fine grained) entropy S_G , given by

$$S_G = - \int d\Gamma \rho(\Gamma, t) [\ln \rho(\Gamma, t) - 1], \quad (35)$$

where Γ is a point in the phase-space of the system, $\rho(\Gamma, t)$ is the phase-space density of the system.

Because of the modified Liouville equation, it holds

$$\frac{dS_G}{dt} = -k \int d\Gamma \rho \alpha = -k \langle \alpha \rangle, \quad (36)$$

with Boltzmann's constant k .

From the eq. 36 it follows that the $\frac{dS_G}{dt}$ is negative. This fact makes it difficult to equate the positive macroscopic, i.e. irreversible thermodynamic entropy production to the negative change of the Gibbs entropy. This situation is usually resolved (Gilbert, Dorfman, 1999) by considering that the negative entropy production inside the system is compensated by a positive entropy production in the thermostat itself, so that the total entropy production is positive, or zero. In nonequilibrium steady state the total entropy production is zero

$$\frac{dS_G}{dt} + \frac{dS_{ter}}{dt} = 0. \quad (37)$$

Then the positive entropy production in the thermostat is equated to the macroscopic entropy production

$$P \equiv \frac{dS_{ter}}{dt} = \frac{\mathbf{J} \cdot \mathbf{E}}{T} = \sigma \frac{E^2}{T}, \quad (38)$$

where \mathbf{J} is the average electric current, σ is the electrical conductivity, T is temperature. The connection to chaotic dynamics is established by considering the change of phase-space. As a result we obtain

$$\frac{dS_G}{dt} = k \sum_j \langle \lambda_j \rangle. \quad (39)$$

From eqs. 37, 38, 39 it follows for ergodic systems

$$\sigma = -\frac{kT}{E^2} \sum_j \lambda_j. \quad (40)$$

This procedure is not quite satisfactory (Rondoni, Cohen, 2000; Gilbert, Dorfman, 1999). In the steady state the phase-space density ρ on the attractor is not a smooth function with smooth derivatives. However, it can be shown by a more careful analyses using the Sinai-Ruelle-Bowen measure which is smooth in the unstable directions and fractal along the stable directions, that the eq. 40 holds.

Another problem concerns the interpretation of the term $\alpha(\mathbf{p}) \cdot \mathbf{p}$ as representing a real physical thermostat, which absorbs the dissipative energy created in the system.

This interpretation is crucial for the identification of the term $\frac{dS_G}{dt}$ with irreversible thermodynamics entropy production. The term $\alpha(\mathbf{p}) \cdot \mathbf{p}$ has nothing to do with a real thermostat (Rondoni, 2000).

Finally we note that it is not surprising that the rate of Gibbs entropy production is negative: The time evolution of the dissipative system equation of motion yields the phase-space contraction. As time elapses the phase space point gets closer and closer to the attractor. Thus the observer who anticipates the state of the system learns more and more about the location of the phase space point as time increases and this gain of information is reflected in a negative change of Gibbs entropy.

The final goal of the attempt to incorporate irreversible thermodynamics into the framework of dynamical system theory is to build a complete description of all quantities occurring in the irreversible thermodynamics in purely dynamical terms. The main quantity in the irreversible thermodynamics is the physical entropy. The fact that the phase-space probability distribution is rearranged by the time evolution, that sets of zero volume take a probability of 1 in the stationary state, makes the Gibbs entropy to diverge to $-\infty$. Thus the Gibbs entropy cannot be identified with the physical entropy. To

overcome this difficulty the various kinds of coarse-grained informational entropies and entropy production were introduced (Gilbert, Dorfman 1999; Kantz, Olbrich 2000; Gaspard, 1998). In the limit of fine graining they become the Gibbs entropy. In the case of thermostatted systems, Gilbert and Dorfman using coarse-grained method had also obtained the eq. 40.

6 Conclusion

LE and KSE were introduced for quantifying chaotic behaviour. The interpretation of these quantities in the framework of the information theory and their relations to the physical notions such as transport coefficients, entropy, entropy production could serve to the better understanding of LE and KSE. The problem of creation and destruction of information was analysed and it was shown how connect the gain of information with KSE, which may be used to characterize the chaotic behaviour of systems. The notion of creation of information associated with prognostic question (by expanding flow) and destruction of information associated with retrospective question is clarified. The LE which is also the measure of chaotic behaviour can be related to the average loss or gain of information. The connection between the dynamical properties of open systems characterized by KSE and LEs, and transport properties of such systems characterized by transport coefficients is illustrated by using i) the escape rate formalism, ii) the Gaussian thermostat method.

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