TIME–AVERAGES AND THE HEAT THEOREM

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In this paper it is illustrated how to compute the time–average of a generic dynamical variable in the limit of large systems. It is also shown how to use this result to deduce an analogue of the second principle of thermodynamics, even in presence of metastable phenomena, for which it is not granted that the standard Gibbs measure can be used.

1. Introduction

The aim of this paper is to discuss the possibility of having a thermodynamic behavior also in presence of metastable phenomena which prevent thermal equilibrium to be reached within a given time scale. We place ourselves in the most general setup, considering an abstract dynamical system with phase space $\mathcal{M}$ and *dynamics* $\Phi : \mathcal{M} \to \mathcal{M}$, where Φ is a suitable map. Now, given a dynamical variable $f : \mathcal{M} \to \mathbb{R}$, in statistical mechanics one is interested in its time average

$$\bar{f}(x_0) = \frac{1}{N} \sum_{n=1}^{N} f(x_n) \ , \qquad x_{n+1} \stackrel{\text{def}}{=} \Phi(x_n) \ .$$

In equilibrium statistical mechanics one considers the limit $N \to +\infty$, but in presence of metastable phenomena one has to consider time averages on some large but still finite time–scale. In the latter case it is meaningful to think of N as a parameter having a fixed "large" value. In this case there is nothing analogous to the ergodic theorem, i.e. the function $\bar{f}(x_0)$ is not almost constant but does depend on the initial datum x_0. Now, if we give an a priori probability distribution $\mu(x_0)$ on the initial data (for example the Lebesgue one), $\bar{f}(x_0)$ turns out to be a random variable, in the sense that it will assume different values with different probabilities. It is then natural to consider the expectation value $< \bar{f} >$ of the time average $\bar{f}(x_0)$ with respect of the initial data distribution, i.e. the quantity

$$< \bar{f} > \stackrel{\text{def}}{=} \int_{\mathcal{M}} \bar{f}(x_0) \, \mathrm{d}\mu \ .$$

In this paper we illustrate the results of paper [1], in which it was shown how the expectation can be computed using a large deviation principle, in the limit of a large system, and it was also shown how an analogue of the second principle of

thermodynamics can be derived. This will be done in Section 3. In the next section we show how to numerically compute the probability distribution function (p.d.f. for short) of the occupation number of a cell, a quantity which plays a fundamental role for computing the thermodynamic quantities of interest (such as entropy). We give also an application to the standard map, in two cases of weak and strong chaos respectively.

2. The p.d.f of the occupation number of a cell.

The time average of the function f can be computed also in the following way (which is more suited for our purposes): consider a partition $\{\mathcal{Z}_j\}$ of the phase space $\mathcal{M}$ into disjoint cells, so that $\mathcal{M} = \bigcup_j \mathcal{Z}_j$, and let $n_j(x_0)$ be the number of points of the orbit $\{x_n\}$ which belong to the cell $\mathcal{Z}_j$ (i.e. the cardinality of the intersection of the orbit with the cell). This number will be called the occupation number in the rest of the paper. Then one has

$$\bar{f}(x_0) = \frac{1}{N}\sum_n f(x_n) \simeq \frac{1}{N}\sum_j n_j(x_0) f_j \ ,$$

f_j being the value of f in a given point of the cell $\mathcal{Z}_j$. This formula shows that the time average of every dynamical variable can be expressed in terms of the random variables $n_j(x_0)$, so that the probability distribution function $F_j(n)$ of the occupation number n_j turns out to have a fundamental role. Let us recall that $F_j(n)$ is the probability that $n_j \leq n$, i.e. the measure of the set of initial data x_0 which give rise to orbits having a number of points n_j in the cell $\mathcal{Z}_j$ less than n. In particular, from the knowledge of $F_j(n)$, one can compute not only the expectation value

$$< n_j >= \int n \, \mathrm{d}F_j \ ,$$

but also all the higher order moments, as the standard deviation and so on.

Note that this probabilistic description is different from the usual one (see for example Ref. [2]), in which one considers the "probability that a given cell $\mathcal{Z}_j$ is occupied". In the latter case one considers "how many initial data" give rise to orbits that are actually in the given cell at a given fixed time, and this fraction is just the probability assigned to the cell. There is nothing as a p.d.f. associated to the cell. This is because one takes no care of the fact that the system can visit the same cell a different number of times during the motion. This fact is crucial for what concerns the time-average of the dynamical variables, but obviously has no importance if one limits oneself to consider their phase–space average at any fixed time.

The function F_j, corresponding to a given cell $\mathcal{Z}_j$, can be numerically computed in the following way: extract a number m of initial data x_0^l , $l = 1, \ldots , m$, at random with respect to the given a priori distribution, then compute the corresponding orbits $\{x_n^l\}$ and let n_j^l be the number of points of the l–th orbit which belong to

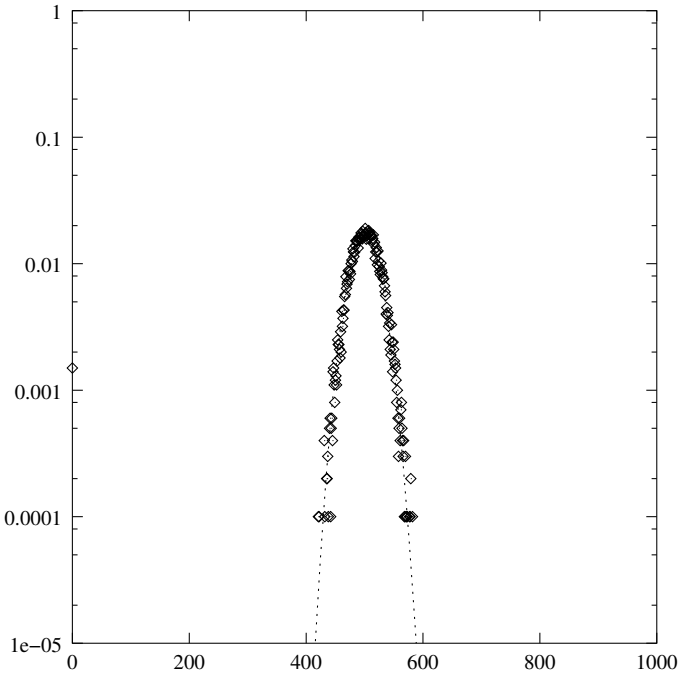

Figure 1. The histogram for $\varepsilon = 1.0$ and the curve $e^{-p}p^k/k!$ versus k, for $p = 500$.

the cell $\mathcal{Z}_j$. Having determined the sequence $\{n_j^l\}$, one builds up the corresponding histogram, i.e. for every $k = 0, \ldots, N$ one reports the number of times (divided by N) the value k appears in the sequence $\{n_j^l\}$. From the histogram, the empirical distribution[a] is then computed. As one increases the number m of initial data the empirical distribution tends to the distribution function $F_j(n)$. As an illustration, Figure 1 and Figure 2 report (in semilogarithmic scale) the histograms built up for the case of the standard map

$$\begin{cases} x' = x + y & \mod 1 \\ y' = y + \varepsilon \sin 2\pi x' & \mod 1 \ , \end{cases}$$

for two different values of ε. We take, as a priori distribution, the uniform distribution on the torus, and we consider the cell $\mathcal{Z}_j = \{(x, y) \in \mathbf{T}^2 : x \in [.4, .5), y \in [.5, .6)\}$. We choose $m = 10^4$ different initial points and the length of any orbit is fixed at $N = 5 \cdot 10^4$. The two figures refer to different values of the parameter ε: Figure 1 corresponds to the case $\varepsilon = 1$, in which the dynamics is very chaotic, while Figure 2 corresponds to the case $\varepsilon = 0.5$, a much less chaotic one. For comparison, in the figures it is also reported (dashed line) the plot of the function $e^{-p}p^k/k!$ versus k, which is the histogram for a Poisson process (namely when the different

[a] We recall that the histogram is nothing that the plot of $F_j(k+1) - F_j(k)$ versus k.

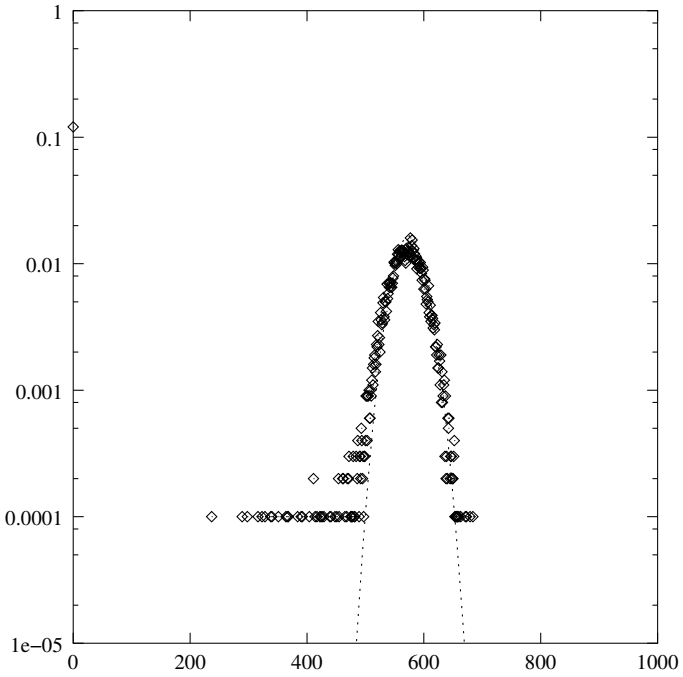

Figure 2. The histogram for $\varepsilon = 0.5$ and the curve $e^{-p}p^k/k!$ versus k, for $p = 575$.

visits of the same cell are independent events). The parameter p is chosen by a best fit. One sees that for $\varepsilon = 1$ the histogram is well approximated by the dashed line, while in the case $\varepsilon = 0.5$ the curve and the histogram exhibit rather relevant differences for small n. This implies that the Laplace transform $\exp(\chi_j(z))$ of $F_j(n)$ (whose importance will be illustrated in the next section) will be different, for large z, from the Laplace transform of a Poisson process.

3. The Thermodynamics.

To arrive to the thermodynamics one needs one more concept: in fact in thermodynamics the expectation value U of the internal energy plays the role of a parameter the value of which can be fixed at will. In particular, as the energy is not bounded from above, then the a priori mean energy $< \bar{\varepsilon} >$ is infinite , and thus, since U is instead finite, one has in general $U \neq < \bar{\varepsilon} >$. In other terms, denoting by ε_j the value of the internal energy in the cell $\mathcal{Z}_j$, one has the condition

$$\frac{1}{N}\sum_j n_j \varepsilon_j = U \quad \text{with} \quad U \neq < \bar{\varepsilon} > \ .$$

This indeed is a condition on the initial data or equivalently on the variables n_j. So, one is confronted with a large deviation problem, inasmuch as one should compute

not the expected value $< \bar{f} >$, but rather the *conditional expectation* $< \bar{f} >_U$ of $\bar{f}$, given the mean energy U. To this end it is sufficient to compute the mean occupation number (which we denote by $\bar{\nu}_j$) when the mean energy is U, because one obviously has

$$< \bar{f} >_U = \frac{1}{N} \sum_j f_j \bar{\nu}_j \ .$$

Note that $\bar{\nu}_j$ satisfies the conditions

$$N = \sum_j \bar{\nu}_j \ , \quad U = \frac{1}{N} \sum_j \varepsilon_j \bar{\nu}_j \ . \tag{1}$$

This problem can be solved, under suitable hypotheses (see Ref. [1]), in the limit of large systems. In other terms, one can provide an asymptotic expansion for the mean occupation number $\bar{\nu}_j$, the remainder of which tends to zero in the thermodynamic limit. If one assumes that the quantities n_j, for different values of j, are independent random variables, one can give a simple expression for the principal term of the expansion. In fact in such a case one has, neglecting the remainder,

$$\bar{\nu}_j = -\chi_j'(\frac{\theta}{N}\varepsilon_j + \alpha) \ , \tag{2}$$

where the prime denotes derivative, and the function $\chi_j(z)$ is the logarithm of the moment function, i.e. is defined by

$$\exp(\chi_j(z)) \stackrel{\text{def}}{=} \int_0^{+\infty} e^{-nz} \, \mathrm{d}F_j \ .$$

The parameters θ and α are determined by imposing the conditions (1), i.e. by requiring

$$N = -\sum_j \chi_j'(\frac{\theta}{N}\varepsilon_j + \alpha) \ , \quad U = -\frac{1}{N} \sum_j \varepsilon_j \chi_j'(\frac{\theta}{N}\varepsilon_j + \alpha) \ .$$

We can now state the main result of the theory. If one defines the exchanged heat as the difference $\delta\mathcal{Q} = \mathrm{d}U - \delta\mathcal{W}$, where $\delta\mathcal{W}$ is the mean work performed by the system when an external parameter is changed, then one finds

$$\delta\mathcal{Q} = \frac{1}{N} \sum_j \varepsilon_j \mathrm{d}\bar{\nu}_j \ .$$

One then finds that this expression admits θ/N as an integrating factor (where θ is the same quantity entering formula (2)). In fact, introducing $\nu_j \stackrel{\text{def}}{=} -\chi_j'(z)$ as an independent variable and the Legendre transform $h_j(\nu)$ of the function $\chi_j(z)$, one indeed has

$$\delta\mathcal{Q} = \frac{N}{\theta} \mathrm{d}\Big(\frac{1}{N} \sum h_j(\bar{\nu}_j)\Big) \ .$$

As a consequence the quantity $S = \sum_j h_j(\bar{\nu}_j)/N$ can be identified with the entropy, and $\beta = \theta/N$ with the inverse temperature. It is easy to verify that

if the p.d.f. of the occupation number corresponds to a Poisson process (i.e. if $F_j(n) = \sum_{k \leq n} e^{-p} p^k / k!$, to which there corresponds $\chi_j(z) = pe^{-z} - p$) one gets

$$\bar{\nu}_j = \frac{N e^{-\beta \varepsilon_j}}{Z(\beta)} \quad \text{with} \quad Z(\beta) = \sum e^{-\beta \varepsilon_j}$$
$$h = -\sum \Big(\nu_j \log \nu_j - \nu_j \log p \Big) \ ,$$

i.e. the Gibbs distribution for the energy and (obviously) the Boltzmann formula for the entropy. Different p.d.f.'s will give rise to different expressions for both the entropy and the energy distribution. In particular, Figure 2 suggests that $\chi_j(z)$ could decrease more slowly than an exponential for increasing z, for example as an inverse power. As an illustration, one can consider the function

$$\chi(z) = p e_q(-z) - p \ ,$$

where $e_q(z) \stackrel{\text{def}}{=} (1 + (1-q)z)^{1/(1-q)}$ is the Tsallis q–deformation of the exponential, and one obtains

$$\bar{\nu}_j = C(\beta_q)(1 + \beta_q (q-1) \varepsilon_j)^{\frac{q}{1-q}}$$
$$h = \frac{1}{q-1} \sum \Big(q \nu_j^{\frac{1}{q}} p^{\frac{q-1}{q}} - \nu_j \Big),$$

where $C(\beta_q)$ is a suitable normalizing constant, and $\beta_q \stackrel{\text{def}}{=} \beta / (1 + (q-1)\alpha)$. This distribution coincides with the Tsallis q–distribution (see Refs. [3]) for the energy, while the expression for the entropy h also coincides with the Tsallis q–entropy S_q if we express h not in terms of $\bar{\nu}_j$, but in terms of the quantities $p_j \stackrel{\text{def}}{=} p^{1/q} q^{1/q-1} \nu_j^{1/q}$.

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