Entropy driven intermitency

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This note reviews some physical aspects of the chaotic hypothesis in nonequilibrium statistical mechanics and attempts at the physical interpretation of the fluctuation theorem as a quantitative intermittency property.

The main assumption, for the foundation of a nonequilibrium statistical mechanics or a theory of developed turbulence, will be:

Chaotic hypothesis: *Asymptotic motions of a chaotic system, be it a system of N particles or a viscous fluid, can be regarded as motions of a mixing Anosov system, for the purposes of computing time averages.*

The point of view goes back to Ruelle,[18],[19], and in this specific form has been proposed in[12]. I shall not define here "mixing Anosov system", see[9]. It will suffice to say that Anosov systems are very well understood dynamical systems in spite of being in a sense the most chaotic: they are so well understood that they can be regarded as the *paradigm* of chaotic systems much as the harmonic oscillators are the paradigm of regular and orderly motions.

This immediately implies the existence and uniqueness of an invariant probability distribution μ which gives the *statistics* if the motions of the system in the sense

$$\lim_{T\to\infty} T^{-1}\int_0^T F(S_t x)\,dt = \int \mu(dy)\,F(y) \tag{1}$$

for *almost all* initial data, *i.e.* outside a set of 0 volume in phase space (volume being measured in the ordinary sense of the Lebesgue measure). Here S_t denotes the time evolution map, solution of the differential equations of motion, and μ is called the *SRB distribution*.

Particular interest will be reserved to *time reversible* systems: *i.e.* systems for which there is an isometry I of phase space such that

$$I^2 = 1, \quad and \quad IS_{-t} = S_t I \tag{2}$$

Denoting $\dot x = f(x)$ the equations of motion and $\sigma(x)$ the divergence $-\mathrm{div}\, f(x) = -\sum_j \partial_{x_j} f_j(x)$ a key quantity to study will be

$$\sigma_+ = \text{time average of } \sigma \tag{3}$$

that shall be called *average entropy production rate* or *average phase space contraction rate*; it will be assumed that $\sigma_+ > 0$ (this quantity is, in general, non negative,[20]).

The main result on $\sigma(x)$ concerns the probability distribution in the stationary state μ of the quantity (an observable, *i.e.* a function of the phase space point x)

$$p = T^{-1}\int_{T/2}^{T/2} \frac{\sigma(S_t x)}{\sigma_+}\,dt \tag{4}$$

which will be called the *$T-$average dimensionless entropy creation rate.* The result is a symmetry property of its probability distribution $\pi_T(p)$: which can be written in the form $\pi_T(p) \stackrel{def}{=} const\, e^{\zeta(p)T+o(T)}$, defining implicitly $\zeta(p)$, as it follows, on general grounds, from the theory of mixing Anosov systems, *cf.*[23], see[1] for a more mathematical statement. The function $\zeta(p)$ is called the *large deviation rate* for the observable p.

Then (see[14]: the delicate continuous time extension of a similar result[12] for discrete time)

Fluctuation theorem: *The "rate function" $\zeta(p)$ verifies*

$$\zeta(-p) = \zeta(p) - p\,\sigma_+ \tag{5}$$

which is a parameterless relation, valid under the above hypotheses of chaoticity and of time reversibility. It is a "mechanical" identity valid for systems with arbitrarily many particles (i.e. $N = 1, 2, \ldots 10^{23}, \ldots$).

Mathematically the above result holds for mixing Anosov flows which are time reversible. The chaotic hypothesis extends the result to rather general systems: of course for such systems it is no longer a theorem much in the same way as the consequences of the ergodic hypothesis in equilibrium statistical mechanics are not theorems for most systems to which they are applied.

Therefore we can say that the chaotic hypothesis implies *in equilibrium* (when the equations of motion are Hamiltonian and therefore $\sigma(x) \equiv 0$) the ergodic hypothesis (quite clearly): hence it implies classical statistical mechanics, starting with Boltzmann's heat theorem which says that $(dU + pdV)/T$ is an exact differential (with U, p, V, T defined as time averages of suitable mechanical quantities, see[9]). Likewise, out of equilibrium and in reversible systems, the chaotic hypothesis implies a general relation that is given by the fluctuation theorem, valid for systems with arbitrarily large numbers of particles. Both the heat theorem and the fluctuation theorem are "universal", *i.e.* parameterless, system independent relations. They could perhaps be considered a curiosity for N small, but certainly the first, at least, is an important property for $N = 10^{23}$.

It becomes, at this point, clear that one should attempt at an interpretation of the fluctuation theorem (5). It is however convenient to analyze it first in more detail to get some familiarity with the physical questions that it is necessary to address to grasp its meaning.

We begin with an attempt at justifying the name "*entropy creation rate*" for σ_+. Without too many comments we quote here the simple but relevant remark,[2], that the so called "*Gibbs entropy*" of an evolving probability distribution which starts, at $t = 0$, as absolutely continuous with density $\rho(x)$ on phase space has the following property

$$-\frac{d}{dt}\int \rho_t(x)\log\rho_t(x)\,dx = \int \sigma(x)\,\rho_t(x)\,dx \tag{6}$$

where $\rho_t(x) = \rho(S_{-t}x)\det\frac{\partial S_{-t}x}{\partial x}$ is the evolving phase space density (here $\partial S_{-t}x/\partial x$ is the matrix of the derivatives of the time evolution map S_t). Since the r.h.s. of (6) formally tends as $t\to\infty$ to the average of σ with respect to the distribution μ, *i.e.* to σ_+, we realize that (6) is a possible justification of the name used for σ_+.

Before proceeding it is also necessary to understand the role of the reversibility assumption in order to see whether it is a serious limitation in view of a possible physical interpretation and physical interest of the fluctuation theorem. Here one can argue that in many cases an irreversible system is "*equivalent*" to a reversible one: in fact several reversibility conjectures have been proposed, see[5],[12],[6] (Sect. 2 and 5),[7] (Sec. 8),[8],[9] (Sec. 9.11),[22].

Rather than trying to be general I shall consider an example, and analyze a Navier–Stokes fluid, in a periodic container of side L, subject to a force with intensity F and with viscosity ν. If $R = FL^3\nu^{-2}$ is the "*Reynolds number*", p is the pressure field, the density is $\rho = 1$, and $\underline{g}$ is a force field of intensity 1 the equations are

$$\begin{aligned}\dot{\underline{u}} &= -R\,\underset{\sim}{u}\cdot\underset{\sim}{\partial}\,\underline{u} + \Delta\,\underline{u} + \underline{g} - \underline{\partial}p\\ \underline{\partial}\cdot\underline{u} &= 0\end{aligned} \tag{7}$$

which are *irreversible* equations. According to the K41 theory (Kolmogorov theory, see[15]) the above equations can be truncated retaining only a few harmonics of the field $\underline{u}$: *i.e.* replacing $\underline{u}(\underline{x}) = \sum_{\underline{k}}\underline{u}_{\underline{k}}\,e^{i\underline{k}\cdot\underline{x}}$ by $\underline{u}(\underline{x}) = \sum_{|\underline{k}|<K(R)}\underline{u}_{\underline{k}}\,e^{i\underline{k}\cdot\underline{x}}$ with $K(R) = R^{3/4}$ so that "effectively" (and accepting the K41 theory) the fluid has $N(R) = O(R^{9/4})$ degrees of freedom.

If R is large (hence the motion is turbulent) the quantity $\mathcal{D} = \int(\underset{\sim}{\partial}\,\underline{u})^2\,d\underline{x}$ fluctuates in time with some average $\langle\mathcal{D}\rangle_{\mu_R}\overset{def}{=}\mathcal{D}(R)$, where μ_R is the probability distribution giving the statistics of the time averages.

We can also consider the following equations, introduced in[8] and called GNS equations,

$$\begin{aligned}\dot{\underline{u}} &= -R\,\underset{\sim}{u}\cdot\underset{\sim}{\partial}\,\underline{u} + \nu(\underline{u})\,\Delta\,\underline{u} + \underline{g} - \underline{\partial}p\\ \underline{\partial}\cdot\underline{u} &= 0\end{aligned} \tag{8}$$

where the "multiplier" $\nu(\underline{u})$ is so defined that $\mathcal{D}(\underline{u})$ is a constant of motion. An elementary calculation yields

$$\nu(\underline{u}) = \frac{\int_V\big(\underset{\sim}{\varphi}\cdot\Delta\,\underline{u} - R\Delta\,\underline{u}\cdot(\underset{\sim}{u}\cdot\underset{\sim}{\partial}\,\underline{u})\big)\,d\underline{x}}{\int_V(\Delta\,\underline{u})^2\,d\underline{x}} \tag{9}$$

which shows that $\nu(\underline{u})$ is *odd* in $\underline{u}$ so that (8) is reversible if time reversal is defined as $(I\,\underline{u})(\underline{x}) = -\underline{u}(\underline{x})$.

Call "local observable" any function $\underline{u}\to F(\underline{u})$ of the velocity field which depends on $\underline{u}$ only via fionitely many of its Fourier compopnents $\underline{u}_{\underline{k}}$; and let $\tilde\mu_{\mathcal{D},R}$ be the SRB distribution for (8). Then the following conjecture was proposed in[8]:

Equivalence conjecture: *If $F(\underline{u})$ is a local observable with non zero average then*

$$\frac{\mu_R(F)}{\mu_{\mathcal{D}(R),R}(F)}\xrightarrow[R\to\infty]{}1 \tag{10}$$

i.e. at large Reynolds number the irreversible NS and the reversible GNS equations are equivalent.

Note the analogy between the conjecture and the equivalence property of statistical ensembles in equilibrium statistical mechanics: here the coefficient of the Laplacian in (7) (which is 1 by our definitions) plays the role of temperature in a canonical ensemble while the quantity $\mathcal{D}$ plays the role of the energy in a microcanonical ensemble: if the energy is suitably tuned the distributions $\mu_R, \mu_{\mathcal{D}(R),R}$ are statistically equivalent as $R\to\infty$ and the Reynolds number R plays the role of the volume and $R\to\infty$ the role of thermodynamic limit.

It is interesting to remark that in nonequilibrium physics the statistical ensembles may be defined not only by the parameters that one regards naturally as control parameters (like energy in the microcanonical ensemble and temperature in the canonical) but *also by the equations of motion* that are used: this is perhaps not so strange because in equilibrium systems no friction is necessary and the equations of motion do not suffer from the ambiguity due to the arbitrariness of the thermostatting mechanisms that remove heat from the system (making possible the evolution towards a statistically stationary state).

The above conjecture is beginning to be tested with results that are at least encouraging, see[17]. Progress in the theory is needed as experiments on fluctuations of entropy production are already available and one would like to interpret them theoretically,[4].

The second question that one has to clarify preliminarly is that the "rate function" $\zeta(p)$ in (5) should be expected to be proportional to some macroscopic parameter measuring the size (like volume or number of degrees of freedom) so that the probability of observing the value p in a stationary state is $\pi_T(p) = const\,e^{\zeta(p)\,T}$ hence it is not observable if $p\neq 1$: any attempt at measuring p

will inexorably lead to $p = 1$ (given that by our normalizations the average value of p is 1).

Therefore one should investigate if, or when, a "*local version*" of the above fluctuation theorem holds telling us some properties, relative to a small volume or to a few degrees of freedom, which could have fluctuations that are frequent enough to be observable.

To get some inspiration we consider an analogous problem: suppose that a high temperature low density gas has density ρ and that it occupies the whole space. Given a volume V we can consider the observable $p = N_V/\rho V$. Then its probability distribution will have the form

$$\pi_V(p) = \, const \, e^{\overline{\zeta}(p)\, V} \tag{11}$$

where the exponent is affected by an error $O(\partial V)$ of the size of the boundary area of V *and* $\overline{\zeta}(p)$ *is* V*–independent.*

This shows that density fluctuations that are not observable in volumes V of macroscopic size do become observable in small enough volumes when the quantity $(\overline{\zeta}(p) - \overline{\zeta}(1))\, V$ becomes reasonably small. Furthermore since $\overline{\zeta}(p)$ is essentially V–independent we can infer that the probability of density fluctuations in a large volume is also measurable, being trivially related to $\overline{\zeta}(p)$ which is visible via the fluctuations in small volumes.

Coming back to our dynamical questions we can ask whether there is at least one model for which one can establish a "local fluctuation theorem" in a sense analogous to the above result on density fluctuations. Indeed there is a class of models that is very suitable for illustration purposes: these are the *chains of coupled maps.* Although their importance is mainly illustrative, they clearly show the possibility of local fluctuation theorems: here it will be enough to refer to the literature,[11],[13].

The conclusion is that if a local fluctuation relation holds then it becomes possible to perform tests of the fluctuation theorem, hence of the chaotic hypothesis.

Therefore we can try to attack the main question of interest here, namely "which is the physical interpretation" of the fluctuation theorem. The key is the following theorem, which is a simple extension of it and holds under the same hypotheses (*i.e.* chaotic hypothesis and time reversibility). It can be regarded as an extension of the Onsager–Machlup theory of fluctuation patterns,[16]. Let F, G be time reversal odd observables (for simplicity and to fix the ideas): $F(Ix) = -F(x), G(IX) = -G(x)$; and let $h, k : [-T/2, T/2] \to R^1$ be two real valued functions or "*patterns*". We call $h'(t) = -h(-t)$, $k'(t) = -k(-t)$ the "*time–reversed patterns*" or "*antipatterns*" of the patterns h, k. If $F(S_t x) = h(t)$ for $t \in [-T/2, T/2]$ we say that F follows the pattern h around the reference point x in the time interval $[-T/2, T/2] \stackrel{def}{=} W_T$. Then, see[10],

Theorem *(extension of Onsager–Machlup theory): The probabilities of the patterns h, k conditioned to a T–average dimensionless entropy production p, see (4), denoted $\pi\big(F(S_t\cdot)\big) = h(t),\, t \in W_T \,\big|\, p\big)$ and $\pi\big(G(S_t\cdot)\big) = k(t),\, t \in W_T \,\big|\, p\big)$ respectively verify*

$$\frac{\pi\big(F(S_t\cdot) = h(t),\, t \in W_T \,\big|\, p\big)}{\pi\big(F(S_t\cdot) = -h(-t),\, t \in W_T \,\big|\, -p\big)} = e^{p\sigma_+ T} \tag{12}$$

and (consequently)

$$\frac{\pi\big(F(S_t\cdot) = h(t),\, t \in W_T \,\big|\, p\big)}{\pi\big(G(S_t\cdot) = k(t),\, t \in W_T \,\big|\, p\big)} = \\ = \frac{\pi\big(F(S_t\cdot) = -h(-t),\, t \in W_T \,\big|\, -p\big)}{\pi\big(G(S_t\cdot) = -k(-t),\, t \in W_T \,\big|\, -p\big)} \tag{13}$$

Hence relative probabilities of patterns in presence of T–average entropy production p are the same as those of the corresponding antipatterns in presence of the opposite T–average entropy production rate.

In other words it suffices to change the sign of the entropy production to reverse the arrow of time. In a reversible system the quantity $\zeta(p)$ measures the degree of irreversibility of a motion observed to have the value p of dimensionless entropy creation rate during an observation time of size T: if we observe patterns over time intervals of size T then the fraction of such intervals in which we shall see an entropy production p rather than 1 (which is the most probable value) will be

$$e^{(\zeta(p)-\zeta(1))T} \tag{14}$$

More generally, in a situation in which a local fluctuation theorem holds and $\zeta(p) = V\overline{\zeta}(p)$ we can divide the volume occupied by the system into small boxes of size V_0, small enough so that one can observe entropy production fluctuations within them, and we can divide the time axis into time intervals of size T. Then

Proposition *(intermittency of fluctuations): The fraction of time intervals in which we shall observe p in a given box V_0 will be $e^{(\overline{\zeta}(p)-\overline{\zeta}(1))\, V_0\, T}$ and this same quantity will be the fraction of boxes V_0 where we shall observe, within a given time interval of size T, entropy production p.*

Normally we shall see $p = 1$ in a fixed box V_0 but "seldom" we shall see $p = -1$ and then, by the above extension of the Onsager–Machlup theory, *everything will look wrong*: every improbable pattern will appear as frequently as we would expect its (probable) antipattern to appear. This will last only for a moment and then things will return normal for a very long time (as the fraction of times in which this can happen in a given bix is $e^{-\overline{\sigma}_+ V_0 T}$). This is a kind of *intermittency* phenomenon.

In fact we see that when a local fluctuation theorem holds we shall see intermittency, in the form of a reversed time arrow, *happening in a small volume V_0 somewhere* in the volume V of the system, provided

$$V\, {V_0}^{-1} e^{-\overline{\sigma}_+ V_0\, T} \simeq 1 \tag{15}$$

furthermore there is a simple relation between fraction of volumes and fraction of times where time reversal occurs: namely they are equal and directly measured by $e^{-\overline{\sigma}_+ V_0\, T}$, *i.e.* by the average entropy creation rate.

We conclude by noting that the above remarks set up a possible way of measuring σ_+ and of attempting to measure $\zeta(p)$ in systems for which it is hard develop a reasonably good numerical simulation and/or an expression for σ_+. The quantity $\overline{\sigma}_+$ can be measured by considering some "current" J associated with the system; *i.e.* an observable $J(x)$ which, among other properties, is odd under time reversal. One then looks at the observable obtained by averaging this current over a time T and averaged over a time T, namely $J_T(x) \stackrel{def}{=} T^{-1} \int_{-T/2}^{T/2} J(S_t x) dt$ and one measures how often J_T takes a value close to the opposite of its (infinite time) average value J_+, assuming that the latter is > 0: this should happen with a frequency $e^{-\overline{\sigma}_+ V_0 T}$ giving us access to $\overline{\sigma}_+$.

Given the special role that entropy generation plays it is very tempting to think that there might be many currents J associated with the system: for each of them one could define $p = J_T/J_+$; then the new quantity p *has the same probability distribution as the variable with the same name that we have associated with the entropy production*. This is true at least for the special case $p = -1$ as just noted: if true in general then we could have easily access to the function $\zeta(p)$ for several values of p. Hence analysizing this "universality" property in special models seems to be an interesting problem.

For a general review on recent developments in non-equilibrium statistical mechanics see[21].

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[1] This means, precisely, that the probability P that p is in an interval of size δ around the value p is such that $\lim_{T\to\infty} T^{-1} \log P = \sup_p \zeta(p)$ with the supremum in the interval δ, for all $p \in (-p_{\max}, p_{\max})$ and $-\infty$ if $p \notin [-p_{\max}, p_{\max}]$. However I shall briefly say that the probability density of the variable p is $\pi_T(p) = const\, e^{\zeta(p)T}$.

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