# The fluctuation theorem beyond linear response theory and an extension to systems with slow dynamics

*Disclaimer: this text was written in 2006: references are not updated and all developments in the field after 2006 are not included*

I started this research at the beginning of my PhD under the supervision of Giancarlo Ruocco and in collaboration with L.Angelani. Initially we performed molecular dynamics simulations. The theoretical results that followed were motivated by these simulations, and were obtained in a series of collaborations with F.Bonetto, L.F.Cugliandolo, G.Gallavotti, A.Giuliani and J.Kurchan. In the following I will briefly recall the statement of the Gallavotti-Cohen fluctuation theorem and the reasons why it attracted much interest in the last decade. Then I will describe our contribution to this subject.

### A. The chaotic hypothesis and the fluctuation relation

The ergodic hypothesis plays a central role in equilibrium statistical mechanics. Although very few systems can be proven to be ergodic, most systems behave effectively as if they were ergodic. In out of equilibrium statistical physics, it is believed that Anosov systems (a particular class of smooth chaotic systems) play the role of ergodic systems in equilibrium statistical physics.

*Anosov systems and the fluctuation theorem* - The fluctuation theorem concerns fluctuations of phase space contraction in reversible hyperbolic (Anosov) systems. If time evolution is described by a differential equation on phase space $M$: $\dot{x} = X(x)$, $x \in M$, or by a map $S : x \to S(x)$ of $M$ one defines the *phase space contraction* as, respectively, $\sigma(x) = -\operatorname{div} X(x)$ or $\sigma(x) = -\log|\det \partial_x S(x)|$. Reversibility means that there is a metric preserving map $I$ of $M$ such that $IS = S^{-1}I$ if $S$ is the time evolution over a certain time $t$ (*e.g.* $t = 1$). *If the system is Anosov*, that is if $M$ is compact and $S$ is smooth and uniformly hyperbolic, see [1–5], the points $x$ will have a well defined statistics (or Sinai-Ruelle-Bowen distribution) $\mu_{srb}$, [5], i.e. almost all points with respect to the volume measure will evolve in time so that *all smooth observables* will have a well defined average equal to the integral over the SRB distribution. The SRB distribution plays in nonequilibrium statistical mechanics the role that the Boltzmann distribution plays in equilibrium. Hence, in particular, the time average of the function $\sigma(x)$ will be asymptotically given by the spatial average with respect to the SRB distribution. In the case of discrete time maps:

$$\sigma_+ \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \sum_{j=0}^{\tau-1} \sigma(S^j(x)) = \int_M \sigma \, d\mu_{srb} \equiv \langle\, \sigma \,\rangle_{srb} \tag{1}$$

and an analogous relation holds in the continuous time case. A general result of Ruelle [5] is that $\sigma_+ \geq 0$. Ruelle's theorem can be thought as a "Boltzmann H theorem" for nonequilibrium statistical mechanics. If $\sigma_+ = 0$ the system conserves the phase space volume and the SRB distribution reduces to the volume measure, i.e. the system is in equilibrium. In the dissipative case $\sigma_+ > 0$, let (in the discrete time case):

$$p(x) = \frac{1}{\tau\sigma_+} \sum_{j=0}^{\tau-1} \sigma(S^j(x)) \tag{2}$$

(an analogous definition is given in the continuous time case). The function $p(x)$ will have average $\langle\, p \,\rangle_{srb} = 1$ and distribution $\pi_\tau(dp)$ such that

$$\pi_\tau(\{p \in \Delta\}) = e^{\tau \max_{p\in\Delta} \zeta_\infty(p) + O(1)} \,, \tag{3}$$

where the correction at the exponent is $O(1)$ w.r.t. $\tau$ as $\tau \to \infty$, i.e. the *large deviation function* $\zeta_\infty(p)$ is well defined. The *Gallavotti-Cohen fluctuation theorem* states that the following fluctuation relation (FR) holds:

$$\zeta_\infty(p) = \zeta_\infty(-p) + p\sigma_+ \qquad \text{for all } |p| < p^* \tag{4}$$

where $\infty > p^* \geq 1$ is a suitable (model dependent) constant, defined by $\zeta_\infty(p) = -\infty$ for $|p| > p^*$. The fluctuation relation was discovered in a numerical simulation in [6] and formulated as a theorem for Anosov systems in [2].

*The chaotic hypothesis and physical implications of the FR* - Hyperbolicity is a paradigm for disordered systems similar to the small oscillations paradigm used for ordered motions: it does not hold exactly in essentially all the physically interesting systems. The *chaotic hypothesis* [1–3, 7, 8] is that nevertheless one can assume that chaotic motions (in the sense of motions with at least one positive Lyapunov exponent) exhibit some average properties of truly hyperbolic motions. This hypothesis is a natural generalization of the ergodic hypothesis, i.e. of the assumption that systems of many particles at equilibrium are well described on average by the microcanonical (or by the Gibbs) distribution, even if they are not really (or they are not proven to be) ergodic. A consequence of the chaotic hypothesis is that (dissipative) deterministic chaotic reversible motions should have fluctuations of phase space contraction verifying Eq. 4.

One interesting example of such motions is given by a system of $N$ interacting particles in $d$ dimensions subjected to nonconservative forces and kept in a stationary state by a *reversible mechanical thermostat*. It will be defined by a differential equation $\dot{x} = X_E(x)$ where $x = (\dot{\underline{q}}, \underline{q}) \in R^{2dN} \equiv M$ (*phase space*) and

$$m\ddot{\underline{q}} = \underline{f}(\underline{q}) + \underline{g}_E(\underline{q}) - \underline{\theta}_E(\dot{\underline{q}}, \underline{q}) \tag{5}$$

where $m$ is the mass of the particles, $\underline{f}(\underline{q})$ describes the internal (conservative) forces between the particles and $\underline{g}_E(\underline{q})$ represents the nonconservative "external" force acting on the system. Finally, $\underline{\theta}_E(\dot{\underline{q}}, \underline{q})$ is a mechanical force that prevents the system to acquire energy indefinitely: this is why we shall call it a *mechanical thermostat*. Systems belonging to this class are frequently used as microscopic models to describe nonequilibrium stationary states induced by the application of a driving force (temperature or velocity gradients, electric fields, etc.) on a fluid system in contact with a thermal bath, [8]. In this context, the phase space contraction rate $\sigma(x)$ has been identified (setting $k_B = 1$) with the *entropy production rate* [1, 6–8], and the fluctuation relation has been successfully tested in several numerical simulations [6, 9–14] and experiments on granular materials and on turbulent flows [15–18]. Having defined the notion of entropy production rate one can define a "duality" between fluxes $\underline{J} = \{J_i\}$ and forces $\underline{E} = \{E_i\}$ using $\sigma(x)$ as a "Lagrangian" [7]:

$$J_i(\underline{E}, x) = \frac{\partial \sigma(x)}{\partial E_i} \tag{6}$$

In the limit $\underline{E} \to \underline{0}$, *i.e.* close to equilibrium, the fluctuation relation leads to Onsager's reciprocity and to Green-Kubo's formulas for transport coefficients [19–21]:

$$\mu_{ij} \equiv \lim_{\underline{E}\to\underline{0}} \frac{\langle J_i \rangle_{\underline{E}}}{E_j} = \int_0^\infty dt \ \langle J_i(t) J_j(0) \rangle_{\underline{E}=\underline{0}} \tag{7}$$

The reasons why the fluctuation relation attracted lot of interest is that it is a *universal* relation (i.e. it contains no model dependent parameters) that reduces to well known universal relations (the Green-Kubo relations) in the linear response regime. Moreover the chaotic hypothesis, that implies the validity of the fluctuation relation for reversible systems, is very powerful: it provides an explicit expression for the invariant measure describing nonequilibrium stationary states of a large class of systems. Thus it is interesting to explore its validity.

*Numerical verification of the chaotic hypothesis* - The simplest check of the applicability of the chaotic hypothesis is a verification of the fluctuation relation: of course even if the check has a positive result this will not "prove" the hypothesis but it will at least add confidence to it. A rather stringent test of the fluctuation relation would be a check which *cannot be reduced to a kind of Green-Kubo relation*; this requires at least one of the two following conditions to be satisfied [14, 24]:

1. the distribution $\pi_\tau(p)$ is distinguishable from a Gaussian, or

2. deviations from the linear response theory, i.e. deviations from the Green-Kubo relation, are observed.

This is very hard to obtain in numerical simulations of Eq. 5 for the following reasons:

1. to observe deviations from linearity in Eq. 7 one has to apply very large forces $E$, then $\sigma_+$ is very large and it becomes very difficult to observe the negative values of $p(x)$ that are needed to compute $\zeta_\infty(-p)$ in Eq. 4;

2. deviations from Gaussianity in $\pi_\tau(p)$ are observed only for values of $p$ that differ significantly (of the order of twice the variance) from 1 and, again, it is very difficult to observe such values of $p$.

Due to the limited computational resources available in the past decade, all numerical computations that can be found in the literature on systems described by Eq. 5 found that the measured distribution $\pi_\tau(p)$ could not be distinguished from a Gaussian distribution in the interval of $p$ accessible to the numerical experiment [6, 9, 10, 14].

The purpose of our work (in collaboration with G. Gallavotti and A. Giuliani) was to test the fluctuation relation, in a numerical simulation of a system described by Eq. 5 (namely, a system of $N = 8$ –in $d = 2$ dimensions– and of $N = 20$ –in $d = 3$– Lennard–Jones-like particles perturbed by a constant force), for large applied force when deviations from linearity can be observed, and the distribution $\pi_\tau(p)$ is appreciably non-Gaussian. This was made possible by the large computational power (two clusters of 18 and 32 biprocessor units) avalaible in the INFM-Soft research center. However, it was still very difficult to reach values of $\tau$ which can be confidently regarded as "close" to the asymptotic limit $\tau \to \infty$; thus to interpret our results we developed a theory of the $o(1)$ corrections to the function $\zeta_\infty(p)$ in order to extract the limiting function $\zeta_\infty(p)$ from the numerical data. In order to compute the finite time corrections, we proposed an algorithm which allows to reconstruct the asymptotic distribution function from measurable quantities at finite time, within a given precision [24]. Our theory of the corrections relies on the symbolic representation of the chaotic dynamics, then it is applicable if one accepts the Chaotic Hypothesis. Taking into account the latter finite time corrections, we successfully tested the fluctuation relation for non–Gaussian distributions and beyond the linear response theory.

Our interpretation of the numerical results is that the chaotic hypothesis can be applied to these systems, also very far from equilibrium, and in particular the fluctuation relation is verified even in regions where its predictions measurably differ from those of linear response theory.

A big open problem we are left with is trying to understand how the fluctuation relation is modified for values of the driving force so high that the attractive set is no more dense in phase space. It is expected, [22, 23], that in such a case $\zeta_\infty(p) - \zeta_\infty(-p)$ is still linear, but the slope is $X\sigma_+$, with $X$ given by the ratio of the dimension of the attractive set and of that of the whole phase space. An estimate of such quantity can be given via the number of negative pairs of exponents in the Lyapunov spectrum. Unfortunately negative pairs begin to appear in the Lyapunov spectrum only for values of the external force so high that no negative fluctuations are observable anymore. We hope that future work will address this point. A recently proposed algorithm to measure large deviations [25] may be useful in this perspective.

### B. Extension of the fluctuation theorem to driven glassy systems

The fluctuation theorem has been extended to a Langevin equation by Kurchan [26] and to generic Markov processes by Lebowitz and Spohn [27]. Thus, at present, the fluctuation relation is believed to be a very general relation that characterizes the fluctuations of the entropy production in out of equilibrium stationary states; moreover, a close connection between the fluctuation relation and the definition of a *nonequilibrium temperature* has been conjectured [7, 28–30].

To exploit this connection, one should consider systems such that the nonequilibrium temperature is not trivially equal to the ambient temperature; for a system coupled to a single thermal bath, this happens if *(i)* the thermal bath has temperature $T$, but the system is not able to equilibrate with the bath, and/or if *(ii)* the bath itself is not at equilibrium, i.e. it does not verify the fluctuation-dissipation relation [31]. The first situation happens, for example, in glassy systems, that never reach equilibrium with the thermal bath; the second situation is realized if one consider the diffusion of a Brownian particle in a complex medium (e.g. a glass, or a granular) [32–34]. In this case the medium, which acts as a thermal bath with respect to the Brownian particle, is itself out of equilibrium. The two situations are closely related as, at least at the mean field level, the problem of glassy dynamics can be mapped in the problem of a single "effective" degree of freedom moving in an out of equilibrium environment [31, 35], and thus situations *(i)* and *(ii)* are described by the same kind of equation, namely a Langevin equation for a single degree of freedom coupled to a complex bath, i.e. a bath that does not verify the fluctuation-dissipation theorem. Finally, note that the simplest situation where the nonequilibrium temperature is not trivial happens when the system is in contact with a certain number of thermal baths at different temperature; the latter can also be seen as a model for a "complex bath" [35].

Our aim was then to discuss the validity of the fluctuation relation for the simplest possible system realizing one of the situations discussed above, namely a Brownian particle subject to a driving force and to a confining potential, and coupled to either a complex (out of equilibrium) bath or to $N$ different baths with different temperature. We found that:

1. the PDF of the entropy production $\sigma(t) = W(t)/\Theta$, where $W(t)$ is the power dissipated by the external force and $\Theta$ is a free parameter with the dimensions of a temperature, does not satisfy the fluctuation relation exactly: if the bath acts on a single time scale the fluctuation relation is verified approximately if $\Theta$ is suitably chosen; if the bath acts on different time scales, the function $[\zeta_\infty(p) - \zeta_\infty(-p)]/\sigma_+$ may have different slopes corresponding to the different temperatures at small $p$ and at large $p$;

2. if a suitable (frequency dependent) *effective temperature* is defined as a property of the bath [31], and if the entropy production rate is defined as the integral over all frequencies $\omega$ of the power injected by the driving

force at frequency $\omega$ divided by the effective temperature at the same frequency, the fluctuation relation holds for the complex bath we considered;

3. The modified fluctuation relation is related, in the linear regime, to the modified Green-Kubo relations in which the effective temperature enters instead of the ambient temperature.

Models like the one we discussed have been recently investigated [32–34] to describe the dynamics of Brownian particles in complex media; Brownian particles are often used as probes in order to study the properties of the medium (e.g. in Dynamic Light Scattering or Diffusing Wave Spectroscopy experiments). Moreover, confining potentials for Brownian particles can be generated using laser beams [36] and experiments on the fluctuations of the power dissipated in such systems are currently being performed [32, 37].

This part of the work is done in collaboration with F. Bonetto, L. Cugliandolo and J. Kurchan and the results have been published in [38]. The analytical results are in good agreement with the numerical simulations on Lennard–Jones systems that motivated them, performed in collaboration with G.Ruocco and L.Angelani and published in [39].

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