Fluctuation theorem revisited

Giovanni Gallavotti

Rutgers Hill Center, I.N.F.N. Roma1, ENS Paris

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Abstract: Recently the “Fluctuation theorem” has been criticized and incorrect incorrect contents have been attributed to it. Here I reestablish and comment the original statements.

Fluctuations

Mathematically the Fluctuation theorem is a property of the phase space contraction of an Anosov map $S$, called time evolution, which is time reversible. The possible connection between the fluctuation theorem and Physics is a different matter that I will not discuss here: there are many places where this is done in full detail, [1–3].

I shall denote by $\Omega$ the phase space (a smooth finite boundaryless manifold) and by $\sigma(x)$ the phase space contraction

$$\sigma(x) = -\log |\det \partial_x S(x)|$$

Time reversal will be an isometry of phase space $I$ such that

$$I S = S^{-1} I, \quad \sigma(Ix) = -\sigma(x)$$

It has been shown that there exists a unique probability distribution, called the statistics of the motion or the SRB distribution, $\mu$ such that for all points $x \in \Omega$, excepted those in a set of 0 volume, it is

$$\lim_{\tau \to \infty} \frac{1}{\tau} \sum_{t=0}^{\tau-1} F(S^t x) = \langle F \rangle = \int_{\Omega} F(y) \mu(dy)$$

for all smooth observables $F$ defined on phase space.

It is intuitive that “phase space cannot expand”; this is expressed by the following result of Ruelle, [4],

**Proposition:** If $\sigma + \langle \sigma \rangle$ it is $\sigma + \geq 0$

Clearly if $S$ is volume preserving it is $\sigma + = 0$. If $\sigma + > 0$ the system does not admit any stationary distribution which is absolutely continuous with respect to the volume.

This motivates calling systems for which $\langle \sigma \rangle > 0$ “dissipative” and calling volume preserving systems “conservative”.

For Anosov systems which are “transitive” (i.e. with a dense orbit), reversible and dissipative one can define the dimensionless phase space contraction, a quantity related to entropy creation rate (see [5]) averaged over a time interval of size $\tau$. This is

$$p = \frac{1}{\sigma + \tau} \sum_{-\tau/2}^{\tau/2-1} \sigma(S^k x)$$

provided of course $\sigma + > 0$.

Then for such systems the probability with respect to the stationary state, i.e. to the SRB distribution $\mu$, that the variable $p$ takes values in $\Delta = [p, p + \delta p]$ can be written as $\Pi(\Delta) = e^{p \max_{p \in \Delta} \zeta(p) + O(1)}$ where $\zeta(p)$ is a suitable function and $O(1)$ refers to the $\tau$-dependence at fixed $p, \delta p$ for all intervals $\Delta$ contained in an open interval $(p^1, p^2)$ (this is often expressed as $\lim_{\tau \to \infty} \frac{1}{\tau} \log \Pi(\Delta) = \zeta(p)$ for $p^1 < p < p^2$). The function $\zeta(p)$ would be called in probability theory the rate function for the large deviations of $\sigma(x)$.

The function $\zeta(p)$ is analytic in $p$ in the interval of definition $(p^1, p^2)$ and convex. In fact more is true and one can prove the following fluctuation theorem:

**Proposition:** In transitive time reversible Anosov systems the rate function $\zeta(p)$ for the phase space contraction $\sigma(x)$ is analytic and strictly convex in an interval $(-p^*, p^*)$ with $+\infty > p^* \geq 1$ and $\zeta(p) = -\infty$ for $|p| > p^*$.

Furthermore

$$\zeta(p) > \zeta(p) - p \sigma +, \quad \text{for} \quad |p| < p^*$$

which is called the “fluctuation relation”.

The result is adapted from a theorem by Sinai who proves analyticity and convexity. Strict convexity follows from a theorem of Griffiths and Ruelle which shows that the only way strict convexity could fail is if $\sigma(x) = \varphi(Sx) - \varphi(x) + c$ where $\varphi(x)$ is a smooth function (typically a Lipschitz continuous function) and $c$ is a constant, see propositions (6.4.2) and (6.4.3) in [6]. The constant vanishes if time reversal holds and $\sigma(x) = \varphi(Sx) - \varphi(S^{-1}x)$ contradicts the assumption that $\sigma + > 0$ (because $\tau^{-1} \sum_{-\tau/2}^{\tau-1} \sigma(S^k x) = \tau^{-1} (\varphi(S^{\tau/2} - 1 x) - \varphi(S^{-\tau/2}x)) \to 0$ as $\tau \to \infty$. The value of $p^*$ must be $p^* \geq 1$ otherwise $p^* < 1$ and the average of $p$ could not be 1 (as it is by its very definition). The fluctuation relation is in [7] and is properly called the fluctuation theorem (a name later
given to other very different relations with remarkable confusion, [8]). The theorem can be extended to Anosov flows (i.e. to systems evolving in continuous time), [9].

Remarks: The relation was discovered in a numerical experiment, [10], and proved in [7]. For finite $\tau$ the function $\zeta(p)$ and $\zeta(-p)$ are replaced by $\zeta_\tau(p), \zeta_\tau(-p)$ which differ from their limits as $\tau \to \infty$ by a quantity bounded by a constant uniformly in any closed interval of $(-p^*, p^*)$

Sometimes one does not consider the above $p$ but a quantity $a = \tau^{-1} \sum_{j=-\tau/2}^{\tau/2-1} \sigma(S^j x)$ and the result can be written

$$\tilde{\zeta}(-a) = \tilde{\zeta}(a) - a, \quad \text{for } |a| < p^* \sigma_+$$

where $\tilde{\zeta}(a)$ is trivially related to $\zeta(p)$. This form dangerously suggests that in the case of systems with $\sigma_+ = 0$ the distribution of the variable $a$ is asymmetric (because the extra condition $|a| < p^* \sigma_+$ might be forgotten, see [11]).

Note that $p^*$ is certainly $< +\infty$ because the variable $\sigma(x)$ is bounded (being continuous on phase space, i.e. on the bounded manifold on which the Anosov map is defined).

However no confusion should be made between $p^* \sigma_+$ and $\sigma_{\text{max}} \equiv \max |\sigma(x)|$: unlike $\sigma_{\text{max}}$ the quantity $p^*$ is a non trivial dynamical quantity, independent on the metric used on phase space to measure distances, hence volume. It is very easy to build examples in which $p^* \sigma_+ < \sigma_{\text{max}}$ and in fact the ratio between the r.h.s and the l.h.s two quantities can be even infinite (e.g. in conservative cases when $p^* \sigma_+ = 0$ but $\sigma(x)$ is not identically 0 because of the metric used.

Note that even in the conservative cases we can define on phase space a time reversal invariant metric, i.e. such that $I$ is an isometry, whose volume elements do not verify Liouville’s theorem, see appendix). This point has not been always understood and the confusion has in fact been made, at least once, in the published literature with nefast consequences.

The fact is that $p^*$ and $\max |a|$ are dynamically determined, non trivial, quantities and one cannot “assume” their value, see comment 13 in reference [11].

Considering more closely the cases $\sigma_+ = 0$ it follows that $\sigma(x) = \varphi(Sx) - \varphi(x) + c$ again by the mentioned result of Griffiths and Ruelle (essentially the same mentioned above) and $c = 0$ by time reversal. Hence the variable

$$a = \frac{1}{\tau} \sum_{j=-\tau/2}^{\tau/2-1} \sigma(S^j x)$$

is bounded and tends uniformly to 0. One could repeat the theory developed for $p$ when $\sigma_+ > 0$ but one would reach the conclusion that $\tilde{\zeta}(a) = -\infty$ for $|a| > 0$ and we see that the result is trivial. In fact in this case it follows that that the system admits an absolutely continuous SRB distribution. The distribution of $a$ is symmetric (trivially by time reversal symmetry) and becomes a delta function around 0 as $t \to \infty$.

Nevertheless the fluctuation relation is non trivial in cases in which the map $S$ depends on parameters $E = (E_1, \ldots, E_n)$ and becomes volume preserving (“conservative”) as $E \to 0$: in this case $\sigma_+ \to 0$ as $E \to 0$ and one has to rewrite the fluctuation relation in an appropriate way to take a meaningful limit.

The result is that the limit as $E \to 0$ of the fluctuation relation in which both sides are divided by $E^2$ makes sense and yields (in the case considered here of transitive Anosov dynamical systems) relations which are non trivial and that can be interpreted as giving Green–Kubo formulae and Onsager reciprocity for transport coefficients, [12].

In fact the very definition of the duality between currents and fluxes so familiar in nonequilibrium thermodynamics since Onsager can be set up in such systems using as generating function the $\sigma_+$ regraded as a function of $E$. Note that the fluxes are usually “currents” divided by the temperature; therefore via the above interpretation one can try to define the temperature even in nonequilibrium situations, [13].

A test

Although a check of the fluctuation relation is difficult nevertheless it has been performed in several cases. Little attention has been dedicated, however, until recently to one rather striking prediction valid under suitable further assumptions which are proposed in [14] where they are called axiom C and pairing rule and are presented as possibly quite general the first, and as at least approximately valid in several examples the second. The prediction of the first assumption is that if under strong forcing (or strong dissipation) the attracting set (i.e. the closure at the attractor) for the dynamics becomes slim and occupies a region of dimensionality lower than that of phase space, then the a new symmetry with the same properties but which leaves the attracting set invariant is generated: “time reversal is unbreakable”, [14, 15]. Hence the area contraction on the attracting set will verify the fluctuation relation.

In general, however, the area elements on the attracting set will be very difficult to measure: but at least in the cases in which the second assumption holds the prediction is that their contraction is related to the total volume contraction $\sigma(x)$ on the full phase space which is much easier to access. Furthermore the fluctuation relation will hold in the form $\zeta(p) = \zeta(-p) - p^* \sigma_+ \gamma$ equal to the ratio of the dimension of the attracting set to the dimension of the full phase space. This in particular implies $\gamma < 1$: which is a surprising and apparently counterintuitive result: a naive view of the attraction mechanism: i.e. a uniform contraction of the transversal
directions would in fact lead to $c > 1$.

The reason why one expects $\gamma > 1$ if the contraction transversal to the attracting set is constant and equal to $\lambda_0$ (a property which, however, is incompatible with the pairing rule) is the following. The total contraction could be written $\sigma(x) = \sigma_0(x) + \lambda_0$ then, setting $c = \frac{\lambda_0}{\sigma_0 + \lambda_0}$ with $\sigma_0 = \sigma_{0+}$, and $\lambda = \frac{\lambda_0}{\sigma_0 + \lambda_0}$, it is $p = c p_0 + \lambda$ and

$$\zeta(p) - \zeta(-p) = \zeta_0 \left( \frac{p - \lambda}{c} \right) - \zeta_0 \left( \frac{-p - \lambda}{c} \right).$$

Developing the expression in powers of $\lambda$ and using the fluctuation relation for $p_0$ and assuming a gaussian distribution for $p_0$ (which is related to the validity of the Green–Kubo relations, see [16]) we get $\zeta(p) - \zeta(-p) = (1 + \lambda) \sigma_+ p$, i.e. $\gamma = 1 + \lambda > 1$ for small $\lambda$ and small $\sigma_{0+}$.

The results in [16] might prelude to the first check of the quite striking prediction that the coefficient $\gamma$ is $< 1$ because in this case the pairing rule seems to be verified within a good approximation (although not exact, [17]).

**Appendix:** No relation between $p^*$, max $|a|$ and $\sigma_{\text{max}} = \max \{|\sigma(x)|\}$: some explicit countereamples

The simplest example (out of many) is provided by the simplest conservative system which is strictly an Anosov transitive system and which has therefore an SRB distribution: this is the geodesic flow on a surface of constant negative curvature, [18]. I discuss here an evolution in continuous time because the system is considered in the literature for such systems, [11] (even simpler examples are possible for time evolution maps).

The phase space $M$ is compact, time reversal is just momentum reversal and the natural metric, induced by the Lobatchesky metric $g_{ij}(q)$ on the surface, is time reversal invariant: the SRB distribution is the Liouville distribution and $\sigma(x) \equiv 0$. However one can introduce a function $\Phi(x)$ on $M$ which is very large in a small vicinity of a point $x_0$, arbitrarily selected, constant outside a slightly larger vicinity of $x_0$ and positive everywhere. A new metric could be defined as $g_{\text{new}}(x) = (\Phi(x) + \Phi(|x|))g(x)$, i.e. $\Phi$ is still time reversal invariant but its volume elements will no longer be invariant under time evolution. The rate of change of phase space volume in the new metric will be $\sigma_{\text{new}}(x) = LF(x)$ where $L$ is the Liouville operator. Since $\Phi$ is arbitrary one can achieve a value of $\sigma_{\text{new}}(x)$ as large as wished by fixing suitably the function $\Phi$.

Nevertheless $a = \frac{1}{T} \int_0^T \sigma_{\text{new}}(Sx) \, dt = \tau^{-1}(F(Sx) - F(x)) \tau^{-\infty} \approx 0$. This contradicts statements existing in the literature, [11], which claim that in such case the quantity $a$ will verify the relation $\zeta(a) = \zeta(-a) - w$: in fact the distribution of $\Phi$ will be a delta function at 0 hence the relation cannot hold with $\zeta(a)$ finite for $a \neq 0$, even though some go as far as claiming that such erroneous conclusion would follow by “repeating”, with minor adaptations, Ruelle’s proof of the fluctuation theorem (which would therefore be incorrect, which is not), see comments 12, 13 and 23 in reference [11].

It has been argued that even if $\sigma_+ > 0$ but small (i.e. the system is close to equilibrium) and the system is Anosov the fluctuation relation will not apply under certain thermostat mechanisms: but the work [18] provides a counterxample (out of many others possible) even to this statement, see [11].

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e-mail: giovanni.gallavotti@roma1.infn.it
web: http://ipparco.roma1.infn.it
Dip. Fisica, U. Roma 1, 00185, Roma, Italia