Fluctuation Theorem

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Fluctuation Theorem:
a simple consequence of a time reversal symmetry; it deals with motions which are chaotic in the strong mathematical sense of being hyperbolic and transitive (ie are generated by smooth hyperbolic evolutions on a smooth compact surface (the "phase space") and with a dense trajectory, also called **Anosov systems**) and "furthermore are time reversible". In such systems any initial data, with the exception of a set of zero volume in phase space, have the same statistical properties in the sense that all smooth observables admit a time average independent of the initial data and expressed as an integral with respect to a probability distribution on phase space, called the "natural stationary state", or simply the "stationary state". The theorem provides, asymptotically in the observation time, a quantitative and parameter free relation between the stationary state probability of observing a value of the average entropy production rate and its opposite. Although there are quite a few examples of mechanical systems which are hyperbolic and transitive in the above mathematical sense, the fluctuation theorem acquires physical interest only in connection with the **chaotic hypothesis**. Under the latter general assumption, combined with time reversal, it predicts a "universal relation" between an entropy creation rate value and its opposite, accessible to simulations and possibly to laboratory experiments. The basis for the physical interpretation of the theorem as a property of stationary states in nonequilibrium statistical mechanics is developed here.

Statistical Mechanics of Nonequilibrium Stationary States. Thermostats

In nonequilibrium statistical mechanics the molecules of a system are subject to nonconservative forces whose work is dissipated in the form of heat supplied to other systems kept at constant temperature: the "thermostats" with which the system is in contact. Under such conditions the systems statistical properties usually reach, after a transient, a "**stationary state**", i.e. they are described by a probability distribution on phase space which

is invariant under time evolution. The study of this situation is a natural extension of "**equilibrium thermodynamics**" where the probability distribution is quite generally simply proportional to the Liouville volume on the energy surface.
Mathematical models for thermostats often involve equations of motion with velocity dependent forces acting on the molecules of the thermostats.

Volume Contraction

Therefore the equations of motion generate evolutions on the phase space X, " i.e." the space of the points representing the microscopic configurations of the molecules of the system "and" of the thermostats. Such motions do not conserve the phase space volume (unlike the case of equilibrium statistical mechanics, where the evolution is Hamiltonian and volume preserving, by "**Liouville's Theorem**"). This is manifested by the non vanishing of the phase space volume contraction rate $\sigma(x)$, which is defined as minus the divergence of the equations of motion for all particles including those of the thermostats, evaluated at the microscopic state $x \in X$ (and it could be > 0 or ≤ 0).
As a rule motion $t \to S_t x$ is observed through **Chaotic Hypothesis/Timing Events|timing events** (also called *Poincaré sections*) in a subset $\Xi \subset X$ of phase space, so that the time evolution of the point $\xi \in \Xi$ takes place in discrete time and is described by a map $\xi \to S\xi$. Then the volume contraction rate is: $\sigma(\xi) \stackrel{def}{=} -\log|\det(\frac{\partial(S\xi)_j}{\partial_{\xi_i}}|$, where i, j label the coordinates of ξ.

Dissipation

In systems that are really out of equilibrium ("i.e." subject to nonconservative forces and/or to thermostats at different temperatures) and dissipative the phase space contraction $\sigma(S_t x)$, or $\sigma(S^n\xi)$ in discrete evolution models, is not only not identically 0 but it has an average σ_+ over $t > 0$ or, respectively, $n > 0$, which is positive.

SRB Statistics

If the "**Chaotic Hypothesis**" is accepted then motions have a well defined statistics μ in the sense that time averages of a generic observable F exist, aside from a set of 0 volume in the phase space X, and are expressed as the x-independent limit:

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T F(S_t x)dt = \int_X F(y)\mu(dy) \overset{def}{=} F_+$$

where μ is the **SRB distribution**. In particular the time average of the phase space contraction rate will be:

$$\sigma_+ = \int_X \sigma(y)\mu(dy).$$

Fluctuation Theorem for Hyperbolic Systems

Consider a "transitive hyperbolic systems" (see also "**Chaotic Hypothesis**"), whose evolution admits a "**time reversal symmetry**", "i.e." there is a smooth **isometry** I of phase space with the property $IS_t = S_{-t}I$ or, in the discrete case, $IS = S^{-1}I$. Assuming $\sigma_+ > 0$, " i.e." supposing the system dissipative in the average, the "time reversal" symmetry is reflected by a symmetry property that can be proved for the large deviations rate (see "**Chaotic Hypothesis**") $\zeta(p)$ of the variable

$$p = \frac{1}{T}\int_0^T \frac{\sigma(S_t x)}{\sigma_+}\,dt$$

or, in the discrete time case,

$$p = \frac{1}{N}\sum_{j=0}^{N-1}\frac{\sigma(S^j\xi)}{\sigma_+},$$

regarded as a random variable with respect to the **SRB probability distribution** μ of the motion; this variable is called "average entropy creation rate", see below. Namely
"'Fluctuation Theorem"' (for Anosov systems): $\zeta(-p) = \zeta(p) - p\sigma_+$, for all p's within the domain of definition $(-p^*, p^*)$ of $\zeta(p)$.
For the domain of definition see "**Chaotic Hypothesis**". The above theorem is very different from other formally similar relations which have been given the same name (at later times, see "Fluctuation Theorem" in Wikipedia for a glimpse of such relations).

The Fluctuation Theorem and Entropy production rate

The physical interest of the above theorem can be seen by considering that, in models of nonequilibrium statistical mechanics systems, the phase space contraction rate has the form:

$$\sigma(x) = \sum_j \frac{Q_j(x)}{k_B T_j} + \dot{R}(x) \stackrel{def}{=} \varepsilon(x) + \dot{R}(x)$$

where $Q_j(x)$ is the amount of work that the system molecules perform per unit time on the molecules of the j-th thermostat whose constant temperature is T_j, k_B is "**Boltzmann constant**", and $\dot{R}(x)$ is a suitable "total time derivative".
Interpreting $Q_j(x)$ as the heat that the molecules of the system inject into the j–th thermostat, the statistics of the observable: $p = \frac{1}{T}\int_0^T \frac{\sigma(S_t x)}{\sigma_+} dt$ approaches as $T \to \infty$ that of: $p' = \frac{1}{T}\int_0^T \frac{\varepsilon(S_t x)}{\varepsilon_+} dt$ because

$$\frac{1}{T}\int_0^T \sigma(S_t x)dt \equiv \frac{1}{T}\int_0^T \varepsilon(S_t x)dt + \frac{1}{T}(R(S_T x) - R(x))$$

the two averages as well as ε_+ and σ_+ are asymptotically the same, at least if $R(x)$ is bounded.
The quantity called $\varepsilon(x)$ above has time averages which are physically measurable, in principle, because they are the heat received per unit time by the thermostats: this is a quantity which can be defined and measured without really knowing the equations of motion: in sharp contrast with the time averages of $\sigma(x)$ which can be measured directly only in simulations.

Fluctuation Relation

Hence if the system evolution is time reversible, which is certainly true in many models but subtle and delicate to establish in experiments, see [BGGZ06], the "fluctuation relation" for the statistical properties of the finite time averages :$p' = \frac{1}{T}\int_0^T \frac{\varepsilon(S_t x)}{\varepsilon_+} dt$ of the "physically observable" dimensionless entropy production rate p', $\zeta(-p') = \zeta(p') - p'\varepsilon_+$, can be expected to hold, for T large with corrections of $O(T^{-1})$, on the basis of the "Chaotic Hypothesis" and of the fluctuation theorem for the (usually not observable) quantity $\frac{\sigma(x)}{\sigma_+}$. Its interest is therefore that it gives an explicit and parameter free relation for the (large) fluctuations of the finite time averages of the entropy production rate $\varepsilon(x)$ in a stationary nonequilibrium state (with statistics given by the **SRB distribution**).

New fluctuation relations have been derived for systems subject to noise, [Ku98,LS99]. It can also be extended to cases in which the quantities $\varepsilon(x)$ and $R(x)$ are not bounded, but its form can change in such cases, [BGG06], [CV03].
The above theorem arose from a new interpretation of the experimental results in [ECM93], given in [GC95], (see [Ga95], [Ru99] for more mathematical versions); the stochastic version was developed in [Ku98], [LS99], see also [CDG06], [BGG06]. A discussion of the relation between the above fluctuation theorem and other results that, later, have been given the same name see [CG99].
The theorem provides, when time reversibility is satisfied, also a criterion to test the **chaotic hypothesis**: the precision with which the relation predicted by the theorem for **Anosov systems** is satisfied becomes a measure of the correctness of the hypothesis. So far this test has been possible only in simulations, given the difficulty of observing very large fluctuation in stationary states.
Historically the concept, and the name of "fluctuation theorem", were introduced in [CG95] and the name has been subsequently adopted, in the literature, to designate other kinds of fluctuations (and some confusion followed).

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See also

Anosov Diffeomorphism, *Chaos*, *Chaotic Hypothesis*, *Fluctuations*, *Entropy*, *Ergodic Theory*, *Smooth Dynamics*

Category:Dynamical Systems | *Statistical Mechanics*