0n the Fluctuation Law(s) for Hamiltonian systems (with equilibrium steady state): A Comment on cond–mat/0008421

Boris Chirikov and Oleg Zhirov
Budker Institute of Nuclear Physics
630090 Novosibirsk, Russia
chirikov @ inp.nsk.su
zhirov @ inp.nsk.su

A generalization of the fluctuation law (FL) ("theorem"), formulated in 1993 by Evans, Cohen and Morriss for a nonequilibrium steady state, on the chaotic Hamiltonian systems with equilibrium steady state in recent publication by Evans, Searles and Mittag (cond–mat/0008421) is briefly discussed. We argue that the physical meaning of this law, as presented in the latter publication, is qualitatively different from the original one. Namely, the original FL concerns the *local* (in time) fluctuations with an intriguing result: a high probability for the "violation" of the Second Law. Instead, the new law describes the *global* fluctuations for which this remarkable unexpected phenomenon is absent or hidden. We compare both types of fluctuations in both classes of Hamiltonian systems, and discuss remarkable similarities as well as the interesting distinctions.

The "Fluctuation Theorem" has been first obtained by Evans, Cohen and Morriss [1] for a particular example of the nonequilibrium steady state, using both the theory as well as numerics. For our purposes it can be represented in the form:

$$\ln\left(\frac{p(\Delta S)}{p(-\Delta S)}\right) = F \cdot \Delta S\,, \qquad F = \frac{2\langle\Delta S\rangle}{\sigma^2} \tag{1}$$

Here $p(\Delta S)$ is the probability of entropy (or entropy–like quantity as in [1, 2]) change ΔS in the ensemble of trajectory segments of a fixed (appropriately scaled) duration τ for the mean change $\langle\Delta S\rangle > 0$ and variance σ^2, and F the fluctuation parameter usually taken to be unity ($F = 1$). We call this type of fluctuations the *local* fluctuations.

By itself, the relation (1) is but a specific reduced representation of the normal probabilistic law, the Gaussian distribution, in a suitable random variable (ΔS):

$$p(\Delta S) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(\Delta S - \langle\Delta S\rangle)^2}{2\sigma^2}\right) \tag{2}$$

shifted with respect to $\Delta S = 0$ due to the permanent entropy production at a constant rate in the nonequilibrium steady state. The FL (1) immediately follows from the normal law (2) but not vice versa. Notice also that this distribution is not universal, yet it is rather typical indeed. However, the surprise (to many) was in that the probability of *negative* ("abnormal") entropy change $\Delta S < 0$ (without time reversal!) is generally not small at all reaching 50% for sufficiently short τ. That is every second change may be abnormal !?

Implicitly, all that is contained in the well developed statistical theory (see, e.g., [3], Section 20, and [4]). Nevertheless, the first direct observation of this phenomenon in a nonequilibrium steady state [1] has so much impressed the authors that they even entitled the paper "Probability of Second Law violations in shearing steady state". In fact, this is simply a sort of peculiar fluctuations discussed in [5].

In our opinion, the main lesson one should learn from the FL is that the entropy evolution is generally *nonmonotonic* contrary to a common belief, still now. The origin of this confusion is, perhaps, in traditional conception of the fluctuations as a charcteristic on the microscopic scale well separated from a much larger macroscopic scale with its averaged quantities like the entropy production rate, for example.

In equilibrium steady state the macroscopic scale with the mean rate $\langle \Delta S \rangle = 0$ traditionally seems to be irrelevant with the entropy trivially conserved. However, in nonequilibrium steady state the macroscopic scale is represented by a finite rate $\langle \Delta S \rangle > 0$, yet the "microscopic" scale of the fluctuations may be well comparable with, and even exceed, the former.

The border of nonmonotonic behavior is at $\Delta S = 0$ (no entropy rise at all) which corresponds to the probability of "abnormal" entropy changes $\Delta S < 0$

$$P_{ab} = \int_{-\infty}^{0} p(s)\, ds\,, \qquad C = \frac{\langle \Delta S \rangle}{\sigma} \tag{3}$$

Here C is a new parameter for the normal/abnormal crossover in the entropy variation sign at $|C| = C_{cro} \sim 1$ when the probability P_{ab} is large.

If a finite–dimensional Hamiltonian system admits the (stable) statistical equilibrium (as is the case in [2]) the overall ($t \to \infty$) average entropy rate $\langle \Delta S \rangle = 0$ for any τ. However, on a finite time scale t_R of a nonequilibrium relaxation to the equilibrium the local $\langle \Delta S \rangle > 0$ as in the nonequilibrium steady state, but temporally. On this time scale the local fluctuations are expected [5] to obey the law similar to the nonequilibrium FL provided $\tau \ll \tau_R$. However, the properties of fluctuations in such a system, studied in [2], turned out to be qualitatively different. Particularly, the celebrated phenomenon of the abnormal fluctuations completely disappeared (?). In our understanding, this crucial change is caused by a different type of the fluctuations studied in [2]: instead to fix $\tau \ll \tau_R$ the fluctuations as a function of time $S(t) = A(t)$ (in [2]) were considered. Such global fluctuations were also studied in a nonequilibrium steady state [5], and found to be rather different, indeed. Particularly, the crossover parameter

$$C(t) = \frac{\langle S(t) \rangle}{\sigma} \tag{4}$$

depends now on the motion time, which is a dynamical variable, rather then on the trajectory segment length τ, which is a parameter of the problem.

It is useful to compare both types of fluctuations for both classes of dynamical systems in nonequilibrium (far–from–equilibrium) states. For the sake of brevity, let us call the new class [2] the stable equilibrium class (SEQ) while the original class (like in [1]) the equilibriumfree, or no–equilibrium one (NEQ). Indeed, the systems with and without the equilibrium steady state have rather different statistical properties of the motion [5]. Notice that, from the physical point of view, both classes are Hamiltonian. In our opinion, the simple models of NEQ with a reversible "friction", being formally dissipative, are physically interesting as far as they simulate the real Hamiltonian infinite–dimensional thermostat.

The local fluctuations in the nonequilibrium *steady state* of NEQ can be determined for any segment length τ, and do not depend on the motion time t. Same fluctuations in SEQ for a *transient, finite–time* nonequilibrium relaxation require the additional condition $\tau \ll \tau_R$ to be measured, and they do depend on the motion time. For $t \gg t_R$ the fluctuations as well as other statistical properties become equilibrium ones. In this case the crossover parameter $C(t) \to 0$

together with the average $\langle \Delta S \rangle \to 0$, and hence half of changes ΔS become "abnormal" as it should be in the statistical equilibrium.

Unlike this, the global fluctuations in NEQ do always depend on time t, and parameter $C(t) \to \infty$ due to $\langle S(t) \rangle \to \infty$. In the limit $t \to \infty$ this implies *zero* probability of abnormal $S(t) < S(0)$ (see [5]). Same fluctuations in SEQ are not exactly the same, and have an interesting peculiarity found in [2]: the *finite* asymptotic probability of abnormal fluctuations. Moreover, this asymptotic value is of the order of the probability for a spontaneous fluctuation of the size comparable with the initial nonequilibrium state of the system which would subsequently relax back to the equilibrium, and so forth ad infinitum. This is not a completely new phenomenon but, apparently, less known one (for discussion see [5] and references therein).

In conclusion, let us mention that we would expect the *rise* of big spontaneous fluctuations, implicitly observed in [2], to obey the law called in [2] "Anti–Fluctuation Theorem" but *without* time reversal.

References

[1] D. Evans, E. Cohen and G. Morriss, Phys. Rev. Lett. **71**, 2401 (1993).

[2] D. Evans, D. Searles and E. Mittag, Fluctuation Theorem for Hamiltonian Systems - Le Chatelier's Principle, cond–mat/0008421.

[3] L.D. Landau and E.M. Lifshitz, *Theoretical Physics*, Vol. X, E.M. Lifshitz, L.P. Pitaevsky, *Physical Kinetics*, Moskva, Nauka (1979).

[4] J. Kurchan, A quantum fluctuation theorem, cond–mat/0007360.

[5] B.V. Chirikov, Big entropy fluctuations in noneqiulibrium steady state: A simple model with Gauss heat bath, nlin.CD/0006033, submitted to JETP.