Big Entropy Fluctuations in Statistical Equilibrium: 
The Fluctuation Law

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

Abstract

The structure of very complicated irregular "microscopic" (local) entropy fluctuations around a big separated "macroscopic" (global) fluctuation in the statistical equilibrium was studied in numerical experiments on a simple 2–freedom strongly chaotic Hamiltonian model described by the modified Arnold cat map. A comparison of transient nonequilibrium rise and relaxation process of the big fluctuation out of the statistical equilibrium with a nonequilibrium steady state in a model without statistical equilibrium is considered and discussed with respect to the so-called Fluctuation Law (or "theorem") introduced and intensively studied recently in the latter case. A new transient fluctuation law was found on the basis of a simple semiempirical theory developed. Preliminary results of numerical experiments on some fractal properties of the "microscopic" fluctuations are presented and briefly discussed.

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1 Introduction: fluctuations in dynamical systems with and without statistical equilibrium

In a previous paper [1] we presented numerical and theoretical results of our studies into the peculiar properties of rare big ("macroscopic", or global) fluctuations out of the statistical equilibrium as different from, and even opposite in a sense to, those of small stationary ("microscopic", or local) ones. Particularly, the former are perfectly regular, on the average, symmetric in time with respect to the fluctuation maximum, and described by simple kinetic equations rather than by a sheer probability of irregular "noise". Moreover, such fluctuations are not only perfectly regular by themselves but also surprisingly stable against any perturbation, both regular and chaotic, whatever its size. At first glance, it looks very strange in a chaotic, highly unstable, dynamics. The resolution of this apparent paradox is in that the dynamical instability of motion does affect the fluctuation instant of time only. As to the fluctuation evolution, it is determined by the kinetics whatever its mechanism, from purely dynamical one to a completely noisy, or stochastic (for discussion see [1, 2]).

A fairly simple picture of big fluctuations in the systems with statistical equilibrium was the basis of old Boltzmann’s fluctuation hypothesis for our Universe. As is well understood by now such a hypothesis is completely incompatible with the present structure of the Universe as it would immediately imply the notorious "heat death" (see, e.g., [3]). The principal solution of this problem, unknown to Boltzmann, is quite clear by now, namely, the "equilibriumfree" models are wanted. Various classes of such models are intensively studied today. Moreover, the celebrated cosmic microwave background tells us that our Universe was born already in the state of a heat death which, however, fortunately to us all became unstable due to the well–known Jeans gravitational instability [4]. This resulted in developing of a rich variety of collective processes, or synergetics, the term recently introduced or, better to say, put in use by Haken [5]. The most important peculiarity of such a collective instability is in that the overall relaxation with ever increasing total entropy is accompanied by an also increasing phase space inhomogeneity of the system, particularly in temperature. In other words, the whole system as well as its local parts become more and more nonequilibrium (for general discussion see, e.g., [6, 7, 8]). We stress that all these inhomogeneous nonequilibrium structures are not big fluctuations like in statistical equilibrium but rather the result of a regular collective instability, so that they are immediately formed under a certain condition. Besides, they are typically dissipative structures in Prigogine's term [9] due to exchange of energy and entropy with the infinite environment. The latter is the most important feature of such processes, and at the same time the main difficulty in studying the dynamics of those models both theoretically and in numerical experiments which are so much simpler for the systems with statistical equilibrium.
In spite of the essential restrictions, the simple models with statistical equilibrium allow us to better understand the mechanism and role of fluctuations in the statistical physics. Particularly, a vague problem of the initial conditions, still the apparently confusing (to many) “freedom”, can be removed in such models. Following our previous paper [1] we take a different approach to the problem: instead discussing the ”true” initial conditions and/or a ”necessary” restriction of those we start our numerical experiments at arbitrary initial conditions (most likely corresponding to the statistical equilibrium), and do observe what the dynamics and statistics of fluctuations is like. Notice, however, that such an approach can be directly applied to the fluctuations in finite systems with statistical equilibrium only (for discussion see [6, 2]). In such, and only such, systems infinitely many big fluctuations grow up spontaneously independent of the initial conditions of the motion. This is similar to the well–known Poincaré recurrences (for discussion see [1]).

Recently, a new class of dynamical models has been developed by Evans, Hoover, Morriss, Nosé, and others (see, e.g., [10]). Some researchers still hope that such brand–new models will help to resolve the ”paradox of irreversibility”. A more serious reason for studying these models is in that they allow for a fairly simple inclusion in a few–freedom model the infinitely dimensional ”thermostat”, or ”heat bath”. This greatly facilitates both numerical experiments as well as the theoretical analysis. The price is the strict restriction of such models to the nonequilibrium steady states only. Moreover, any collective processes of interacting particles are also excluded, just those responsible for the very existence of the nonequilibrium steady states. In a more complicated Nosé - Hoover version of those models these severe restrictions can be partly, but not completely, lifted. Whether it would be sufficient for the inclusion of collective processes remains, to our knowledge, an open question.

On the other hand, a nonequilibrium steady state studied in the new models is but a little, characteristic though, piece of the chaotic collective processes. In [2] it was conjectured that the regularities in the fluctuations found in a nonequilibrium steady state can be applied, at least qualitatively, to a small part of a big fluctuation in a statistical equilibrium on both sides of the maximum. This conjecture was one of the motivations for the present studies. The result turned out to be more interesting than expected (Section 5). The conjecture was partly confirmed, indeed, but a new surprising peculiarity of fluctuations was found which appears to be even more generic, and which has been accidentally missed in [2].

2 The model

In the present studies we make use of the same model as in [1]. For reader’s convenience we briefly repeat its description. It is specified by the Arnold cat map
(see [11, 12]):

\[
\begin{align*}
p & = p + x \mod 1 \\
x & = x + p \mod 1
\end{align*}
\]  

which is a linear canonical map on a unit torus. It has no parameters, and is chaotic and even ergodic. The rate of the local exponential instability, the Lyapunov exponent \( \lambda = \ln \left( \frac{3}{2} + \sqrt{5}/2 \right) = 0.96 \), implies a fast correlation decay (relaxation) with characteristic time \( t_r \sim 1/\lambda \approx 1 \). Throughout the paper \( t \) denotes the time in map's iterations.

As in [1] we use a minor modification of this map:

\[
\begin{align*}
p & = p + x - 1/2 \mod C \\
x & = x + p - C/2 \mod 1
\end{align*}
\]  

where \( C \gg 1 \) is a circumference of the phase space torus. This allows us to study big fluctuations with diffusive rise/relaxation kinetics in \( p \) and characteristic time \( t_p \sim C^2/12D_p \gg 1 \) where \( D_p = 1/12 \) is the diffusion rate. The relaxation time in \( x \) does not depend on \( C \) and remains short \((t_r \sim 1)\) so that subsequent values of \( x \) are nearly uncorrelated. This allows to restrict the statistical properties of the motion to the action \( p \) only. For example, the distribution function becomes

\[
f(x, p) \rightarrow f(p) = \int_0^1 f(x, p) \, dx
\]

The size of a big fluctuation in \( p \) is characterized by the standard deviation \( \sigma(t) \) for a group of \( N \) trajectories (or noninteracting particles).

Below, as in [1], we shall consider a particular case of big fluctuations, namely one with the prescribed position in the phase space:

\[
x_{fl} = x_0 = \frac{1}{2}, \quad p_{fl} = p_0 = \frac{C}{2}
\]

at the (unstable) fixed point \( x_0 = 1/2 \), \( p_0 = C/2 \) of map (2.2). Then, the variance \( v \) of the size in \( p \) is determined by the relation

\[
v = \sigma^2 = \langle p^2 \rangle - p_0^2
\]

where brackets \( \langle ... \rangle \) denote the averaging over \( N \) trajectories. In ergodic motion at equilibrium \( v = v_E = C^2/12 \). In what follows we will use the dimensionless measure \( \tilde{v} = v/v_E \rightarrow v \), and omit tilde.

The variable \( v(t) \) is especially convenient in diffusive approximation of the kinetic equation as it is varying in proportion to time. Yet, its relation to the fundamental conception of entropy is also important. The standard definition of the entropy, which can be traced back to Boltzmann, reads in our case:

\[
S(t) = -\langle \ln f(p) \rangle + S_0 \approx \frac{1}{2} \ln v(t)
\]
where \( f(p) \) is a coarse–grained distribution function, \( S_0 \) stands for an arbitrary constant, and the latter relation is a very simple and convenient approximation found in \([1]\) under the condition that the distribution \( f(p) \) is the standard Gauss law (see Section 3 below):

\[
f(p) = \frac{\exp\left(-\frac{(p-p_0)^2}{2\sigma^2}\right)}{\sqrt{2\pi\sigma^2}}
\]

and the constant \( S_0 \) is set to:

\[
S_0 = -\frac{1}{2} \ln (2\pi e) \approx -1.4189 \approx -\sqrt{2}
\]

Approximation in (2.6) holds on the most part of the big fluctuation except a relatively small domain near the equilibrium where the distribution in \( p \) approaches the homogeneous one. The exact entropy (with constant (2.8)) in equilibrium is

\[
S_E = -\frac{1}{2} \ln \left(\frac{\pi e}{6}\right) \approx -0.18
\]

instead of zero in approximation (2.6). The difference is relatively small, the smaller the bigger is the fluctuation. In the main part of big fluctuation our simple relation for the entropy reproduces the exact one to a surprising accuracy (see Fig.4 in \([1]\)).

Notice that the distribution calculated from any finite number of trajectories is always a coarse–grained one. However, the direct application of the exact relation in Eq.(2.6) requires too many trajectories, especially for the fluctuation of a small size. A great advantage of our aproximation is in that the computation of \( S \) does not require very many trajectories as does the distribution function. In fact, even a single trajectory is sufficient as Fig.1 in \([1]\) demonstrates!

A finite number of trajectories used for calculating the variance \( \sigma^2 \) is a sort of the coarse–grained distribution, as required in relation (2.6), but with a free bin size which can be arbitrarily small.

Now we can turn to the main subject of this paper, the so–called fluctuation law (or Fluctuation "theorem"). We begin with the fundamental statistical property of the dynamical model, the distribution function in \( p \).

3 The fluctuation law: \( p \)–distribution

The "Fluctuation Theorem" has been first obtained by Evans, Cohen and Morriss \([13]\) 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:

\[
\ln \left( \frac{f(\Delta S)}{f(-\Delta S)} \right) = \eta \cdot \Delta S, \quad \eta = \frac{2\langle \Delta S \rangle}{\sigma^2}
\]
Here \( f(\Delta S) \) is the probability of entropy (or entropy–like quantity as in [13]) change \( \Delta S \) in the ensemble of trajectory segments of a fixed (appropriately scaled) duration \( t_s \) for the mean change \( \langle \Delta S \rangle > 0 \) and variance \( \sigma^2 \), and the fluctuation parameter \( \eta = 1 \) usually taken to be unity.

By itself, the relation (3.1) is but a specific reduced representation of the normal probabilistic law, the Gaussian distribution, in a suitable random variable \( \Delta S \):

\[
f(\Delta S) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left( -\frac{(\Delta S - \langle \Delta S \rangle)^2}{2\sigma^2} \right)
\]

(3.2)

shifted with respect to \( \Delta S = 0 \) due to the permanent entropy production at a constant rate in the nonequilibrium steady state. The fluctuation law (3.1) immediately follows from the normal law (3.2) but not vice versa. However, the surprise (to many) was in that the probability of negative ("abnormal" or "wrong") entropy change \( \Delta S < 0 \) (without time reversal!) is generally not small at all reaching 50% for sufficiently short \( t_s \). That is every second change may be "wrong"!

Implicitly, all that is contained in the well developed statistical theory (see, e.g., [14], Section 20, and [15]). Nevertheless, the first direct observation of this phenomenon in a nonequilibrium steady state [13] 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 [2].

In our opinion, the main lesson one should learn from the Fluctuation law 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 characteristic 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 the nonequilibrium steady state the macroscopic scale is represented by a finite rate \( \langle \Delta S \rangle > 0 \), yet the "microscopic" scale of the fluctuations can 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 "wrong" entropy changes \( \Delta S < 0 \)

\[
P_{wr}(F) = \int_{-\infty}^{0} f(s, F) \, ds
\]

(3.3)

Here \( F = \langle \Delta S \rangle / \sigma \) is a new parameter for the "right/wrong" crossover in the entropy variation sign at \( |F| = F_{cro} \sim 1 \) when the probability \( P_{wr} \) is large.

If a finite–dimensional Hamiltonian system admits the (stable) statistical equilibrium as in our model (2.2) here the overall \( (t \to \infty) \) average entropy rate \( \langle \Delta S \rangle = 0 \)
for any \( t_s \). However, on a finite time scale \( t_p \sim C^2 \) (see Section 2) 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 fluctuations were conjectured \( \mathcal{A} \) to obey the law similar to the nonequilibrium one provided \( t_s \ll t_p \).

The entropy–like quantity in our problem is variance \( v \), Eq.(2.5), which monotonically depends on the entropy (2.6). The time dependence \( v(t) \) in a big fluctuation was computed as follows (for details see \( \mathcal{A} \)). The data were obtained from simultaneous running of \( N \) trajectories for very long time in order to collect sufficiently many fluctuations for the reliable separation of the regular part of the fluctuation, or the kinetic subdynamics in Balescu’s term (see \( \mathcal{A} \) and references therein), from the stationary fluctuations, the main subject of the present studies (see below). The separation was done by the plain averaging of individual \( v_i(t) \) values \( (i = 1, \ldots, n) \) over all \( n \) fluctuations collected in a run. The size of the fluctuations was fixed by the condition that current

\[
\langle v(t) \rangle < v_b \tag{3.4}
\]

at some time instant \( t \approx t_i \), the moment of a fluctuation. This condition determines, in fact, the border of the whole fluctuation domain: \( 0 < v < v_b \). The event of entering this domain is the macroscopic ”cause” of the fluctuation whose obvious ”effect” will be subsequent relaxation to the equilibrium. However, and this is the main point of our philosophy, the second ”effect” of the same ”cause” was preceding rise of the fluctuation in apparent contradiction with the ”causality principle” (for discussion see \( \mathcal{A} \)). In any event, the second effect requires the permanent memory of trajectories within some time window \( w \). Typically, \( w \gtrsim C^2 \), the total diffusion time, was chosen (see Section 2). After fixing the current \( t_i \) value the computation within the same window \( w \) had been continued, and only then the search for the next fluctuation was resumed.

Two examples of big global fluctuations are shown in Fig.1. They differ by the number of separate fluctuations in each run for averaging. While for a larger \( n = 1137 \) the dependence \( \langle v(\tau) \rangle \) looks rather smooth, in the second run, with \( n = 32 \) only, the stationary local fluctuations around the averaged global one are clearly seen.

The average anti–diffusive/diffusive kinetics from/to the statistical equilibrium (horizontal straight line) is shown by the two wiggly curves. A smooth solid line is semiempirical relation (3.13) to be discussed below together with the expected kinetics near the maximum, Eq.(3.14), (two oblique straight lines). The mean variance \( \langle v(t - t_i) \rangle \) is doubly averaged in both the number of trajectories \( N \) (see Eq.(2.5)) and that of recurrent fluctuations \( n \).

In this Section we consider the statistics of the original dynamical variable, the dimensionless action \( \tilde{p} = 2\sqrt{3}p/C \rightarrow p \) (see Section 2), with respect to the fixed fluctuation position \( p_0 = \sqrt{3} \), or of the quantity \( u = p - p_0 \). Its two first moments,
in the limit $N \cdot n \to \infty$, are
$$\langle u(\tau) \rangle = 0, \quad \langle u^2(\tau) \rangle = \langle v(\tau) \rangle$$

Neglecting all dynamical correlations (see Section 2) would imply the standard Gaussian distribution
$$G(u) = \frac{\exp(-u^2/2v(\tau))}{\sqrt{2\pi v(\tau)}} = \frac{\exp(-g^2/2)}{\sqrt{2\pi}}$$

(cf. Eq.(2.7)) provided a free (unbounded) anti–diffusion/diffusion. Moreover, in a new, Gaussian, variable $g = u/\sqrt{v}$ the distribution would not depend on time either. This allows for a considerable increasing of the statistics in computation of the actual distribution $f(u)$ by summing up the data in a certain interval of $\langle v(\tau) \rangle$ shown in Fig.1.

The result is presented in Fig.2 in the form of the ratio $f(u)/G(u)$ as a function of the Gaussian variable $g^2 = u^2/v$. Within a moderate $g^2 \lesssim 5$ the ratio is close to unity as expected for a free $x$–uncorrelated diffusion. However, for larger deviations the ratio is progressively decreasing while the shape of distribution $f(u)$ remains Gaussian within this region. Qualitatively, it is similar to the distortion observed in a nonequilibrium steady state (see [2], Figs.2 and 3) but of the opposite sign. Moreover, the crossover between the two regions
$$g^2_{\text{cro}} \approx 4.5$$
is nearly the same in both processes, and also for the both examples in Fig.2 here. In [2] it was conjectured that the origin of such a distortion might be some peculiar effect of dynamical correlations in $x$ which are small but nonzero (Section 2). Yet, this still remains an open question.

In addition, the second crossover does appear which is not as ”universal” as the first one but also demonstrates the local Gaussian shape of the empirical distributions that is a straight line in the semi–log scale. The first crossover does not depend on the averaging domain but the slope of the distribution above the crossover (in the second region) does so. To the contrary, the second crossover depends on the averaging conditions but the slope in the third region does not. Apparently, the third region represents the effect of the boundary condition on the long tails of the distribution. All these interesting peculiarities of a very specific ”triple” Gaussian distribution require further studies.

In the first region $g^2 \lesssim 5$, which comprises approximately 97% of the total probability, the distribution is reasonably close to the Gaussian one, and this explains a surprising accuracy of simple relation (2.6) for the entropy (see [2], Fig.6).

Near the equilibrium the distribution can be calculated from a simple diffusion equation:
$$\frac{\partial f(\tau, u)}{\partial t} = \frac{D}{2} \cdot \frac{\partial^2 f(\tau, u)}{\partial u^2}$$

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Near the equilibrium the distribution can be calculated from a simple diffusion equation:
where $D = 1/C^2$ is the diffusion rate. For periodic boundary conditions $f(\tau, u + 2\sqrt{3}) = f(\tau, u)$, used in numerical experiments with model (2.2), and for the fluctuation symmetry with respect to $u = 0$ (see (3.4)) the eigenfunctions and eigenvalues of Eq.(3.8) are respectively:

$$\phi_m = \cos \left( \frac{\pi m u \sqrt{3}}{\sqrt{3}} \right), \quad \gamma_m = \frac{D}{2} \cdot \frac{\pi^2 m^2}{3} = \frac{\pi^2 m^2}{6 C^2} \quad (3.9)$$

where $m = 0, 1, \ldots$ is any integer.

In the first approximation, we can assume the initial distribution $f(0, u) = \delta(u)$ to be a $\delta$–function. Then, the solution of diffusion equation (3.8) on both sides of the fluctuation maximum at $\tau = 0$ is represented by a series:

$$f(|\tau|, u) = \frac{1}{2\sqrt{3}} + \frac{1}{\sqrt{3}} \sum_{m=1}^{\infty} e^{-\gamma_m |\tau|} \cos \left( \frac{\pi m u \sqrt{3}}{\sqrt{3}} \right) \quad (3.10)$$

Here the first term describes the ergodic equilibrium, and the others do so for the rising/decay of a big fluctuation, on the average.

Moreover, we could further approximate the initial $\delta$–function by a Gaussian distribution

$$\delta(u) \approx \frac{\exp \left( -\frac{u^2}{2v_b} \right)}{\sqrt{2\pi v_b}} \quad (3.11)$$

where $v_b \ll 1$ is the size of the fluctuation domain (3.4). Then, one would expect the Gaussian distribution to persist up to $|\tau| \sim 1/\gamma_1 \sim C^2$ when lower modes of the solution (3.10) come into play. In fact, according to our numerical experiments the Gaussian distribution is considerably distorted also for small $|\tau| \lesssim 50$. Apparently, this distortion is caused by the selection condition (3.4) which cut out large distribution fluctuations.

Near the equilibrium the solution provides a simple relation for the main quantity in the problem, the variance

$$v(|\tau|) = \langle u^2 \rangle \approx 1 - \frac{12}{\pi^2} \cdot \exp \left( -\frac{\pi^2 |\tau|}{6 C^2} \right) \quad (3.12)$$

which is close to a semiempirical relation in Fig.1:

$$v_f(|\tau|) \approx 1 - \exp \left( -\frac{|\tau|}{0.65 C^2} \right) \quad (3.13)$$

Particularly, the most important factor in the exponential (3.12) $6/\pi^2 = 0.608$ is only 6% less than the empirical one 0.65 in (3.13). On the other hand, both expressions, Eqs.(3.12) and (3.13), are also close to a simple relation $v(|\tau|) \approx |\tau|/C^2$, directly derived from the diffusion rate $D = 1/C^2$, upon a small correction

$$v_f(|\tau|) \approx |\tau|/C^2 + 0.05, \quad |\tau| \lesssim w/2 \quad (3.14)$$
introduced in [1] to describe the effect of a finite fluctuation size at $\tau = 0$ determined by the selection condition (3.4).

In conclusion of this Section we stress again that in spite of considerable deviations on the tails the distribution $f(u)$ remains close to the normal (Gauss) law in its main part comprising 97% of the total probability. This will be essential in the next Section.

Now we can turn to the main problem of the present studies, the fluctuations of our entropy–like quantity, the variance $v(\tau)$.

4 The fluctuation law: 
"Wrong" macroscopic entropy variations of both signs

The so–called "Fluctuation Law", recently introduced in the studies of the nonequilibrium steady state, was discussed at the beginning of previous Section. In our problem it can be related to an entropy–like quantity, the variance $v(\mid \tau \mid)$. So, first of all, we consider here the statistics of this variable.

4.1 $\chi^2$–distribution

Under condition of the normal distribution in $u$, which is a good approximation (see previous Section), the statistical properties of the sum of $u^2$ values are described by the so–called $\chi^2$–distribution (see, e.g., [17]):

$$\chi(s) = \frac{s^m e^{-s}}{\Gamma(m+1)} \to \chi(m) \cdot \exp \left[ -(s - m)^2 / 2m \right]$$

(4.1)

where random quantity

$$s = \frac{1}{2} \sum_{i=1}^{k} u_i^2 = \frac{k \tilde{v}}{2}$$

(4.2)

$\Gamma(x)$ is the gamma–function, $m = k/2 - 1$, and variance $\tilde{v} = v / \langle v(\mid \tau \mid) \rangle \to v$ is the random variable now normalized to its mean according to the Gaussian distribution in $p$ (Section 3). Again, we omit tilde in what follows (cf. Section 2). The first expression in (4.1) is the exact distribution with three main characteristics:

$$s_{max} = m, \quad \langle s \rangle = m + 1, \quad v_s = \langle s^2 \rangle - \langle s \rangle^2 = \frac{2}{k} \langle s \rangle^2 = \frac{k}{2}$$

(4.3)

the maximum of probability density, mean $s$, and its variance. One should not confuse the latter, which is a characteristic of the random variable $s$, with another
variance $\tilde{v} \rightarrow v$ described above. The latter expression in (4.1) is a Gaussian approximation to the former for large number $k \gg 1$ of terms in sum (4.2). Notice the shift $\langle s \rangle - s_{\text{max}} = 1 \ll k$. The approximation was chosen in such a way to provide the best Gaussian description for the distribution cap that is most important in our studies below. To this end, both the position and height of the top as well as the second derivative over there were fixed to be exactly equal in the two distributions. Interestingly, the two normalizing factors, in Eq.(4.1) and the standard Gaussian one, are very close

$$\chi(m) \cdot \sqrt{2\pi m} = 1 - \frac{1}{12m} + ... \quad (4.4)$$

even for small $m$.

In Fig.3 a comparison of the two distributions for $k = 10$ is shown. The very cap looks perfect but the progressive deviation below is primarily due to asymmetry of the $\chi^2$-distribution. In what follows we restrict ourselves to this optimized Gaussian approximation.

Now, we need to transform the distribution to the main dynamical (and chaotic) variable in our problem, the random variance $v = 2s/k$, Eq.(4.2). We obtain:

$$\chi(v) \approx \exp \left[ -\frac{(v - v_0)^2}{2\sigma_v^2} \right] \frac{1}{\sqrt{2\pi\sigma_v^2}} \quad (4.5)$$

where

$$v_0 = \frac{m}{m+1} = 1 - \frac{2}{k}, \quad \sigma_v^2 = \frac{m}{(m+1)^2} \approx \frac{2}{k} \quad (4.6)$$

the distribution maximum, and $v$ variance, respectively. Again, notice a small shift $v_0 - \langle v \rangle = -2/k \approx -\sigma_v^2$.

As was explained in Section 3 the variance $v(\tau)$ was computed in numerical experiments by the two averagings. First, in each realization of the big fluctuation the current averaging is done over a group of $N \lesssim 10$ trajectories. On this stage $k = N$ should be substituted in Eq.(4.6). Since technically it is very difficult to increase $N$ the accuracy of our approximation (4.5) is generally rather poor (see Fig.3). Moreover, this trouble goes over to the second averaging of $n$ successive realizations of the big fluctuation, no matter how large is the number $n$. As different realizations are statistically independent, formally the parameter $k = N \cdot n$ increases by $n$ times but the problem is in actual deviation of the approximation (4.5) from the true unknown distribution except, hopefully, the distribution cap. In any event, all we can do at the moment is applying Eq.(4.5) with the latter value of $k = Nn$.

### 4.2 The probability of ”wrong” entropy variation

In the nonequilibrium steady state the entropy is always increasing on the average, and the ”wrong” variation means sporadic decreases of the entropy on some finite
time intervals (see, e.g., and references therein). In our problem of a big finite fluctuation out of statistical equilibrium the situation is more interesting. Namely, the entropy is both decreasing and increasing, on the average, during the corresponding anti–diffusion and diffusion stage of the fluctuation, and respectively the ”wrong” entropy variation is both its temporary increase or decrease.

Here we present some preliminary results of numerical experiments on the local fluctuations around the big (global) fluctuation as explained in Section 3.

The computation procedure of obtaining the data for the fluctuation law was as follows. The whole time window $2w$ was subdivided in a number of segments of length $t_s$ (iterations), and a change $\Delta v(\tau)$ of the doubly average variance (our entropy–like quantity) on each one was calculated. To suppress still large local fluctuations a new double averaging was applied. The first one was defined as

$$\overline{\Delta v(\tau_j)} = \frac{1}{t_s} \sum_{\tau=\tau_j}^{\tau_j+t_s} \Delta v(\tau)$$

(4.7)

Since successive $\Delta v(\tau)$ are not independent this averaging turned out to be insufficient. The second one was done over $L$ successive segments:

$$\overline{\Delta v(\tau_i)} = \frac{1}{L} \sum_{j=1}^{L} \Delta v(\tau_j)$$

(4.8)

with the final result ascribed to $\tau_i = \tau_j + t_sL/2$, the center of the full averaging interval.

Of two different formulation of the fluctuation law, Eqs.(3.2) and (3.3), we have chosen the latter one for the integral probability as more reliable because of much less fluctuations. For calculation of probability $P_{wr}$ of ”wrong” $\Delta v(\tau)$ the number of segments satisfying the condition

$$\tau \cdot \Delta v(\tau) < 0$$

(4.9)

was counted.

An example of time dependence for such a probability is presented in Fig.4 for segment length $t_s = 30$ and averaging moving window size $L = 30$ using the data in Fig.1 with $n = 32$ and $N = 4$. The empirical results are shown by points the number of which is $2w/t_s \approx 650$. For large $|\tau| \gtrsim 2000$ the probability $P_{wr} \approx 0.5$ oscillates around 50% as expected in the equilibrium. However, near the fluctuation maximum the probability of ”wrong” entropy changes rapidly drops almost down to zero. This is a result of the average (macroscopic) entropy destruction/production in course of anti–diffusion/diffusion.

The upper solid curve in Fig.4 represents a simple theory described above (with $b = 1$, see Eq.(4.10)). It is based on Eq.(3.3) with the distribution $f(s) \approx \chi(v)$.
in the Gaussian approximation (4.5). Then, the fluctuation parameter in Eq.(3.3) becomes:

\[ F(\tau) = \frac{|\langle \Delta v_f \rangle|}{\sigma_f} \approx \frac{t_s(1 - v_f(\tau))/aC^2}{v_f(\tau)\sqrt{2\sigma_v^2/b}} \] (4.10)

Here the average change and the variance \( \sigma_f^2 \) are expressed via the semiempirical function \( v_f(\tau) \) with parameter \( a = 0.65 \), Eq.(3.13), and parameter \( \sigma_v^2 \) with \( k = nN \) in Eq.(4.5) as follows:

\[ \langle \Delta S \rangle \rightarrow |\langle \Delta v_f \rangle| \approx t_s dv_f(\tau) d\tau \approx t_s(1 - v_f(\tau)) \frac{1}{aC^2} \frac{\sigma_v^2}{b} v_f^2 = 4v_f^2 \frac{nN}{b} \] (4.11)

In the latter relation the factor 2 is introduced assuming statistically independent fluctuations on both ends of the segment \( t_s \). The calculation of theoretical probability \( P_{\text{wr}} \) was performed by the same double averaging, Eqs.(4.8), of the integral (3.3) with parameter (4.10) as for the empirical data.

The exact function (3.3) is unknown, as was explained above, but under assumption of Gaussian \( v \) fluctuations it becomes the standard error integral which can be explicitly calculated. Moreover, we managed to find a very simple and surprisingly accurate approximation for the error integral which in a particular case of Eq.(3.3) takes the form:

\[ P_{\text{wr}}(F) \approx \exp \left( -\frac{F^2}{2} \right) \frac{2}{2(F + 1)} \] (4.12)

A comparison with the exact integral is shown in Fig.5. The relative accuracy \( |\Delta P/P| < 0.05 \) is better than 5% in a huge range of \( P \gtrsim 10^{-4} \) larger than 5 orders of magnitude! Asymptotically, as \( F \rightarrow \infty \) the error \( |\Delta P/P| \rightarrow \sqrt{\pi/2} - 1 \approx 0.25 \) increases but still remains surprisingly small.

Coming back to the comparison of theory (4.12) with the empirical data in Fig.4 we see that the agreement is rather poor. Qualitatively, the theory describes the phenomenon but considerably overestimates the probability of the "wrong" entropy changes. This is why we have had to introduce an empirical factor \( b \) into our simple theory (4.10). To achieve the agreement with the empirical data we have to take the value of this factor as large as \( b = 30 \) (the lower solid curve in Fig.4). It hardly could be explained by a distortion of the Gaussian distribution we neglected. To understand the origin of such a discrepancy we have undertaken a study of various statistical properties of the \( v \) fluctuations.

### 4.3 Various \( v \)-statistics

We begin with the so-called current fluctuations that is the fluctuations at a fixed \( \tau \). These fluctuations are approximately described by the optimized Gaussian distribution (4.5) in dimensionless variable \( v/\langle v(\tau) \rangle \approx v/v_f(\tau) \) where \( v_f \) is given by
the approximate relation (3.13). The first two moments of the distribution were computed, namely the expected mean shift specific for the optimized Gaussian distribution
\[
\langle v - 1 \rangle \approx \sigma_v^2 \pm \sigma_v
\]
and the variance
\[
\langle \sigma_v^2 \rangle \approx \frac{2}{k} = \frac{2}{nN}
\]
which also determines the standard deviation for the shift in Eq.(4.13). The empirical specific shift turned out to be, indeed, very close to theoretical one, the ratio of both being 1.05. However, the corresponding ratio 0.36 for the variance itself indicates a considerable disagreement with the theory. To further elucidate this point we have computed the time dependence for both characteristics using our standard procedure of the double averaging (Section 4.2). The results presented in Fig.6 clearly demonstrate a regular increase of both the shift and variance at small \(|\tau|\), just in the region which is most important in our studies (see Fig.4). Partly, it is explained by a poor approximation (3.13) we use. To cope with this difficulty we have even omitted the region \(|\tau| < 200\) in averaging but this did not help in full.

In any event, the observed threefold decrease of the current variance cannot explain the thirtyfold (!) decrease required to agree the theory with the empirical data in Fig.4. So, we turned to investigation of the main parameter of the theory \(F(\tau)\), Eq.(4.10). To this end, we have computed different segment fluctuations in comparison with the theoretical prediction. Specifically, we calculated three average ratios (see Eqs.(4.7) and (4.8)):

\[
\left[ \frac{\Delta v}{\Delta v_f} \right]_R = \frac{1}{L} \sum \frac{\Delta v}{\Delta v_f}
\]
for the average change \(\Delta v\) per segment,

\[
\left[ \frac{\langle (\Delta v)^2 \rangle}{\sigma_f^2} \right]_R = \frac{1}{L} \sum \frac{\sigma^2}{\sigma_f^2}
\]
for the variance of \(\Delta v\) per segment, and

\[
\left[ \frac{F^2}{(\Delta v_f)^2} \right]_R = \frac{1}{L} \sum \left( \frac{\Delta v}{\sigma^2} \right)^2 \cdot \frac{\sigma_f^2}{(\Delta v_f)^2}
\]
for the ratio of the former that is for the fluctuation parameter squared. The theoretical quantities with sub \(f\) were taken from Eq.(4.11) and applied to the second averaging only.

The results are presented in Fig.7 for three values of the segment length \(t_s = 20, 30, 40\). The first ratio (4.15a) for the mean \(\Delta v\) is shown by the middle solid
curves, and it seems in a reasonable agreement with the theory. On the contrary, the variance (4.15b) (lower dashed curves) is about two orders of magnitude less than expected except the central region of small |τ| where it is much larger and strongly depends on ts. Particularly, for ts = 30 the variance is close to the theoretical one in disagreement with the upper theoretical curve in Fig.4. The difference between the two series of data is in the averaging procedure. In Fig.7 it was a separate averaging of the variance only while in Fig.4 the averaging included the ratio of the mean change squared to the variance of ∆v. The latter is characterised by the third ratio (4.15c) shown in Fig.7 by the upper solid curves. This data do better describe the fluctuation parameter F(τ). Yet, the empirical parameter b ∼ 100 is now at least three times as big compared with b = 30 in Fig.4. Apparently, the remaining discrepancy is explained by still more complicated averaging of the probability Pwr(F) as well as other approximations in the theory.

In spite of all these difficulties the theory developed provides a consistent picture of the segment fluctuations including their most intriguing part of the “wrong” entropy changes. Moreover, an approximate scaling of the empirical data can be inferred from Eq.(4.10) with respect to the dimensionless variable τ/ts. At least, this is possible in the range ts = 20 − 40 where the curves in all three groups in Fig.7 are close (besides small |τ| for the second ratio which is unimportant for the final conclusion).

The scaling is based on a simple approximation \( v_f(τ) \approx |τ|/C^2 \) (see Eq.(3.14)) which holds for \( v < 0.5 \), or \( |τ| < C^2/2 \). Then, Eqs.(4.10) and (4.11) imply

\[
F(τ) \approx \frac{t_s/C^2}{(|τ|/C^2) \cdot \sqrt{4/nNb}} = \frac{t_s}{|τ|} \cdot \sqrt{\frac{nNb}{4}}
\]  

(4.16)

This scaling is shown in Fig.8 for the interval ts = 10 − 40, and b = 30 (cf. Fig.4). In spite of some divergence of the theoretical curves for large \( |τ|/t_s \sim C^2/2t_s \) the scaling describes the probability Pwr(τ/ts) fairly well within the fluctuations, except perhaps the case for ts = 10.

5 Conclusion: A new conjecture

In the present paper we report the preliminary results of our investigation into the local (segment) fluctuations in the transient steady state supported by a big regular fluctuation out of the statistical equilibrium (see Fig.1). One of the motivations for these studies was a conjecture \[2\] that the fluctuation properties, particularly the fluctuation law, formulated and intensively investigated in the nonequilibrium steady state, are similar to those in the transient steady state of a dynamical system with statistical equilibrium. Our original goal was either to confirm or to disprove this
conjecture. A preliminary answer to this question, we have reached so far, turns out to be more interesting than just the plain yes or no.

In the nonequilibrium steady state the entropy is always increasing on the average, and the "wrong" variation means sporadic decreases of the entropy on some finite time intervals (see, e.g., [10, 2] and references therein). In our problem the entropy is not only increasing, on the average, during the corresponding diffusion stage of a big fluctuation but also decreasing on the previous stage of anti–diffusion, so that the notions "right" and "wrong" exchange upon crossing the fluctuation maximum.

We did observe, indeed, such a generalized fluctuation law (in our formulation (3.3), see Figs.4 and 8). Moreover, we have developed a simple theory, Eqs.(4.12) and (4.10), which qualitatively describes this law. However, to reach a quantitative agreement with the empirical data we had to introduce into the theory a surprisingly big fitting parameter $b = 30$ instead of expected $b = 1$.

Investigation into this difficulty revealed that the problem is in unexpectedly small variance of the segment fluctuations of the entropy–like change $\Delta v$ (see Fig.7). Thus, the main physical question to be answered is the origin and mechanism of such a strong suppression of the segment fluctuations.

A possible answer to this question, suggested by a careful inspection of the fluctuation structure in Fig.1, is the following. Indeed, the wiggly curve in this figure demonstrates some very complicated fractal structure of the local fluctuations. For the problem in question, the most important feature of this structure is a large variety of its time scales up to that of the underlying big fluctuation itself. This is especially clear from the picture of the maximal local fluctuations presented in Fig.9 for two separated realizations of a big fluctuation. Here, without averaging over many realizations, it is even difficult to discern the local fluctuations from global ones, particularly by their shape. Notice that both can be not only negative with respect to the equilibrium but also positive, up to $v(\tau) = 3$ (see Section 2). In the latter extreme case all the trajectories are concentrated near $p = 0 \ mod \ 1$ that is the position of such fluctuations differs from one for $\langle v(\tau) \rangle \ll 1$ studied in this paper. This would require redifinition of the variance $v (2.5)$, and of approximate relation (2.6) for the entropy. In any case, the entropy of a big fluctuation does first decrease, and only then grows back to the equilibrium, contrary to an immediate impression from Fig.9.

Essentially, the mechanism of large–scale local fluctuations is the same as (or, at least, very similar to) that for the big fluctuations that is in both cases it is the anti–diffusion/diffusion with roughly the same rate. This would imply the strong correlations between the values of $v(\tau)$ for different $\tau$ in spite of statistically independent realizations of $v(\tau)$ for any fixed $\tau$. Apparently, these very correlations is the ultimate origin of considerable suppression of the segment fluctuations.
An example of this correlation is presented in Fig. 10. It describes the difference

\[ v_c = v(\tau) - \langle v(\tau) \rangle \approx v(\tau) - v_f(\tau) \]  \hspace{1cm} (5.1)

where \( v_f \) is approximation (3.13). Since the latter is rather poor for small \( \tau \) the calculation of correlation was performed starting at \( \tau_0 = 300 \) in a window \( T = 2^{13} = 8192 \) which is the period of \( v_c(\tau) \) for subsequent Fourier transforms. The correlation obtained in such a way is well described by a simple empirical relation

\[ K(t) \approx K_f(t) = A \cdot \exp(-t/t_K) + R \]  \hspace{1cm} (5.2)

where \( t = |\tau - \tau'| \), \( A = 0.9 \), \( R = 0.1 \), and the characteristic time of approximately exponential decay \( t_K = 250 \).

Within the range of the segment length \( t_s \leq 40 \) in Fig. 8 the correlation decay is less than 20\%, and this explains the observed approximate scaling. However, the origin of a long residual correlation \( R \), comprising both the free diffusion as well as the equilibrium (cf. Fig. 1), remains unclear.

Certainly, a more complete mathematical analysis and physical interpretation are still to be done.

Another interesting question is why the local fluctuations in a nonequilibrium steady state do not show any suppression (see, e.g., Fig. 2 in [2]). By eye, the time dependence of the entropy there (Fig. 4 in [3]) looks like a fractal one similar to that in Fig. 1 above. What is the difference?

We conjecture that the main origin of an essentially different fractal structure in [2] is in a “minor” modification of the dynamical model there. Namely, like in the present paper and in previous publication [1] the model included parameter \( C \) but just for the main study of the nonequilibrium steady state it was set to one (\( C = 1 \)) without paying much attention to this particular case. As a result, the relaxation of local fluctuations in \( p \) became ballistic (fast) as in \( x \), and hence the correlations were suppressed which ensured the standard Gaussian statistics of the fluctuations.

For the problem under consideration here this choice would be very difficult in case of the diffusive kinetics of the global (big) fluctuations. But then, with \( C \gg 1 \), the local fluctuations become also diffusive (see Figs. 1 and 9), hence strong correlations and suppression of the latter resulting, particularly, in a considerable decrease of the probability of “wrong” entropy variation.

We conjecture that for large parameter \( C \gg 1 \) in the model for nonequilibrium steady state the statistics of the local fluctuations, particularly the fluctuation law, will be much more interesting for investigation, and more difficult too. Certainly, the whole problem deserves farther studies.
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Figure captions

Fig.1 Two big fluctuations averaged over different numbers of repetitions (reurrences) in each run (see text): wiggly lines show the time dependence of the mean variance $\langle v(t - t_i) \rangle$ around the fluctuation maxima; a smooth solid line is semiempirical relation, Eq.(3.13), for the anti-diffusion/diffusion kinetics of fluctuation; two oblique straight lines represent the expected diffusive kinetics near the maximum, Eq.(3.14), and the horizontal straight line is the equilibrium. Run parameters and results are respectively: $C = 50$, $N = 5/4$, $v_b = 0.0256 / 0.0034$, $n = 1137 / 32$, $w = 10000$. Average period between successive fluctuations $\langle P \rangle \approx 7.7 \times 10^5 / 2.3 \times 10^6$ iterations. Two short dotted lines at the bottom indicate the range of the measurement of $p$-distribution in Fig.2.

Fig.2 A triple "Gaussian" distribution for a big global fluctuation. The ratio of empirical to the standard Gaussian distribution vs. the Gaussian variable $g^2 = u^2/v$ is shown for two averaging domains (see Fig.1): $\tau = 50 - 350$ (wiggly line) and $\tau = 50 - 100$ (dots). Oblique straight lines demonstrate the Gaussian shape in all three regions of the empirical distributions. Run parameters and results are respectively: $C = 50$, $N = 5$, $v_b = 0.0256$, $n = 32598$, $w = 10000$, $\langle P \rangle \approx 7.7 \times 10^5$; averaging bin size $\Delta u = 0.05$.

Fig.3 Comparison of $\chi^2$-distribution (solid line) and its best Gaussian approximation (dotted line), Eq.(4.1): $k = 10$ ($m = 4$).

Fig.4 Probability of "wrong" entropy change in ensemble of trajectory segments for a big fluctuation in Fig.1: $n = 32$, $t_s = L = 30$; points are empirical data; upper solid curve is theory, Eq.(4.12), with empirical parameter in Eq.(4.10) $b = 1$; lower curve is the same for $b = 30$.

Fig.5 Comparison of the exact integral (3.3) for the Gaussian distribution $f(s)$ (solid curve) with approximation (4.12) (circles); dashed line is relative accuracy of the approximation.

Fig.6 Empirical time dependence of the shift, Eq.(4.13) (solid line), and that of the standard deviation (two dashed curves) for the data in Fig.1 with $n = 32$, $t_s = L = 30$. The dashed horizontal straight line is the mean reduced shift $\langle (v/v_f - 1) \rangle nN/2$, and the two dotted lines show the averaged standard deviation. The central part of the time dependence $|\tau| < 200$ is omitted in averaging (see text).

Fig.7 Time dependence of the segment fluctuations for data in Fig.1 with $n = 32$, $L = 30$, and $t_s = 20, 30, 40$. Middle curves show the first reduced mo-
moment, Eq.(4.15a); the lower ones are for the second moment, Eq.(4.15b), and the upper for the fluctuation parameter $F^2$, Eq.(4.15c).

Fig.8 An approximate scaling of the fluctuation law $P_{wr}(\tau/t_s)$ for data in Fig.1 with $n = 32$, $L = 30$, and $t_s = 10, 20, 30, 40$ (symbols). The theory with empirical parameter $b = 30$, Eq.(4.16), is presented by solid lines.

Fig.9 Two different realizations of a big fluctuation are shown by wiggly lines, black and gray with dots. A smooth solid line is semiempirical relation (3.13) for the averaged big fluctuation, and two oblique straight lines represent diffusive kinetics near the maximum, Eq.(3.14).

Fig.10 Correlation of local fluctuations (5.1) within the window $\tau = 300 - 8492$ for data in Fig.1 with $N = 4$, $n = 32$ (thick line), and its approximation by empirical relation (5.2) (thin line).
$P_{wr}(\tau \Delta v < 0)$

$\tau = t - t_i$
$P(F) < 0.05$

$P = 0.5 \exp(-F^2/2)/(F+1)$

$|\Delta P/P| < 0.05$
\[ P_{\text{wr}}(\tau \Delta v < 0) \]

- \( \tau/t_s = 40 \)
- \( \tau/t_s = 30 \)
- \( \tau/t_s = 20 \)
- \( \tau/t_s = 10 \)

- theory
$K_f(t) = 0.9 \cdot \exp(-t/250) + 0.1$