Viscosity, Reversibility, Statistical Ensembles (in a Navier-Stokes fluid)

I. General introduction to "non equilibrium stationarity"

Equilibrium Physics theory is based on
(H1) the *Ergodic Hypothesis*, **EH** (*i.e.* initial data x typically *evolve covering a dense set* in phase space), and
(H2) on taking for granted that the *only invariant volume is Liouville's volume*, [1, 2].

(H1)&(H2) are extremely powerful and lead to identify the probability distributions (PDF) that give the averages of macroscopic observables. The distributions (synonim="ensembles") depend on a few parameters and their collection describes completely the possible equilibrium states of a given system.

The two assumptions can be criticized and their inadequacy becomes manifest when trying to build a theory of the stationary non equilibrium states.

A system in a stationary state is out of equilibrium if it evolves under the action of non conservative forces whose work is dissipated as heat ceded to external thermostats, which might be phenomenologically realized via constraints or dissipative forces, or ideally via infinite reservoirs.

Examples are a gas enclosed in two counterrotating heat conducting cylinders, a viscous incompressible fluid driven by a (non conservative force), ... **BUT**:

(H1) certainly cannot hold, in general, when a system is out of equilibrium as in such cases dissipation reduces the part of phase space where the evolution can dwell, at least if forcing is strong enough.

(H2) motions of most macroscopically relevant system are chaotic, most initially close configuration evolve in time diverging at exponential rate: *i.e.* motions are *"hyperbolic"*.

However in chaotic systems there are **∞-many** ways of measuring the volume $\mu(\Delta)$ of phase space sets Δ: which are invariant and therefore could 'claim' to the interpretation of frequency of visit to cells Δ.

So the Liouville volume loses its privileged place: for lack of uniqueness and because in general in chaotic systems frequency of visit $\mu(\Delta)$ cannot even be supposed given by $\int_\Delta \rho(x)dx$ for some non constant density ρ.

Furthermore even in equilibrium Liouville's volume is not the only invariant volume and its special role is sometimes ascribed to the fact that it is invariant:

a **shaky argument** because its metric invariance is accompanied by "wild" deformation of the volumes shape. Even the well established equilibrium ensembles have to be explained anew.

The chaoticity of motions of systems of thermodyamic interest (unexpectedly) proposes, from Ruelle's work, an answer to both problems, [3, 4].

(a) Any laboratory measurement is based on a "protocol for the set up": inevitably the protocol generates initial states that have some randomness, which depends on the protocol, **in spite of attempts at avoiding uncertainty**.

A basic assumption is that a given protocol generates data which depend on several unkown quantities: nevertheless all protocols designed to study a given system are supposed to have some randomess expressible as a PDF which has a density $\rho_P(x)$: the **density is not known** but the **assumption is that it exists**. Formally:

(a) *a protocol for an experiment (or simulation) on a system produces intial data affected by a (usually very small) uncertainty whose PDF has a density on phase space.*

(b) if the evolution is chaotic, which is generally the case in the systems of interest for thermodynamics, then it is a hyperbolic evolution. Formally:

In the vicinity of the attractor the evolution is hyperbolic.

In particular this applies when system is conservative.

Assumptions (a),(b) offer a solution to the above two key problems which is provided by the properties of the hyperbolic motions.

As in the theory of ordered motions we use the paradigm of the harmonic oscillators (*e.g.* to model pendulum, elastic chains and strings, rigid motion, integrable systems...), likewise in the theory of chaotic motions the paradigm is the *hyperbolic motion*, of which the simplest example are the Anosov systems, which entered the scene of Physics in the '960's.

Like the harmonic oscillators case, their properties are very elementary although not really well known yet in the field, see [5, p.219].

In great generality the property of such systems is that if the initial data x are chosen with a distribution $\rho(x)dx$ which has a density ρ on phase space, no matter which ρ is, will evolve in time visiting, as $\mathbf{t} \to \infty$, any number of prefixed volume elements Δ with a frequency $\mu(\Delta)$

independent of ρ ! .

This remains true even when evolution is very dissipative and motions approach an attractor not dense in phase space.[6, 7, 8]

This gives the possibility of solving both problems (1) and (2), including the cases of equilibrium.

The property **(b), chaos,** and **(a), unknown but existent randomess of initial data**, solves the problem of the frequency $\mu(\Delta)$ of visit to sets Δ: uniquely, as a theorem on chaotic evolution (*i.e.* hyperbolic ev.).

Hence in the case of conservative systems it identifies the Liouville volume as the privileged volume measurement.

Therefore Liouville volume is **not** privileged because it stands obviously out the wide variety of invariant volumes that exist with "equal rights" as soon as the system exhibits chaotic motions,

rather because the data have intrinsically some randomness with a PDF (typically not invariant) but which has a density $\rho_P(x)$ (typically $\rho_P(x)$ is concentrated on a very small vicinity of what the protocol is designed for).

The (a),(b) assumption therefore (via the simple hyperbolic motions theory) assign a unique PDF determining the statistical properties of the (few) observables of interest.

Hence, whether in equilibrium or in stationary non equilibrium, the states of a system are identified with a well determined collection of PDFs.

At this point new horizons open up, and the role of the Liouville's distribution is more clearly understood.

Equilibrium and non equilibrium statistical analysis have been remarkably unified: given a system and an equation of evolution for it the frequency of visit to cells Δ is uniquely determined.

Furthermore different evolution equations for the same system can lead to different PDF's for the stationary state which nevertheseess assign the same average to the thermodynamic observables.

Thus the existence of equivalent distributions and equations, well known in equilibrium (canonical, grand canonical, microcanonical ensembles ..) can be envisaged for stationary non equilibrium description as part of a more general theory of ensembles.

II. A special example of wide interest.

Consider the 2D Navier Stokes equation for an incompressible fluid in a periodic container of side 2π.

Velocity $\mathbf{u}(\mathbf{x})$ is expressed via a Fourier's series:

$$\mathbf{u}(\mathbf{x}) = \sum_{\vec{0}\neq\mathbf{k}=(k_1,k_2)\in Z^2} u_{\mathbf{k}} e(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}, \qquad e(\mathbf{k})\cdot\mathbf{k}=0$$

with $u_{\mathbf{k}} = \overline{u}_{-\mathbf{k}}$, $\mathbf{k}^\perp = (k_2, -k_1)$, $e(\mathbf{k}) = \frac{i\mathbf{k}^\perp}{|\mathbf{k}|}$. Hence NS is

$$\dot{u}_{\mathbf{k}} = \mathcal{E}(u)_{\mathbf{k}} - \nu\mathbf{k}^2 u_{\mathbf{k}} + f_{\mathbf{k}}, \qquad \mathbf{NS^{irr}}$$

$$\mathcal{E}(u)_{\mathbf{k}} = -\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}} \frac{(\mathbf{k}_2^2-\mathbf{k}_1^2)\,(\mathbf{k}_1^\perp\cdot\mathbf{k}_2)}{2|\mathbf{k}_1||\mathbf{k}_2||\mathbf{k}|} u_{\mathbf{k}_1} u_{\mathbf{k}_2},$$

the forcing will be taken s.t. $\sum_{\mathbf{k}} |f_{\mathbf{k}}|^2 = 1$ and $f_{\mathbf{k}} = 0$ except for $|\mathbf{k}| < K$, so f is a "large scale force", *e.g.* $f_{\mathbf{k}} = 0$ except for $\mathbf{k} = \pm(2,-1)$. So there is only one parameter $\nu \equiv \frac{1}{R}$ viscosity or Reynolds number.

Incompressibility condition and viscosity play the role of thermostats: they are phenomenological properties.

The first regulates the temperature (relating pressure, temperature, density via the eq. of state) and the viscosity controls the energy dissipation (proportional to the "enstrophy", $\mathcal{D}(\mathbf{u}) = \sum_{\mathbf{k}} \mathbf{k}^2 |u_{\mathbf{k}}|^2$).

So we have a Euler fluid subject to phenomenological constraints. And we can think of replacing one of them, *e.g.* viscosity, with a different constraint which achieves the same result of bounding the dissipation.

This, for instance, could be replacing "official NS eq." by

$$\dot{u}_{\mathbf{k}} = \mathcal{E}(u)_{\mathbf{k}} - \alpha(\mathbf{u})\mathbf{k}^2 u_{\mathbf{k}} + f_{\mathbf{k}} \qquad \mathbf{NS^{rev}}$$

with viscosity ν replaced by a multiplier $\alpha(\mathbf{u})$ designed so that enstrophy $\mathcal{D}(u) = \sum_{\mathbf{k}} |\mathbf{k}|^2 |\mathbf{u}_{\mathbf{k}}|^2$ **is exactly conserved**.

In the 2D case, this means that

$$\alpha(\mathbf{u}) = \frac{\sum_{\mathbf{k}} \overline{f}_{\mathbf{k}} \mathbf{k}^2 u_{\mathbf{k}}}{\sum_{\mathbf{k}} \mathbf{k}^4 |u_{\mathbf{k}}|^2}$$

In 3D the expression of α is a little more involved: nevertheless all what will be said in the 2D case applies to 3D with the appropriate $\alpha(\mathbf{u})$.

Denote $t \to S_t^{rev,N}\mathbf{u} = \mathbf{u}(t)$ the evolution for the new eq. and $t \to S_t^{irr,N}\mathbf{u}$ the evol. for the official NS eq.: where N is a UV cut-off introduced to eliminate problems about existence of solutions: (not arising in 2D unlike in 3D).

The equations above are to be understood by setting $\mathbf{u}_{\mathbf{k}} = 0$ if $|k_i| > N$.

N will have the role that the container volume V plays in Statistical Mechanics, while the observables which depend only on the modes $u_{\mathbf{k}}$ with $|\mathbf{k}| < L$, “large scale observables”, play the role of the local observables in Stat. Mech., which depend only on the particles located in a volume $L \ll V$.

Of course we shall be interested in properties of large scale observables which become N-independent as $N \to \infty$, just as in the theory of the thermodynamic limit in SM.

The evolutions of the two equations are chaotic at least if R is large and if the dissipation En is large.

Actually both equations should be regarded as phenomenological versions of a fundamental equation which is the Hamiltonian microscopic equation: whose motions are certainly chaotic and reversible.

Therefore given N and $\nu = \frac{1}{R}$ or the Enstrophy En, and assuming (Ha),(Hb) above, we associate with each ν, N or each En, N resp. the unique PDF $\mu_R^{irr,N}$ or $\mu_{En}^{rev,N}$, stationary distribution implied by the hyperbolicity, *i.e.* by chaos near the attractor.

The collection of the distributions represents all stationary states of the two evolutions: and can be called the irreversible ensembles or resp. the reversible ensembles at cut-off N for the NS flow.

The **conjecture** is (in 2D or 3D):

There is a $1-1$ correspondence between R and En such that for all large scale observables, *i.e.* functions $O_L(\mathbf{u})$ of the velocity field $\mathbf{u}$ depending only on $u_{\mathbf{k}}$ with $|\mathbf{k}|<L$, it is

$$\lim_{N\to\infty}\mu_R^{irr,N}(O_L)=\lim_{N\to\infty}\mu_{En}^{rev,N}(O_L)$$

and the correspondence is $R\longleftrightarrow En$ is defined by:

$$\mu_R^{irr,N}(\sum_{\mathbf{k}}\mathbf{k}^2|u_{\mathbf{k}}|^2)=En$$

in complete analogy with the thermod. limit in SM.

An **exact** consequence,[9], hence a first test, is the relation;

$$\lim_{N\to\infty}\mu_{En}^{rev,N}(\alpha)=\nu$$

A test is ($\nu = \frac{1}{R} = 1/2048$, $N = 31$, *i.e.* 3968 modes):

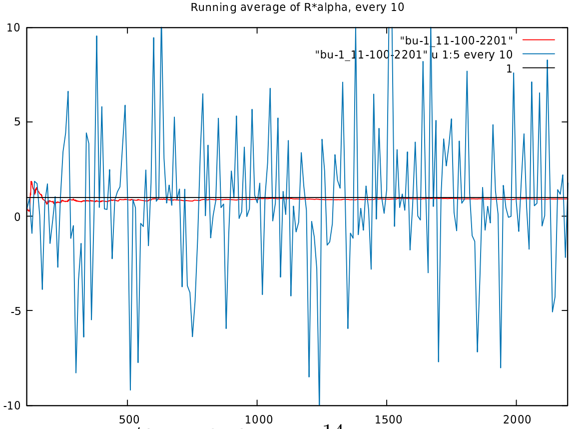

Fig.1: time units $2/h$ with $h = 2^{-14}$ RK4 integrator. Blue fluctuations = time evolution of $R\alpha(t)$ in*reversible evol.* (NS_{rev}); red line yields, at time t, "running average" $R\alpha(t)$, $\langle\, R\alpha(t)\,\rangle \xrightarrow[t\to\infty]{} 1$. Reached within 10% amid fluctuations 150 times as large in a short run. Horizontal visual aid at height 1.

Reversibility of NS^{rev} suggests testing validity of "Fluctuation Relation", (FR). But new problems arise:

FR proposes a universal relation for the observable

$$p = \frac{1}{\tau}\int_0^\tau \frac{\sigma(\mathbf{u}(t))}{\sigma_+}dt, \qquad \sigma_+ = \langle\, \sigma(\mathbf{u}(t))\,\rangle$$

where $\sigma(\mathbf{u})$ = phase space contraction (*i.e.* "divergence")

$$\sigma(\mathbf{u}) = \sum_{\mathbf{k}} \partial_{u_{\mathbf{k}}}(\alpha(\mathbf{u})\mathbf{k}^2 u_{\mathbf{k}})$$

Namely probability density of p should obey "large deviation rule" *i.e.* be $\propto e^{\tau s(p)}$ for τ large, with

$$s(p) - s(-p) = \tau\, p\, \sigma_+, \qquad \text{“}FR''$$

But evol. must be chaotic and time revers. on attractor.

For R large motion is (empirically) chaotic.

However time reversal is not implied by the reversibility of the equation: the attracting set $\mathcal{A}$ might fail to be dense on phase space.

So its time reversal image might be disconnected from $\mathcal{A}$ and the time reversal symmetry will be spontaneously broken for motions on $\mathcal{A}$ (which, at stationarity, are the only relevant).

This is a real problem at large N, as most $u_{\mathbf{k}}$ might be "damped away": as indicated by considering the Lyapunov exponents structure, illustrated by the following figure.

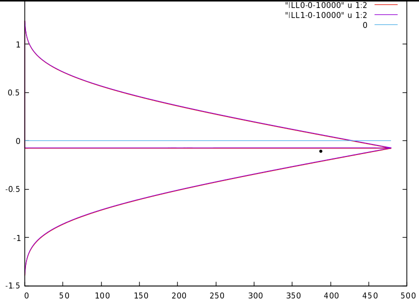

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Fig.5: Local Lyap. spectrum in 960 modes in NS_{rev} and NS_{irr} flows at $R = 2048$, **superposed**. The $n = 4N(N+1)$ exponents $\lambda_0, \ldots \lambda_{n-1}$ are drawn reporting for each $k = 0, \ldots, k_{\frac{n}{2}-1}$ the $\lambda_k, \lambda_{n-1-k}$ and $\frac{1}{2}(\lambda_k + \lambda_{n-1-k})$ for each $k = 0, \ldots \frac{n}{2} - 1$ Spectra are averaged over 800 time units sampled every 4 (quite short): before $t = 800/h$ running average values become stable, although the individual exponents are still fluctuating.

Overlap of Lyap. exp. for $NS^{irr,N}$ and $NS^{rev,N}$ indicates possible equiv. extension to selected not large scale observ.

warning 1 Is the “pairing” between $\lambda_k, \lambda_{n-1-k}$ approximately realized only in a range of R and N. Check?

warning 2 Are the global Lyap. exp. paired?

The above pairing (if confirmed for the global exp.) could be interpreted, [10, 9, 11], to mean that the pairs of negative exponents control the approach to the attracting set: so that do not contribute to the $\sigma(t)$.

Thus the simplest is to study cases in which there is approximate pairing and all pairs have opposite sign: so that it can be supposed that the attracting set is dense and hyperbolic: then time reversal applies and FR should hold.

Coincidence of local exponents for rever. and irrever. evol., exhibited above, induces to test FR at least when $d_\pm = d$, which happens at low N.

The local Lyapunov spectrum in a $7x7$ truncation of NS: with all pairs of opposite sign':

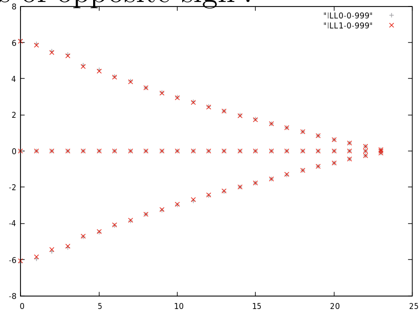

Fig.2: Local Lyapunov spectra for *both* NS_{irr} *and* NS_{rev} flows with $d = 48$ modes, $R = 2048$. Rapid computation with only 1000 samples taken every $4/h$ time steps of time $h = 2^{-13}$ and averaged: the values give the $d/2$ exponents λ_k, the λ_{d-1-k}, and $\frac{1}{2}(\lambda_k + \lambda_{d-1-k})$; it shows the approximate pairing and the equal number of non negative and negative exp.

Therefore, at least in this case the attracting set appears to be whole phase space and FR should hold for **the reversible case**.

Lyap. spectra equivalence of NS^{rev} and NS^{irr} is not part of the conjecture: hence it is worth testing the FR also in the NS^{irr}: where it certainly cannot be, *a priori*, applied because evolution is irreversible.

However phase space volume contraction for reversible ev. is an observable also for irrev. evolution:

$$\sigma_{rev}(\mathbf{u}) = \sum_{\mathbf{k}} \partial_{\mathbf{u_k}}(\alpha(\mathbf{u})\mathbf{k}^2 u_{\mathbf{k}})$$

and is natural to ask whether equivalence (already surprising for the Lyap. exp.) extends to the fluctuation of $\sigma_{rev}(\mathbf{u})$ viewed as observable for NS^{irr}.

Possibility of FR for $\sigma_{rev}(\mathbf{u})$ has been discussed in earlier works and here I do not try to justify why the result, described in the following Fig., below was expected.

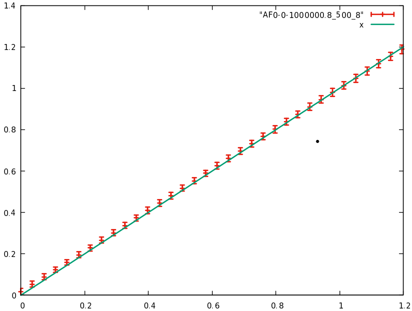

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Fig.4: The PDF for FR in NS^{irr}, red, with 48 modes, $R = 2048$. The τ is chosen 8, the slope of the graph increases with τ reaching 1 at about $\tau \sim 2$. The graph is derived from registering the flow every $8/h$ time steps of size $h = 2^{-13}$. The blue line $f(x) = x$ is a visual aid. The corresponding reversible FR essentially overlaps with the above.

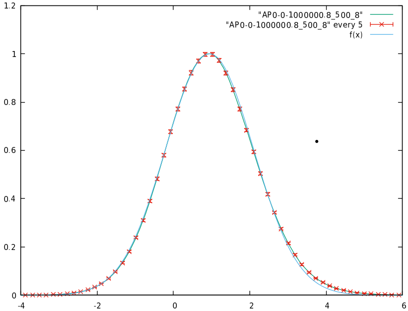

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Fig.4: Test FR in NS^{irr}, red, with 48 modes (7×7), $R=2048$. The τ is chosen 8, the slope of the graph increases with τ reaching 1 at about τ 2. The graph is built with 10^6 data, divided into 500 bins, obtained sampling the flow every $8/h$ time steps of size $h=2^{-13}$. The blue line $f(x)=e^{-a(x-b)^2}$ fitted via a,b, normalized to 1. The corresponding reversible FR essentially overlaps with the above.

III. What about larger N?, and other comments

The case with 224 modes (15×15), from Lyap. spectrum and pairing, would still yield a slope deviation from 1 by $\sim 2\%$ assuming that local Ly. exp. coincide with the true exp. (which is not expected) and would be very difficult to distinguish from the errors.

The case with 960 modes(31×31) should show a deviation of at least 20%: however the computer time is for the moment too long, already for studying the local Lyapunov exponents.

This is unfortunate since already in [9, 11] a scenario, in the frame of the Chaotic Hypothesis, has been proposed to test the FR in strongly dissipative irrever. evol. The scenario has many items that need to be tested and cannot be presented here.

Finally a question asked often is: why to change NS equation to study another (particularly if equivalent).

(1) for the same reason why in equil. several ensembles are considered, although equivalent: and studying equivalence led to better understanding about phase transitions, long range forces, finite size effects, scaling properties...

Other comments;

(2) the NS equation is phenomenological: viscosity is not a property of molecules (which evolve via reversible eq.). It is questioned whether in 3D Obuk.Kol. scaling theory remains among the predictions of the rev. NS equation. This problem (open) might also shed light on the statistical properties dwelling above the Kolmogorov scale.

(3) in 3D NS^{irr} might have no regular solution and even no constructive solution at all for mildly general initial data. NS^{rev} has no mathematical problems: but the princple of difficulties conservation operates. By its dire action the multiplier α can become < 0, eliminating hope to control limit $N \to \infty$. The advantage is that the limit needs not exist as the conjecture refers only to observables of large scale.

(4) negative fluctuations for α signal a regime of high turbulence: it is in this regime that it would be very interesting to test statistics at scales behind Kolm. scale.

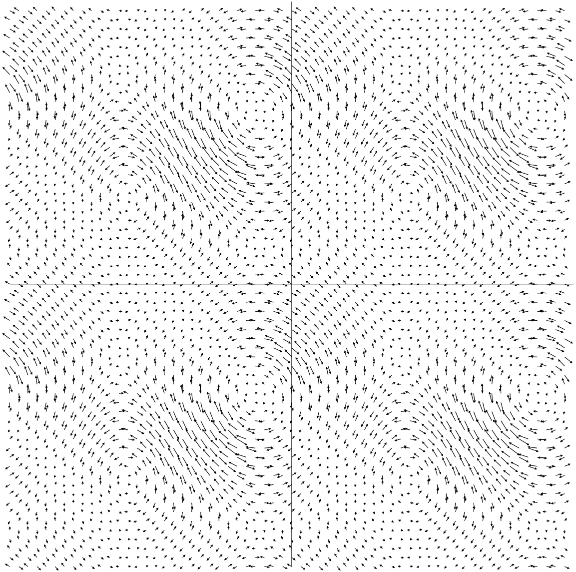

Fig.6: 960 modes (31 $\times$ 31), R=2048, 4 identical movie frames periodically repeated for visual aid; with 4 vortices each.

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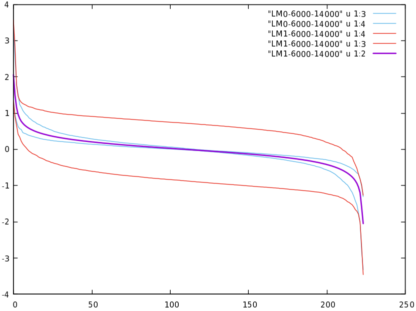

Fig.7: 2^{17}-Local Ly.Ex. for 224 modes (15×15): R=2048. The red curves are the loci of the largest and mallest L.E. in 8000 shots of the velocity field in NS^{rev}. The blue curves are the same for NS^{irr}. The central violet line is the graphs of L.E. of BOTH, superposed *i.e.* 'coinciding' on the graph scale.

The difference $|\lambda_k^{rev} - \lambda_k^{irr}|$ is reported in the Fig.8

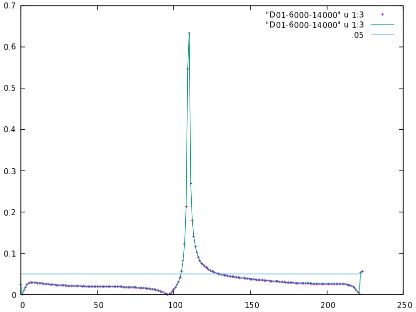

Fig. 8: the difference $2\frac{|\lambda_k^{rev}-\lambda_k^{irr}|}{|\lambda_k^{rev}|+|\lambda_k^{irr}|}$ between corresponding L.E. for NS^{rev} and NS^{irr}. The green line interpolates the actual values represented by the dots, and the bar marks the .05 level.

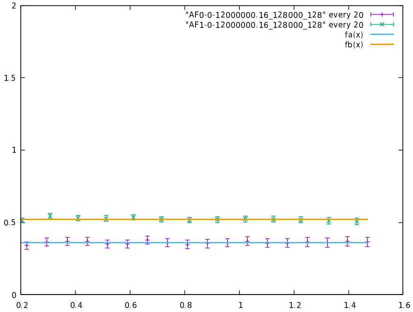

Fig.9: Evidence (?) for the Chaotic hypothesis: Fluctuation Relation, for $x = p\sigma_+\tau$, *i.e.* $\frac{\log P_\tau(x) - \log P_\tau(-x)}{x} = const$. Green data are for NS^{rev}, red data for the NS^{irr}; the straight lines, yellow and blue, are the best fit to a constant.

FR holds but the value of the constant, **if equivalence for σ agree in the average and if pairing holds**, should be $\frac{n_+}{n}$, $n_+ = 2{*}$number of L.E. > 0, $n = a$ total number of L.E. This is correct only up to $\sim 20\%$, **hence not OK** $\Rightarrow$ why?

Question: the integration is done at low precision (due to run-time length) and the experiment should be repeated at higher precision. Here the divergence is recorded every 2 time unit ($i.e.$ $2\delta t^{-1} = 2 * 2^{13}$) up to $t \simeq 1.56\, 10^5$ ($t = 2^7 * 128 = 2^{14}$).

Or, simply, σ is not a local observable and might not be covered by equivalence: just as the L.E. case which agree in average but exhibit different fluctuations.