Hypotheses for Fluctuation Relations in Nonequilibrium Systems

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For isoenergetic SLLOD, E.C.M. (1993) proposed and tested this relation:

$$\frac{\mu_i}{\mu_{i^*}} = \frac{\exp\left[-\sum_n^+ \lambda_{i,n}\tau\right]}{\exp\left[-\sum_n^+ \lambda_{i^*,n}\tau\right]} = \exp\left[Nd\langle\alpha_i\rangle_\tau\tau\right]$$

i, i^* conjugate segments length τ; $d =$ dimension;
$\lambda_i =$ finite time Lyapunov exp.

$$\langle\alpha_i\rangle_\tau \propto -\sum_n \lambda_{i,n} \propto \text{average e.p.r.}$$

$$\begin{cases} \dot{\mathbf{q}}_i = \mathbf{p}_i/m + \mathbf{n}_x \gamma y_i \ , \quad i = 1, ..., N \\ \dot{\mathbf{p}}_i = \mathbf{F}_i - \mathbf{n}_x \gamma p_{yi} - \alpha \mathbf{p}_i \end{cases}$$

$$\alpha_{IE} = \frac{-\gamma P_{xy} V}{\sum_{i=1}^{N} \mathbf{p}_i^2/m}, \ \ \alpha_{IK} = \frac{\sum_{i=1}^{N} (\mathbf{F}_i . \mathbf{p}_i - \gamma p_{xi} p_{yi})}{\sum_{i=1}^{N} \mathbf{p}_i^2/m}$$

$$\sigma_{IE} = c \ \alpha_{IE}, \quad \sigma_{IK} = c \ \alpha_{IK} - \frac{\gamma P_{xy}^{K} V}{\sum_{i=1}^{N} \mathbf{p}_i^2/m}$$

In 1994, Evans and Searles first of papers deriving relations similar to that of E.C.M. for

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Original ESR for DF, virtually no hypotheses: only time reversibility.
Transient: non-invariant, distributions. Numerical and mathematical support for Steady State.

In 1995, Gallavotti and Cohen, inspired by ECM:

Chaotic Hypothesis: *A reversible N-particle system in a stationary state can be regarded as transitive Anosov system, for calculations of its macroscopic properties.*

Markov partition; attribute weight to cell C_i

$\Lambda^{-1}_{w_i,u,\tau} = 1/|$Jacobian dynamics restricted to $W^u|$

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THM for phase space contraction rate.

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dissipation or e.p.r.? (most often tested)
Could one rely on different mechanisms?

Puzzling result. GCFT hard to verify at low shear γ, IK–SLLOD.

In fact, harder and harder the closer and closer to equilibrium (E.S. J. Chem. Phys. 2000, Z.R.A. cond-mat/0311583, D.K. nlin.CD/0401036),

although closer to equilirium implies higher chaos, hence CH should have been better verified (M.R. 2003, very high γ).

What happens close to equilibrium?

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Why? Easy to see in simple systems

$$\sigma = \sigma_d + \sigma_c = O(F_e^2) + \sigma_c(F_e = 0)$$

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As in ESR & E. To be tested (Gilbert ’06).

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Question: For only a few special observables (not all phase functions), and a special result, could one do without Anosov structure and full knowledge of SRB measure?

ES tried a different approach: rely on Liouville equation only, and extend work on TFR.

Phase space $\mathcal{M}$, evolution $S^\tau : \mathcal{M} \to \mathcal{M}$;

reversibility $iS^\tau\Gamma = S^{-\tau} i\Gamma$;

regular measure $d\mu(\Gamma) = f(\Gamma)d\Gamma$;

odd observable $\phi : \mathcal{M} \to I\!R$,

$$\overline{\phi}_{t_0,t_0+\tau}(\Gamma) = \frac{1}{\tau}\int_{t_0}^{t_0+\tau} \phi(S^s\Gamma)ds = \frac{1}{\tau}\phi_{t_0,t_0+\tau}(\Gamma)$$

Dissipation function for TRI f:

$$\overline{\Omega}_{t_0,t_0+\tau}(\Gamma) = \frac{1}{\tau}\left[\ln\frac{f(S^{t_0}\Gamma)}{f(S^{t_0+\tau}\Gamma)} - \int_{t_0}^{t_0+\tau} \Lambda(S^s\Gamma)ds\right]$$

$\Lambda = -\sigma =$ phase space expansion rate.

Suitable $f \Rightarrow \Omega =$ e.p.r. $= F_e J/k_B T$ or energy dissipation rate. $f(\Gamma) = 1/|\mathcal{M}| \Rightarrow \Omega = \Lambda$

Let $\delta > 0$, $t_0 = 0$, $\quad A_\delta^+ = (A - \delta, A + \delta)$

$$A_\delta^- = (-A - \delta, -A + \delta)$$

Consider

$$\frac{\mu(C(\overline{\Omega}_{0,\tau} \in A_\delta^+))}{\mu(C(\overline{\Omega}_{0,\tau} \in A_\delta^-))} = \frac{\int_{C(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f(\Gamma) d\Gamma}{\int_{C(\overline{\Omega}_{0,\tau} \in A_\delta^-)} f(\Gamma) d\Gamma} ,$$

Observe that

$$C(\overline{\Omega}_{0,\tau} \in A_\delta^-) = iS^\tau C(\overline{\Omega}_{0,\tau} \in A_\delta^+)$$

introduce the transformation $\Gamma = iS^\tau X$

Choose f so that $f(\Gamma) = f(i\Gamma)$.

Some algebra yields the ESTFR

$$\frac{\mu(C(\overline{\Omega}_{0,\tau} \in A_\delta^+))}{\mu(C(\overline{\Omega}_{0,\tau} \in A_\delta^-))} =$$

$$\frac{\int_{C(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f(\Gamma) d\Gamma}{\int_{C(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f(S^\tau X) \exp\left(\Lambda_{0,\tau}(X)\right) dX} =$$

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$$\frac{\int_{C(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f(\Gamma) d\Gamma}{\int_{C(\overline{\Omega}_{0,\tau} \in A_\delta^+)} \exp\left[-\Omega_{0,\tau}(X)\right] f(X) dX} =$$

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$$= \left\langle \exp\left(-\Omega_{0,\tau}\right) \right\rangle^{-1}_{\overline{\Omega}_{0,\tau} \in A_\delta^+} = \mathbf{e}^{[\mathbf{A} + \epsilon(\delta, \mathbf{A}, \tau)]\tau}$$

Consider now

$$\frac{\mu(C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+))}{\mu(C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^-))} = \frac{\int_{C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+)} f(\Gamma) d\Gamma}{\int_{C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^-)} f(\Gamma) d\Gamma}$$

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and take $t = t_0 + \tau + t_0$. Then

$$C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^-) = iS^t C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+)$$

If $W \in C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+)$, and $\Gamma = iS^tW$, like before we have

$$\frac{\mu(C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+))}{\mu(C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^-))} = \langle \exp\left(-\Omega_{0,t}\right)\rangle^{-1}_{\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+}$$

The special case $\overline{\phi}_{t_0,t_0+\tau} = \overline{\Omega}_{t_0,t_0+\tau}$, yields

$$\frac{\mu(C(\overline{\Omega}_{t_0,t_0+\tau} \in A_\delta^+))}{\mu(C(\overline{\Omega}_{t_0,t_0+\tau} \in A_\delta^-))} = \langle \exp\left(-\Omega_{0,t}\right)\rangle^{-1}_{\overline{\Omega}_{t_0,t_0+\tau} \in A_\delta^+}$$

$$= e^{[A+\epsilon(\delta,t_0,A,\tau)]\tau} \left\langle e^{-\Omega_{0,t_0}-\Omega_{t_0+\tau,2t_0+\tau}} \right\rangle^{-1}_{\overline{\Omega}_{t_0,t_0+\tau} \in A_\delta^+}$$

Exact result, for all t_0, τ, δ, and observable pairs $A, -A$. It rests only on time reversibility of S^t, and $f(iS^t\Gamma) \neq 0$ if $f(\Gamma) \neq 0$.

Move now evolution from sets to measures, using

$$\mu_{t_0}(S^{t_0}E) = \int_{S^{t_0}E} f_{t_0}(W)dW =$$

$$= \int_E f(X)dX = \mu(E)$$

Some algebra yields

$$\frac{\mu_{t_0}(C(\overline{\phi}_{0,\tau} \in A_\delta^+))}{\mu_{t_0}(C(\overline{\phi}_{0,\tau} \in A_\delta^-))} = \frac{\mu_{t_0}(S^{t_0}C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+))}{\mu_{t_0}(S^{t_0}C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^-))}$$

$$= \frac{\mu(C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+))}{\mu(C(\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^-))}$$

$$= \langle \exp\left(-\Omega_{0,t}\right)\rangle^{-1}_{\overline{\phi}_{t_0,t_0+\tau} \in A_\delta^+}$$

and letting $\overline{\phi}_{t_0,t_0+\tau} = \overline{\Omega}_{t_0,t_0+\tau}$

$$\frac{1}{\tau}\ln\frac{\mu_{t_0}(C(\overline{\Omega}_{0,\tau}\in A_\delta^+))}{\mu_{t_0}(C(\overline{\Omega}_{0,\tau}\in A_\delta^-))} = A + \epsilon(\delta, t_0, A, \tau) +$$

$$-\frac{1}{\tau}\ln\left\langle e^{-\Omega_{0,t_0}-\Omega_{t_0+\tau,2t_0+\tau}}\right\rangle_{\overline{\Omega}_{t_0,t_0+\tau}\in A_\delta^+}$$

If $\mu_{t_0} \to \mu_\infty$, should change from statement on ensemble of trajectories, f_{t_0}, however long t_0, to statement concerning also statistics generated by a single typical trajectory: the ESSFR.

Given any tolerance $\gamma > 0$ we would like to write:

$$A - \gamma \leq \frac{1}{\tau} \ln \frac{\mu_{t_0}(C(\overline{\Omega}_{0,\tau} \in A_\delta^+))}{\mu_{t_0}(C(\overline{\Omega}_{0,\tau} \in A_\delta^-))} \leq A + \gamma \,,$$

for allowed $A, -A$, and small δ, large t_0, τ.

Some assumption is necessary.

Chaos/properties of interesting observables help.

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But for bounded Ω, as in many situations, no extra assumptions: $|\Omega| \leq \Omega^*$, for $\Omega^* > 0$,

$$e^{-2t_0\Omega^*} \leq \left\langle e^{-\Omega_{0,t_0} - \Omega_{t_0+\tau, 2t_0+\tau}} \right\rangle_{\overline{\Omega}_{t_0, t_0+\tau} \in A_\delta^+} \leq e^{2t_0\Omega^*}$$

Taking $\delta < \gamma$, we have $|\epsilon| < \gamma$, hence ESSFR is satisfied if

$$\tau \geq \frac{2t_0\Omega^*}{\gamma - \delta} .$$

It only remains to ask how $C(\overline{\Omega}_{0,\tau} \in A_\delta^+)$, is related to support $\mathcal{A}$ of μ_∞: $\mathcal{A} \cap C(\overline{\Omega}_{0,\tau} \in A_\delta^+)$. We consider two cases:

i. $\mathcal{A} = \mathcal{M}$: one obtains the ESSFR as $C(\overline{\Omega}_{0,\tau} \in A_\delta^+) = \mathcal{A} \cap C(\overline{\Omega}_{0,\tau} \in A_\delta^+)$

ii. Unique attractor $\mathcal{A}$ (and repeller), mild condition yields same result.

$\Omega^* < \infty$ not serious restriction: isokinetic electric or colour current, some isoenergetic, hard particles, Anosov...

Low probability near Ω-singularities, correlations decay, large N not exploited: so ESSFR expected for interesting cases with unbounded Ω.

Bound A^* on observable fluctuations depends on system and observable.

At equilibrium, $\Omega = JF_e/k_BT = 0$

hence, symmetry of $\phi = J$ in whole range.

Conclusions.

1. SSFRs for dissipation function and other functions (also p.s.c.r.) only from TRI, convergence to steady state and boundedness of Ω.

3. Reasonable approach? If so, TRI suffices: different perspetcitve, possible different results (e.g. ϕ) along with those stemming from CH.