Deterministic thermostats and Fluctuation Relations

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For isoenergetic shear, Evans-Cohen-Morriss (1993) proposed and tested this relation:

$$\frac{\mu(\overline{\Omega}_\tau = A)}{\mu(\overline{\Omega}_\tau = -A)} = \frac{\exp\left[-\sum_n^+ \lambda_{A,n}\tau\right]}{\exp\left[-\sum_n^+ \lambda_{-A,n}\tau\right]} = \exp\left[A\tau\right]$$

$\overline{\Omega}_\tau$ average entropy production rate in *long* segment length τ; λ_i = finite time Lyapunov exp.

$$-\sum_n \lambda_{i,n} \propto \text{average entropy production rate}$$

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Virtually no hypotheses: only time reversibility
Transient: non-invariant distributions. Numerical and mathematical support for Steady State.

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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

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

$w_i = \{S^t x_i\}_{t=-\tau/2}^{\tau/2}$, large τ, $x_i \in C_i$.

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Theorem for phase space contraction rate.

Q.: which systems look like Anosov?

Similarly to ergodicity, microscopic dynamics such that deviations from Anosov unobservable.

Different mechanisms?

Indeed, there are difficulties. For instance: convergence times diverge while approaching equilibrium and GCFR domain shrinks to $\{0\}$.

Why? Easy to see in simple systems

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

Anosov, strong; FR, for phase space contraction.

Evans-Searles tried a different approach: rely on Liouville equation only, for reversible systems.

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 $\Omega : \mathcal{M} \to I\!R$,

Dissipation function for TRI f:

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

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

Suitable (equilibrium) $f \Rightarrow$

$\Omega =$ dissipation rate $= F_e J/k_B T$

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 $\Gamma = iS^\tau X$

Some algebra yields Evans-Searles Transient FR

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

$$= \mathbf{e}^{[\mathbf{A}+\epsilon(\delta,\mathbf{A},\tau)]\tau}$$

$$\epsilon \leq \delta$$

Interesting, although transient, like Jarzynski & Crooks FRs. Experiments.

Now, let averaging start at time t_0

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

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

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

Change coordinates: $\Gamma = iS^t W$.

Move evolution from sets to measures:

$$\mu_{t_0}(S^{t_0}E) = \mu(E)$$

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

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

$\mu_{t_0} \to \mu_\infty$, should change from statement on ensemble of trajectories, f_{t_0}, even long t_0, to statement concerning also statistics of single typical trajectory: the Steady State Evans-Searles FR.

Trouble: $t_0 \to \infty$ before τ in

$$\left\langle e^{-\Omega_{0,t_0}} \cdot e^{-\Omega_{t_0+\tau,2t_0+\tau}} \right\rangle$$

Some assumption is necessary.

For observable A, and $t_0 \to \infty$

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

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$$= \left\langle e^{-\Omega_{t_0+\tau,2t_0+\tau}} \right\rangle = \left\langle e^{-\Omega_{0,t_0}} \right\rangle_{t_0+\tau} = 1$$

$$\left\langle e^{-\Omega_{0,t_0}} \right\rangle = \int e^{-\Omega_{0,t_0}(\Gamma)} f(\Gamma) d\Gamma = \int f_{t_0}(\Gamma) d\Gamma = 1$$

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Range of A around $[0, \langle \Omega \rangle]$.

Conclusions.

1. Steady sate FR for dissipation function within physical times only from reversibility and correlations decay. These are the physical reasons.

2. Boundedness of Ω + transitivity may suffice. No need for (approximate) anosovicity, only boundedness of steady state mean of $e^{-\Omega_{0,t_0}}$: 1 at equilibrium, $O(F_e^2)$ corrections if close.

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But: stochastic approach does not explain how irreversibility arises (Kurchan).

Ambiguities in identification of observables.

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Which physical mechanisms determine FRs?
Like ergocity is too little and too much;
anosovicity is too little and too much.