Friction, reversibility, fluctuations in nonequilibrium and chaotic hypothesis (V.Lucarini & GG)

Stationary states: $\Rightarrow$ probab. distrib. on phase space.

Collections of stationary states $\Rightarrow$ ensembles $\mathcal{E}$: in equilibrium give the statistics (canonical, microc., &tc).

Can this be done for stationary nonequilibrium? Motion:

$$\dot{x}_j = f_j(x) + F_j - \nu\,(Lx)_j, \qquad \nu > 0,\ j = 1, \ldots, N$$

$L > 0$ dissipation matrix: e.g. $(Lx)_j = x_j$, $\nu > 0$ (friction), $f(x) = f(-x)$ (time reversal)

Chaotic hypothesis: "think of it as an Anosov system" (Cohen,G)

(analogue of the periodicity≡ergodicity hypothesis of Boltzmann, Clausius, Maxwell, and possibly as unintuitive)

Time reversal symmetry is violated by friction.

BUT it is a fundamental symmetry: $\Rightarrow$ possible to restore?

How? in which sense? Start from a special case:

the Lorenz96 eq. (periodic b.c.)

$$\dot{x}_j = x_{j-1}(x_{j+1} - x_{j-2}) + F - \nu x_j, \qquad j = 0, \ldots, N-1$$

Vary ν and let μ_ν stationary distrib. Let $\overline{E} = \langle \sum_j \dot{x}_i^2 \rangle_{\mu_\nu}$:
this is "ensemble" (viscosity ensemble)
Equivalent ensembles conjecture: replace ν by

$$\alpha(x) = \frac{\sum_i F x_i}{\sum_i x_i^2}$$

New Eq. has $E(x) = \sum_i x_i^2$ as exact constant of motion

$$\dot{x}_j = x_{j-1}(x_{j+1} - x_{j-2}) + F - \alpha(x) x_j,$$

and volume contracts by $\sum \partial_j (a(x) x_j)$

$$\sigma(x) = (N-1)\alpha(x), \quad p = \tau^{-1} \int_0^\tau \sigma(x(t)) dt / \langle \sigma \rangle$$

Equivalent ensembles (conjecture):

Stationary states $\widetilde{\mu}_E$ label by $E \Rightarrow \widetilde{\mathcal{E}}$ ("energy ensemble").

$$\mu_\nu \sim \widetilde{\mu}_E \longleftrightarrow E = \mu_\nu(E(\cdot)) \longleftrightarrow \nu = \widetilde{\mu}_E(\alpha(\cdot))$$

Give the same statistics in the limit of large $R = \frac{F}{\nu^2}$.

Analogy canonical μ_β = microcanonical $\widetilde{\mu}_E$ if

$$\mu_\beta(E(.)) = E \longleftrightarrow \widetilde{\mu}_E(K(.)) = \frac{3}{2\beta}N$$

in the limit of large volume (fixed density or specific E).

Why? several reasons. Eg. chaoticity implies

$$\alpha(x(t)) = \frac{\sum_i F x_i}{\sum_i x_i^2} \qquad \text{"self − averaging"}$$

Tests performed at $N = 32$ (with checks up to $N = 512$) and high R (at $R > 8$, system is very chaotic with > 20 Lyap.s exponents and at larger R it has $\sim \frac{1}{2}N$ L.e.)

1) $\mu_{\overline{E}}(\alpha) = \nu \longleftrightarrow \mu_\nu(E) = \overline{E}$

2) If g is reasonable ("local") observable $\frac{1}{T}\int_0^T g(S_t x)dt$ has same statistics in both

3) The "Fluctuation Relation" holds for the fluctuations of phase space vol (reversible case): reflect chaotic hypothesis

4) Found its N-independence and ensemble independence (Livi,Politi,Ruffo)

5) In so doing found or confirmed several scaling and pairing rules for Lyapunov exponents (somewhat surprising) and checked a local version of the F.R.

Scaling of energy-momentum (irreversible model):

$$E = \sum_i x_i^2, \qquad M = \sum_i x_i$$

$$\frac{\overline{E}^i_R}{N} \sim c_E R^{4/3}, \quad \frac{\overline{M}^i_R}{N} \sim 2c_E R^{1/3} \quad c_E = 0.59 \pm 0.01$$

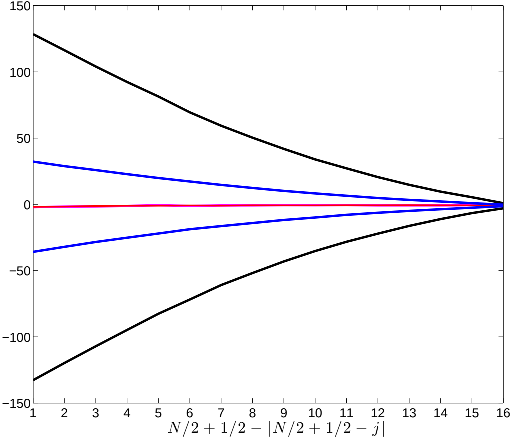
$$\frac{std(E)^i_R}{N} = \frac{\left(\overline{E^2}^i_R - (\overline{E}^i_R)^2\right)^{1/2}}{N} = \tilde{c}_E R^{4/3}, \quad \tilde{c}_E \sim 0.2 c_E$$

$$\frac{std(M)^i_R}{N} = \tilde{c}_M R^{2/3} \quad \tilde{c}_E \sim 0.046 \pm 0.001$$

$$t^{i,M}_{dec} \sim c_M R^{-2/3} \quad c_M = 1.28 \pm 0.01$$

The first two confirm Lorenz96, the 3d,4th "new", 5th is the "decorrelation" time $\langle\, M(t)M(0)\, \rangle$

Irreversible model Lyapunov exponents arranged pairwise



Black: Lyap. exp.s $R = 2048$
Magenta: $\pi(j) = (\lambda_j + \lambda_{N-j+1})/2$.
Blue: Lyap. exp.s $R = 256$
value of $\pi(j)$ at $R = 252$ (invisible below magenta).

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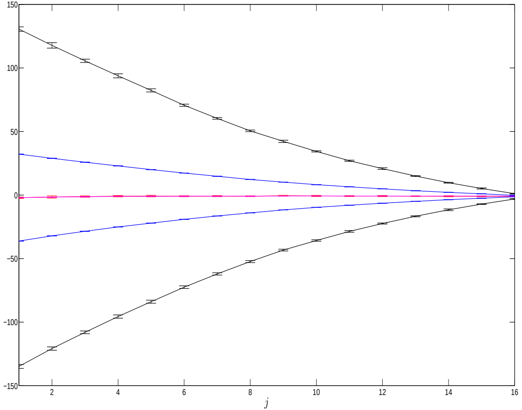

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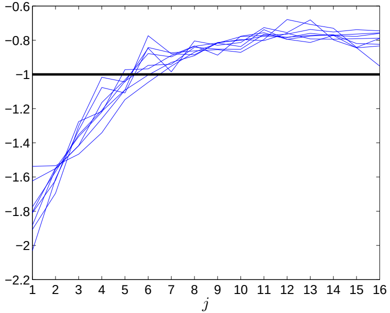
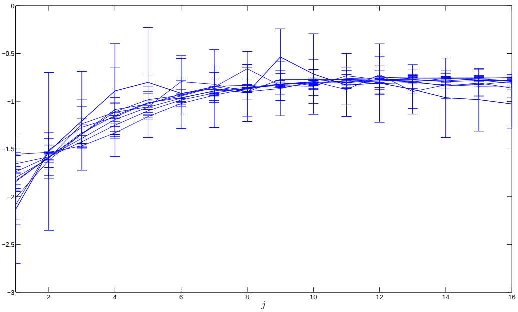
Pairing accuracy. Irreversible model.



Blue: $\pi(j) = (\lambda_j + \lambda_{N-j+1})/2$, $8 < R < 2048$, $N = 32$.

Almost constant: as it can be seen if compared to λ_j. The small variation reflects the fact that the spectrum shows an asymptotic shape.

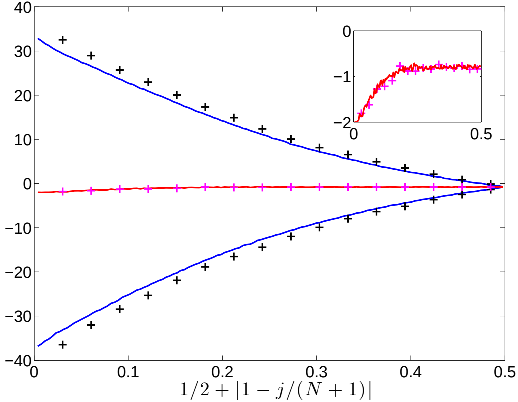
Pairing accuracy. Irreversible model.



Blue: $\pi(j) = (\lambda_j + \lambda_{N-j+1})/2$, $8 \leq R \leq 2048, N = 32$.

Almost constant: as it can be seen if compared to λ_j. The small variation reflects the fact that the spectrum shows an asymptotic shape.

Continuous limit of Lyapunov Spectrum (LPR): asymptotics in $N = 32, 256$ at R fixed:

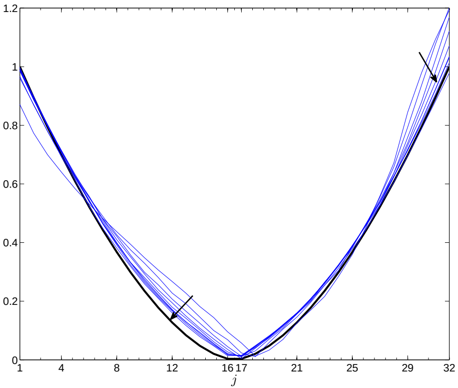


$R = 256$: λ_j for $N = 256$ and Black mark $N = 32$
red line $\pi(j) = (\lambda_j + \lambda_{N-j+1})/2$
for $N = 256$ and marker for $N = 32$; zoom

Scaling Lyapunov Spectrum: $8 \le R = 2^n \le 2048$

$$x = \frac{j}{N+1} \;\Rightarrow\; |\lambda(x) + \pi(x)| \sim c_\lambda \, |2x - 1|^{5/3} \, R^{2/3}$$

$$\sim |\lambda(x) + 1| \sim c_\lambda \, |2x - 1|^{5/3} \, R^{2/3}, \quad c_\lambda \sim 0.8$$



Blue: $|\lambda_j + 1| / (c_\lambda R^{2/3})$, Black: $|2j/(N+1) - 1|^{5/3}$

Dimension of Attractor

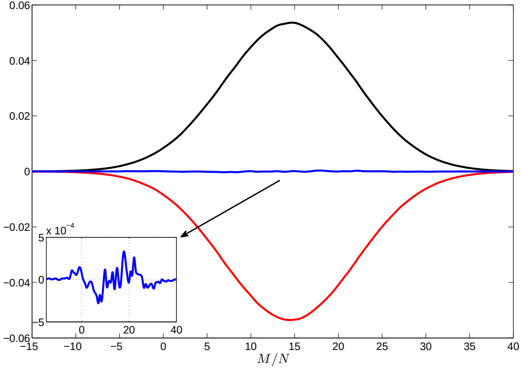
The $|\lambda(x)+1| \sim c_\lambda \, |2x-1|^{5/3} \, R^{2/3}$ yields the full spectrum: hence can compute the KY dimension

$$N - d_{KY} = \frac{N}{1 + c_\lambda R^{\frac{2}{3}}} \xrightarrow[R\to\infty]{} 0, \qquad \forall\ N$$

attractor has a dimension virtually indistinguishable from that of the full phase space.

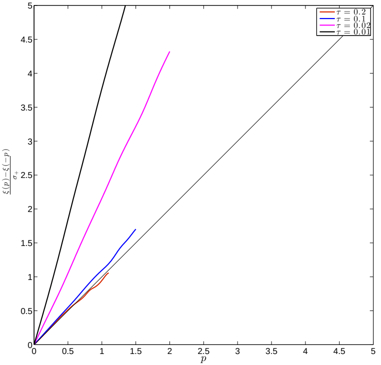
However SRB distribution deeply different from equidistribution (often confused with ergodicity): made clear by the equivalence (if holding) and the validity of the Fluctuation Relation needs test

Reversible-Irreversible ensembles equivalence:



Black: pdf for M/N rev, $R = 2048$. Blue − pdf for M/N irrev for $R = 2048$. Red black + blue line. Note vertical scales.

Check Fluctuation Relation (FR)



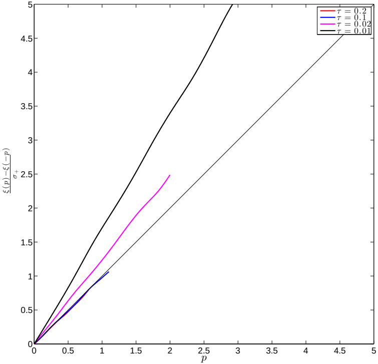
$$p = \frac{1}{\tau}\frac{\int_0^\tau \sigma(x(t))dt}{\langle\, \sigma \,\rangle_{srb}}$$

$$\frac{1}{\tau\overline{\sigma}_R}\log\frac{P_\tau^R(p)}{P_\tau^R(-p)} = 1 \quad ???$$

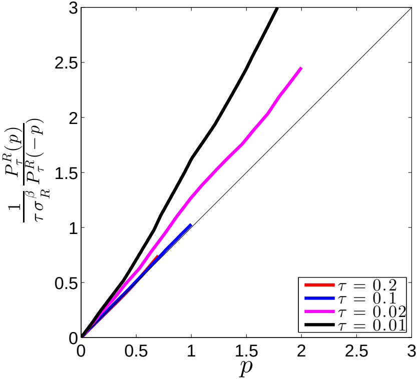
F.R. slope $c(\tau) \xrightarrow[R\to\infty]{} 1,\ R = 512$

$$c(\tau) = 1 + \left(\frac{t^{r,\sigma}_{dec,R}}{\tau}\right)^{4/3} = 1 + \left(\frac{c_\sigma}{\tau}\right)^{4/3} R^{-8/9}$$

Check Fluctuation Relation



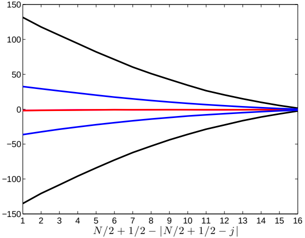
F.R. $R = 2048$, approach 1 as $\tau \uparrow$ beyond decorrelation time



Local F.R. for $R = 2048$

$$\frac{1}{\tau} \log \frac{P^R_\tau(p)}{P^R_\tau(-p)} = \overline{\sigma^\beta}_R p + O(\tau^{-1}) = \beta \overline{\sigma}_R p + O(\tau^{-1})$$

Lyapunov exp. reversible ≡ irrev



Red: Lyap exps $R = 2048$. Magenta $(\lambda_j + \lambda_{N-j+1})/2$. Blue Lyaps $R = 256$. Black: $(\lambda_j + \lambda_{N-j+1})/2$

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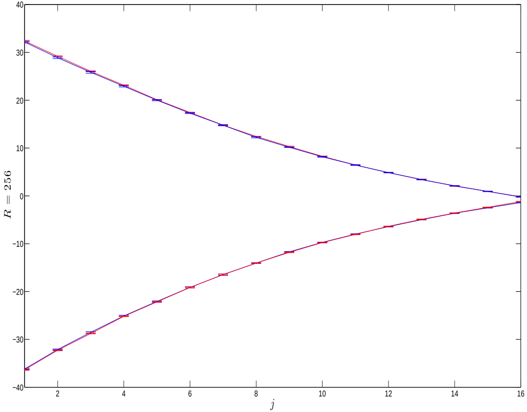

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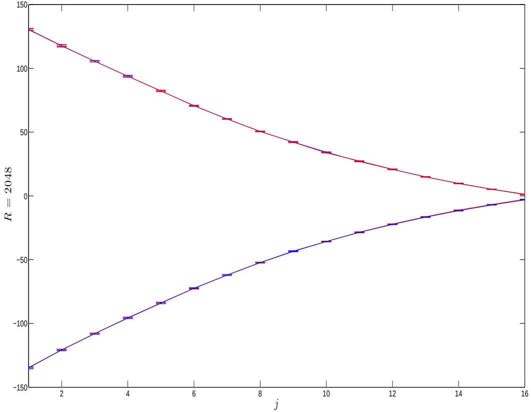

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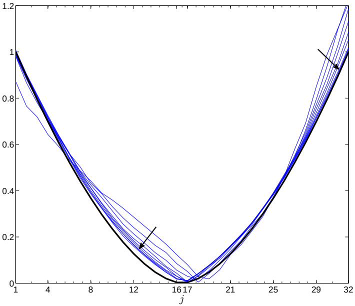
Reversible pairing



Blue $|\lambda_j + 1|/(c_\lambda F^{2/3})$ for F (growing as arrows) ≥ 8 to ≤ 2048. Black: $|2j/(N+1) - 1|^{5/3}$

Equivalent Ensembles (more) general theory

$E(x)$ observable s.t. $\sum_{j=1}^{N} \partial_j E(x)(Lx)_j = M(x) > 0 \;\; x \neq 0$.
E.g. $L = 1,\; E(x) = \frac{1}{2}\sum_j x_j^2, \Rightarrow M(x) = x^2$.

$$\dot{x}_j = f_j(x) + F_j - \nu (Lx)_j, \qquad \nu > 0,\; j = 1, \ldots, N$$

$$\dot{x}_j = f_j(x) + F_j - \alpha(x)(Lx)_j, \qquad \alpha(x) \stackrel{def}{=} \frac{\sum_{j=1}^{N} F_j \partial_j E}{M(x)}$$

Dissipation balanced on $E(x) \Rightarrow E(x(t)) = const$

Define $\mathcal{E}$ and $\widetilde{\mathcal{E}}$: conjectured is equivalence at large forcing (when both satisfy Chaotic hypothesis for $\langle\, \alpha(x(t))\alpha(x(0))\,\rangle$ is finite).

Lorenz96 is one example
Other examples: NS equation (periodic container $\mathcal{O}$)

with viscosity ν

$$\dot{\vec{u}} + (\vec{u}\cdot\boldsymbol{\partial})\vec{u} = -\boldsymbol{\partial} p + \vec{g} + \nu\Delta\vec{u} = 0, \qquad \boldsymbol{\partial}\cdot\vec{u} = 0$$

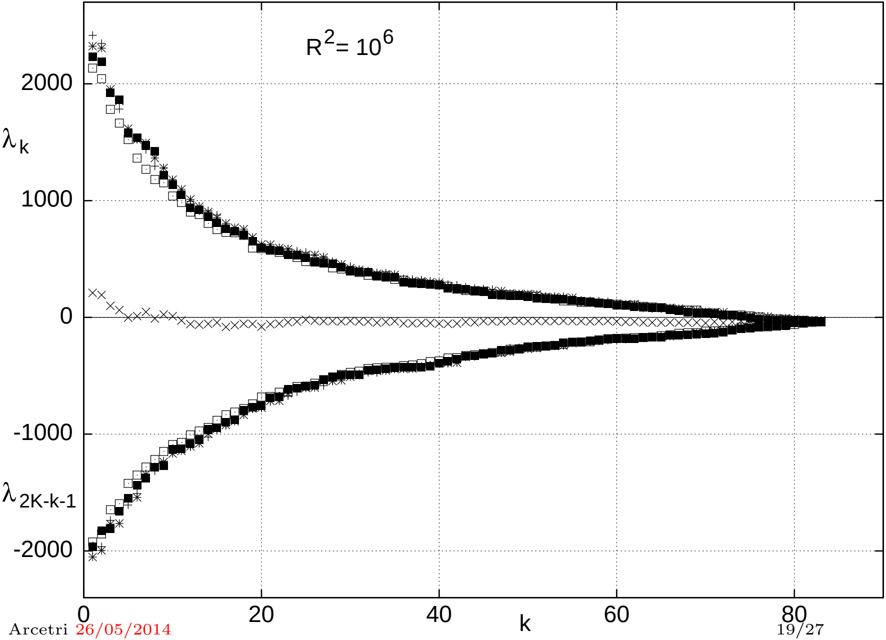
and equivalent eq. balanced on the "dissipation" observable $E(\vec{u}) = \int_{\mathcal{O}} (\partial\vec{u}(x))^2 dx$

$$\dot{\vec{u}} + (\vec{u}\cdot\boldsymbol{\partial})\vec{u} = -\boldsymbol{\partial} p + \vec{g} + \alpha(\vec{u})\Delta\vec{u}, \qquad \boldsymbol{\partial}\cdot\vec{u} = 0$$

$$\alpha(\vec{u}) \stackrel{def}{=} \frac{\sum_{\vec{k}} \vec{k}^2\, \vec{g}_{\vec{k}}\cdot\vec{u}_{-\vec{k}}}{\sum_{\vec{k}} \vec{k}^4 |\vec{u}_{\vec{k}}|^2}, \qquad D = 2$$

If $D = 3$ similar expression (more involved because vorticity is not conserved in inviscid case)

$N = 168$: $R^2 = 10^6$; viscous NS $(+)$,energy $(*)$, enstr $(\boxdot)$



Lyap exps $N = 168$: $R^2 = 10^6$, force on $\pm(4,-3), \pm(3,-4)$

viscous $(+)$ at force on $\pm(4,-3), \pm(3,-4)$
$(\times) = (\lambda_k + \lambda'_k)/2$
energy $(*)$
enstrophy $(\boxdot)$, or
palinstrophy $(\blacksquare)$.

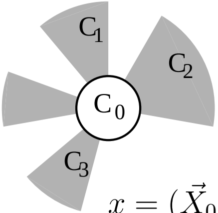
Runs lengths $T \in [125, 250]$, units of $1/\lambda_{max}$, λ_{max}.

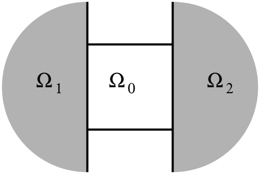
Error bars identified with symbols size.

Overlap of the 4 spectra (approximate, because of numerical fluctuations in quantities that should be exact constants)

NS too $\Rightarrow$ hints at extending equivalence to spectra.

Particle system: thermostats and ensembles





$$x = (\vec{X}_0, \dot{\vec{X}}_0, \vec{X}_1, \dot{\vec{X}}_1, \ldots, \vec{X}_\nu, \dot{\vec{X}}_\nu)$$

Equations of motion

$$m\ddot{\vec{X}}_{0i} = -\partial_i U_0(\vec{X}_0) - \sum^{j>0} \partial_i U_{0,j}(\vec{X}_0, \vec{X}_j) + \partial_i \Psi(\vec{X}_j) + \Phi_i(\vec{X}_0)$$

$$m\ddot{\vec{X}}_{ji} = -\partial_i U_j(\vec{X}_j) - \partial_i U_{0,j}(\vec{X}_0, \vec{X}_j) + \partial_i \Psi(\vec{X}_j)$$

$$U_j(\vec{X}_j) = \sum_{q,q'\in\vec{X}_j} \varphi, \; U_{0,j}(\vec{X}_0, \vec{X}_j) = \sum_{q\in\Omega_0, q'\in\Omega_j} \varphi, \; \Psi(X) = \sum_q \psi(q)$$

Initial state: infinite Gibbs at density δ_j and temp. β_j^{-1}

Time evolution

Thermostats should admit evolution but are ∞

Enclose all particles in a ball Λ_n (side $2^n r_\varphi$) $\Rightarrow$

Then time evolution exists $x \to S_t^{(n,0)} x \Rightarrow$

it should exist also $\lim_{n\to\infty} S_t^{(n,0)} x = S_t^{(0)} x$ **??**

and is thermostats temperature defined for $t > 0$?
More generally are intensive quantities constants of motion?

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} K_{j,\Lambda}(x(t)) = \frac{d}{2}\beta_j^{-1}\delta_j$$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} N_{j,\Lambda}(x(t)) = \delta_j$$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} U_{j,\Lambda}(x(t)) = u_j$$

Temp., density, energy dens. **should** be fixed $\forall t, j > 0$

Entropy production: thermostats entropy increases by

$$\sigma_0(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)}, \qquad Q_j \stackrel{def}{=} -\dot{\vec{X}}_j \cdot \partial_{\vec{X}_j} U_{0,j}(\vec{X}_0, \vec{X}_j))$$

Alternative models (Λ_n–regularized thermostats)

$$m\ddot{\vec{X}}_{0i} = -\partial_i U_0(\vec{X}_0) - \sum^{j>0} \partial_i U_{0,j}(\vec{X}_0, \vec{X}_j) + \partial_i \Psi(\vec{X}_j) + \Phi_i(\vec{X}_0)$$

$$m\ddot{\vec{X}}_{ji} = -\partial_i U_j(\vec{X}_j) - \partial_i U_{0,j}(\vec{X}_0, \vec{X}_j) + \partial_i \Psi(\vec{X}_j) - \alpha_{j,n}\dot{\vec{X}}_{ji}$$

With $\alpha_{j,n}$ s.t. $U_{j,\Lambda_n} + K_{j,\Lambda_n} = E_{j,\Lambda_n}$ is exact constant

$$\alpha_{j,n} \stackrel{def}{=} \frac{Q_j}{d\, N_j k_B T_j(x)}, \qquad Q_j \stackrel{def}{=} -\dot{\vec{X}}_j \cdot \partial_j U_{0,j}(\vec{X}_0, \vec{X}_j)$$

with $m\dot{\vec{X}}_j^2 \stackrel{def}{=} 2K_{j,\Lambda_n}(x) \stackrel{def}{=} d\, N_j k_B T_j(x)$= Thermostats temperature

Entropy

$$Q_j \stackrel{def}{=} -\dot{\vec{X}}_j \cdot \partial_{\vec{X}_j} U_{0,j}(\vec{X}_0, \vec{X}_j), \quad \textit{heat}$$

$$\sigma_0(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)}, \quad \textit{Hamiltonian entropy production}$$

$$\sigma(\mathbf{x}) = \sum_{\mathbf{j>0}} \frac{\mathbf{Q_j}}{\mathbf{k_B T_j(x)}} + \beta_{\mathbf{0}}(\dot{\mathbf{K}}_{\mathbf{0}} + \dot{\mathbf{U}}_{\mathbf{0}} + \dot{\mathbf{\Psi}}_{\mathbf{0}}) \stackrel{\mathbf{def}}{=} \sigma_{\mathbf{0}}(\mathbf{x}) + \dot{\mathbf{F}}(\mathbf{x})$$

Theorem (Presutti, G): *with* μ_0*–probability* $1, \forall t > 0$

$$\lim_{n\to\infty} S_t^{(n,1)} x = \lim_{n\to\infty} S_t^{(n,0)} x, \quad \frac{d\mu_t(dx)}{dt} = -\sigma(x)\,\mu_t(dx)$$

Remarkable: *Entropy production* = *volume contraction* + *a time derivative*: possible to define entropy prod. in Hamilt. context: it coincides with the definition of entropy as phase space contraction ("up to a derivative", of course)

Equivalence? (in therm. lim. $\Lambda_n \to \infty$)

Idea: $Q_j \stackrel{def}{=} -\dot{\vec{X}}_j \cdot \partial_j U_{0,j}(\vec{X}_0, \vec{X}_j)$ is $O(1)$
(Williams,Searles,Evans 2004)

hence $\alpha_{\mathbf{j}} = \frac{\mathbf{Q_j}}{\mathbf{d\,N_j k_B T_{j,n}(x)}} \Rightarrow 0$ as $n \to \infty$.

But is $T_{j,n}(x) \geq c > 0$ **??**

Theorem (Presutti, G): *with μ_0–probability* 1

$\frac{\mathbf{K_{j,\Lambda_n}(x)}}{|\mathbf{\Lambda_n \cap \Omega_j}|} \geq \frac{1}{4}\, d\, \delta_j\, k_B T_j$ *(hence $\alpha \xrightarrow[n\to\infty]{} 0$).*

Entropy production = volume contraction + a time derivative

In nonequilibrium several quantities are defined up to an additive time derivative, as in equilibrium several quantities are defined up to a an additive constant

Macroscopic constants of motion

$\Rightarrow$ (average of σ) $\equiv$ (average of σ_0)

All this **provided** $\beta_j(x)$ is a constant of motion as $n \to \infty$ and $\beta_j(S_t x) = \beta_j$

In other words: very generally phase space contraction can be identified with physically defined entropy production.

Theorem: *Let Γ be a pair potential and $\varphi + \varepsilon\Gamma$ be superstable for $|\varepsilon|$ small and $P(\varphi + \varepsilon\Gamma)$ (twice) differentiable at $\varepsilon = 0$ (i.e. "no phase trans."))*

$$g(S_t x) \stackrel{def}{=} \lim_{\Lambda_n \to \infty} \frac{1}{\Lambda_n \cap \Omega_j} \sum_{q,q' \in x} \Gamma(q(t) - q'(t)) = g$$

with μ_0-probability 1 and for all $t > 0$: i.e. $g(x)$ constant of motion.

$\Rightarrow$ Infinitely many constants of motion.

References [1, 2]

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