Anomalous and standard behaviour with and without chaos in 1-d

Lamberto Rondoni – Politecnico di Torino

A. Gamba, C. Giberti, C. Paneni, D. Searles, C. Vernia

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http://www.rarenoise.lnl.infn.it/

Outline

Usually one assumes that the macroscopic irreversible behaviour emerges from deterministic reversible microscopic dynamics, which appears stochastic at the mesoscopic level of observation, thanks to some form of microscopic *chaos*.

At the mesoscopic level of observation, irregular microscopic motions are perceived as noise (Onsager-Machlup), if mesoscopic scales are well sperated from microscopic and macroscopic ones.

Mesoscopic behaviour is characterized by irreversibility and fluctuations.

Which form of microscopic chaos is required?
It depends on property of interest.
It depends on kind of interactions.

Bertini, De Sole, Gabrielli, Jona-Lasinio, Landim generalize Onsager-Machlup to fluctuations of nonequilibrium steady states of Markov processes in Local Equilibrium (JSP **107**, 635 (2002)).
Claims of wide applicability.

Consider stochastic particle systems with hydrodyamic description for vector of macroscopic observables

$$\partial_t \varrho = \nabla \cdot [D(\varrho) \nabla \varrho] \equiv \mathcal{D}(\varrho)$$
$$\varrho = \varrho(x, t)$$

whose evolution tends to unique steady state $\bar{\varrho}$.

Theory asserts that spontaneous fluctuations are governed by **adjoint** hydrodynamic equation:

$$-\partial_t \varrho = \mathcal{D}^* (\varrho)$$

Then, provided $\mathcal{D}$ decomposes as

$$\mathcal{D}(\varrho) = \frac{1}{2}\nabla \cdot \left(\chi(\varrho) \nabla \frac{\delta \mathcal{S}}{\delta \varrho} \right) + \mathcal{A}$$

where $\mathcal{S}$ is the entropy, χ Onsager's matrix, and $\mathcal{A}$ a non-dissipative ($\perp$ thermodynamic force) term, one has

$$\mathcal{D}^* (\varrho) = \mathcal{D} (\varrho) - 2\mathcal{A}$$

Question: can nonequilibrium deterministic reversible dynamics lead to $\mathcal{D}^* \neq \mathcal{D}$, for the fluctuations of certain observabels?

Consider $\varrho = n$-dimensional vector with
deterministic, reversible, dissipative dynamics:

$$\dot{\varrho} = \mathcal{D}(\varrho) \ ,$$

where $\mathcal{D} =$ is a vector field with one attracting fixed point $\hat{\varrho}$
(and one repelling fixed point), and
$\varrho_i(t) =$ observable in position i
$\hat{\varrho} =$ steady state.

Add Gaussian noise: $\dot{\varrho} = \mathcal{D}(\varrho) + \xi$

$\langle \xi(t) \rangle = 0,$
$\langle \xi_i\,(t)\,\xi_j\,(t') \rangle = K_{ij}\delta\,(t - t');$ K symmetric, positive definite.

As in O-M, most likely path yields hydrodynamics, in $n \to \infty$ limit.

Decompose deterministic part, $\mathcal{D}$, in two contributions:

- time-odd, contributing to transport;
- time-even, not contributing to transport.

$$\mathcal{D}(\varrho) = -\frac{1}{2} K \nabla_\varrho V(\varrho) + \mathcal{A}(\varrho), \quad \langle K \nabla_\varrho V, \mathcal{A} \rangle = 0$$

∇_ϱ = differentiation w.r.t. components of ϱ.

$\nabla_\varrho V$ = thermodynamic force.
$\hat{\varrho}$ minimizes V

K = Onsager matrix (with derivatives).
$\langle x, y \rangle = x^T K^{-1} y$;

Probability of path γ from ϱ^i to ϱ^f: $P(\gamma) \propto \exp\left\{-J_{[t_i,t_f]}(\varrho)\right\}$

$$J_{[t_i,t_f]}(\varrho) = \frac{1}{2}\int_{t_i}^{t_f} \left\langle \dot{\varrho} + \frac{1}{2}K\nabla_\varrho V - \mathcal{A}, \dot{\varrho} + \frac{1}{2}K\nabla_\varrho V - \mathcal{A} \right\rangle \mathrm{d}t$$

$$= \frac{1}{2}\int_{t_i}^{t_f} \left\langle \dot{\varrho} - \frac{1}{2}K\nabla_\varrho V - \mathcal{A}\,,\ \dot{\varrho} - \frac{1}{2}K\nabla_\varrho V - \mathcal{A} \right\rangle \mathrm{d}t + \left[V^f - V^i\right]$$

Minimization leads to laws for relaxation and for fluctuation paths:

$$\dot{\varrho} = \mathcal{D}(\varrho) = -\frac{1}{2}K\nabla_\varrho V + \mathcal{A}(\varrho)$$

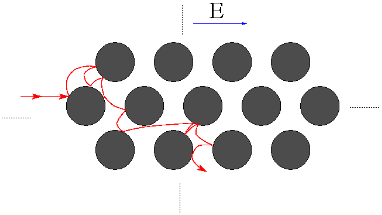
$$-\dot{\varrho} = \mathcal{D}^*(\varrho) = -\frac{1}{2}K\nabla_\varrho V - \mathcal{A}(\varrho)$$

Asymmetry (not present in O-M) due to

time reversal parity of non-dissipative term $\mathcal{A}$.

Nonequilibrium Lorentz Gas

$\dot{\mathbf{x}} = \mathbf{p}$; $\quad \dot{\mathbf{p}} = \varepsilon \hat{\mathbf{x}} - \alpha \mathbf{p} \quad \alpha = \varepsilon p_x$



Dissipative, TRI;

for small ε: hyperbolic, ergodic measure weighs differently trajectories with opposite currents:

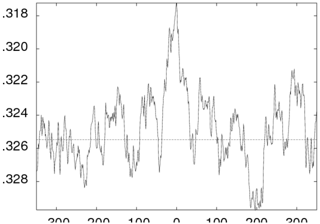
temporal symmetry broken on statistical level.

Phase space graining $\Rightarrow$ conjugation with Markov process.

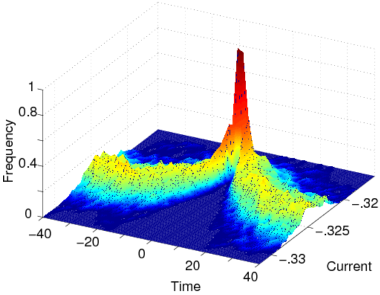
No results on symmetry of generator of Markov chain, which, in any case,

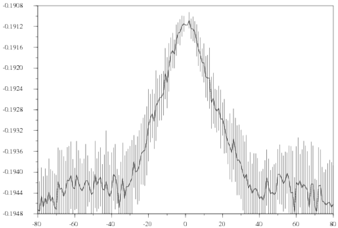
concerns phase space, not real space.

Current fluctuations



No asymmetry of most likely path





$$J(t) = \sum_{i=1}^{N} \frac{p_{i,x}}{N} \ , \quad \mathbf{p}_i = (p_{i,x}, p_{i,y}) \ , \quad p_{i,x}^2 + p_{i,y}^2 = 1$$

Between collisions $\dot{p}_{i,x} = \varepsilon \left(1 - p_{i,x}^2\right)$ and

$$\dot{J} = \varepsilon \left(1 - NJ^2\right) + \frac{\varepsilon}{N} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} p_{i,x} p_{j,x}$$

If collisions only produce noise, randomizing the p's, large N deterministic part of dynamics is (correlation term vanishes):

$$\dot{J} \approx \varepsilon \left(1 - NJ^2\right)$$

with attractor $\hat{J} = 1/\sqrt{N}$, repeller $\tilde{J} = -1/\sqrt{N} \Longrightarrow \mathcal{A} = 0$

Peculiar situation for symmetric paths.

Chaos not sufficient; correlations, hence interactions, needed.

Nonequilibrium FPU chain of Lepri, Livi, Politi (Phys. D 1998);
chaos and correlations due to interactions:

$$q_0 = q_{N+1} = 0; \qquad \ddot{q}_l = f_l - f_{l+1}, \quad l = 2, \ldots N$$

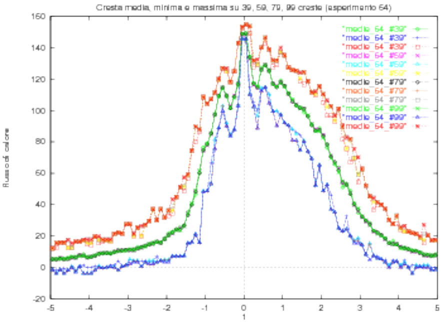
$$f_l = -V'(q_l - q_{l-1}); \quad V(x) = \frac{x^2}{2} + \beta \frac{x^4}{4}$$

$$\ddot{q}_1 = -\zeta_L \dot{q}_1 + f_1 - f_2; \quad \ddot{q}_N = -\zeta_R \dot{q}_N + f_N - f_{N+1}$$

ζ_L, ζ_R Nosé-Hoover at different T and equal response time.

High frequency modes like stochastic perturbation.

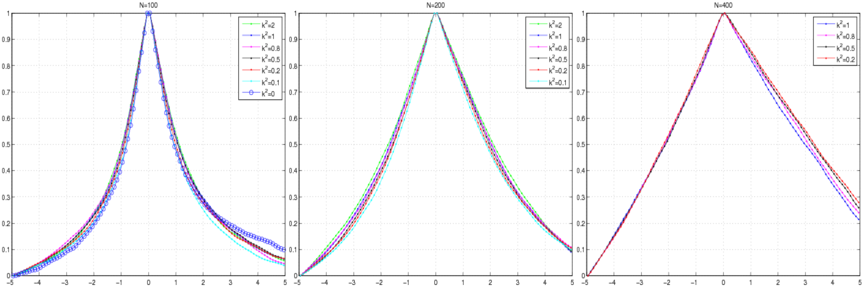
Local heat flux
$N = 66$
$T_R = 20$
$T_L = 70$
J on 10 sites
threshold: 3σ



Average, maximum and minimum envelope of crests of 39, 59, 79 and 99 histograms.
Each histogram from $\approx 2.5 \cdot 10^4$ paths.

Clear asymmetry; it suffices to consider mean fluctuation.

What about other interactions? E.g. hard instead of x^4 potential:

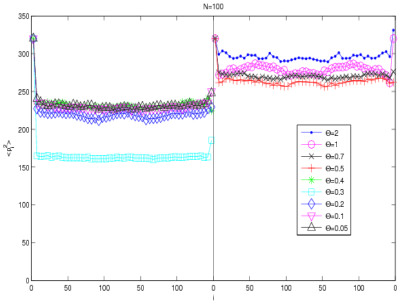


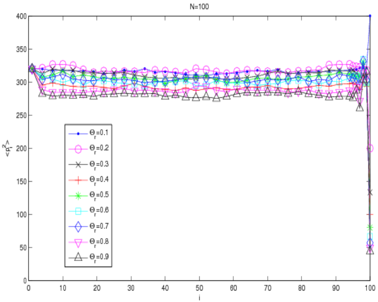
Average fluctuations of density in center of chains, for $N = 100$, $N = 200$, $N = 400$, and different values of elastic constant, k^2.

Fluctuations temporally asymmetric and not sensibly affected by the value of k^2.

Harmonic chain temperature profile in nonequilibrium steady state.

Strong particle-thermostat coupling for small relaxation time θ.





Local virial property holds.

Decreasing θ settles profile much closer to T_ℓ than T_r.

Discontinuity between $\theta = 0.5$ and $\theta = 0.3$.

$\theta = 0.3$ leads to bulk profile at $(T_\ell + T_r)/2$ as in RLL.

With $\theta_\ell = 1$ and decreasing θ_r, system equilibrates with hot thermostat independently of θ_r.

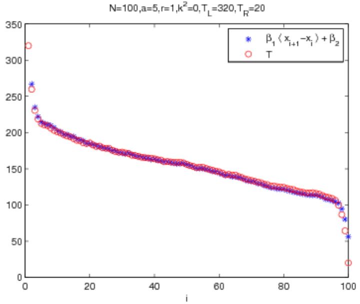
Pure harmonic chains without thermostats are hamiltonian, integrable, Lyapunov exponents vanish. With $T_r = 20$ and T_ℓ:

T_ℓ	λ_1	$\langle\chi\rangle$
420	$.00771 \pm 0.5(-4)$	2.7988
370	$.00769 \pm 0.6(-4)$	2.5737
320	$.00779 \pm 0.7(-4)$	2.3382
220	$.00792 \pm 0.5(-4)$	1.7644
120	$.00928 \pm 0.1(-3)$	1.0726
80	$.01101 \pm 0.1(-3)$	0.7194
50	$.01338 \pm 0.2(-3)$	0.3775
20	$.01328 \pm 0.1(-3)$	6.5453e-005

$N = 100$, $k^2 = 1$, largest Lyapunov exponent is positive and decreases, average phase space contraction rate grows with T_ℓ.

λ_1 and $\langle \chi \rangle$ for hard particles with $k^2 = 0$, $N = 100$ and $T_r = 20$. Integrable case without thermostats.

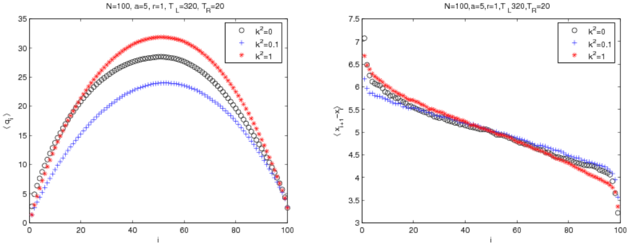
T_ℓ	λ_1	$\langle \chi \rangle$
320	.01641	8.41388
220	.01931	4.93916
120	.01978	2.05788
80	.02441	1.02030
50	.02983	0.33846
20	.03157	0.04161



Chaotic like in purely harmonic cases, but here a nonequilibrium temperature profile sets in.

Chaos (and virial property) insufficient for local equilibrium.

LTE? Fourier law? Peculiarities of 1-d systems: definitions based on small fluctuations about equilibrium positions frustrated by $O(N)$ fluctuations. Also temperature gradients yield large mean displacements from equilibrium positions.



Nonequilibrium induces asymmetry: particles shift towards cold side: density gradient, hence pressure gradient.

Inverse mass density, may be correlated to kinetic temperature.

In steady state:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[\kappa(x)\frac{\mathrm{d}\,T}{\mathrm{d}x}\right] = 0 \ , \quad \text{i.e.} \quad \frac{\mathrm{d}\,T}{\mathrm{d}x} = \frac{\mathrm{C}_1}{\kappa(x)}$$

As $\langle q_i \rangle$ approximated by parabola, try q_ℓ, q_r small > 0 in

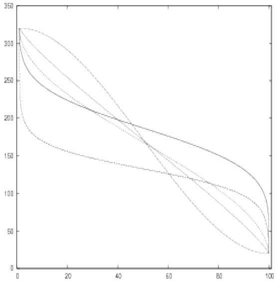
$$\kappa(x) \propto [(x - q_\ell)(N + q_r - x)]^\alpha$$

E.g. $\alpha = 1$:

$$T(x) = C_1 \log \frac{x - q_\ell}{N + q_r - x} + C_2$$

In general:

$$\overline{\kappa} = \frac{1}{N}\int_0^N \kappa(x)\ \mathrm{d}x \sim N^{2\alpha}$$



Discussion

1. Chaos not fundamental in 1-d. In NESS, hard collisions occur practically randomly; break correlations favouring standard behaviour more efficiently than generic chaos.
2. Temperature gradients alter bulk behaviour, even when it resembles noninteracting particles. Robust nonlocality in NESS.
3. Asymmetric fluctuation paths ubiquitous in deterministic TRI dynamics with proper interactions. Microscopic theory? Attempt in terms of correlation functions in PSR 2008.
4. Assuming Fourier's law, thermal conductivity divergence related to deviations of positions from equilibrium.
5. Strong dependence on microscopic dynamics: no genuine LTE (as in stochastic systems). May be typical of 1-d.
6. Experimental consquences.

GaR Phys.A 04; GiRV Phys.A 06, Phys.D 07; PSR JCP 06, 08