New concepts emerging from a linear response theory for nonequilibrium

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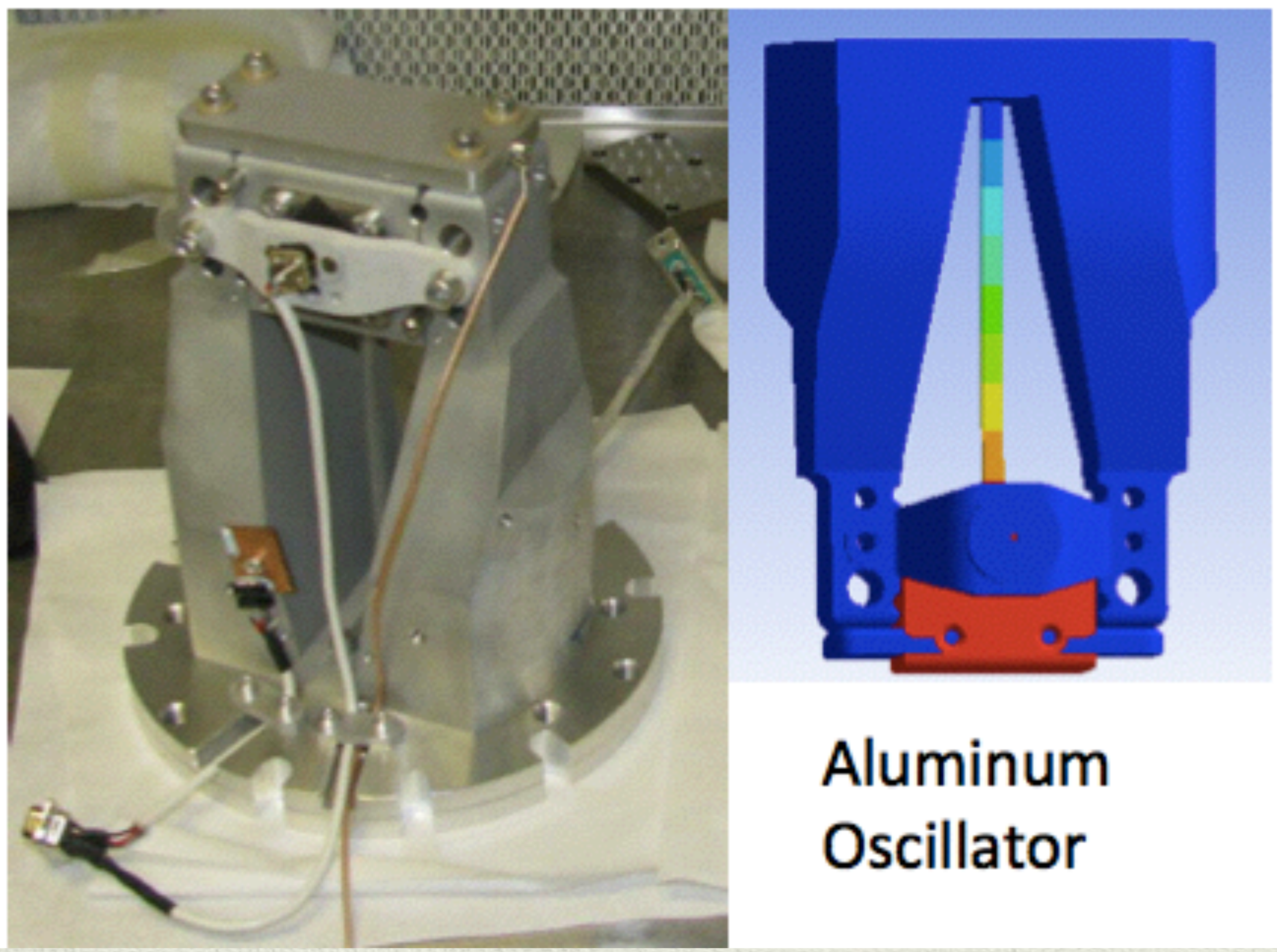
Overview

- Linear response
- Linear response to temperature kicks
- Entropy production and *something else*
- Time-symmetric quantities: how many?

A macroscopic FPU?

- capacitive readout of oscillator vibration
- Possibility to apply thermal gradient



Livia Conti, Lamberto Rondoni, et al: www.rarenoise.lnl.infn.it

Linear response for FPU?

- How does a Fermi-Pasta-Ulam chain react to a change in one temperature?
- Nonequilibrium specific heat $\neq$ variance of the energy
- Compressibility in nonequilibrium?

Fluctuation-Dissipation Th.: Kubo

$$\frac{d\langle A(t)\rangle}{dh_s} = \frac{1}{T}\frac{d}{ds}\langle A(t)V(s)\rangle \qquad E \to E - h_s V$$

- An observable A(t) reacts to the appearance of a potential V(s)
- $\frac{1}{T}\frac{d}{ds}V(s)$ is the entropy production from -V

Out of equilibrium: many FDT

- a1) perturb the density of states and evolve (Agarwal, Vulpiani & C, Seifert & Speck, Parrondo &C,…)
- a2) "bring back" the observable to the perturbation (Ruelle)
- b) probability of paths (Cugliandolo &C, Harada-Sasa, Lippiello &C, Ricci-Tersenghi, Chatelain, Maes, …)
- short review: Baiesi & Maes, New J. Phys. (2013)

Path probability (Markov), $P(\omega)$

$$\omega \to \{x_s\} \quad \text{for} \quad 0 \leq s \leq t$$

- Overdamped Langevin

$$dx_s = \mu\, F(s)\, ds + \sqrt{2\mu T}\; dB_s$$

- Discrete states C, C′, …with jump rates

$$W(C \to C')$$

Diffusion

- Probability of a sequence $dx_0, dx_1, dx_2, \ldots$

$$dP_i = (2\pi dt)^{-1/2} \exp\left\{\frac{(dB_i)^2}{2dt}\right\}$$

$$= (4\pi\mu T dt)^{-1/2} \exp\left\{\frac{[dx_i - \mu F(i)]^2}{4\mu T dt}\right\}$$

$$P(\omega) = \lim_{dt\to 0} \Pi_i dP_i$$

Diffusion + perturbation

$$dx_s = \mu\, F(s)\, ds + h_s \mu \frac{\partial V}{\partial x}(s) ds + \sqrt{2\mu T}\; dB_s$$

- Perturbation changes the path probability
- Ratio of path probabilities is finite for $dt \to 0$

$$\frac{P^h(\omega)}{P(\omega)}$$

Susceptibility (h>0 for s>0)

Generator

$$\frac{P^h(\omega)}{P(\omega)} = \exp\left\{ \frac{h}{2T}[V(t) - V(0)] - \frac{h}{2T}\int_0^t \boxed{L} V(s)ds \right\}$$

$$\langle A(t)\rangle^h - \langle A(t)\rangle = \left\langle A(t)\left[\frac{P^h(\omega)}{P(\omega)} - 1\right]\right\rangle$$

- Susceptibility

$$\chi_{AV}(t) = \lim_{h\to 0} \frac{\langle A(t)\rangle^h - \langle A(t)\rangle}{h}$$

Markov generator

- In this case: $$L = \mu F \frac{\partial}{\partial x} + \mu T \frac{\partial^2}{\partial x^2}$$

$$\langle LV \rangle = \frac{d}{dt} \langle V \rangle$$

- interpret as expected variation:

$$LV(x) = \left\langle \frac{dV}{dt} \right\rangle \Big|_x$$

Response function

$$\chi_{AV}(t) = \int_0^t R_{AV}(t,s)ds$$

$$R_{AV}(t,s) = \frac{1}{2T}\left[\frac{d}{ds}\langle V(s)A(t)\rangle - \langle LV(s)A(t)\rangle\right]$$

- 1/2 entropy production
- minus 1/2 “expected” entropy production

Response function

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Entropic term

Frenetic term

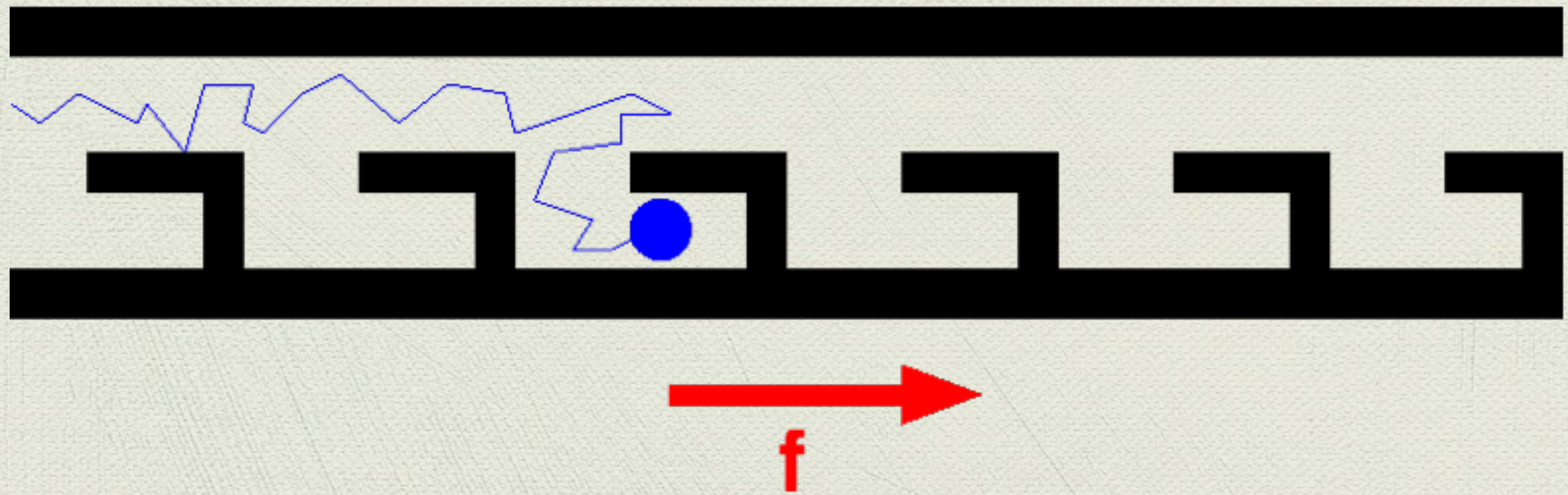
Baiesi, Maes, Wynants, PRL (2009)
Lippiello, Corberi, Zannetti, PRE (2005)

Negative response

- The sum of the two terms may be <0

$$R_{AV}(t,s) = \frac{1}{2T}\left[\frac{d}{ds}\langle V(s)A(t)\rangle - \langle LV(s)A(t)\rangle\right]$$

- Example: negative mobility for strong forces



Baerts, Basu, Maes, Safaverdi, PRE (2013)

Negative mobility

Giant Negative Mobility of Janus Particles in a Corrugated Channel

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(Dated: May 29, 2014)

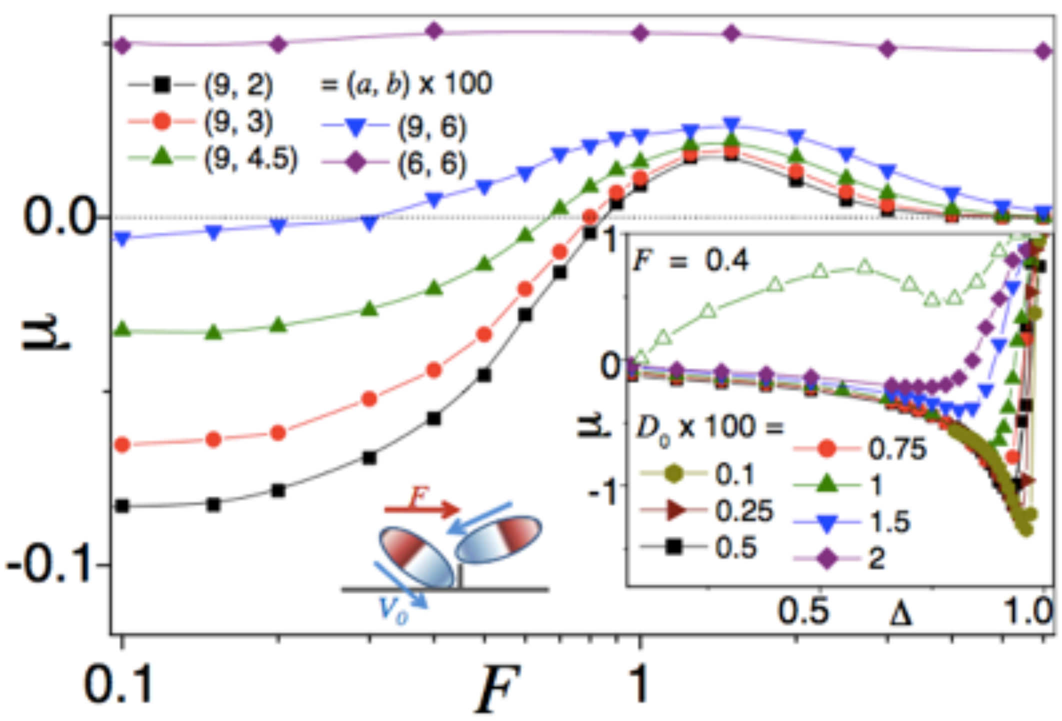

FIG. 2: (Color online) Mobility $\mu(F)$ of a prolate JP driven along a septate channel for different values of its semiaxes a and b (see legend). Compartment parameters: $x_L = y_L = 1$ and $\Delta = 0.16$; self-propulsion parameters: $v_0 = 1$ and $D_\theta = D_0 = 0.03$. Inset: μ vs Δ for $F = 0.4$, $a = 0.09$, $b = 0.03$ and different D_0 (solid symbols). The curve (empty triangles) for the oblate JP with $a = 0.03$, $b = 0.09$ at $D_0 = 0.01$ is plotted for comparison. All the remaining parameters are as in the main panel. Sketch: a prolate JP tumbling over a winglet of the channel wall under the action of the drive (see text).

- The structure of R(t,s) is different for inertial systems
- Achieved in a standard path-space comparison, with different drift terms (Radon-Nicodym derivative, Girsanov Th.)

$$dx_s = \boxed{\mu\, F(s)\, ds} + \sqrt{2\mu T}\; dB_s$$

- The structure of R(t,s) is different for inertial systems
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What happens if we change the noise term?

Mathematical problem

- The response to T kicks involves changing the noise term!
- $\dfrac{P^h(\omega)}{P(\omega)}$ not well defined for different noises
- However: we are interested in the limit h—> 0

T(1+h), small deviation from T

$$\frac{dP_t^h}{dP_t} = (2\pi T(1+h)dt)^{-1/2} \exp\left\{ -\frac{[dx_t - \mu F(t)dt]^2}{4\mu T(1+h)dt}) \right\} / dP_t$$

$$= \exp\left\{ \frac{h}{2T} \left[\boxed{-T + \frac{(dx_t)^2}{2\mu dt}} + \frac{\mu}{2} F^2(t)dt + \mu T \frac{\partial F}{\partial x}(t)dt - F(t) \circ dx_t \right] \right\}$$

Dangerous term (mathematically)

entropy production, as before

new terms

$$= \exp\left\{ \frac{h}{2}[dS - B_S\, dt] + \frac{h}{2}[dM - B_M\, dt] \right\}$$

Four terms:

heat flux / temperature

- Entropy production $$dS(t) = \boxed{\frac{dQ(t)}{T}} = -\frac{1}{T}F(t) \circ dx_t$$
- Expected entropy production $$B_S(t)dt = \boxed{-\frac{\mu}{T}\left[F^2(t) + T\frac{dF}{dx}(t)\right]dt}$$

[Sekimoto, Stochastic Energetics]

- Activity (?) $$dM(x_t) \equiv \frac{1}{T}\left[\frac{(dx_t)^2}{2\mu dt} - T\right]$$
- Expected activity (?) $$B_M(t)dt \equiv \langle dM\rangle(x_t) = \frac{\mu}{2T}F^2(t)dt$$

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Time symmetric

- Activity (?) $$dM(x_t) \equiv \frac{1}{T}\left[\frac{(dx_t)^2}{2\mu dt} - T\right]$$
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Dynamical activity

- Very relevant in kinetically constrained models
- Count the **number** of jumps between states
- time-symmetric quantity

Lecomte, Appert-Rolland, van Wijland, PRL (2005)
Merolle, Garrahan, D. Chandler, PNAS (2005)

Relation with activity

- The $(dx)^2$ term should scale as the number of successful jumps in an underlying random walk description

Susceptibility

Susceptibility

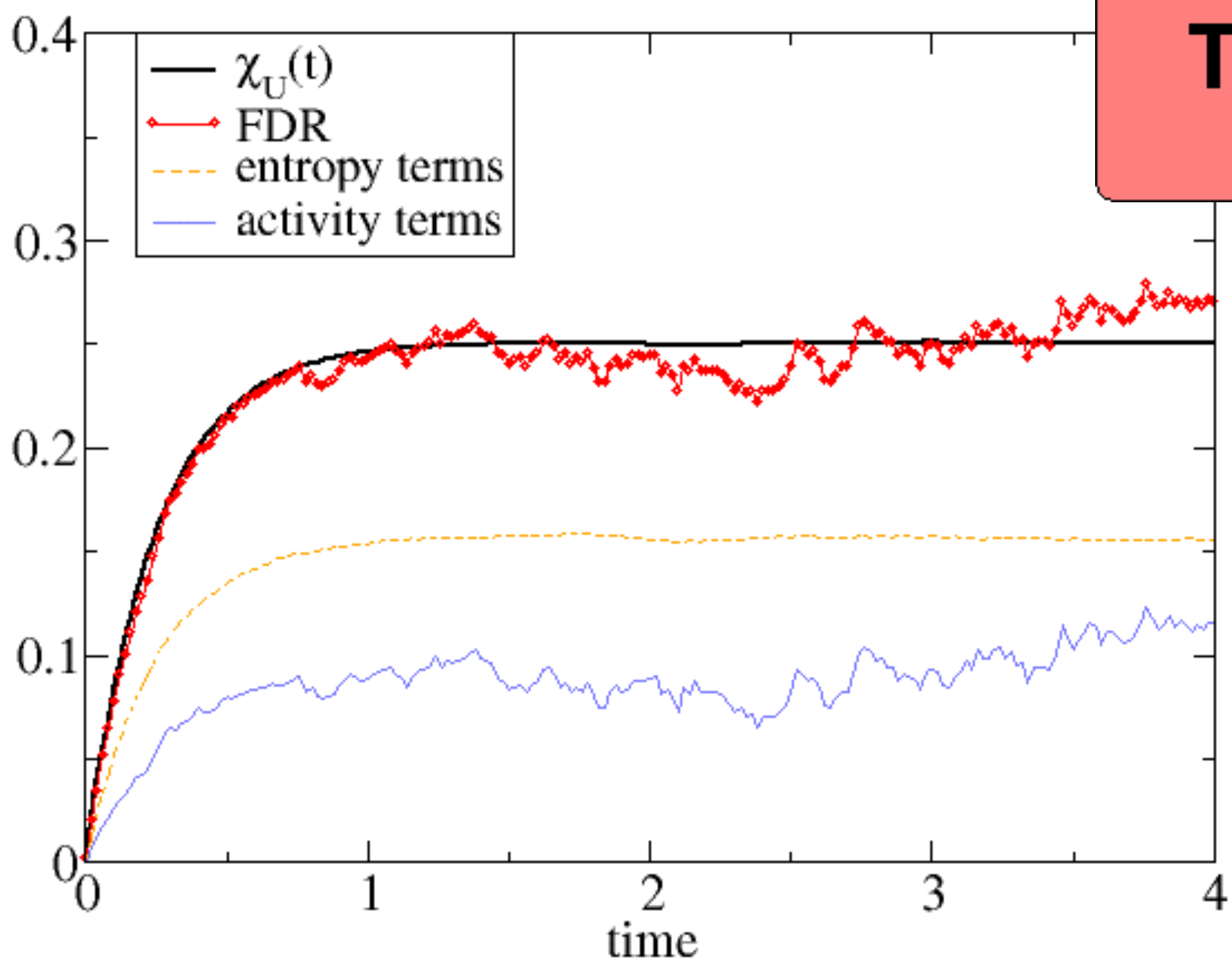
$$\chi_A(t) = \frac{1}{2T}\left\langle A(t)\left[\underbrace{S(t)}_{\text{antisymmetric (entropy produced)}} \underbrace{- \int_0^t B_S(s)ds + M(t) - \int_0^t B_M(s)ds}_{\text{symmetric terms (frenetic contributions + activity)}}\right]\right\rangle$$

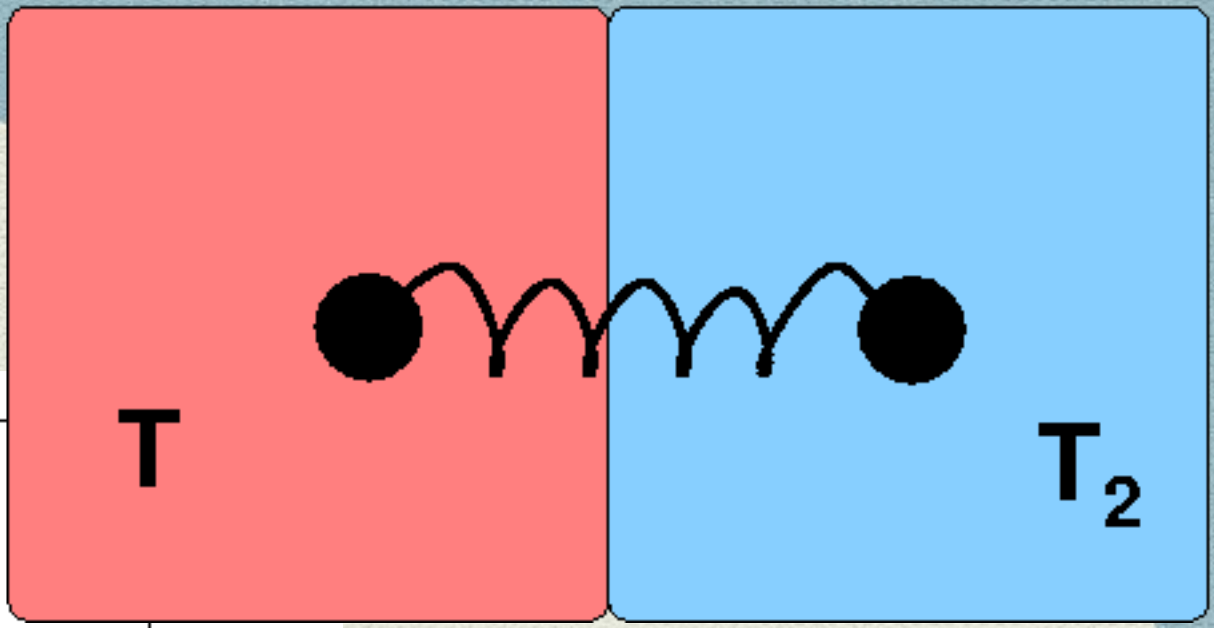
antisymmetric
(entropy produced)

symmetric terms
(frenetic contributions + activity)

Example: harmonic spring

- Susceptibility of the internal energy





Inertial dynamics

$$dx_t = v_t dt$$

$$m\, dv_t = F(x_t)dt - \gamma v_t dt + \sqrt{2\gamma T}\, d\mathcal{B}_t$$

- Harada-Sasa/stochastic energetics for the entropy production terms

$$T\, dS(x_t, v_t) = m v_t \circ dv_t - F(x_t) v_t dt$$

$$T\, B_S(x_t, v_t) = \frac{\gamma}{m}[T - m v_t^2]$$

Harada-Sasa for transients/jumps: Lippiello, Baiesi, Sarracino, PRL (2014)

Inertial dynamics

$$T\, dM(x_t, v_t) = \frac{(m\, dv_t)^2}{2\gamma dt} - T - \frac{m}{\gamma} F(x_t) dv_t$$

$$T\, B_M(x_t, v_t) = \frac{\gamma}{2}\left[v_t^2 - \left(\frac{F(x_t)}{\gamma}\right)^2\right]$$

Susceptibility

$$\chi_A(t) = \frac{1}{2T}\left\langle A(t)\left[S(t) - \int_0^t B_S(s)ds + M(t) - \int_0^t B_M(s)ds\right]\right\rangle$$

antisymmetric

symmetric terms

Conclusions

- General scheme: probability of trajectories -> physics
- Time-symmetric quantities in response formulas
- Not only dissipation, but also “activation”
- Name(s): dynamical activity, frenesy, traffic, …
- Attempt to compare trajectories with different T