Stochastic thermodynamics and martingale theory for a model physical system of particles

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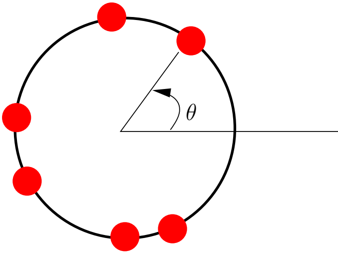
- Simone Pigolotti (OIST, Japan)
- Édgar Roldán (ICTP, Italy)
- Stefano Ruffo (SISSA, Italy)

References:

- J. Stat. Phys. **143**, 543 (2011); J. Stat. Mech.: Theory Exp. P11003 (2013); EPL **113**, 60008 (2016); EPL **124**, 60006 (2018)

Model

- N interacting point particles on a circle:
  Confg. $\mathcal{C} \equiv \{\theta_i\}$
- Long-ranged interparticle potential:
  $\mathcal{V}(\mathcal{C}) \equiv \frac{1}{2N} \sum_{i,j=1}^{N} [1 - \cos(\theta_i - \theta_j)]$
- Potential due to external field h:
  $\mathcal{V}_{\mathrm{ext}}(\mathcal{C}; h) \equiv -h \sum_{i=1}^{N} \cos \theta_i$
- Net potential $V(\mathcal{C}; h) = \mathcal{V} + \mathcal{V}_{\mathrm{ext}}$



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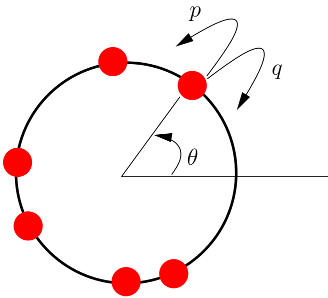
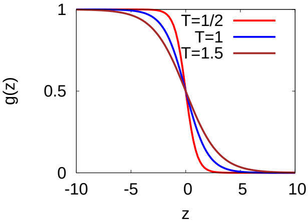
- Dynamics: Stochastic Markovian at temperature $T = 1/\beta$
  1. Every particle in time $\mathrm{d}t$ *attempts* to hop by amount $0 < \phi < 2\pi$:
     (i) $\theta_i \to \theta_i + \phi$ with prob. p
     (ii) $\theta_i \to \theta_i - \phi$ with prob. $1-p$
  2. New position accepted with probability $g(\Delta V(\mathcal{C}))\mathrm{d}t$, where
     $$g(z) = (1/2)[1 - \tanh(\beta z/2)]$$
  3. N attempted hops $\equiv 1$ time step





(Gupta, Dauxois, Ruffo (2011)

Fokker-Planck limit and stationary state

- Fokker-Planck limit $\phi \ll 1$
- $N \to \infty$: motion of a single particle in a self-consistent mean field

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = (2p-1)\phi - \frac{\phi^2\beta}{2}\frac{\partial\langle v\rangle[\rho](\theta;h)}{\partial\theta} + \phi\eta(t)$$

  Gaussian, white noise: $\overline{\eta(t)} = 0$, $\overline{\eta(t)\eta(t')} = \delta(t-t')$

- Time evolution of the single-particle distribution

$$\frac{\partial\rho}{\partial t} = -\frac{\partial}{\partial\theta}\left[\left((2p-1)\phi - \frac{\phi^2\beta}{2}\frac{\partial\langle v\rangle[\rho](\theta;h)}{\partial\theta}\right)\rho\right] + \frac{\phi^2}{2}\frac{\partial^2\rho}{\partial\theta^2}$$

- $\langle v\rangle[\rho](\theta;h) \equiv -m_x[\rho]\cos\theta - m_y[\rho]\sin\theta - h\cos\theta$ is the mean-field potential

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- $\langle v\rangle[\rho](\theta;h) \equiv -m_x[\rho]\cos\theta - m_y[\rho]\sin\theta - h\cos\theta$ is the mean-field potential
- Self-consistent mean fields $(m_x[\rho], m_y[\rho]) \equiv \int \mathrm{d}\theta\ (\cos\theta, \sin\theta)\rho(\theta,t)$
- Exact stationary state

$$\rho_{\rm ss}(\theta;h) = \rho_{\rm ss}(0;h)e^{-g(\theta)}\left[1 + (e^{-\frac{4\pi(2p-1)}{\phi}} - 1)\frac{\int_0^\theta \mathrm{d}\theta' e^{g(\theta')}}{\int_0^{2\pi}\mathrm{d}\theta' e^{g(\theta')}}\right];$$

$g(\theta) \equiv -2(2p-1)\theta/\phi + \beta\langle v\rangle[\rho_{\rm ss}](\theta;h)$;

$\rho_{\rm ss}(0;h)$ fixed by normalization $\int_0^{2\pi}\mathrm{d}\theta\ \rho_{\rm ss}(\theta;h) = 1$

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- 1. $p = 1/2 \Rightarrow$ Equilibrium stationary state $\rho_{\mathrm{ss}} \propto \exp(-\beta\langle v\rangle)$
  2. $p \neq 1/2 \Rightarrow$ Nonequilibrium stationary state

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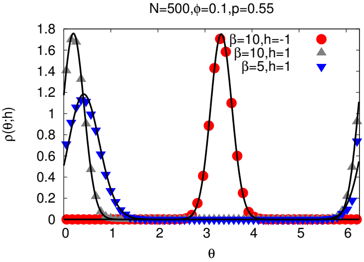
- Numerical check: Measure $m_{x,y}$ in simulations



Equilibrium initial condition: Work done by external field

- Start in equilibrium at $h = h_0$
- Change field in time over duration $\tau \ll \tau_{\mathrm{eq}}$;
  at the α-th time step: $h_\alpha = h_0 + \Delta h \, \alpha/\tau$
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- Reverse protocol:
  system in equilibrium at h_τ, then change h as $h_\alpha = h_\tau - \Delta h \; \alpha/\tau$;

$$W_{\rm R} = \frac{1}{\tau} \sum_{\alpha=1}^{\tau} \sum_{i=1}^{N} \cos\theta_i^{(\alpha)}$$

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-
  1. $\{\theta_i^{(\alpha)}\}_{\rm F}$ and $\{\theta_i^{(\alpha)}\}_{\rm R}$ different due to initial conditions and stochastic evolution
  2. $W_{\rm F} \propto N$ and $W_{\rm R} \propto N$
  3. Different distributions for work per particle: $P_{\rm F}(W_{\rm F}/N)$ and $P_{\rm R}(W_{\rm R}/N)$

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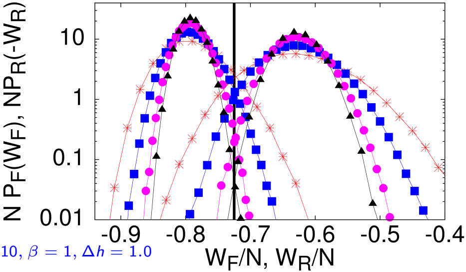

$\phi = 0.1$, $h_0 = 1.0$, $\tau = 10$, $\beta = 1$, $\Delta h = 1.0$

$N = 50, 100, 200, 300$

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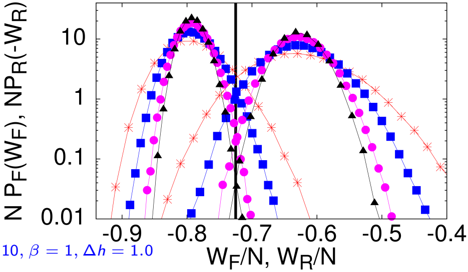

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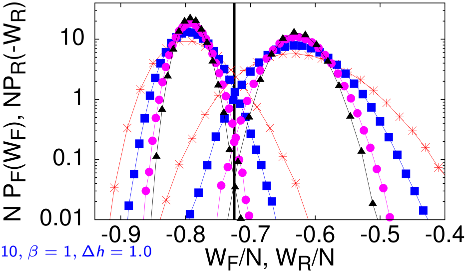

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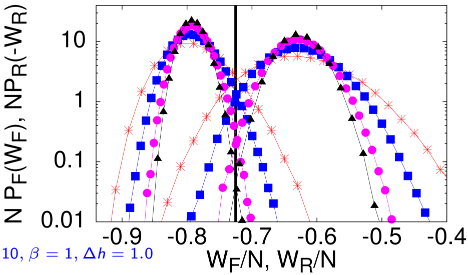

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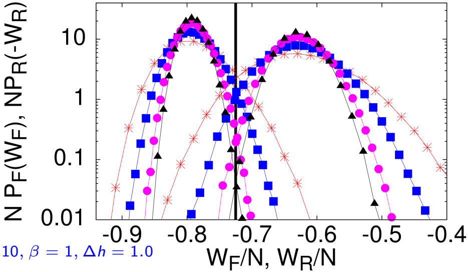

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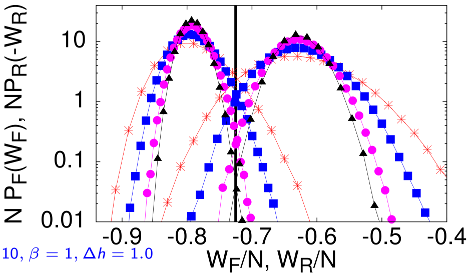

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- In our case, intersection at $\Delta\mathcal{F}/N$, the free-energy change per particle; can be computed from $\rho_{\rm eq}(\theta; h)$
- Perfect match underlines the effective single-particle nature of the N-particle dynamics for large N in the Fokker-Planck limit $\phi \ll 1$ *(Gupta, Dauxois, Ruffo (2016))*

Nonequilibrium initial condition: Generalizing Jarzynski

- $p \neq 1/2$ in our model; Start with NESS at $h = h_0$, change field over time τ as $h_\alpha = h_0 + \Delta h \; \alpha/\tau$.

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$$Y \equiv \int_0^\tau \mathrm{d}t\ \frac{\mathrm{d}h(t)}{\mathrm{d}t} \frac{\partial \Phi}{\partial h}(\mathcal{C}(t); h(t)); \quad \Phi(\mathcal{C}; h) \equiv -\ln \rho_{\mathrm{ss}}(\mathcal{C}; h)$$

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  3. $\langle \exp(-Y) \rangle = 1 \Rightarrow \langle \exp(-\beta W) \rangle = \exp(-\beta \Delta \mathcal{F})$ (Jarzynski)

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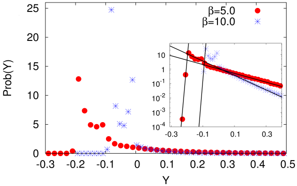

- In our case,

$$Y_i \approx \sum_{\alpha=1}^{\tau} \ln \left(\frac{\rho_{\mathrm{ss}}(\theta_i^{(\alpha)}; h_{\alpha-1})}{\rho_{\mathrm{ss}}(\theta_i^{(\alpha)}; h_\alpha)} \right)$$

- $p = 0.55$, $N = 500$, $\phi = 0.1$, $h_0 = 1.0$, $\Delta h = 0.15$, $\tau = 15$

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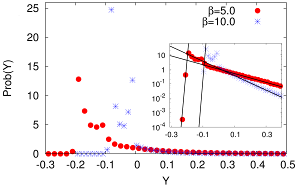

- In our case,

$$Y_i \approx \sum_{\alpha=1}^{\tau} \ln \left(\frac{\rho_{\rm ss}(\theta_i^{(\alpha)}; h_{\alpha-1})}{\rho_{\rm ss}(\theta_i^{(\alpha)}; h_\alpha)} \right)$$

- $p = 0.55$, $N = 500$, $\phi = 0.1$, $h_0 = 1.0$, $\Delta h = 0.15$, $\tau = 15$

Nonequilibrium initial condition: Generalizing Jarzynski

- $p \neq 1/2$ in our model; Start with NESS at $h = h_0$, change field over time τ as $h_\alpha = h_0 + \Delta h\ \alpha/\tau$.
- Hatano-Sasa:

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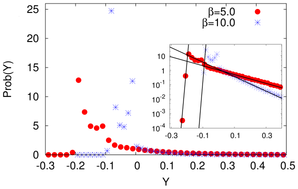

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- Combined use of N-particle dynamics and exact single-particle stationary state distribution
- Results further highlight the effective mean-field nature of the N-particle dynamics for large N.

(Gupta, Dauxois, Ruffo (2016))

Housekeeping heat

- Motion of a particle in a mean-field:

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = F(\theta; h) + \eta(t)$$

$F(\theta; h) \equiv (2p-1)\phi - \frac{\phi^2\beta}{2}\frac{\partial\langle v\rangle[\rho](\theta;h)}{\partial\theta}$

Gaussian, white noise: $\overline{\eta(t)} = 0,\ \overline{\eta(t)\eta(t')} = 2D\delta(t-t');\ D = \frac{\phi^2}{2}$

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- Work done by $f(\theta; h)$ in time $t = \int_0^t \mathrm{d}t'\ \dot{\theta}(t') f(\theta(t'); h(t'))$; Dissipated into the environment as the Housekeeping Heat

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$$-Q_t^{\mathrm{hk}} = \int_0^t \mathrm{d}t' \; \dot{\theta}(t') \left(F(\theta(t'); h(t')) - D \frac{\partial \ln \rho_{\mathrm{ss}}(\theta(t'); h(t'))}{\mathrm{d}\theta} \right)$$

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- What we show:
$$\langle e^{\beta Q_t^{\mathrm{hk}}} | \theta_{[0,\tau]} \rangle = e^{\beta Q_\tau^{\mathrm{hk}}} \text{ for any } t \geq \tau$$

In a general Markovian nonequilibrium process under arbitrary time-dependent driving, the exponentiated housekeeping heat is a martingale *(Chétrite, Gupta, Neri, Roldán (2018))*

Housekeeping heat

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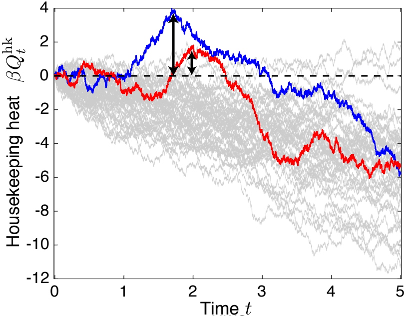

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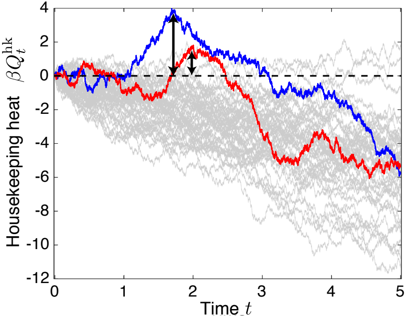

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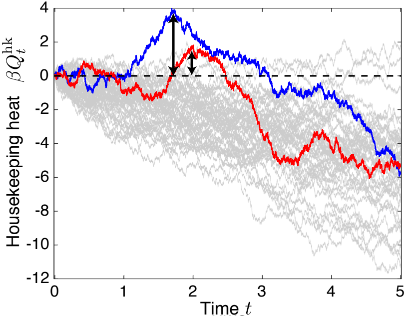

- On the average, heat is given to the environment........*But* there are instances when heat is absorbed from the environment
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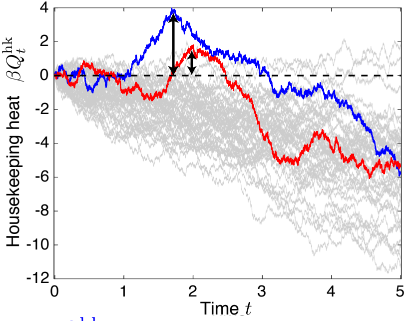

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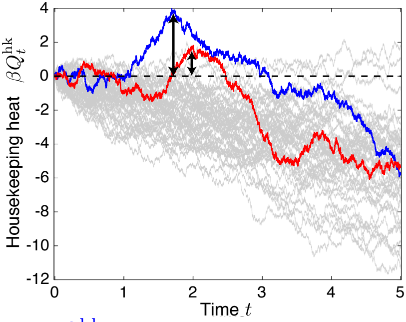

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$$\mathrm{Prob}[Q_{\max,t}^{\rm hk} \leq q] \leq 1 - e^{-\beta q}; \quad \langle Q_{\max,t}^{\rm hk} \rangle \leq k_B T$$

(Chétrite, Gupta, Neri, Roldán (2018))

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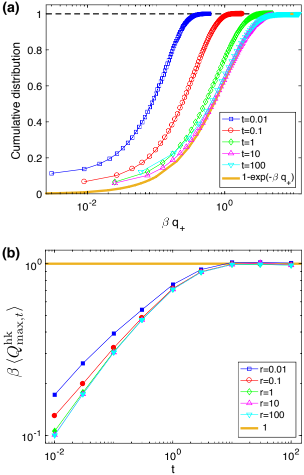

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- Holds for general Markovian processes with arbitrary time-dependent driving

Take-home messages

- Implementing concepts of stochastic thermodynamics gives valuable insights into the nature of the stationary state
- Applying Martingale theory yields universal results that restrict nature of physical processes, e.g., heat exchanges with the environment
- What next ?? Experimental tests, Application to quantum systems,...