Out-of-equilibrium physics in spontaneous synchronization

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References

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Coworkers

  

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Plan

- Spontaneous synchronization
- Kuramoto and Sakaguchi models, the role of noise
- Inertia and the connection with statistical mechanics
- Equilibrium and out-of-equilibrium
- Complete phase diagram: First and second order phase transition
- Hysteresis and bistability
- Linear stability analysis
- Intermezzo on HMF
- A stochastic discrete model
- Out of equilibrium fluctuations
- Summary

What is synchronization?

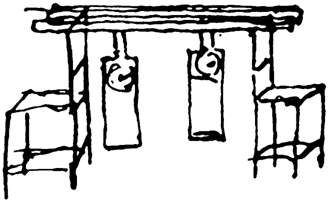
Synchronization is the **adjustment** of the **rhythm** of **active, dissipative** oscillators caused by a **weak interaction**.

Prerequisite: Each oscillator persists in its motion thanks to an **external source of energy**.

Active oscillators

- generates **periodic oscillations**
- **absence** of periodic forces
- **dissipative** dynamical system
- **autonomous** differential equation
- **limit cycle** in phase space

Christiaan Huygens



Christiaan Huygens first observed the synchronization of two **clocks** in 1656

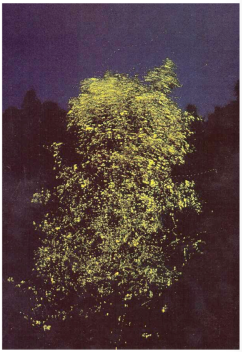
Radio communication

... in more recent times

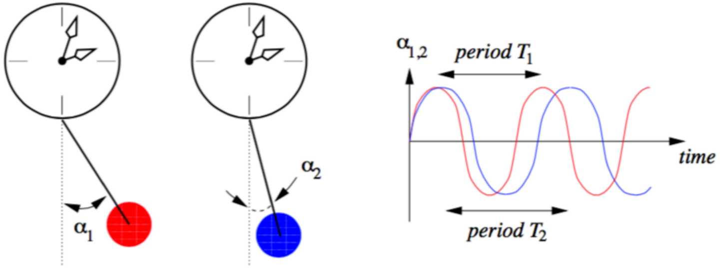
W. J. Eccles and J. H. Vincent (1920) discover synchronization in a **triod**.
The theory is then developed by Edward Appleton and Balthasar Van de Pol (1922-1927) setting the foundations for modern **radio communication**.

Flashing fireflies

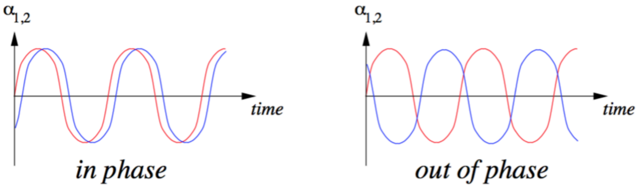


Englebert Kaempfer observes in Siam (1680) synchronization in **flashing fireflies**
Jean-Jacques Dourtous de Mairan discovers **circadian rhythms** in the movement of **bean leaves** (1729).

In absence of coupling

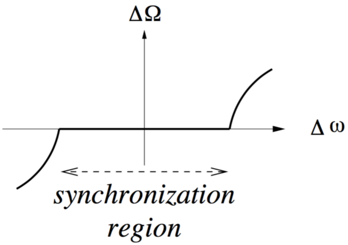


Weak coupling



$$\omega_1 < \Omega < \omega_2.$$

Synchronization region



$\Delta\omega$ difference in unperturbed frequencies

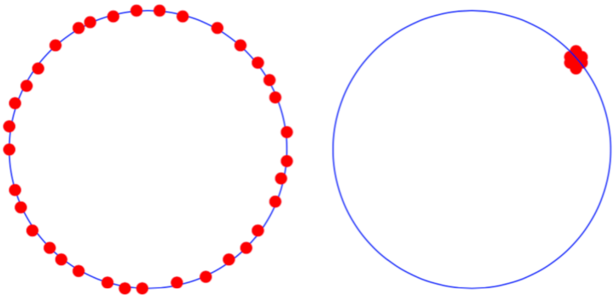
$\Delta\Omega$ difference in observed frequencies

Phase

$$\varphi = \varphi_0 + \frac{2\pi}{T}\int_0^{\theta}\frac{d\theta}{\dot{\theta}}$$

$$\varphi = \varphi_0 + 2\pi\frac{t - t_0}{T}$$

Many phases



Stuart-Landau

Weakly nonlinear dynamics near a bifurcation

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = i\omega Q + (\alpha - \beta|Q|^2)Q$$

$\alpha, \beta, \omega \in \mathbb{R}$

$$Q = \rho e^{i\theta}$$

$\rho, \theta \in \mathbb{R}$ and $\theta \in [-\pi, \pi]$

$$\begin{aligned} & \mathrm{d}\rho/\mathrm{d}t|_{\rho=\rho_{\text{stable}}} = 0 \\ & \mathrm{d}\rho/\mathrm{d}t|_{\rho<\rho_{\text{stable}}} > 0 \\ , \qquad & \mathrm{d}\rho/\mathrm{d}t|_{\rho>\rho_{\text{stable}}} < 0 \end{aligned}$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega.$$

Coupled Stuart-Landau oscillators

$$\frac{\mathrm{d}Q_i}{\mathrm{d}t} = i\omega_i Q_i + (\alpha - \beta|Q_i|^2)Q_i + \sum_{j=1, j\neq i}^{N} K_{ij} Q_j,$$

$K_{ij} > 0$

Three simplifying premises

1. large number of oscillators: $N \to \infty$,
2. the coupling $K_{ij}\ \forall\ i, j$ scaling as $K_{ij} = K/N$ with K finite, implying thereby that every oscillator is coupled *weakly* and with equal strength to every other oscillator, and
3. the limit $\alpha, \beta \to \infty$, while keeping α/β fixed and finite, and, moreover, $\omega_i\ \forall\ i$ being finite.

Kuramoto limit

$$Q_i = \rho_i e^{i\theta_i}$$

Each ρ_i relaxes over a time of $O(1/\beta)$ to its limit-cycle value $\sqrt{\alpha/\beta}$.

The long-time dynamics corresponds to self-sustained limit-cycle oscillations for each oscillator, which is described by the evolution equation

$$\frac{\mathrm{d}\theta_i}{\mathrm{d}t} = \omega_i + \frac{\tilde{K}}{N} \sum_{j=1}^{N} \sin(\theta_j - \theta_i).$$

The ω_i are N *quenched* random variables extracted from the distribution $g(\omega)$.

These are the governing dynamical equation of the Kuramoto model

The Kuramoto transition

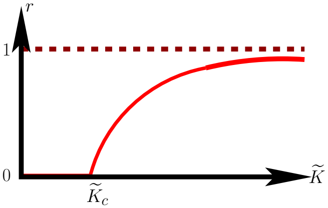
Let $g(\omega)$ be unimodal and symmetric around the average $\langle\omega\rangle$ with *width* σ.

By going to the *comoving frame* rotating with frequency $\langle\omega\rangle$, one may consider the ω_i's to have zero mean.

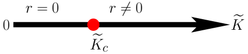
Kuramoto's order parameter

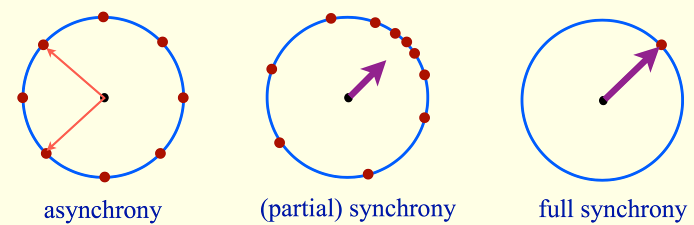
$$\mathbf{r}(t) = r(t)e^{i\psi(t)} \equiv \frac{1}{N}\sum_{j=1}^{N} e^{i\theta_j(t)},$$

- High $\tilde{K}$: Synchronized phase , $r > 0$
- Low $\tilde{K}$: Incoherent phase, $r \approx 0$.



Phase distribution





Fixed-point and drifting phases

The dynamics in terms of $r(t)$ and $\psi(t)$

$$\frac{\mathrm{d}\theta_i}{\mathrm{d}t} = \omega_i + \tilde{K} r \sin(\psi - \theta_i).$$

Phase difference $\phi_i = \theta_i - \psi$.

Two types of oscillators

1. Fixed point $\dot{\phi}_i = 0$,$\phi_i = \arcsin(\omega_i / \tilde{K} r_{st})$ if $|\omega_i| \leq \tilde{K} r_{st}$
2. Drifting $\dot{\phi}_i \neq 0$ if $|\omega_i| > \tilde{K} r_{st}$

where r_{st} is the stationary value reached by $r(t)$.
Let us introduce $\rho(\theta, \omega, t)$, the fraction of oscillators with frequency ω, phase θ at time t in the $N \to \infty$ limit, with normalization

$$\int_{-\pi}^{\pi} \mathrm{d}\theta \; \rho(\theta, \omega, t) = 1 \; \forall \; \omega, t$$

Self consistent equation for the order parameter $r_{\rm rs}$

One observes that $\rho(\theta, \omega, t)$ converges to a time independent form $\rho_{\rm st}(\theta, \omega)$ and the stationary order parameter is given by

$$r_{\rm st} = \int d\theta \int d\omega \; g(\omega) e^{i\theta} \rho_{\rm st}(\theta, \omega).$$

The separation between fixed-point and drifting oscillators allows one to write the stationary distribution in an $r_{\rm rs}$-dependent form

$$\rho_{\rm st}(\theta, \omega; r_{\rm st}) = \begin{cases} \rho_{\rm st}^{fp} \text{ if } |\omega| \leq \tilde{K} r_{\rm st} \\ \rho_{\rm st}^{dr} \text{ if } |\omega| > \tilde{K} r_{\rm st} \end{cases}$$

and therefore write a self-consistent equation for the stationary order parameter $r_{\rm rs}$

$$r_{\rm st} = \int d\theta \int d\omega \; g(\omega) e^{i\theta} \rho_{\rm st}(\theta, \omega; r_{\rm st}).$$

Solution of the self-consistent equation

Due to the symmetry $g(\omega) = g(-\omega)$ of the frequency distribution

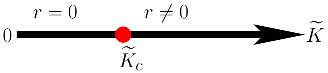
$$\rho_{\rm st}(-\theta, -\omega; r_{\rm st}) = \rho_{\rm st}(\theta, \omega; r_{\rm st})$$
$$\rho_{\rm st; r_{st}}(\theta + \pi, -\omega, ; r_{\rm st}) = \rho_{\rm st}(\theta, \omega; r_{\rm st})$$

and guessing the form of $\rho_{\rm st}^{fp}, \rho_{\rm st}^{dr}$ one can perform the integral in ω and rewrite the self-consistent equation as

$$r_{\rm st} = \tilde{K} r_{\rm st} \int_{-\pi/2}^{\pi/2} \mathrm{d}\theta \ \cos^2\theta \ g(\tilde{K} r_{\rm st} \sin\theta)$$

This equation has always the solution $r_{\rm st} = 0$ and at $\tilde{K} = \tilde{K}_c = 2/\pi g(0)$ a $r_{\rm st} \neq 0$ solution bifurcates supercritically, continuously from zero, and reaches $r_{\rm st} = 1$ in the $\tilde{K} \to \infty$. Near $\tilde{K} = \tilde{K}_c$, $r_{\rm st} \approx (\tilde{K} - \tilde{K}_c)^{1/2}$.

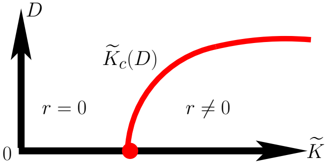
The Sakaguchi model



Stochastic fluctuations of the ω_i in time

$$\frac{d\theta_i}{dt} = \omega_i + \frac{\tilde{K}}{N} \sum_{j=1}^{N} \sin(\theta_j - \theta_i) + \eta_i(t)$$

$$< \eta_i(t) >= 0 \, , \, < \eta_i(t)\eta_j(t') >= 2D\delta_{ij}\delta(t - t')$$



Kuramoto model with inertia and noise

Two dynamical variables: θ_i (Phase); v_i (Angular velocity)

$$\frac{d\theta_i}{dt} = v_i$$

$$m\frac{dv_i}{dt} = -\gamma v_i + \omega_i + \frac{K}{N}\sum_{j=1}^{N}\sin(\theta_j - \theta_i) + \eta_i(t)$$

where m is the inertia and γ the friction constant and $\eta_i(t)$ is a Gaussian white noise.

Motivation:

- An adaptive frequency can explain the slower approach to synchronization observed in a particular firefly (the Pteropyx mallacae) `Ermentrout (1991)`
- Phase dynamics in electric power distribution networks in the mean-field limit `Filatrella, Nielsen and Pedersen (2008), Rohden, Sorge, Timme and Witthaut (2012), Olmi and Torcini (2014)`

Rescaling

One can analyze the model in the reduced parameter space (T, σ, m)

$$\frac{d\theta_i}{dt} = v_i$$

$$\frac{dv_i}{dt} = F_i + \eta_i(t) = -\frac{1}{\sqrt{m}} v_i + \sigma\omega_i + \frac{1}{N}\sum_{j=1}^{N} \sin(\theta_j - \theta_i) + \eta_i(t)$$

where now:

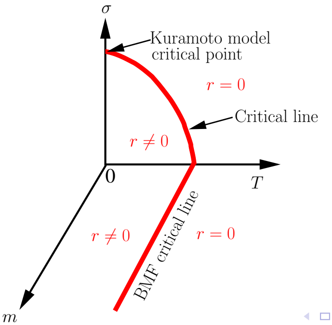
- $g(\omega)$ has zero average and unit width
- $< \eta_i(t)\eta_j(t') >= \frac{2T}{\sqrt{m}}\delta_{ij}\delta(t-t')$

Two steps

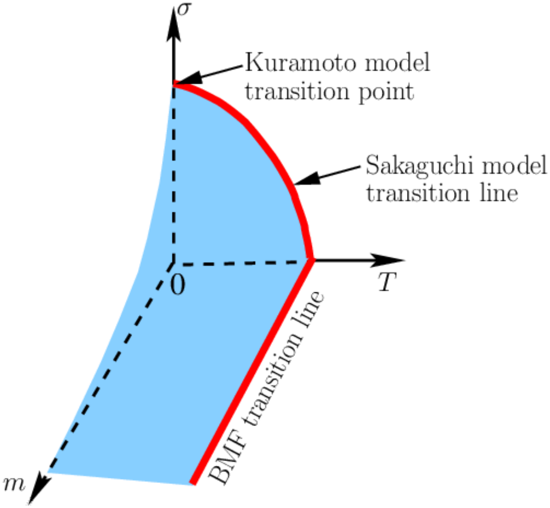
- Subtracting average motion: $\theta_i \Rightarrow \theta_i + < \omega > t$,$v_i \Rightarrow v_i + < \omega > t$, $\omega_i \Rightarrow \omega_i + < \omega >$
- Rescaling: $t' = t\sqrt{K/m}$,$v_i' = v_i\sqrt{m/K}$,$1/\sqrt{m'} = \gamma/\sqrt{Km}$, $\sigma' = \gamma\sigma/K$, $T' = T/K$.

Critical lines at equilibrium ($\sigma = 0$) and non equilibrium ($\sigma > 0$)

- `Kuramoto:` $m = T = 0$, $\sigma > 0$, $\sigma_c = \pi g(0)/2$
- `Sakaguchi:` $m = 0$, $T > 0$, $\sigma > 0$,
  $2 = \int_{-\infty}^{\infty} d\omega\ g(\omega)[T/(T^2 + \omega^2\sigma_c^2]$
- `Brownian Mean Field Model:` $\sigma = 0$ Hamiltonian system + heat-bath Chavanis (2013)

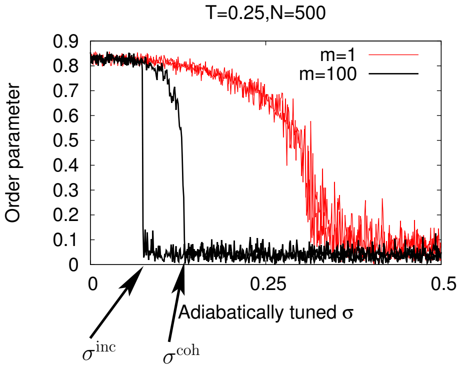


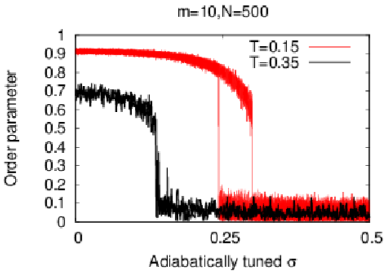
Phase diagram



Gaussian $g(\omega)$

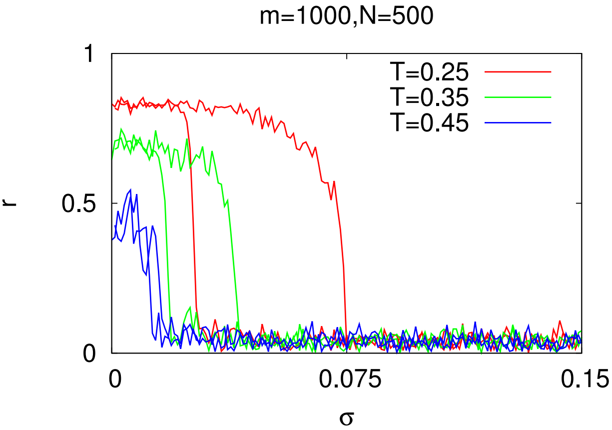
Hysteresis for Gaussian $g(\omega)$





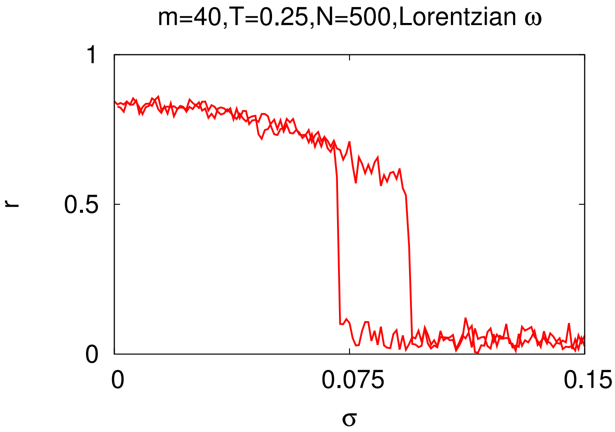
Adiabatically tuned σ

Hysteresis for Gaussian $g(\omega)$ when approaching the BMF limit $T = 0.5$



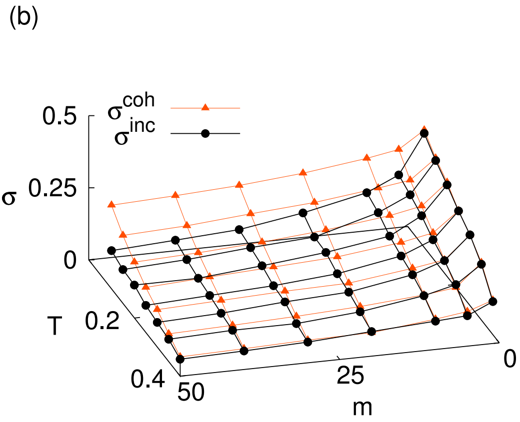
Adiabatically tuned σ

Hysteresis for Lorentzian $g(\omega)$



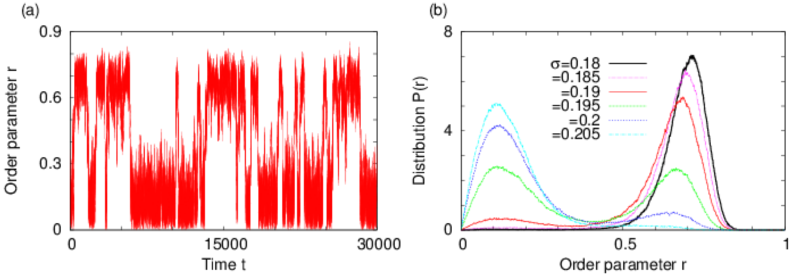
Adiabatically tuned σ

Coexistence region



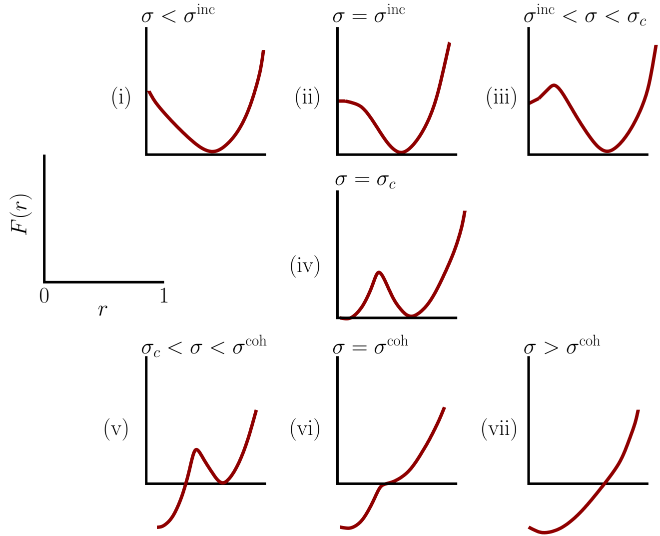
The actual phase transition point lies in between
$\sigma^{inc}(m, T) < \sigma_c(m, T) < \sigma^{coh}(m, T)$

Bistability

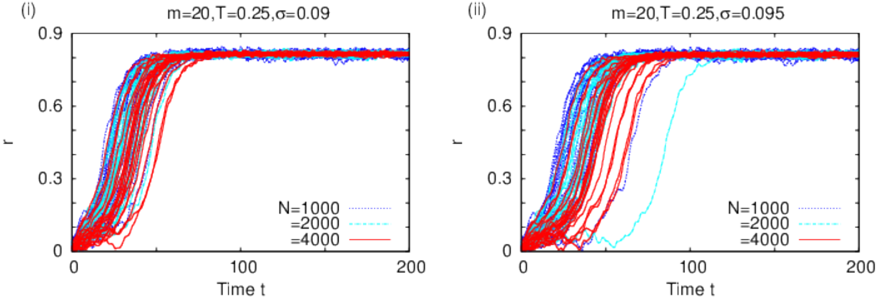


For $m = 20$, $T = 0.25$, $N = 100$, and a Gaussian $g(\omega)$ with zero mean and unit width, (left) shows, at $\sigma = 0.195$, r vs. time in the stationary state, while (right) shows the distribution $P(r)$ at several σ's around $\sigma_c = 0.195$.

Landau picture

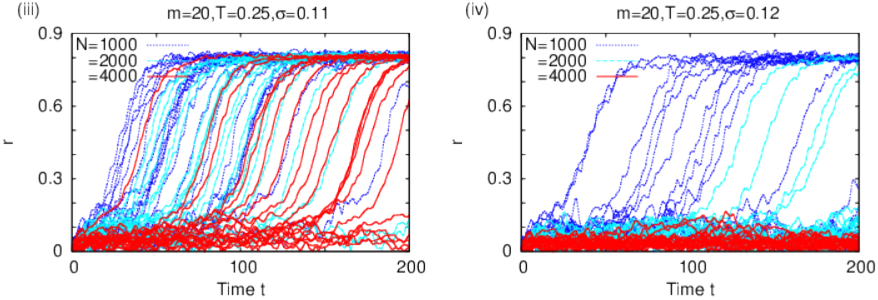


Below $\sigma^{\rm inc}(m, T)$



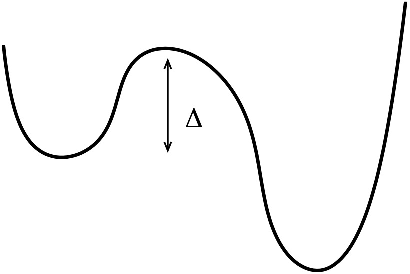
$m = 20$, $T = 0.25$,$\sigma = 0.09$(left),$\sigma = 0.095$(right)

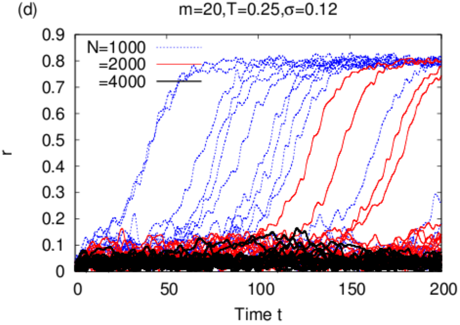
Above $\sigma^{\mathrm{inc}}(m, T)$



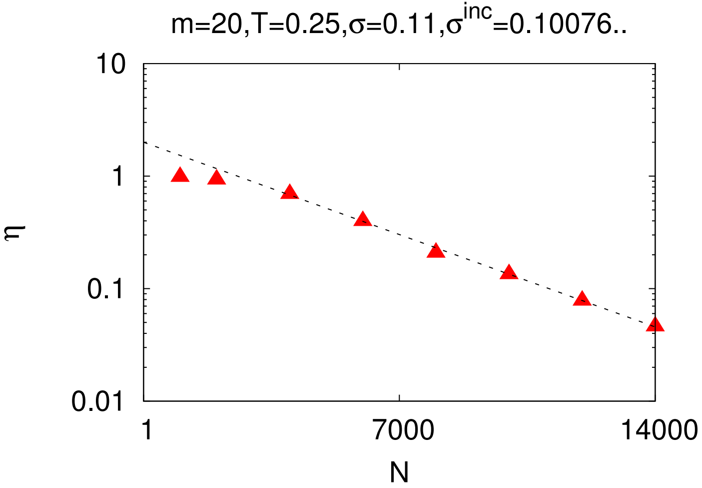
$m = 20$, $T = 0.25$,$\sigma = 0.11$(left),$\sigma = 0.12$(right)

Mean-field metastability





Fraction of initial incoherent states reaching the synchronized state



$m = 20$, $T = 0.25$,$\sigma = 0.11$

Detailed balance

Fokker-Planck equation for the N-body distribution

$$\frac{\partial f_N(\mathbf{x})}{\partial t} = -\sum_{i=1}^{2N} \frac{\partial [A_i(\mathbf{x}) f_N(\mathbf{x})]}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{2N} \frac{\partial^2 [B_{i,j}(\mathbf{x}) f_N(\mathbf{x})]}{\partial x_i \partial x_j}$$

$\mathbf{x} = (\theta_1, \ldots, \theta_N; v_1, \ldots, v_N)$ $\mathbf{A}(\mathbf{x}) = (v_1, \ldots, v_N; F_1, \ldots, F_N)$ $B_{i,j} = \delta_{i,j} 2T$

Detailed balance conditions (Risken)

$$\epsilon_i \epsilon_j B_{i,j}(\epsilon \mathbf{x}) = B_{i,j}(\mathbf{x}) \ , \ \epsilon_i A_i(\epsilon \mathbf{x}) f_N^s(\mathbf{x}) = -A_i(\mathbf{x}) f_N^s(\mathbf{x}) + \sum_{j=1}^{2N} \frac{\partial [B_{i,j}(\mathbf{x}) f_N^s(\mathbf{x})]}{\partial x_j}$$

where $\epsilon_i = \pm 1$ is the parity with respect to time reversal and f_N^s is a stationary solution of the Fokker-Planck equation.
These conditions can be satisfied only when $\sigma = 0$ and, as a consequence $f_N^s \propto \exp(-H/T)$

$N \to \infty$ continuum limit

Single-particle distribution $f(\theta, v, \omega, t)$: Fraction of oscillators at time t and for each ω which have phase θ and angular velocity v (Periodic in θ and normalized).
Evolution by Kramers equation

$$\frac{\partial f}{\partial t} = -v\frac{\partial f}{\partial \theta} + \frac{\partial}{\partial v}\Big(\frac{v}{\sqrt{m}} - \sigma\omega - r\sin(\psi - \theta)\Big)f + \frac{T}{\sqrt{m}}\frac{\partial^2 f}{\partial v^2},$$

with self-consistent order parameter

$$r\exp(i\psi) = \iiint d\theta dv d\omega g(\omega)\exp(i\theta)f(\theta, v, \omega, t)$$

Homogeneous ($r = 0$) solution

$$f^{\rm inc} = \frac{1}{2\pi}\frac{1}{\sqrt{2\pi T}}\exp\left(-\frac{(v - \sigma\omega\sqrt{m})^2}{2T}\right)$$

Linear stability results

Stability analysis gives σ^{inc}:
$f(\theta, v, \omega, t) = f^{\mathrm{inc}}(\theta, v, \omega) + e^{\lambda t}\delta f(\theta, v, \omega)$

$$\frac{2T}{e^{mT}} = \sum_{p=0}^{\infty} \frac{(-mT)^p(1+\frac{p}{mT})}{p!} \int_{-\infty}^{+\infty} \frac{g(\omega)d\omega}{1+\frac{p}{mT}+i\frac{\sigma\omega}{T}+\frac{\lambda}{T\sqrt{m}}}.$$

`Acebron, Bonilla and Spigler (2000)`

- At most one solution with a positive real part.
- Neutral stability $\Rightarrow \lambda = 0$ gives the stability surface $\sigma^{\mathrm{inc}}(m, T)$.
- Similarly, one can define $\sigma^{\mathrm{coh}}(m, T)$.
- The two surfaces enclose the first-order transition surface $\sigma_c(m, T)$.
- Taking proper limits, the surface $\sigma^{\mathrm{inc}}(m, T)$ meets the critical lines on the (T, σ) and (m, T) planes.
- The intersection of the surface with the (m, σ) plane gives an implicit formula for $\sigma^{\mathrm{inc}}_{\mathrm{noiseless}}(m, \sigma)$.

Summary of the first part

- Kuramoto model from the point of view of equilibrium and non equilibrium statistical mechanics
- First-order phase transition in presence of inertia (full phase diagram).
- In absence of quenched randomness $\sigma = 0$ the stationary probability distribution is the Boltzmann-Gibbs product measure $\exp(-(K+U)/T) = \exp(-K/T)\exp(-U/T)$. The phase transition is characterized by the potential energy U only and it is the same for underdamped or overdamped dynamics.
- In presence of quenched randomness $\sigma \neq 0$ the system is out of equilibrium and the stationary measure is not a product measure and the phase transition depends on the damping coefficient.

A stochastic model of long-range interacting particles

N interacting particles ($i = 1, 2, \ldots, N$) moving on a unit circle, with angles θ_1.

Microscopic configuration

$$\mathcal{C} = \{\theta_i; i = 1, 2, \ldots, N\}$$

The particles interact via the potential

$$\mathcal{V}(\mathcal{C}) = \frac{K}{2N} \sum_{i,j=1}^{N} [1 - \cos(\theta_i - \theta_j)]$$

$K = 1$ in the following. External fields h_i

$$\mathcal{V}_{\rm ext}(\mathcal{C}) = \sum_{i=1}^{N} h_i \cos\theta_i$$

The fields h_i's may be considered as quenched random variables with a common distribution $P(h)$.

The net potential energy is therefore

$$V(\mathcal{C}) = \mathcal{V}(\mathcal{C}) + \mathcal{V}_{\rm ext}(\mathcal{C})$$

The stochastic dynamics

All particles sequentially attempt to move backward (forward) on the circle

$$\theta_i \to \theta_i' = \theta_i + f_i \text{ with probability p}$$
$$\theta_i \to \theta_i' = \theta_i - f_i \text{ with probability q=1-p}$$

The f_i are quenched random variables, each particles carries its own f_i.
However, particles effectively take up the attempted position with probability $g(\Delta V(\mathcal{C}))\Delta t$

$$\Delta V(\mathcal{C}) = (1/N)\sum_{j=1}^{N}[-\cos(\theta_i' - \theta_j) + \cos(\theta_i - \theta_j)] - h_i[\cos\theta_i' - \cos\theta_i]$$

$$g(z) = (1/2)[1 - \tanh(\beta z/2)]$$

Overdamped motion of particles in contact with a heat-bath at inverse temperature β and in presence of an external field. For $p \neq q$ the particles move asymmetrically under the action of an external drive.

Master equation in continuous time

$P = P(\{\theta_i\}; t)$ be the probability to observe the configuration $\mathcal{C} = \{\theta_i\}$ at time t and take the limit $\Delta t \to 0$

$$
\begin{aligned}
\frac{\partial P}{\partial t} = \sum_{i=1}^{N} \Big[& \\
& + P(\ldots, \theta_i - f_i, \ldots; t) pg(\Delta V(\mathcal{C}[(\theta_i - f_i) \to \theta_i])) + \\
& + P(\ldots, \theta_i + f_i, \ldots; t) qg(\Delta V(\mathcal{C}[(\theta_i + f_i) \to \theta_i])) - \\
& - P(\ldots, \theta_i, \ldots; t) \Big\{ pg(\Delta V(\mathcal{C}[\theta_i \to (\theta_i + f_i)])) + qg(\Delta V(\mathcal{C}[(\theta_i) \to (\theta_i - f_i)])) \Big\} \Big]
\end{aligned}
$$

At long times, the system settles into a stationary state $P_{\mathrm{st}}(\{\theta_i\})$.

- Equilibrium: For $p = 1/2$, the particles move in a symmetric manner. The system has an equilibrium stationary state $P_{\mathrm{eq}}(\{\theta_i\}) \propto e^{-\beta V(\{\theta_i\})}$. Detailed balance is satisfied.
- Non Equilibrium: For $p \neq 1/2$, the particles have a preferred direction, The system at long times settles into a nonequilibrium stationary state, characterized. Detailed balance is violated leading to nonzero probability currents in phase space.

Fokker-Planck limit and Langevin equation

We assume that $f_i \ll 1 \; \forall \; i$. Taylor expanding in powers of f_i's and retaining terms up to second order

$$\frac{\partial P}{\partial t} = -\sum_{i=1}^{N} \frac{\partial J_i}{\partial \theta_i},$$

where the probability current J_i for the i-th particle is given by

$$J_i \quad = \quad \left[(2p-1)f_i + \frac{f_i^2 \beta}{2}\left(\frac{1}{N}\sum_{j=1}^{N} \sin \Delta\theta_{ji} + h_i \sin \theta_i\right)\right] P - \frac{f_i^2}{2}\frac{\partial P}{\partial \theta_i}.$$

The corresponding Langevin equation is

$$\dot{\theta}_i = (2p-1)f_i + \frac{f_i^2 \beta}{2}\left(\frac{1}{N}\sum_{j=1}^{N} \sin(\theta_j - \theta_i) + h_i \sin \theta_i\right) + f_i \eta_i(t),$$

where $\eta_i(t)$ is a random noise with

$$\langle \eta_i(t) \rangle = 0, \qquad \langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij}\delta(t - t').$$

Equilibrium vs. non equilibrium

- Equilibrium: For $p = 1/2$ the system settles into an equilibrium stationary state $P_{\mathrm{eq}}(\{\theta_i\})$ which makes $J_i = 0$ individually for each i.
- Non Equilibrium: For $p \neq 1/2$, the system reaches a non-equilibrium stationary state. However, in the special case when the jump length is the same for all the particles and there is no external field ($f_i = f$ and $h_i = 0 \, \forall \, i$), one may make a Galilean transformation, $\theta_i \to \theta_i + [(2p-1)f/2]t$, so that in the frame moving with the velocity $[(2p-1)f/2]$, the Langevin equation takes a form identical to the one for $p = 1/2$, and the stationary state has again the equilibrium measure $P_{\mathrm{eq}}(\{\theta_i\})$.

The $N \to \infty$ limit and the single-particle distribution

In the thermodynamic limit $N \to \infty$ with $h_i = h$, let us introduce the single-particle distribution $\rho(\theta; f, t)$, the density of particles with jump length f which are at location θ on the circle at time t. ρ is periodic $\rho(\theta; f, t) = \rho(\theta + 2\pi; f, t)$ and normalized

$$\int_0^{2\pi} d\theta \; \rho(\theta; f, t) = 1 \;\; \forall \;\; f.$$

In terms of $\rho(\theta; f, t)$, the Langevin equation reads

$$\dot{\theta} = (2p - 1)f + \frac{f^2 \beta}{2}\Big(m_y \cos\theta - m_x \sin\theta + h \sin\theta\Big) + f\eta(t),$$

where

$$(m_x, m_y) = \int d\theta df \; (\cos\theta, \sin\theta)\rho(\theta; f, t)\mathcal{P}(f),$$

and

$$\langle \eta(t) \rangle = 0, \quad \langle \eta(t)\eta(t') \rangle = \delta(t - t').$$

This stochastic dynamics is very similar to the one of the Sakaguchi model.

Single-particle Fokker-Planck equation

The single-particle Fokker-Planck equation satisfied by $\rho(\theta; f, t)$ may be obtained from the Langevin equation

$$\frac{\partial \rho}{\partial t} = -\frac{\partial j}{\partial \theta}$$

where the probability current j is given by

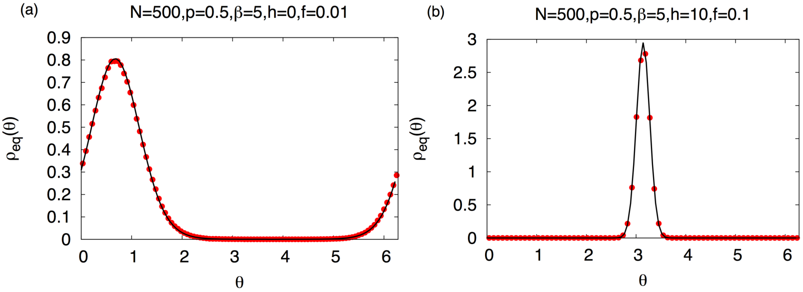
$$j = \Big[(2p-1)f + \frac{f^2\beta}{2}\Big(m_y \cos\theta - m_x \sin\theta + h \sin\theta\Big)\Big]\rho - \frac{f^2}{2}\frac{\partial \rho}{\partial \theta}.$$

The stationary solution $\rho_{\rm st}$ is

$$\rho_{\rm st}(\theta; f) = \rho(0; f) e^{2(2p-1)\theta/f + \beta(m_x \cos\theta + m_y \sin\theta - h\cos\theta)}$$
$$\times \left[1 + (e^{-4\pi(2p-1)/f} - 1)\frac{\int_0^\theta d\theta' e^{-2(2p-1)\theta'/f - \beta(m_x \cos\theta' + m_y \sin\theta' - h\cos\theta')}}{\int_0^{2\pi} d\theta' e^{-2(2p-1)\theta'/f - \beta(m_x \cos\theta' + m_y \sin\theta' - h\cos\theta')}}\right]$$

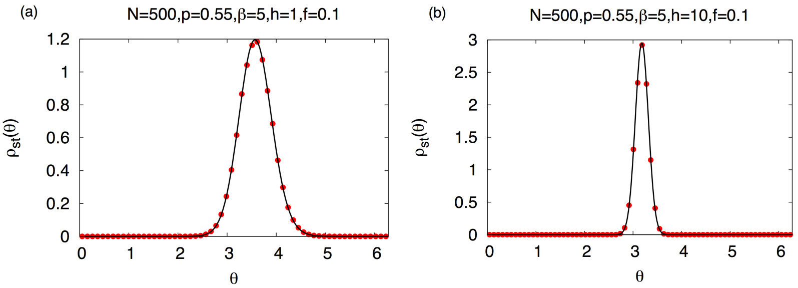
where $(m_x, m_y) = \int d\theta df (\cos\theta, \sin\theta)\rho_{\rm st}(\theta; f)\mathcal{P}(f)$, and the constant $\rho(0; f)$ is fixed by the normalization condition.

Numerical results: Equilibrium $p = 1/2$



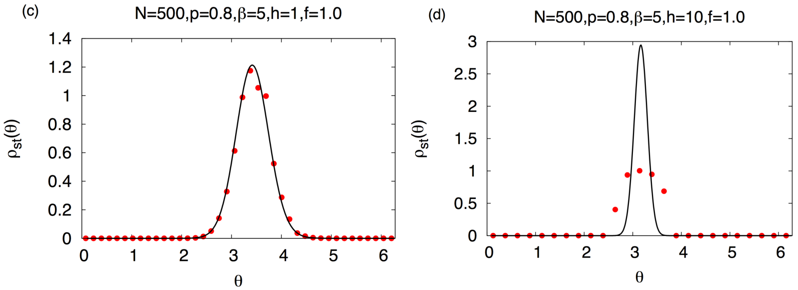
Panel (a) $f = 0.01$, $h = 0$
Panel (b) $f = 0.1$, $h = 10$

Numerical results: Non Equilibrium $p = 0.55$ $f = 0.1$



$f = 0.1$

Numerical results: Non Equilibrium $p = 0.55$ $f = 1$



$f = 1$

Fluctuation theorems: Nonequilibrium work relations

Gas-piston setup with $N \sim 10^{23}$ particle (Macroscopic). The piston is rapidly pushed into the gas and then pulled at the initial position (work is positive if done against the system)

$$W > 0$$

Microscopically (in a gas with few particles), we could observe $W < 0$, but, on average

$$\langle W \rangle > 0$$

The second principle can be formulated as an equality (Jarzynski)

$$\langle e^{-W/(k_B T)} \rangle = 1$$

If the piston is manipulated in a time symmetric manner (Crooks)

$$\frac{P(W)}{P(-W)} = \langle e^{W/(k_B T)} \rangle$$

Protocol

$$t = 0\,[\lambda = A, T] \qquad \text{equilibrium} \;\; \rightarrow \;\; t = \tau\,\lambda = B\,\text{non equilibrium}$$
$$\rightarrow \;\; t = \tau^*\;[\lambda = B, T]\,\mathrm{equilibrium}$$

No external work is done on the system in the time interval $\tau < t < \tau^*$.

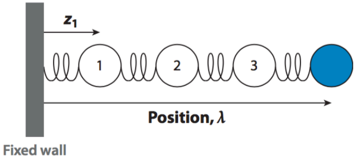
Clausius inequality (Second Law of Thermodynamics)

$$W \geq \Delta F = F_{B,T} - F_{A,T}$$

where F is the Helmholtz free energy. When the parameter λ is varied slowly (adiabatic transformation) $W = \Delta F$.

Important: Fluctuation theorems are valid also when the system is isolated after it is equilibrated at time $t = 0$.

Microscopic model



$$H(\mathbf{x};\lambda) = \sum_{i=1}^{3} \frac{p_i^2}{2m} + \sum_{i=0}^{3} U(z_{k+1} - z_k)$$

where $\mathbf{x} = (z_1, z_2, z_3, p_1, p_2, p_3)$ and the boundary conditions are $z_0 = 0,\ z_4 = \lambda(t)$

$$W = \int dW = \int_A^B \mathrm{d}\lambda \frac{\partial H}{\partial \lambda}(\mathbf{x},\lambda) = \int_0^t \mathrm{d}t \dot{\lambda} \frac{\partial H}{\partial \lambda}(\mathbf{x}(\mathbf{t}), \lambda(t))$$

$$\mathcal{H}(\mathbf{x},\mathbf{y},\lambda) = H(\mathbf{x};\lambda) + H_{env}(\mathbf{y}) + H_{int}(\mathbf{x},\mathbf{y})$$

Boltzmann-Gibbs distributions

If the interaction with the bath H_{int} is sufficiently weak

$$p^{eq}_{\lambda,T}(\mathbf{x}) = \frac{1}{Z_{\lambda,T}} \exp\left[-H(\mathbf{x};\lambda)/(k_B T)\right] \ , \ Z_{\lambda,T} = \int \mathrm{d}\mathbf{x} \exp\left[-H(\mathbf{x};\lambda)/(k_B T)\right]$$

If H_{int} is instead "large"

$$p^{eq}_{\lambda,T} \propto \exp\left(-H^*/k_B T\right) \ , \ H^*(\mathbf{x};\lambda) = H(\mathbf{x};\lambda) + \phi(\mathbf{x},T)$$

where $\phi(\mathbf{x},T)$ is the free-energy cost of inserting the system into the thermostat. The free energy associated with the equilibrium state is

$$F_{\lambda,T} = -k_B T \ln Z_{\lambda,T}$$

For a "swarm" of independent trajectories $(\mathbf{x}_1(t), \mathbf{x}_2(t), \ldots, (0 < t < \tau)$ one can compute the corresponding work $W_1, W_2, \ldots,$ and determine the distribution $P(W)$, which must respect

$$\langle W \rangle = \int \mathrm{d}W P(W) W \geq \Delta F = F_{B,T} - F_{A,T}$$

Proof of Jarzynski for an isolated system

After preparing the system in the initial equilibrium state, we disconnect it from the environment and perform work by varying λ from A to B. The statistics of work is determined by the statistics over the initial state

$$\langle e^{-W/(k_B T)} \rangle = \int \mathrm{d}\mathbf{x}(0) p^{eq}_{A,T}(\mathbf{x}(0)) e^{-W/(k_B T)}$$

Since $\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t}$, the work is given by

$$W = H(\mathbf{x}(\tau), B) - H(\mathbf{x}(0), A)$$

Changing variables from initial to final

$$\langle e^{-W/(k_B T)} \rangle = \frac{1}{Z_{A,T}} \int \mathrm{d}\mathbf{x}(\tau) |\partial \mathbf{x}(\tau)/\partial \mathbf{x}(0)|^{-1} \exp\left(-H(\mathbf{x}(\tau); B)/(k_B T)\right)$$

Using Liouville theorem $|\partial \mathbf{x}(\tau)/\partial \mathbf{x}(0)| = 1$, one finally gets

$$\langle e^{-W/(k_B T)} \rangle = \frac{Z_{B,T}}{Z_{A,T}} = e^{-(F_{B,T} - F_{A,T})/(k_B T)}$$

Hatano-Sasa, Jarzynski and Crooks

Protocol $\{\lambda(t)\}_{0\leq t\leq\tau}; \lambda(0)\equiv\lambda_1, \lambda(\tau)\equiv\lambda_2\}$

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

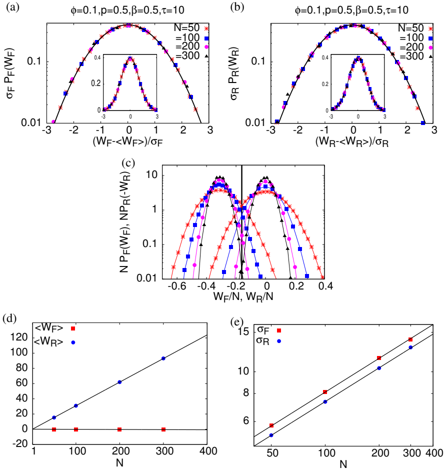
Y is dissipated work.

$$\left\langle e^{-Y}\right\rangle = 1.$$

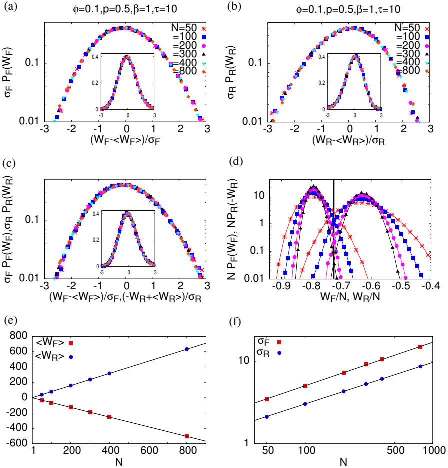
$$\left\langle e^{-\beta W}\right\rangle = e^{-\beta\Delta F},$$

$$\frac{P_{\mathrm{F}}(W_{\mathrm{F}})}{P_{\mathrm{R}}(-W_{\mathrm{F}})} = e^{\beta(W_{\mathrm{F}}-\Delta F)}.$$

Work distributions for homogeneous state

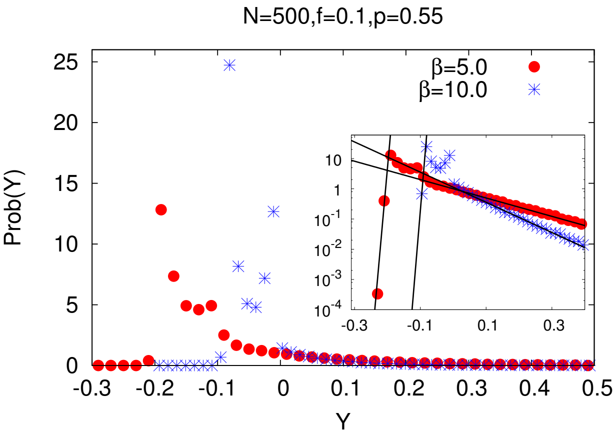


Work distributions for inhomogeneous state



$$P_{\mathrm{F,R}}(W_{\mathrm{F,R}}) \sim \frac{1}{\sigma_{\mathrm{F,R}}} g_{\mathrm{F,R}}\left(\frac{W_{\mathrm{F,R}} - \langle W_{\mathrm{F,R}}\rangle}{\sigma_{\mathrm{F,R}}}\right) \quad g_{\mathrm{F}}(x) = g_{\mathrm{R}}(-x)$$

Hatano-Sasa distribution



Summary

- Kuramoto model from the point of view of equilibrium and non equilibrium statistical mechanics
- First-order phase transition in presence of inertia (full phase diagram)
- Long-range interactions, the HMF model and the Vlasov equation
- Check of out-of-equilibrium fluctuations: effective one-body

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View of the gulf of Trieste from SISSA