# Non equilibrium free energies in systems with long range interactions and models of geophysical turbulence

#### F. BOUCHET – ENS-Lyon and CNRS

#### May 2014 - GGI - Firenze

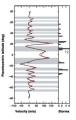
F. Bouchet CNRS–ENSL Non equilibrium free energies in mean field systems.

# Collaborators and Ongoing Projects

- Large deviations, instantons non-equilibrium phase transition for quasi-geostrophic turbulence: J. Laurie (Post-doc ANR Statocean), O. Zaboronski (Warwick Univ.)
- Large deviations in two time scale problems: jet formation in Geostrophic Turbulence: C. Nardini, T. Tangarife (ENS-Lyon), and E. Van den Eijnden (NYU)
- Rare events, large deviations, and extreme heat waves in the atmosphere: J. Wouters (ENS-Lyon)
- Numerical computation of large deviation for transition trajectories in the Ginzburg Landau equation: J. Rolland and E. Simonnet (INLN-Nice)
- Large deviations, non-equilibrium free energies, and current fluctuation for particles with long range interactions:
   K. Gawedzki, and C. Nardini (ENS-Lyon).

#### Jupiter's Zonal Jets We look for a theoretical description of zonal jets



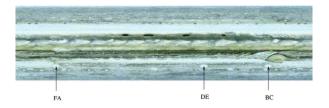


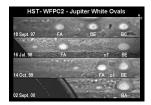
Jupiter's atmosphere

Jupiter's zonal winds (Voyager and Cassini, from Porco et al 2003)

How to theoretically predict such a velocity profile?

#### Has One of Jupiter's Jets Been Lost ? We look for a theoretical description of zonal jets



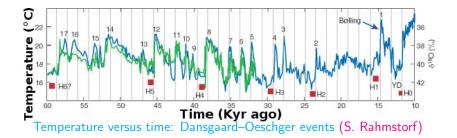


Jupiter's white ovals (see Youssef and Markus 2005)

The white ovals appeared in 1939-1940 (Rogers 1995). Following an instability of the zonal jet ?

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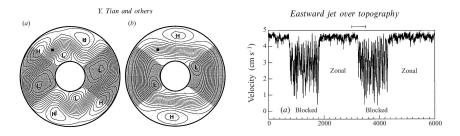
#### Abrupt Climate Changes Long times matter



- What is the dynamics and probability of abrupt climate changes?
- Predict attractors, transition pathways and probabilities.
- Study a hierarchy of models of ocean circulation and of turbulent atmospheres.

#### Phase Transitions in Rotating Tank Experiments The rotation as an ordering field (Quasi Geostrophic dynamics)

#### Transitions between blocked and zonal states



Y. Tian and col, J. Fluid. Mech. (2001) (groups of H. Swinney and M. Ghil)

# The Main Issues

- How to characterize and predict the attractors in extended systems with long range interactions?
- In case of multiple attractors, can we compute their relative probability?
- Can we compute the transition pathways and the transition probabilities?

# Large Deviations and Free Energies for Macroscopic Variables

- We all know the importance of the concepts of entropy and free energy in equilibrium statistical mechanics.
- Free energy of a macrostate (for instance the velocity field, the density  $\rho$ , the one particle distribution function, etc.)

$$\mathcal{P}_{N}[\rho] \underset{N \to \infty}{\sim} \frac{1}{Z} e^{-N\frac{\mathscr{P}[\rho]}{k_{B}T}},$$
  
with  $Z = \int \mathscr{D}[\rho] e^{-N\frac{\mathscr{P}[\rho]}{k_{B}T}}$ 

• The free energy is

$$F(T) = -k_B T \log(Z(T)) = \min_{\{\rho \mid \int \rho = 1\}} \mathscr{F}[\rho].$$

• How to generalize these concepts to non-equilibrium problems?

#### The Driven and Overdamped Mean Field Model

• Langevin dynamics for an overdamped Hamiltonian system with long range interactions

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N} \sum_{m=1}^N \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT}\eta_n.$$

• F is a constant force driving the system out of equilibrium (F = 0 : equilibrium problem).

# Outline

- The Driven Overdamped Model with Mean Field Interactions
  - The model and the Non linear Fokker-Planck equation
  - Large deviation of the empirical density
  - Action minimisation, Hamilton Jacobi, and transverse decomposition for the non-equilibrium free energies
- 2 Two easy solutions for the free energy computation
  - Sanov's theorem and large deviations
  - The equilibrium case (F=0)
  - The independent particle case ( $\epsilon = 0$  and  $F \neq 0$ )
- 3 Perturbative expansion of the free energies
  - Leading order correction to the free energy
  - Series expansion and solvability conditions
  - Numerical computation of large deviations

The model and the Non linear Fokker-Planck equation Large deviation of the empirical density Action minimisation, Hamilton Jacobi, and transverse decon

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#### The Driven and Overdamped Mean Field Model

• Langevin dynamics for an overdamped Hamiltonian system with long range interactions

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N} \sum_{m=1}^N \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT}\eta_n.$$

- x<sub>n</sub> ∈ T = [0, 2π[ the one dimensional circle (generalization to diffusions over the torus T<sup>d</sup> in dimension d is straightforward). N particles.
- $\langle \eta_n \eta_m \rangle = \delta^{nm} \delta(t-t').$
- The onsite potential *U* and the interaction potential *V* are periodic functions.
- F is a constant force driving the system out of equilibrium (F = 0 : equilibrium problem).

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The Non-Linear Fokker–Planck Eq. (Vlasov Mac–Kean Eq.)

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N} \sum_{m=1}^{N} \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT} \frac{\mathrm{d}\beta_n}{\mathrm{d}t}$$

- The empirical density  $\rho_N(x) = \frac{1}{N} \sum_{n=1}^N \delta(x x_n)$ .
- For large *N*, a mean field approximation gives the Non-Linear Fokker Planck equation:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\frac{\partial}{\partial x} \left[ \mathscr{J} \left[ \rho \right] \right] \text{ with } \mathscr{J} \left[ \rho \right] = \left( F - \frac{\mathrm{d}U}{\mathrm{d}x} - \varepsilon \frac{\mathrm{d}}{\mathrm{d}x} V * \rho \right) \rho - k_B T \frac{\partial \rho}{\partial x}, \\ \text{ with } (V * \rho)(x) &\equiv \int \mathrm{d}x_1 \rho(x_1) V(x - x_1). \end{aligned}$$

• We assume that a stationary solution of the non-linear Fokker–Planck equation exists:

$$\frac{\partial}{\partial x}\left[\left(-F+\frac{\mathrm{d}U}{\mathrm{d}x}+\varepsilon\frac{\mathrm{d}}{\mathrm{d}x}V*\rho_{\varepsilon,F}\right)\rho_{\varepsilon,F}+k_BT\frac{\partial\rho_{\varepsilon,F}}{\partial x}\right]=0.$$

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# The PDF of the Empirical Density

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N} \sum_{m=1}^{N} \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT} \frac{\mathrm{d}\eta_n}{\mathrm{d}t}$$

• Empirical density:

$$\rho_N(t,x) = \frac{1}{N} \sum_{n=1}^N \delta(x-x_n).$$

• "Probability Density Function" of the empirical density:

$$\mathscr{P}_{\mathsf{N}}[\rho] \equiv \langle \delta(\rho - \rho_{\mathsf{N}}) \rangle_{\mathsf{N}},$$

(the probability density to observe  $\rho_N$  to be equal to  $\rho$ , where  $\rho$  is a function of x).

• Formally defined through the average of any observable  $\mathscr{A}$ :

$$\langle \mathscr{A}[\rho] \rangle_{N} = \int \mathscr{D}[\rho] \mathscr{A}[\rho] \mathscr{P}_{N}[\rho].$$

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## Large Deviations of the Empirical Density

• Empirical density

$$\rho_N(t,x) = \frac{1}{N} \sum_{n=1}^N \delta(x-x_n).$$

• If the empirical density PDF verifies

$$\frac{1}{N}\log \mathscr{P}_{N}\left[\rho_{N}=\rho\right] \underset{N\to\infty}{\sim} -\frac{\mathscr{F}\left[\rho\right]}{k_{B}T},$$

we call this a large deviation result with rate N and large deviation functional  $-\mathscr{F}/k_BT$ .

• Loosely speaking, we have

$$\mathscr{P}_{N}[\rho_{N}=\rho] \underset{N\to\infty}{\sim} C \mathrm{e}^{-N\frac{\mathscr{F}[\rho]}{k_{B}T}}$$

- Then  $\mathscr{F}[\rho]$  is the free energy of the macrostate  $\rho$ .
- What is the large deviation rate function of the overdamped mean field model?

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An Exact Evolution Equation for the Empirical Density

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N} \sum_{m=1}^{N} \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT} \frac{\mathrm{d}\eta_n}{\mathrm{d}t}$$

- The empirical density  $\rho_N(x) = \frac{1}{N} \sum_{n=1}^N \delta(x x_n)$ .
- With Ito formula, we get the formal equation

$$\frac{\partial \rho_N}{\partial t} = -\frac{\partial}{\partial x} \left( \mathscr{J} \left[ \rho_N \right] \right) + \frac{\partial}{\partial x} \left( \sqrt{\frac{2k_B T}{N} \rho_N} \eta \right),$$

with  $\langle \eta(t,x)\eta(t',x')
angle=\delta(t-t')\delta(x-x').$ 

- This is a stochastic partial differential equation with weak noise
- Path integral formulation (Onsager–Machlup) or Freidlin–Wentzell theory.

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Action for the Large Deviations of the Empirical Density

$$\frac{\partial \rho_N}{\partial t} = -\frac{\partial}{\partial x} \left( \mathscr{J} \left[ \rho_N \right] \right) + \frac{\partial}{\partial x} \left( \sqrt{\frac{2k_B T}{N} \rho_N} \xi \right).$$

• Then the stationary PDF for the empirical distribution verifies a large deviation principle with

$$\mathscr{F}[\rho] = \min_{\{r(t,x) \mid r(-\infty,x) = \rho_{\varepsilon,F} \text{ and } r(0,x) = \rho\}} \mathscr{A}[r]$$

where  $\rho_{\varepsilon,F}$  is the stationary distribution of the non-linear Fokker-Planck equation, with

$$\mathscr{A}[r] = \frac{1}{4} \int_{-\infty}^{0} \mathrm{d}t \left\langle \frac{\partial r}{\partial t} + \frac{\partial}{\partial x} \mathscr{J}[r], \frac{\partial r}{\partial t} + \frac{\partial}{\partial x} \mathscr{J}[r] \right\rangle_{r}$$

 The stationary large deviations functional can be obtained solving an difficult variational problem (D.A. Dawson and Gärtner, 1987).

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## Action and Scalar Product

$$\mathscr{A}[r] = \frac{1}{4} \int_{-\infty}^{0} \mathrm{d}t \int \mathrm{d}x \left\langle \frac{\partial r}{\partial t} + \frac{\partial}{\partial x} \mathscr{J}[r], \frac{\partial r}{\partial t} + \frac{\partial}{\partial x} \mathscr{J}[r] \right\rangle_{r},$$

with

$$\langle r_1, r_2 \rangle_r = \int \mathrm{d}x_1 \mathrm{d}x_2 \, C_\eta^{-1} \left( x_1 - x_2 \right) r_1(x_1) r_2(x_2) = \int \mathrm{d}x \, r_1(x) \left( \frac{\partial}{\partial x} \left[ r \frac{\partial}{\partial x} \right] \right)^{-1} (r_2)(x).$$

• In the following we will consider the gradient of a functional  $\mathscr{V}$ with respect to this scalar product, defined by  $\delta \mathscr{V} = \langle \operatorname{grad}_r \mathscr{V}, \delta \rho \rangle_r$ 

We get

$$\operatorname{grad}_{r} \mathscr{V} = -\frac{\partial}{\partial x} \left[ r \frac{\partial}{\partial x} \frac{\delta \mathscr{V}}{\delta \rho(x)} \right].$$

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## Hamilton-Jacobi Equation

The solution of the variational problem

$$\mathscr{F}[\rho] = \min_{\left\{r(t,x) \mid r(-\infty,x) = \rho_{\varepsilon,F} \text{ and } r(0,x) = \rho\right\}} \mathscr{A}[r]$$

with

$$\mathscr{A}[r] = \frac{1}{4} \int_{-\infty}^{0} \mathrm{d}t \int \mathrm{d}x \left\langle \frac{\partial r}{\partial t} + \frac{\partial}{\partial x} \mathscr{J}[r], \frac{\partial r}{\partial t} + \frac{\partial}{\partial x} \mathscr{J}[r] \right\rangle_{r},$$

is a solution of the Hamilton-Jacobi equation

$$\langle \operatorname{grad}_{r} \mathscr{F}, \operatorname{grad}_{r} \mathscr{F} \rangle_{r} + \left\langle \operatorname{grad}_{r} \mathscr{F}, -\frac{\partial}{\partial x} \mathscr{J}[r] \right\rangle_{r} = 0.$$

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Non-Equilibrium Free Energy and Transverse Decomposition

With some natural hypothesis insuring unicity, we have equivalence between the three properties:

- ${f 0}$   ${\mathscr F}$  is a local minima of the action variational problem
- 2  ${\mathscr F}$  solves the Hamilton Jacobi equation

$$\langle \operatorname{grad}_{r} \mathscr{F}, \operatorname{grad}_{r} \mathscr{F} \rangle_{r} + \left\langle \operatorname{grad}_{r} \mathscr{F}, -\frac{\partial}{\partial x} \mathscr{J}[r] \right\rangle_{r} = 0.$$

There exists a transverse decomposition

$$-\frac{\partial}{\partial x}\mathscr{J}[r] = -\operatorname{grad}_{r}\mathscr{F} + \mathscr{G} \text{ with } \langle \operatorname{grad}_{r}\mathscr{F}, \mathscr{G} \rangle_{r} = 0.$$

Bertini, DeSole, Gabrielli, Jona-Lasinio and Landim

Sanov's theorem and large deviations The equilibrium case (F=0) The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

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Sanov's theorem and large deviations The equilibrium case (F=0) The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

# Sanov's Theorem

- Let us consider N independent and identically distributed variables  $\{x_n\}$  with PDF P(x).
- What is the large deviation of the empirical density  $\rho_N(x) = \frac{1}{N} \sum_{n=1}^N \delta(x x_n)$ ?
- Sanov's theorem:

$$\frac{1}{N}\log \mathscr{P}_{N}[\rho] \underset{N \to \infty}{\sim} - \int \rho \log \left(\frac{\rho}{P}\right) dx \equiv \mathscr{S}_{KB}[\rho \| P]$$

• Or equivalently

$$\langle \delta(\rho - \rho_N) \rangle_N \equiv \int \prod_{n=1}^N dx_n P(x_n) \, \delta(\rho - \rho_N) \mathop{\sim}_{N \to \infty} C e^{-N \int \rho \log\left(\frac{\rho}{P}\right) dx}$$

- The large deviation rate functional is the Kullback–Leibler entropy. If  $P = 1/2\pi$ ,  $\mathscr{S}_{KB}[\rho || P] = \mathscr{S}[\rho] = -\int \rho \log(\rho) dx$ .
- The most probable PDF is P.

Sanov's theorem and large deviations **The equilibrium case (F=0)** The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

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Sanov's theorem and large deviations **The equilibrium case (F=0)** The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

Equilibrium (F = 0): the Gibbs Distribution

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = -\frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N}\sum_{m=1}^N \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT}\eta_n.$$

• It is a Langevin dynamics with Hamiltonian

$$H_N(x_1,...,x_N) = \sum_{n=1}^N U(x_n) + \frac{1}{2N} \sum_{n,m=1}^N V(x_n - x_m).$$

• We know that the *N*-particle stationary measure is the Gibbs measure with PDF

$$P_N^S(x_1,...,x_N) = \frac{1}{Z_N} e^{-\frac{H_N}{k_B T}}.$$

• We want to compute

$$\mathscr{P}_{N}^{S}[\rho] = \langle \delta(\rho - \rho_{N}) \rangle_{N} = \frac{1}{Z_{N}} \int \prod_{n=1}^{N} \mathrm{d}x_{n} \,\delta(\rho - \rho_{N}) \,\mathrm{e}^{-\frac{H_{N}(x_{1},\dots,x_{N})}{k_{B}T}}.$$

Sanov's theorem and large deviations **The equilibrium case (F=0)** The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

Large Deviations of the Empirical Density at Equilibrium

$$\mathscr{P}_{N}[\rho] = \frac{1}{Z_{N}} \int \prod_{n=1}^{N} \mathrm{d}x_{n} \,\delta(\rho - \rho_{N}) \,\mathrm{e}^{-\frac{H_{N}(x_{1},\dots,x_{N})}{k_{B}T}}$$

• We use the mean field "approximation" for the Hamiltonian

$$H_{N} \underset{N \to \infty}{\sim} N \mathscr{H}[\rho] \equiv N \left[ \int \rho U + \frac{1}{2} \int \rho (V * \rho) \right].$$

Then

$$\mathscr{P}_{N}^{S}[\rho] \underset{N \to \infty}{\sim} \frac{1}{Z_{N}} e^{-N\frac{\mathscr{K}[\rho]}{k_{B}T}} \int \prod_{n=1}^{N} dx_{n} \,\delta\left(\rho - \rho_{N}\right) \underset{N \to \infty}{\sim} \frac{1}{Z} e^{-N\frac{\mathscr{F}_{eq}[\rho]}{k_{B}T}},$$

with

$$\mathscr{F}_{eq}[\rho] = \mathscr{H}[\rho] + k_B T \int \rho \log(\rho) \, \mathrm{d}x.$$

• E. Caglioti, P. L. Lions, C. Marchioro, M. Pulvirenti, *Commun. Math. Phys.*,1992.

## Equilibrium Solution and Gradient Flow

• What is the relation between the equilibrium solution

$$\mathscr{F}_{eq}[\rho] = \mathscr{H}[\rho] + k_B T \int \rho \log(\rho) \, \mathrm{d}x.$$

and the transverse decomposition?

• We can check directly that

$$-\frac{\partial}{\partial x}\mathscr{J}_{F=0}\left[\rho\right]=-\mathrm{grad}_{\rho}\mathscr{F}_{eq}$$

F. Otto - C. Villani

• In the equilibrium case, the non-linear Fokker-Planck equation is a gradient flow with respect to the "noise scalar product".

The driven overdamped mean field model<br/>Two easy solutionsSanov's theorem and large deviations<br/>The equilibrium case (F=0)Perturbative Non-eq. free energies.The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

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Sanov's theorem and large deviations The equilibrium case (F=0) The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

## $\varepsilon = 0$ : A Trivial Non-Equilibrium Case

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) + \sqrt{2k_BT}\frac{\mathrm{d}\eta_n}{\mathrm{d}t}.$$

Empirical density

$$\rho_N(t,x) = \frac{1}{N} \sum_{n=1}^N \delta(x-x_n).$$

• We assume that the initial N-particle PDF is

$$P_N(x_1,...,x_N,t=0) = \prod_{n=1}^N \rho_0(x_n).$$

• The *N* particles are statistically independent. We can apply Sanov's theorem.

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Sanov's theorem and large deviations The equilibrium case (F=0) The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

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#### $\varepsilon = 0$ : A Trivial Non-Equilibrium Case

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) + \sqrt{2k_BT}\frac{\mathrm{d}\eta_n}{\mathrm{d}t}.$$

• The N-particle PDF is  $P_N(x_1,...,x_N,t=0) = \prod_{n=1}^N \rho_0(x,t)$ , where  $\rho_0$  is the solution to the one particle Fokker-Planck equation

$$\frac{\partial \rho_0}{\partial t} = \frac{\partial}{\partial x} \left[ \left( -F + \frac{\mathrm{d}U}{\mathrm{d}x} \right) \rho_0 + k_B T \frac{\partial \rho_0}{\partial x} \right] = FP[\rho_0].$$

• Using Sanov's theorem we conclude

$$\frac{1}{N}\log \mathscr{P}_N\left[\rho_N=\rho,t\right] \underset{N\to\infty}{\sim} -\frac{\mathscr{F}[\rho,t]}{k_B T} = -\int \rho(x)\log\left(\frac{\rho(x)}{\rho_0(t,x)}\right) \mathrm{d}x.$$

• If  $\rho_{0,F}$  is the stationary distribution of the one particle Fokker-Planck equation, we have

$$\mathscr{F}_{\varepsilon=0}[\rho] = k_B T \int \rho(x) \log\left(\frac{\rho(x)}{\rho_{0,F}(x)}\right) dx.$$

Sanov's theorem and large deviations The equilibrium case (F=0) The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )

Equilibrium Solution and Transverse Decomposition

We can directly check that

$$-\frac{\partial}{\partial x}\mathscr{J}_{\varepsilon=0}\left[\rho\right]=-\mathsf{grad}_{\rho}\mathscr{F}_{\varepsilon=0}+\mathscr{G}_{\varepsilon=0}\left[\rho\right]$$

with

$$\left\langle \mathsf{grad}_{\rho}\mathscr{F}_{\varepsilon=0},\mathscr{G}_{\varepsilon=0}\right\rangle _{\rho}=0$$

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#### The Non-Equilibrium Interacting Case

$$\frac{\mathrm{d}x_n}{\mathrm{d}t} = F - \frac{\mathrm{d}U}{\mathrm{d}x}(x_n) - \frac{\varepsilon}{N} \sum_{m=1}^N \frac{\mathrm{d}V}{\mathrm{d}x}(x_n - x_m) + \sqrt{2k_BT} \frac{\mathrm{d}\eta_n}{\mathrm{d}t}.$$

- The N-particle PDF is not known a-priori.
- No detailed balance, currents in the stationary state.
- What to do then ?

Leading order correction to the free energy Series expansion and solvability conditions Numerical computation of large deviations

# Outline

- The Driven Overdamped Model with Mean Field Interactions
   The model and the Non linear Fokker-Planck equation
  - Large deviation of the empirical density
  - Action minimisation, Hamilton Jacobi, and transverse decomposition for the non-equilibrium free energies
- 2 Two easy solutions for the free energy computation
  - Sanov's theorem and large deviations
  - The equilibrium case (F=0)
  - The independent particle case ( $\varepsilon = 0$  and  $F \neq 0$ )
- Operational expansion of the free energies
  - Leading order correction to the free energy
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#### Perturbative expansion of the free energy

• We suppose

$$-\frac{\partial}{\partial x}\mathscr{J}[\rho] = -\operatorname{grad}_{\rho}\mathscr{F}_{0} + \mathscr{G}_{0}[\rho] + \varepsilon \mathscr{P}[\rho]$$

with

$$\left<\operatorname{\mathsf{grad}}_{\rho}\mathscr{F}_{0},\mathscr{G}_{0}\right>_{
ho}=0$$

- We look for the solution  $\mathscr{F}_{\varepsilon}$  of either, the action minimization, the Hamilton-Jacobi equation or the transverse decomposition.
- Can we find  $\mathscr{F}_1$  such that

$$\mathscr{F}_{\varepsilon} = \mathscr{F}_{0} + \varepsilon \mathscr{F}_{1} + O(\varepsilon^{2})?$$

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Zero Order Fluctuation Path Zero order minimizer of the action.

• The minimizer of the action corresponding to the zero order free energy problem

$$-rac{\partial}{\partial x}\mathscr{J}_0[
ho]=- ext{grad}_{
ho}\mathscr{F}_0+\mathscr{G}_0[
ho]$$

is a fluctuation path  $R_0[\rho, t]$ : a time reversed solution to the relaxation equation for the dual dynamics.

It solves

$$\frac{\partial R_0}{\partial t} = \operatorname{grad}_{R_0} \mathscr{F}_0 + \mathscr{G}_0[R_0]$$

with  $R_0[\rho, -\infty] = \rho_0$  (an attractor of the zero order dynamics) and  $R_0[\rho, 0] = \rho$ .

Freidlin-Wentzell book.

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# First Order Non-Equilibrium Free Energy

- When we have a variational problem, inserting the zero order minimizer in the action, we immediately obtain the first order minima.
- Using this remark, we obtain

$$\mathscr{F}_{1}[\rho] = -\varepsilon \int_{-\infty}^{0} \left\langle \mathsf{grad}_{R_{0}[\rho]} \mathscr{F}_{0}[R_{0}[\rho]], \mathscr{P}[R_{0}[\rho]] \right\rangle_{R_{0}[\rho]}$$

• The first order non-equilibrium free energies can be expressed as an integral over the relaxation paths.

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#### Solution at Order 1 for the Mean Field Models

$$\mathscr{F}^{\leq 2}[\rho] = \int \left[\rho\left(\frac{\varepsilon}{2}V*\rho\right) + k_B T\rho \ln \frac{\rho}{\rho_{0,F}}\right] + \frac{\varepsilon}{2} \int \int dx_1 dx_2 \rho(x_1)\rho(x_2) f_1(x_1,x_2).$$

with  $f_1$  the unique solution to

$$\frac{1}{\rho_{0,F}(x_1)}FP_{0,x_1}\left[\rho_{i,0}(x_1)f_1'(x_1,x_2)\right] + \frac{1}{\rho_{0,F}(x_2)}FP_{0,x_2}\left[\rho_{0,F}(x_2)f_1'(x_1,x_2)\right] = \dots$$
$$\dots j_0V'(x_1 - x_2)\left[\frac{1}{\rho_{0,F}(x_1)} - \frac{1}{\rho_{0,F}(x_2)}\right].$$

 A non local free energy: conjugated effects of the non-equilibrium driving and of the two-body interactions.

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# Series Expansion and Solvability Conditions

• The first order solution can be generalized to all order to get the expansion

$$\mathscr{F}_{\varepsilon}[\rho] = \sum_{n=0}^{\infty} \varepsilon^n \mathscr{F}_n[\rho],$$

- We have natural recurrence relation to express all  $\mathscr{F}_n[\rho]$  as integrals over the relaxation paths corresponding to the previous order fluctuation paths.
- The convergence of these integrals at each order, is equivalent to solvability conditions that appear the Hamilton-Jacobi equation when expanding in power of  $\varepsilon$ .
- We have proven that these solvability conditions are verified at all order (existence of the series expansion).

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# Non-Equilibrium Free-Energy of the Mean Field Models

- We got some explicit results for the computation of the non-equilibrium free energy of the driven overdamped HMF model.
- The free energy can be easily computed for two cases: the equilibrium case and the independent particle case.
- We have developed a theory of perturbative expansions of action minimisation and Hamilton-Jacobi equation, valid in a broad context.
- This theory, applied to the mean field models, show that at order one (and above) the non-equilibrium free energy is a non local functional of the field due either to non-equilibrium effects or to two body interactions.

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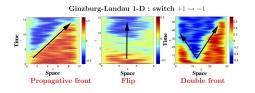
# Outline

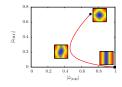
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Numerical Computation of Rare Events and Large Deviations Computation of least action paths (instantons) and/or multilevel splitting





Multilevel-splitting: Ginzburg-Landau transitions (with E. Simonnet and J. Rolland) 2D Navier-Stokes instantons (with J. Laurie)

• Rare events and their probability can now be computed numerically in complex dynamical systems.

Leading order correction to the free energy Series expansion and solvability conditions Numerical computation of large deviations

# Summary and Perspectives

- Explicit computations of non-equilibrium free energies (large deviations for the empirical density) for the dynamics of particles with mean field interactions (two limit cases, and perturbative expansions)
- A general theory for series expansion of free energies within each basin of attractions of the unperturbed dynamics.
- Non-equilibrium statistical mechanics and large deviation theory will be useful to understand turbulence in Geophysical Fluid Dynamics.

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