Non-Equilibrium Free Energies for Particle Systems and Turbulent Flows

F. BOUCHET – ENS-Lyon and CNRS

Statistical Mechanics of Self-Gravitating Particles.
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Collaborators

- Non-Equilibrium free energy of a driven system with long range interactions: K. Gawedzki and C. Nardini (ENS-Lyon and Florence).
- Instantons and large deviations for the 2D Navier-Stokes equations: J. Laurie (Post-doc ANR Statocean), O. Zaboronsky (Warwick).
- Kinetic theory of geostrophic jets: T. Tangarife (ENS-Lyon) and C. Nardini.
- Large deviations for systems with connected attractors: H. Touchette (Queen Mary Univ, London).
- Large deviations and Monte-Carlo simulations of the 2D Euler and Shallow Water eq.: M. Potters (Utrecht university) and A. Licari (ENS-Lyon).
- Large deviations and Monte-Carlo simulations of the 3D axisymmetric Euler eq.: S. Thalabard (CEA Saclay).

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 ρ, the one particle distribution function, etc.)

$$\mathscr{P}_N[\rho] \underset{N\to\infty}{\sim} \frac{1}{Z} e^{-N\frac{\mathscr{F}[\rho]}{k_B T}},$$

$$\text{with } Z = \int \mathscr{D}[\rho]\, e^{-N\frac{\mathscr{F}[\rho]}{k_B T}}.$$

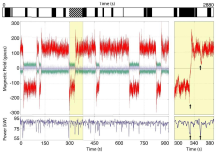
- The free energy is

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

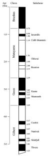
- How to generalize these concepts to non-equilibrium problems?

Random Transitions in Geophysical Turbulence

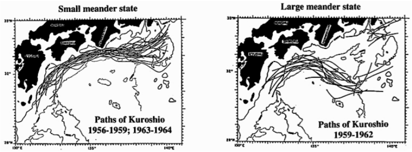
A huge number of turbulent flows have a bistable or multistable behavior



VKS experiment



Earth



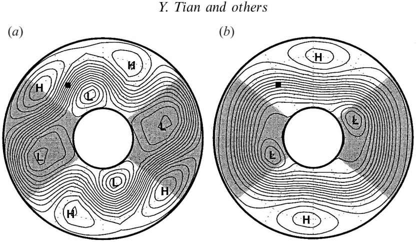
Kuroshio current

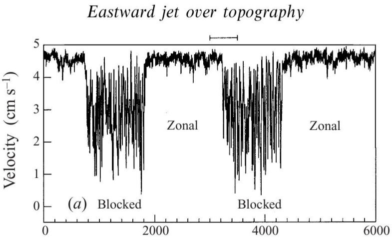
Other examples:

- Turbulent convection, Van Karman, and Couette turbulence.
- Multistability in the atmosphere, weather regimes, and so on.

Phase Transitions in Rotating Tank Experiments
(Quasi Geostrophic dynamics)

Transitions between blocked and zonal states



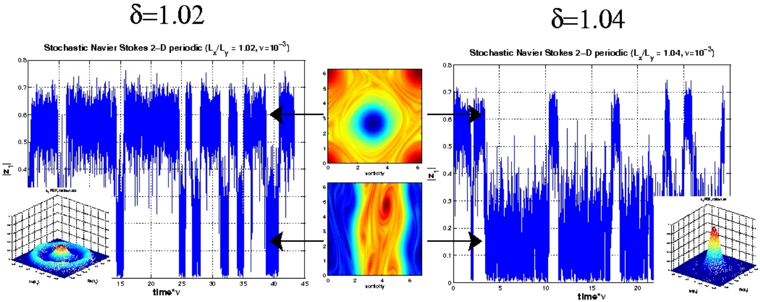


Y. Tian and col, J. Fluid. Mech. (2001) (groups of H. Swinney and M. Ghil)

The 2D Stochastic-Navier-Stokes Eq.

Non equilibrium phase transitions

$$\frac{\partial \omega}{\partial t} + \mathbf{v}.\nabla\omega = \nu\Delta\omega - \alpha\omega + \sqrt{\sigma} f_s .$$



Order parameter : $z_1 = \int dxdy \exp(iy)\omega(x,y)$.

For unidirectional flows $|z_1| \simeq 0$, for dipoles $|z_1| \simeq 0.6 - 0.7$

The Driven and Overdamped Mean Field Model

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

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

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

Outline

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The Driven and Overdamped Mean Field Model

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

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

- $x_n \in T = [0, 2\pi[$ the one dimensional circle (generalization to diffusions over the torus T^d in dimension d is straightforward). N particles.
- $\langle \zeta_n \zeta_m \rangle = \delta^{nm}\delta(t - t')$.
- 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).

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

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

- 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 Vlasov Mac-Kean Eq.:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left[\left(-F + \frac{\mathrm{d}U}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}V * \rho\right)\rho + k_B T\frac{\partial \rho}{\partial x}\right],$$

$$\text{with } (V * \rho)(x) \equiv \int \mathrm{d}x_1\, \rho(x_1) V(x - x_1).$$

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

$$\frac{\partial}{\partial x}\left[\left(-F + \frac{\mathrm{d}U}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}V * \rho_i\right)\rho_i + k_B T\frac{\partial \rho_i}{\partial x}\right] = 0.$$

Outline

The PDF of the Empirical Density

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

- Empirical density:

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

- "Probability Density Function" of the empirical density:

$$\mathscr{P}_N[\rho] \equiv \langle \delta(\rho - \rho_N) \rangle_N,$$

  (the probability density to observe ρ_N to be equal to ρ, where ρ is a function of x).
- Formally defined through the average of any observable $\mathscr{A}$:

$$\langle \mathscr{A}[\rho] \rangle_N = \int \mathscr{D}[\rho]\, \mathscr{A}[\rho]\, \mathscr{P}_N[\rho].$$

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

$$\frac{1}{N}\log\mathscr{P}_N[\rho] \underset{N\to\infty}{\sim} -\frac{\mathscr{F}[\rho]}{k_B T},$$

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

- Loosely speaking, we have

$$\mathscr{P}_N[\rho] \underset{N\to\infty}{\sim} C\mathrm{e}^{-N\frac{\mathscr{F}[\rho]}{k_B T}}.$$

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

Outline

1. The Driven Overdamped Model with Mean Field Interactions
   - The model and the Vlasov Mac-Kean equation
   - Large deviation of the empirical density
   - Sanov's theorem and large deviations
2. Non-Equilibrium Free Energies for the mean field model
   - Dawson–Gärtner result
   - A functional Hamilton-Jacobi equation
   - Solution for the stationary Hamilton-Jacobi equation
3. Large deviations for turbulent flows
   - Phase Transitions for the 2D Stochastic Navier-Stokes equations
   - Path integrals and large deviations
   - Instantons for the 2D Stochastic Navier-Stokes equations

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:

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

- Or equivalently

$$\langle\delta(\rho-\rho_N)\rangle_N \equiv \int\prod_{n=1}^{N}\mathrm{d}x_n P(x_n)\,\delta(\rho-\rho_N) \underset{N\to\infty}{\sim} C\mathrm{e}^{-N\int\rho\log\left(\frac{\rho}{P}\right)\mathrm{d}x}.$$

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

Equilibrium: the Gibbs Distribution

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

- 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

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

- We want to compute

$$\mathscr{P}_N^S[\rho] = \langle \delta(\rho - \rho_N) \rangle_N = \frac{1}{Z_N}\int \prod_{n=1}^{N}\mathrm{d}x_n\, \delta(\rho - \rho_N)\,\mathrm{e}^{-\frac{H_N(x_1,...,x_N)}{k_B T}}.$$

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

$$\mathscr{P}_N^S[\rho] \underset{N\to\infty}{\sim} \frac{1}{Z_N}\mathrm{e}^{-N\frac{\mathscr{H}[\rho]}{k_B T}}\int \prod_{n=1}^{N}\mathrm{d}x_n\,\delta(\rho-\rho_N) \underset{N\to\infty}{\sim} \frac{1}{Z}\mathrm{e}^{-N\frac{\mathscr{F}[\rho]}{k_B T}},$$

with

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

- E. Caglioti, P. L. Lions, C. Marchioro, M. Pulvirenti, *Commun. Math. Phys.*,1992.
- F. Bouchet, J. Barré, J. Stat. Mech., 2005.

$V=0$ and $F\neq 0$: A Trivial Non-Equilibrium Case

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

- 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.

$V=0$: A Trivial Non-Equilibrium Case

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

- The N-particle PDF is $P_N(x_1,...,x_N,t=0)=\prod_{n=1}^N\rho_0(x,t)$, where ρ_0 is the solution to the one particle Fokker-Planck equation

$$\frac{\partial\rho_0}{\partial t}=FP_0\left[\rho_0\right]\text{ with }FP_0\left[\rho\right]\equiv\frac{\partial}{\partial x}\left[\left(-F+\frac{\mathrm{d}U}{\mathrm{d}x}\right)\rho+k_BT\frac{\partial\rho}{\partial x}\right].$$

- Using Sanov's theorem we conclude

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

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

$$\mathscr{F}_S\left[\rho\right]=k_BT\int\rho(x)\log\left(\frac{\rho(x)}{\rho_{0,i}(x)}\right)\mathrm{d}x.$$

The Non-Equilibrium Interacting Case

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

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

Outline

An Exact Evolution Equation for the Empirical Density

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

- With Ito formula, we get

$$\frac{\partial \rho_N}{\partial t} = \left[\left(-F + \frac{\mathrm{d}U}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}(V * \rho_N)\right)\rho_N + k_B T\frac{\partial \rho_N}{\partial x}\right] + \sqrt{\frac{2k_B T}{N}\rho_N}\xi,$$

with $\langle \zeta(t,x)\zeta(t',x')\rangle = \delta(t-t')\delta(x-x')$.

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

Freidlin–Wentzell theory or Onsager Machlup Formalism

Classical Large Deviations for SDE or SPDE

$$dx = f(x)dt + \sqrt{\nu}dW.$$

- Hypothesis: the deterministic dynamics has isolated attractors.

  Large deviation results:

$$P(X) \sim \exp\left(-\frac{V(X)}{\nu}\right) \text{ to mean } \lim_{\nu\to 0} \nu \log P = -V.$$

$$\text{with } V(X) = \inf_{t>0} \inf_{\{x(t)|x(0)\in 0 \text{ and } x(t)=X\}} L[x],$$

$$\text{and } L[x] = \frac{1}{2}\int_0^t ds\,(\dot{x} - f(x))^2.$$

Application of Instanton or Freidlin–Wentzell Theory

$$\frac{\partial \rho_N}{\partial t} = j\left[\rho_N\right] + \sqrt{\frac{2k_B T}{N}\rho_N}\xi .$$

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

$$\mathscr{F}\left[\rho\right] = \min_{\left\{\tilde{\rho}(t,x) | \tilde{\rho}(-\infty,x)=\rho_S \text{ and } \tilde{\rho}(0,x)=\rho\right\}} \mathscr{I}\left[\tilde{\rho}\right],$$

where ρ_s is the stationary distribution of the non-linear Fokker-Planck equation, with

$$\mathscr{I}\left[\tilde{\rho}\right] = \frac{1}{4}\int_{-\infty}^{0} \mathrm{d}t \int \mathrm{d}x \left(\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial j\left[\tilde{\rho}\right]}{\partial x}\right)\left(\frac{\partial}{\partial x}\left[\tilde{\rho}\frac{\partial}{\partial x}\right]\right)^{-1}\left(\frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial j\left[\tilde{\rho}\right]}{\partial x}\right).$$

D.A. Dawson and Gärtner, 1987

- The stationary large deviations functional can be obtained solving an intricate variational problem.

Outline

A Simpler Approach: Temporal Evolution of $\mathscr{F}$

- We can derive, from scratch, using Ito formula, the evolution equation for any observable

$$\left\langle \mathscr{A}\left[\rho\right]\right\rangle_N=\int\mathscr{D}\left[\rho\right]\mathscr{A}\left[\rho\right]\mathscr{P}_N\left[\rho,t\right].$$

- From this, we get the equation for verified by $\mathscr{P}_N$ and by $\mathscr{F}\left[\rho,t\right]=\lim_{N\rightarrow\infty}\frac{1}{N}\log\mathscr{P}_N\left[\rho,t\right]$

$$\frac{\partial\mathscr{F}}{\partial t}=\int\mathrm{d}x\left\{\left(\frac{\partial}{\partial x}\left(\frac{\delta\mathscr{F}}{\delta\rho(x)}\right)\right)^2-j\left[\rho\right](x)\frac{\partial}{\partial x}\left(\frac{\delta\mathscr{F}}{\delta\rho(x)}\right)\right\}.$$

- This is a functional Hamilton-Jacobi equation.

The Functional Hamilton-Jacobi Equation

Trivial solutions

$$\frac{\partial \mathscr{F}}{\partial t} = \int \mathrm{d}x \left\{ \left(\frac{\partial}{\partial x} \frac{\delta \mathscr{F}}{\delta \rho} \right)^2 - j[\rho] \frac{\partial}{\partial x} \frac{\delta \mathscr{F}}{\delta \rho} \right\}$$

- Check of the results for the trivial cases:
- We check that if $F = 0$, the equilibrium free energy $\mathscr{F}[\rho] = \mathscr{H}[\rho] + k_B T \int \rho \log(\rho)\, \mathrm{d}x$ is a solution.
- We check that if $V = 0$, the free energy we got from Sanov's theorem is a solution

$$\mathscr{F}[\rho] = k_B T \int \mathrm{d}x\, \rho(x) \log\left(\frac{\rho(x)}{\rho_0(x,t)} \right).$$

Outline

Solution for the Stationary Hamilton-Jacobi Eq.

$$I[\mathscr{F}][\rho] \equiv \int \mathrm{d}x \frac{\delta \mathscr{F}}{\delta \rho(x)}[\rho] \left\{ FP_0[\rho] + \varepsilon \rho (V' * \rho) - \frac{\mathrm{d}}{\mathrm{d}x}\left[\rho \frac{\mathrm{d}}{\mathrm{d}x} \frac{\delta \mathscr{F}}{\delta \rho(x)}[\rho] \right] \right\}.$$

- We want to solve

$$I[\mathscr{F}] = 0.$$

- We look for a Taylor expansion

$$\mathscr{F}[\rho] = \int \left[\frac{1}{2}\rho (V * \rho) + k_B T \rho \ln(\rho/\rho_{i,0}) \right] + \sum_{n=1}^{\infty} \varepsilon^n \mathscr{F}_n[\rho].$$

Taylor Series Solution of the Stationary Hamilton-Jacobi

- We expand. We get a hierarchy of non homogeneous linear problems
$$I_L\left[\mathscr{F}_n\right] = \mathscr{H}_n\left[\mathscr{F}_{n-1},...,\mathscr{F}_1\right],$$
with
$$I_L\left[\mathscr{F}\right]\left[\rho\right] \equiv \int \mathrm{d}x\,\frac{\rho}{\rho_{i,0}} FP_0\left[\rho_{i,0}\frac{\delta\mathscr{F}}{\delta\rho(x)}\right].$$
- Proof of the existence of the expansion : what is the kernel of $I_L\left[\mathscr{F}\right]$ and is $\mathscr{H}_n\left[\mathscr{F}_{n-1},...,\mathscr{F}_1\right]$ in the image of I_L (solvability condition)?

Solvability Condition

- We have proven that the solvability condition is satisfied for all order up to $n = 4$ included.
- We expect that the minima of $\mathscr{F}$ is $\rho_{i,\varepsilon}$ the stationary solution to the non-linear Fokker-Planck equation :

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\delta\mathscr{F}}{\delta\rho(\theta)}[\rho_{i,\varepsilon}] = 0.$$

- We have proven that the solvability condition at order $n+1$ is satisfied if and only if

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\frac{\delta\mathscr{F}^{\leq n}}{\delta\rho(\theta)}\left[\rho_{i,\varepsilon}^{\leq n}\right] = \mathscr{O}\left(\varepsilon^{n+1}\right).$$

Solution at Order 2

$$\mathscr{F}^{\leq 2}[\rho] = \int \left[\rho \left(\frac{1}{2} V * \rho \right) + k_B T \rho \ln \frac{\rho}{\rho_{i,0}} \right] + \frac{1}{2} \int \int dx_1 dx_2 \, \rho(x_1) \rho(x_2) f_1(x_1, x_2).$$

with f_1 the unique solution to

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

$$\dots j_0 V'(x_1 - x_2) \left[\frac{1}{\rho_{i,0}(x_1)} - \frac{1}{\rho_{i,0}(x_2)} \right].$$

- Conjugated effect of the non-equilibrium driving and of the two-body interactions.

Non-Equilibrium Free-Energy of the Driven Overdamped HMF model

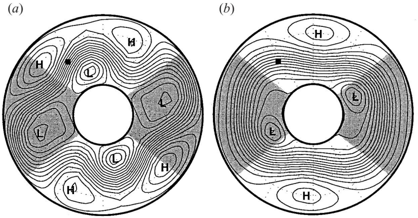
- We got some explicit results for the computation of the non-equilibrium free energy of the driven overdamped HMF model.
- This follows the results obtained by Derrida, Bodineau, Lebowitz, ... , and people from the group of Jona-Lasinio in Rome.
- Our results are for a somewhat more physical model ...
- Can we generalize this to turbulence problems?

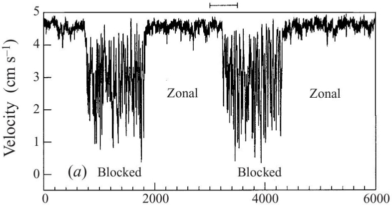
Outline

Phase Transitions in Rotating Tank Experiments
(Quasi Geostrophic dynamics)

Transitions between blocked and zonal states

Y. Tian and others





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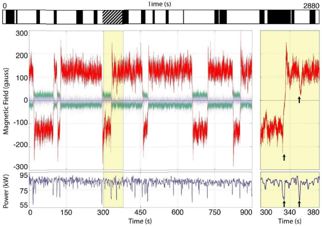
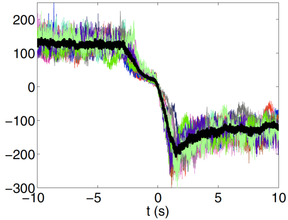
Random Transitions in Geophysical Turbulence

Magnetic Field Reversal (Turbulent Dynamo, MHD Dynamics)



Magnetic field timeseries



Zoom on reversal paths

(VKS experiment)

In turbulent flows, transitions from one attractor to another often occur through a predictable path.

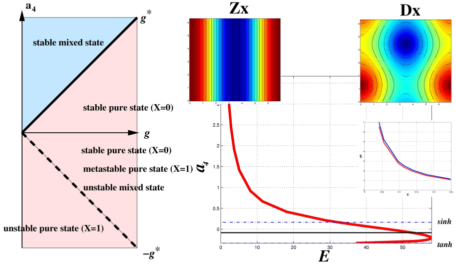
The 2D Stochastic-Navier-Stokes (SNS) Equations

- The simplest model with large scale self-organization of the flow
$$\frac{\partial \omega}{\partial t}+\mathbf{u}.\nabla\omega=\nu\Delta\omega-\alpha\omega+\sqrt{2\alpha}f_s$$
where $\omega=(\nabla\wedge\mathbf{u}).\mathbf{e}_z$ is the vorticity, f_s is a random force, α is the Rayleigh friction coefficient.
- We study the regime with time scale separations:

turnover time $= 1 \ll 1/\alpha =$ forcing or dissipation time.

- Analogies with geophysical flows (Quasi Geostrophic and Shallow Water layer models).

Statistical Equilibria for the 2D-Euler Eq. (doubly periodic)

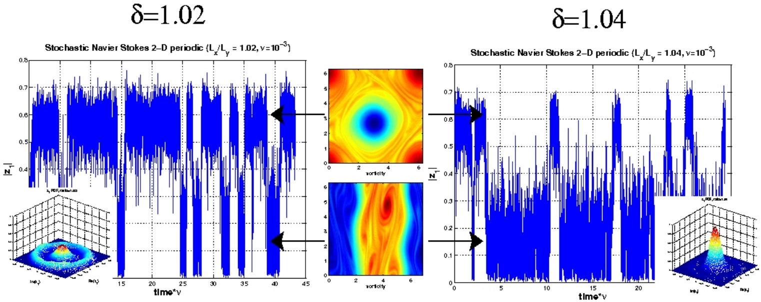


Bifurcation analysis : degeneracy removal, either by the domain geometry (g) or by the nonlinearity of the vorticity-stream function relation (f, parameter a_4).

Derivation: normal form for an Energy-Casimir variational problem. A general degeneracy removal mechanism.

Non-Equilibrium Phase Transition

The time series and PDF of the order parameter



Order parameter : $z_1 = \int dxdy \exp(iy)\omega(x,y)$.

For unidirectional flows $|z_1| \simeq 0$, for dipoles $|z_1| \simeq 0.6 - 0.7$.

F. Bouchet, and E. Simonnet, PRL (2009)

Outline

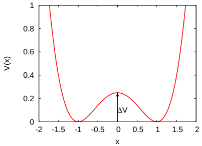
Path Integrals And Large Deviations In Non-Equilibrium Statistical Mechanics

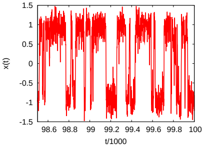
- Aim: entropy and free energy encode all the statistics of the equilibrium system. How to define and compute similar quantities for non-equilibrium systems?
- Answer: large deviations for ensembles of dynamical paths = non-equilibrium and dynamical free energies
- How to compute those?

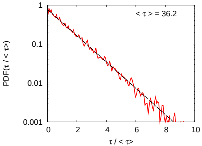
Kramer's Problem: a Pedagogical Example for Bistability

Historical example: Computation by Kramer of the Arrhenius law for a bistable mechanical system with noise

$$\frac{dx}{dt} = -\frac{dV}{dx}(x) + \sqrt{2D}\eta(t) \ \text{Rate}: \ \lambda = A\exp\left(-\frac{\Delta V}{RT}\right) \ \text{with } RT \propto 2D$$







The problem was solved by Kramers (30'). Modern approach: path integral formulation (instanton theory, physicists) or large deviation theory (Freidlin-Wentzell, mathematicians)

Path Integrals for ODE – Onsager Machlup (50')

$$\frac{dx}{dt} - f(x) = +\sqrt{2D}\eta(x,t)$$

- Path integral representation of transition probabilities:

$$P(x_0, x_T, T) = \int_{x(0)=x_0}^{x(T)=x_T} \mathscr{D}[x] \exp\left(-\frac{\mathscr{S}[T,x]}{2D}\right)$$

$$\text{with } \mathscr{S}[T,x] = \frac{1}{2}\int_0^T \mathrm{d}t \left\{ [\dot{x} - f(x)]^2 - 2Df'(x) \right\}.$$

- Instanton: the most probable path with fixed boundary conditions

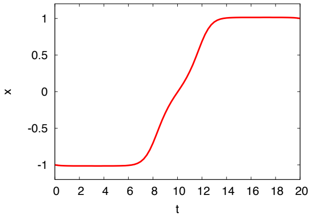
$$S(T, x_0, x_T) = \min_{\{x | x(0)=x_0 \text{ and } x(T)=x_T\}} \{\mathscr{S}[T,x]\}$$

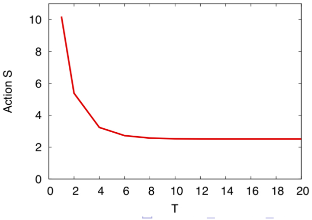
- Saddle point approximation (WKB) gives large deviations results:

$$\log P(x_0, x_T, T) \underset{D \to 0}{\sim} -\frac{S(T, x_0, x_T)}{2D}$$

What to Do with Path Integrals ?

- Solving the equations in the saddle point approximation using theory or numerical optimization (gradient methods)
- Transition rates and transition trajectories are given by minima and minimizers of the action
- It explains why most transition trajectories concentrate close to a single one (instanton trajectory)





Outline

The Action of the 2D Stochastic Navier-Stokes

$$\frac{\partial \omega}{\partial t}+\mathbf{u}.\nabla\omega=\nu\Delta\omega-\alpha\omega+\sqrt{2\alpha}f_s \text{ with } \left\langle f_s(\mathbf{x},t),f_s(\mathbf{x}',t')\right\rangle = C(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

$$\mathscr{S}[T,x]=\frac{1}{2}\int_0^T \mathrm{d}t \int_{\mathscr{D}} \mathrm{dxdx'}\, p(\mathrm{x},\mathrm{t})C(\mathrm{x}-\mathrm{x}')p(\mathrm{x}',\mathrm{t})$$

$$\textit{with } p=\frac{\partial \omega}{\partial t}+\mathbf{u}.\nabla\omega+\alpha\omega-\nu\Delta\omega$$

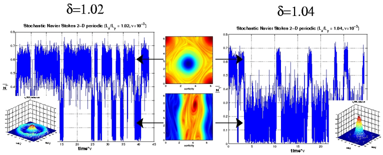
- Theory: we can compute explicitly and study the stability of many instantons (parallel to parallel flows, spatial white noise, Laplacian eigenmodes, etc.)
- Numerical minimization of the action (using gradient methods)

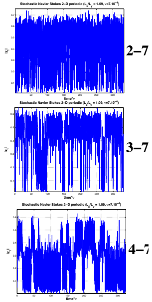
Instantons from Dipole to Parallel Flows

- We can numerically compute instantons connecting dipoles to parallel flows
- They depend on the force spectrum
- Not much

Degenerate Forces Prevent Bistability

- Definition: $C_{\mathbf{k}} = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, C(\mathbf{x}) \exp(i\mathbf{k}.\mathbf{x})$. The force is degenerate if $C_{\mathbf{k}} = 0$ for some $\mathbf{k}$, non-degenerate otherwise





Order parameter : $z_1 = \int dxdy \exp(iy)\omega(x,y)$. Direct numerical simulations for different force spectrums

- Possible relations with weather regimes in the atmosphere

Conclusions from Instanton Analysis

- We can numerically compute instantons for simple turbulent flows
- The result depends much on the force spectrum
- There is no large deviations for transitions between attractors for non-degenerate forces
- No bistability for non-degenerate forces

Conclusion

- Explicit computation of non-equilibrium free energy for an overdamped system with long range interactions.
- Numerical computations of instantons and large deviations for the 2D stochastic Navier-Stokes equations.
- Kinetic theory of zonal jets for the 2D stochastic Navier-Stokes equations and quasi-geostrophic jets.
- Perspectives : explicit computation of large deviations for quasi-linear approximation of quasi-geostrophic jet formation.