Instanton trajectories for random transitions in turbulent flows

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Résumé. De nombreux écoulements turbulents ont plusieurs attracteurs et un comportement bistable ou multistable (la transition entre deux attracteurs est un évènement rare). C'est le cas par exemple pour la dynamique du champs magnétique terrestre, cycles de Milankovich pour le climat, la multistabilité des courants océaniques, les écoulements de Couette et de Rayleigh–Besnard turbulents, un grand nombre d'autres exemples expérimentaux, etc. Pour aucun écoulement turbulents, il n'existe actuellement de théorie satisfaisante pour décrire les attracteurs eux mêmes et la dynamique et le taux de transition du passage d'un attracteur à un autre. Les méthodes traditionnelles pour les systèmes proches de l'équilibres (théorie de Kramer) ou pour des systèmes avec un nombre de degrés de liberté relativement petit (grandes déviations) ne s'appliquent pas aux écoulements turbulents. Dans cet exposé, nous décrirons des résultats récents dans le cadre de la turbulence bidimensionnelle, basés sur des approches de mécanique statistique et de théorie des instantons en théorie des champs (prédisant des grandes déviations).

1 Introduction

Many turbulent flows can evolve and self-organize towards two or more very different states. In some of these systems, the transition between two of such states is rare and occurs relatively rapidly. Such systems include magnetic field reversals in the Earth or in MHD experiments [1], 2D turbulence [2], atmospheric flows [3], and for paths of ocean currents [4], Van Karman flows [5], and many other experiments. The understanding of these transitions is an extremely difficult problem due to the large number of degrees of freedoms, large separation of timescales and the non-equilibrium nature of these flows. It is important to develop a non-equilibrium theory in order to understand this phenomena.

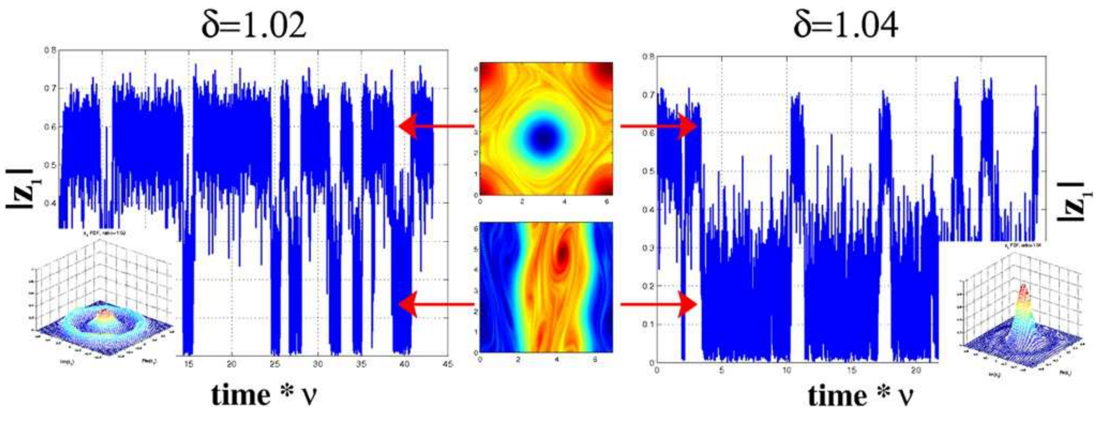

Figure 1. Figure taken from [8] showing rare transitions (illustrated by the Fourier component of the largest y mode) between two large scale attractors of the periodic 2D Navier-Stokes equations. The system spends the majority of its time close to the vortex dipole and parallel flows configurations.

However, for forced-dissipated turbulent systems it is unclear how to define the set of attractors for the dynamics. Although, in the limit of weak forcing and dissipation, one would expect that the set of attractors would converge to the ones of the deterministic equation. In the case of the 2D Euler equations, equilibrium statistical mechanics in the form of the Robert–Miller–Sommeria (RMS) theory [6,7] allows the prediction of the set of attractors for the dynamics. These attractors are a subset of the steady states of the 2D Euler equations.

Moreover, simulations of the 2D Navier-Stokes equations in the weak force and dissipation limit showed that the dynamics actually concentrate around precisely the set attractors for the 2D Euler equations [8]. Interestingly, the same simulation showed sporadic non-equilibrium phase transitions, where the system spontaneously switches between two apparently stable steady states resulting in a complete change in the macroscopic behaviour. If the forcing and dissipation is weak, then these transitions are actually extremely rare, occurring on a timescale much longer than the dynamical timescale.

In this proceeding, will discuss how instanton theory can explain these non-equilibrium phase transitions by allowing for the compututation of the transition probability for observing such a rare transition and determining the most probable trajectory (instanton) between two sets of attractors. These results are of fundamental importance as the transition probability contains a vast amount of information, for instance, one can estimate the timescale of observing such a trajectory and compute the reaction rate of the transition - a key quantity used in the field of transitions in chemical reactions.

The main objective is to present the initial applications of instanton theory to non-equilibrium phase transitions in the 2D Navier-Stokes equations, where we wish to predict the transition probability and compute the instantons for transitions between two steady states of the 2D Euler equations. The motivation for this was the observation of rare transitions in the numerical simulation of the 2D Navier-Stokes equations in [8]. Fig. 1 shows bistability and rare transitions between two attractors in a numerical simulation of the stochastically forced 2D Navier-Stokes equation in a periodic rectangular box taken from [8]. The system has evolved to an apparent non-equilibrium steady state, in which most of the time, the system's dynamics is concentrated around two sets of attractors, namely the vortex dipole and parallel flow. However, at long time intervals, the system sporadically switches between these two large scale attractors. Our aim is to understand this switching behaviour with instanton theory.

As preliminary results, we prove that transitions between two steady states are not rare events in the weak forcing-dissipation limit for the 2D Navier-Stokes equations with non-degenerate noise. This is a consequence of the fact that there are no two well-defined sets of attractors in the 2D Navier-Stokes equations. However, independently of this transition problem, we can show that transitions to high energy steady states are rare events and derive a non-trivial large deviation result for these transitions in the 2D Navier-Stokes equations. For this, the energy of the states $\mathscr{E}[\omega] = E$ has the role of the large deviation parameter in the limit as $E \to \infty$.

2 The 2D Euler and stochastic Navier-Stokes equations

We present the equations of motion for describing 2D and geophysical turbulent flows, described by the 2D Navier-Stokes equations with stochastic forcing. In the limit when forcing and dissipation goes to zero, the 2D Navier-Stokes equations reduce to the 2D Euler equations. We will give some details on the special properties that both of these equations have and how they influence the dynamics. Equilibrium statistical mechanics in the form of the RMS theory can be used to predict the most probable macrostate in which the flow will self-organize for the 2D Euler equations. Unfortunately, this theory cannot be applied for non-equilibrium systems where forcing and dissipation are present. Instead, we plan on utilizing instanton theory to gain insight into the non-equilibrium behaviour of these systems. We are interested in the non-equilibrium dynamics associated to the 2D stochastically forced Navier-Stokes equations on a periodic domain $\mathscr{D} = [0, 2\delta\pi) \times [0, 2\pi)$ with aspect ratio δ :

$$\frac{\partial \omega}{\partial t} + \mathbf{v} \cdot \nabla \omega = -\alpha \omega + \nu \Delta \omega + \sqrt{2\alpha} \eta, \tag{1a}$$

$$\mathbf{v} = \mathbf{e}_z \times \nabla \psi, \quad \omega = \Delta \psi, \tag{1b}$$

where ω, $\mathbf{v}$ and ψ are respectively the vorticity, the non-divergent velocity and the streamfunction defined up to a constant, which is set to zero without loss of generality. We have included an addition linear friction term $-\alpha\omega$ to describe large scale dissipation. We consider non-dimensional equations, where a typical energy is of order 1 (see [9]) such that ν is the inverse of the Reynold's number and α is the inverse of a Reynold's number based on the large scale friction. We assume that the Reynold's numbers satisfy $\nu \ll \alpha \ll 1$. In the limit of weak forcing and dissipation : $\lim_{\alpha\to 0}\lim_{\nu\to 0}$, the 2D Navier-Stokes equations converge to the 2D Euler equations for finite time, but the type of forcing and dissipation determines to which set of attractors the dynamics evolve to over a very long time. The curl of the forcing $\eta(\mathbf{x}.t)$ is a white in time Gaussian field defined by $\langle \eta(\mathbf{x}, t)\eta(\mathbf{x}', t')\rangle = C(\mathbf{x} - \mathbf{x}')\delta(t - t')$, where C is the correlation function of a stochastically homogeneous noise.

The 2D Euler equations are given by Eq. (1) with forcing and dissipation set to zero, i.e. when $\alpha = \nu = 0$. The kinetic energy of the flow is given by

$$\mathscr{E}[\omega] = -\frac{1}{2}\int_{\mathscr{D}} \mathrm{d}\mathbf{x}\,\omega\psi,$$

The energy is conserved, i.e. $\mathrm{d}\mathscr{E}/\mathrm{d}t = 0$, and is one of the invariants of the 2D Euler equations. The 2D Euler equations also conserve an infinite number of functionals, called Casimirs. They are related to the degenerate structure of the infinite-dimensional Hamiltonian system and can be understood as invariants arising from Noether's theorem. These functionals are of the form

$$\mathscr{C}_s[\omega] = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\; s(\omega), \tag{2}$$

where s is any sufficiently regular function. These infinite number of conserved quantities are responsible for the equations having an infinite (continuous) set of steady states (see section 2 in [9]). Physically, these states are important because some of them act as attractors for the dynamics. Any of the infinite number of steady states of the 2D Euler equation satisfy $\mathbf{v}\cdot\nabla\omega = 0$.

3 Instanton theory

The application of instanton theory to non-equilbrium problems has been studied theoretically for gradient dynamics of Brownian particles in a potential [10], and numerically for non-interacting system of magnetic particles [11] and for thermally activated reversals in the Ginzburg-Landau model [12]. Instanton theory utilizes the saddle-point approximation to a path integral representation for the transition probability. This results in the most probable trajectory (instanton) being given by the minimizer of an action functional $\mathcal{A}$. This is analogous to the more mathematically rigorous theory developed by Freidlin and Wentzell [13]. To illustrate instanton theory, let us consider a diffusion process described by an Itô stochastic differential equation (SDE)

$$\dot{\omega}_i = -F_i(\omega) + \sqrt{2\alpha}\eta_i, \tag{3}$$

where η_i, $1 \le i \le n$ are independent Gaussian white noises with $\langle \eta_i(t)\eta_j(t')\rangle = \delta_{i,j}\delta(t - t')$, α is the noise amplitude and $\mathbf{F} : \mathbb{R}^n \to \mathbb{R}^n$ is a uniformly Lipschitz function. Then one can represent the transition probability for observing a trajectory between two states, $\omega(0) = \omega_0$ and $\omega(T) = \omega_T$, in time T as

$$P(\omega_T, T; \omega_0, 0) \;=\; \int \mathscr{D}[\omega]\; e^{-\frac{1}{2\alpha}\mathcal{A}[\omega]}. \tag{4}$$

Formula (4) is a path integral for the transition probability of observing a trajectory from state ω_0 at time $t = 0$ to state ω_T at time $t = T$. The right-hand side represents a summation over all possible paths linking the two states which have some probability distribution represented by the exponential. The action $\mathcal{A}$ of the SDE (3) is given by $\mathcal{A}[\omega] = (1/2)\int_0^T \mathrm{d}t\; [\dot{\omega} + \mathbf{F}(\omega)]^{\mathbf{2}}$. The quadratic form of the action $\mathcal{A}$ is a consequence of the Gaussian statistics of the noises η_i.

A large deviation result can be derived in the limit of vanishing noise $\alpha \to 0$ by application of the saddle-point approximation of the path integral, which states that in the limit of $\alpha \to 0$, the main contribution to the path integral will arise from the trajectory that globally minimizes the action $\mathcal{A}[\omega]$. This leads to the large deviation principle

$$\lim_{\alpha\to 0} -\alpha \log(P) = \frac{1}{2} \inf_{T>0} A[\omega_0, \omega_T, T], \tag{5}$$

where $A[\omega_0, \omega_T, T] = \mathcal{A}[\omega^*]$ is the minimum of the action $\mathcal{A}[\omega]$ with ω satisfying the boundary conditions $\omega(0) = \omega_0$ and $\omega(T) = \omega_T$. The minimizer ω^* in known as the instanton and corresponds to the most probable transition trajectory between the two states in time T.

3.1 The 2D Navier-Stokes action

In this subsection, we discuss the application of large deviation theory to the 2D Navier-Stokes equations (1). The initial step is the construction of the action functional associated to Eqs. (1). The action functional is given by

$$\begin{aligned}\mathcal{A}[\omega] &= \frac{1}{2}\int_0^T \mathrm{d}t \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}' \;\left[\dot{\omega} + \mathbf{v}\cdot\nabla\omega + \alpha\omega - \nu\Delta\omega\right](\mathbf{x}) C(\mathbf{x}-\mathbf{x}') \left[\dot{\omega} + \mathbf{v}\cdot\nabla\omega + \alpha\omega - \nu\Delta\omega\right](\mathbf{x}') \\ &= \frac{1}{2}\int_{\mathscr{D}} \mathrm{d}t\; \mathcal{L}[\omega, \dot{\omega}],\end{aligned} \tag{6}$$

where $\mathcal{L}$ is the Lagrangian associated to the action $\mathcal{A}$.

If a large deviation result exists, then departure from the optimal trajectory is rare and the optimal action $\mathcal{A}[\omega^*]$ gives the large deviation result. The minimizer, or instanton, ω^* satisfies the Euler-Lagrange equations associated to the Lagrangian (6). Specifically, this instanton trajectory is a solution of

$$\dot{q} + \mathbf{v}\cdot\nabla q = \Delta^{-1}(\mathbf{e}_z\cdot[\nabla\omega\times\nabla q]) + \alpha q - \nu\Delta q, \tag{7a}$$

$$q(\mathbf{x}) = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}'\; p(\mathbf{x}')C(\mathbf{x}-\mathbf{x}'), \tag{7b}$$

$$p = \dot{\omega} + \mathbf{v}\cdot\nabla\omega + \alpha\omega - \nu\Delta\omega, \tag{7c}$$

subject to the boundary conditions $\omega(0) = \omega_0$ and $\omega(T) = \omega_T$. The Euler-Lagrange equations (7) are usually ill-posed for initial value problems. However, they should be verified by all critical points of $\mathcal{A}$ which correspond to a special set of initial conditions that solve the boundary value problem.

3.2 Transitions between steady states

We have already mentioned that the 2D Navier-Stokes equations with weak forcing and dissipation evolves towards steady states, which are attractors of the 2D Euler dynamics. Rare transitions have been numerically observed between a vortex dipole and a parallel flow (see Fig. 1 and [8]). We present in the following subsections several simplified cases of transitions in the 2D Navier-Stokes equations that can be treated analytically [14].

One of the key properties of the 2D Euler equations is that the ensemble of steady states are connected. This is readily seen by the fact that any steady state ω_T (such that $\mathbf{v}_T\cdot\nabla\omega_T = 0$) is connected to zero through the path $\omega(\mathbf{x}, t) = \gamma(t)\omega_T$ with $\gamma(0) = 0$ and $\gamma(T) = 1$. This places the 2D Navier-stokes equations (in the limit of weak forcing and dissipation) outside the scope of applying Freidlin–Wentzell theory. The consequence of this, is that for large times the minimum of $\mathcal{A}$ is of order α. Therefore, transitions from one state to another are not rare events and there is no large deviation result. We will now present a simple example to illustrate this.

3.3 Instanton from 0 to ω_T with zero viscosity and Gaussian white noise forcing

We will consider an instanton trajectory starting at zero and going to a final steady state ω_T such that $\mathbf{v}_T \cdot \nabla\omega_T = 0$.

In order for us to obtain an explicitly solvable solution, we consider the 2D Navier-Stokes action with a forcing profile corresponding to white in space noise : $C(\mathbf{x}-\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$. A further simplification we consider is to set viscosity to zero : $\nu = 0$, this is to ensure that the dissipation for any arbitrary state remains uniform on all the modes [1]. For Gaussian white noise, the Euler-Lagrange equations (7) simplify to

$$\dot{p} + \mathbf{v} \cdot \nabla p = \Delta^{-1}(\mathbf{e}_z \cdot [\nabla\omega \times \nabla p]) + \alpha p, \tag{8a}$$

$$p = \dot{\omega} + \mathbf{v} \cdot \nabla\omega + \alpha\omega. \tag{8b}$$

We make an ansatz for the instanton trajectory, and show that this satisfies the Euler-Lagrange equations (8). We consider the ansatz :

$$\omega(\mathbf{x},t) = \gamma(t)\omega_T(\mathbf{x}), \quad \text{then} \quad p(\mathbf{x},t) = [\dot{\gamma}(t) + \alpha\gamma(t)]\,\omega_T(\mathbf{x}), \tag{9}$$

where γ parametrizes the path and has the following boundary conditions : $\gamma(0) = 0$ and $\gamma(T) = 1$. The ansatz states that the instanton will diffuse through the continuous set of steady states. Substitution of the ansatz (9) into the Euler-Lagrange equations (8), we find that Eq. (9) is an instanton (solution to the Euler-Lagrange equation) if

$$\ddot{\gamma} = \alpha^2\gamma, \quad \text{with} \quad \gamma(0) = 0,\ \gamma(T) = 1. \tag{10}$$

We can solve the evolution equation (10) subject to the boundary conditions to determine the instanton trajectory. The instanton trajectory is then given by

$$\omega^*(\mathbf{x},t) = \frac{\sinh(\alpha t)}{\sinh(\alpha T)}\omega_T(\mathbf{x}). \tag{11}$$

We remark, that by showing the instanton solves the Euler-Lagrange equation, we have only proved that the trajectory (11) is a critical point of the action, and not the global minimizer.

Now that we have the formula for the instanton, Eq. (11), we can compute the action corresponding to the instanton trajectory (11)

$$A[\omega_T, T] = \mathcal{A}[\omega^*] = \frac{\alpha e^{\alpha T}}{2\sinh(\alpha T)} \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \omega_T^2. \tag{12}$$

We observe that the action (12) is proportional to the enstrophy of the final state ω_T. However, there is no large deviation principle for (12), as the right-hand side of Eq. (5) will vanish. This is because the instanton trajectory does not correspond to a rare event, as it corresponds to the diffusion across a continuous set of steady states via an Ornstein–Uhlenbeck process.

We expect to observe a similar result for any non-degenerate force correlation $C(\mathbf{x}-\mathbf{x}')$, non-degenerate in the sense that the force acts over all modes of ω. This is because the optimum transition trajectories will always correspond to the diffusion across continuous sets of steady states via an Ornstein–Uhlenbeck process linking two states. These types of transitions are not rare events. We expect a large deviation result to exist when the saddle–point approximation is valid, i.e. there exists a large parameter corresponding to a rare trajectory.

We conjecture, that if there are degeneracies in $C(\mathbf{x}-\mathbf{x}')$, i.e. such that the forcing does not directly influence the modes in which the transition must occurs, then we expect that other modes must be excited, via the nonlinear term $\mathbf{v} \cdot \nabla\omega$, in order to influence the modes involved in the transition. In this case, it should produce a non-trivial instanton transition trajectory that isn't described by an Ornstein–Uhlenbeck process through a continuous set of steady states. Subsequently, a large deviation result consistent with formula (5) should exist.

1. For more specific types of ω_T, we can include viscosity and a arbitrary $C(\mathbf{x}-\mathbf{x}')$, e.g. instantons between parallel flows.

3.4 Rare trajectories to high energy states

In the previous subsection, we showed an example of a transition between zero and an arbitrary steady states will not produce a large deviation result in the vanishing forcing-dissipation limit $\alpha \to 0$. However, by considering another large deviation parameter, namely the energy E, we can derive a large deviation principle for a rare transition between zero and a high energy steady state. To show the large deviation result, we are required to parametrize a steady state with respect to its energy $\mathscr{E}(\omega) = E$. For any given steady state $\omega(\mathbf{x})$, we can parametrize it such that $\omega(\mathbf{x}) = \sqrt{E}\omega_1(\mathbf{x})$, where ω_1 is the corresponding steady state that has unit energy $\mathscr{E}(\omega_1) = 1$. By considering the result from the previous subsection, namely Eq. (12), then for an instanton trajectory starting at zero, one can derive a large deviation principle (5) for transitions to final states with $E \to \infty$, i.e.

$$\lim_{E\to\infty} -\frac{1}{E}\log(P) = \frac{1}{2}\int_{\mathscr{D}} \mathrm{d}\mathbf{x}\,\omega_1^2. \tag{13}$$

Eq. (13) states that in the limit of large energy states, the logarithm of the transition probability is proportional to the energy E times the enstrophy of the state. Physically, this implies that the most probable rare transitions will occur between steady states which have minimum enstrophy. The above result can be generalized to an arbitrary forces defined by an arbitrary correlation $C(\mathbf{x} - \mathbf{x}')$ for several types of transitions, i.e. for the rare transitions between two parallel flows or between two vortex steady states with the same eigenmodes in both spatial dimensions [14].

Références

1. M. Berhanu, R. Monchaux, S. Fauve, N. Mordant, F. Petrelis, A. Chiffaudel, F. Daviaud, B. Dubrulle, L. Marie & F. Ravelet, Magnetic field reversals in an experimental turbulent dynamo. *Europhysics Letters* **77**, 59001 (2007)
2. J. Sommeria, Experimental study of the two-dimensional inverse energy cascade in a square box, *Journal of Fluid Mechanics*, **170**, 139-168 (1986)
3. R. E. Weeks, Y. Tian, J. S. Urbach, K. Ide, H. L. Swinney & M. Ghil, Transitions between blocked and zonal flows in a rotating annulus with topography, *Science*, **278**, 1598–1601 (1997)
4. M. J. Schmeits & H. A. Dijkstra, Bimodal behavior of the Kuroshio and the Gulf stream, *Journal of Physical Oceanography*, **31**, 3435-3456 (2001)
5. F. Ravelet, L. Marié, A. Chiffaudel & F. Daviaud, Multistability and memory effect in a highly turbulent flow : experimental evidence for a global bifurcation, *Physical Review Letters*, **93**, 164501 (2004)
6. J. Miller, Statistical mechanics of Euler equations in two dimensions, *Physical Review Letters* **65**, 2137-2140 (1990)
7. R. Robert & J. Sommeria, Statistical equilibrium states for two-dimensional flows, *Journal of Fluid Mechanics*, **229**, 291-310 (1991)
8. F. Bouchet & E. Simmonet, Random changes of flow topology in two-dimensional and geophysical turbulence, *Physical Review Letters*, **102**, 1-4, (2009)
9. F. Bouchet & A. Venaille, Statistical mechanics of two-dimensional and geophysical flows, *Physics Reports*, à paraître.
10. B. Caroli, C. Caroli & B. Roulet, Diffusion in a bistabel potential : The functional integral approach, *Journal of Statistical Physics*, **26**, 83-111 (1981)
11. D. Berkov, Numerical calculation of the energy barrier distribution in disordered many-particle systems : the path integral method, *Journal of Magnetism and Magnetic Materials*, **186**, 199-213 (1998)
12. W. E, W. Ren & E. Vanden-Eijnden, Minimum action method for the study of rare events, *Communcations in Pure and Applied Mathematics*, **57**, 637-656 (2004)
13. M. I. Freidlin & A. S. Wentzell, *Random perturbations of dynamical systems*, Springer (1998)
14. F. Bouchet & J. Laurie, Instanton theory and rare transitions in the 2D Navier-Stokes equations, en préparation.