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Statistical mechanics approaches to self organization of 2D flows: fifty years after, where does Onsager's route lead to?

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Self organization of two-dimensional and geophysical turbulent flows is of paramount importance for atmosphere and ocean applications. Following Onsager, we explain why statistical mechanics can explain and predict these phenomena. The most recent theoretical developments in statistical mechanics use large deviation theory as a fundamental tool. We present large deviation results for both equilibrium and non-equilibrium problems for two-dimensional turbulent flows.

I. INTRODUCTION

Self-organization of two-dimensional and geophysical flows

Atmospheric and oceanic flows are three-dimensional (3D), but are strongly dominated by the Coriolis force and mainly balanced by pressure gradients (geostrophic balance). The turbulence that develops in such flows is called geostrophic turbulence. Models describing geostrophic turbulence have the same type of additional invariants as those of the two-dimensional (2D) Euler equations. As a consequence, energy flows backward and the main phenomenon is the formation of large scale coherent structures (jets, cyclones and anticyclones). One such example is the formation of Jupiter's Great Red Spot, Fig. 1.

FIG. 1. Picture of Jupiter's Great Red Spot - a large scale vortex situated between bands of atmospheric jets. Photo courtesy of NASA: http://photojournal.jpl.nasa.gov/catalog/PIA00014.

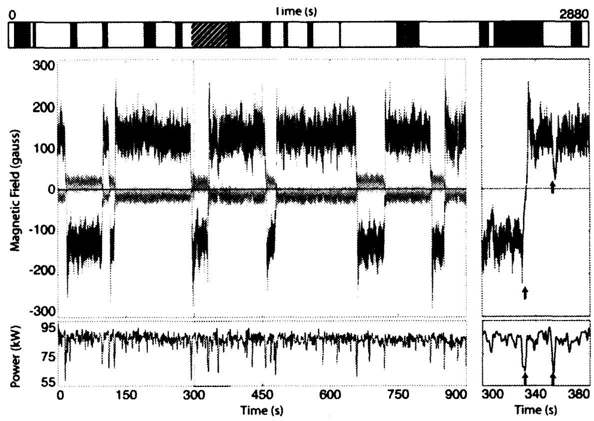

FIG. 2. Figure taken from [1] showing random transitions between meta-stable orientations of the magnetic field in an experimental turbulent dynamo. The main azimuthal component of the magnetic field is shown in red.

The analogy between 2D turbulence and geophysical turbulence is further emphasized by the theoretical similarity between the 2D Euler equations, describing 2D flows, and the layered quasi-geostrophic or shallow water models, describing the largest scales of geostrophic turbulence: both are transport equations for a scalar quantity by a non-divergent flow, conserving an infinite number of invariants.

The formation of large scale coherent structures is a fascinating problem and an essential part of the dynamics of Earth's atmosphere and oceans. This is the main motivation for setting up a theory for the self-organization of 2D turbulence.

Statistical mechanics of the self-organization of two-dimensional and geophysical flows: Onsager's route

Any turbulence problem involves a huge number of degrees of freedom coupled via complex nonlinear interactions. The aim of any theory of turbulence is to understand the statistical properties of the velocity field. It is thus extremely tempting to attack these problems from a statistical mechanics point of view.

Statistical mechanics is indeed a very powerful theory that allows us to reduce the complexity of a system down to a few thermodynamic parameters. As an example, the concept of phase transition allows us to describe drastic changes of the whole system when a few external parameters are changed. Statistical mechanics is the main theoretical approach we develop in this proceeding. It succeeds in explaining many of the phenomena associated with 2D turbulence [2].

This may seem surprising at first, as it is a common belief that statistical mechanics is not successful in handling turbulence problems. The reason for this belief is that most turbulence problems are intrinsically far from equilibrium. For instance, the forward energy cascade in 3D turbulence involves a finite energy dissipation, no matter how small the viscosity (anomalous dissipation) (see for instance Onsager's insightful consideration of the non-conservation of energy by the 3D Euler equations [3])

As a result of the finite energy flux, the flow cannot be considered close to some equilibrium distribution. By contrast, 2D turbulence does not suffer from the anomalous dissipation of the energy, so equilibrium statistical mechanics, or close to equilibrium statistical mechanics makes sense when small fluxes are present.

The first attempt to use equilibrium statistical mechanics ideas to explain the self-organization of 2D turbulence arise from Onsager in 1949 [4] (see [3] for a review of Onsager's contributions to turbulence theory). Onsager worked with the point-vortex model, a model made of singular point vortices, first used by Lord Kelvin and which corresponds to a special class of solutions of the 2D Euler equations. The equilibrium statistical mechanics of the point-vortex model has a long and very interesting history, with wonderful pieces of mathematical achievements [4–11].

The generalization of Onsager's ideas to the 2D Euler equations with a continuous vorticity field, taking into account all invariants, has been proposed in the beginning of the 1990s [12–15], leading to the Robert–Sommeria–Miller theory (RSM theory). The RSM theory includes the previous Onsager theory and determines within which limits the theory will give relevant predictions and results.

Over the last fifteen years, the RSM equilibrium theory has been applied successfully to a large class of problems, for both the 2D Euler and quasi-geostrophic equations. This includes many interesting applications, such as the predictions of phase transitions in different contexts, a model for the Great Red Spot and other Jovian vortices, and models of ocean vortices and jets. A detailed description of the statistical mechanics of 2D and geophysical flows and of these applications is presented in the review [2].

For statistically stationary turbulent flows, power input through external forces balance energy dissipation on average. In the limit of very small forces and dissipation, compared to conservative terms of the dynamics, it is expected to find a strong relation between these non-equilibrium flows and some of the states predicted by equilibrium statistical mechanics. In order to give a precise meaning to this general idea, and to deal with far from equilibrium situations, it is essential to develop a non-equilibrium statistical mechanics. As we discuss below, this has been the subject of recent key advances in the applications of statistical mechanics to turbulent flows.

A contemporary approach to statistical mechanics: large deviation theory

At the time he was scientifically active, Onsager made a large number of decisive contributions to statistical mechanics theory: solutions of the 2D Ising model, reciprocity relations, contributions to the statistical mechanics of electrolytes and turbulence, and so on. Since that time the theoretical approaches for treating statistical mechanics problems have been completely renewed. One of the main changes has been the use of the language of large deviation theory in more than 20 years. For instance, recent results in the understanding of equilibrium statistical mechanics problems, proving fluctuations theorems (Onsager's reciprocity relations generalized far from equilibrium), and in dealing with non-equilibrium statistical mechanics problems, are all large deviation results.

Interestingly, as is discussed in this proceeding, the route proposed by Onsager in his 1949 paper [4], in order to understand the self-organization of two-dimensional flows, led a few decades later to some of the first applications of large deviation theory to equilibrium statistical mechanics problems.

The theory of large deviations concerns itself with the asymptotic behaviour of the exponential decay of the probabilities of rare or extreme events. The associated limiting parameter is usually taken to be the number of observations or particles, but can be other parameters, such as vanishing noise or the temperature of a chemical reaction, or large time. Large deviation theory can be considered a generalization of the central limit theorem, but with the refinement of including information about the behaviour of the tails of the probability density. The main result of large deviation theory is the large deviation principle, a result describing the leading asymptotic behaviour of the tails or large deviations of the probability distribution in the limit $N \to \infty$. For instance, the large deviation principle for a random variable S_N is

$$\lim_{N\to\infty} -\frac{1}{N}\log[P(X_N = x)] = I(x), \tag{1}$$

where P is the probability density for the random variable X_N, and $I(x)$ is called the rate function. For instance, if $X_N = (1/N)\sum_{i=1}^{N} x_i$, where x_i are independent identically distributed random variables then $I(x)$ is given by Cramér's theorem.

The aim of this proceeding is to explain and derive heuristically large deviation results for the equilibrium statistical mechanics of the 2D Euler equations (equilibrium) and for the 2D Navier-Stokes equations with stochastic forces (non-equilibrium). In the equilibrium case, the large deviation results provide an explanation of the mean field variational problem that has been extensively discussed during the RIMS-workshop held in Kyoto in 2011. In this case, the rate function is then related to the entropy of the macrostates.

Large deviation theory in 2D turbulence, the equilibrium mean field variational problem, and the probability of rare events for non-equilibrium situations

The first large deviation results in 2D turbulence have been obtained in the context of the RSM theory for the 2D Euler equations. Michel and Robert [16] have studied the large deviation of Young measures and have suggested that the entropy of the RSM theory is the analogue of a large deviation rate function. By considering a prior distribution for the vorticity invariants, in a framework where the invariants are considered in a canonical ensemble rather than in a microcanonical one, Boucher and collaborators [17] have given a derivation of a large deviation result based on finite dimensional approximations of the vorticity field.

We present in section III a heuristic construction of microcanonical invariant measures for the 2D Euler equations. This construction primarily follows the initial ideas of the previous works [16, 17], but is much more simplified. Moreover, for pedagogical reasons, the reading of this heuristic presentation does not imply any knowledge of large deviation theory and avoids any technical discussion. These measures are constructed using finite dimensional approximation of the vorticity field, where N^2 is the number of degrees of freedom. N^2 is then the large deviation parameter and the entropy appears as the analogue of the large deviation rate function, defined up to a constant.

In order to state the main result discussed in section III, let us define $p(\mathbf{x},\sigma)$ as the local probability to observe vorticity values equal to σ at point $\mathbf{x}$: $p(\mathbf{x},\sigma) = \langle\delta(\omega(\mathbf{x}) - \sigma)\rangle$, where δ is the Dirac delta function. We consider averaging $\langle\cdot\rangle$ over the microcanonical measure. Then the large deviation rate function for $p(\mathbf{x},\sigma)$ is $S(E_0) - S[p, E_0]$ where

$$S[p, E_0] = \begin{cases} \mathscr{S}[p] \equiv & \int_{\mathscr{D}} \mathrm{d}\mathbf{x} \sum_k p_k \log p_k \ \text{ if } \mathscr{N}[p] = 1, \ \forall k \ A[p_k] = A_k, \ \text{ and } \mathscr{E}[\overline{\omega}] = E_0 \\ -\infty & \text{otherwise,} \end{cases} \tag{2a}$$

and

$$S(E_0) = \sup_{\{p \mid \mathscr{N}[p]=1\}} \left\{\mathscr{S}[p] \mid \mathscr{E}[\bar{\omega}] = E_0, \forall k \ A[p_k] = A_k\right\}, \tag{2b}$$

with E_0,A_k and $\mathcal{N}$, the energy, the vorticity distribution, and the probability normalization defined in section III respectively.

The interpretation of this result is that the most probable value for the local probability is the maximizer of the variational problem (2b), and that the probability to observe a departure from this most probable state is exponentially large, with parameter N^2 and rate function (2a). Furthermore, the classical mean field equation for the streamfunction ψ can be derived from (2a), as discussed in reference [18].

From a historical perspective, it is interesting to note that Onsager considered the point vortex model rather than the 2D Euler equations, in order to properly define the microcanonical measure without having to deal with the mathematical aspects of defining measures over functional spaces. Large deviation results for equilibrium measures have also been derived recently for the point vortex model. Starting from either canonical measures, or approximate microcanonical measures for the system of N point vortices, a series of mathematical papers have proven that when $N \to \infty$, the one particle distribution function converges to the solution of a mean-field variational problem [6, 7, 10], as was first guessed by physicists [5]. This type of mean field variational problem was one of the main subjects of the RIMS-workshop held in Kyoto in 2011. The rate of this convergence, and the study of the probability of departures from this mean field equilibrium is given by a large deviation result proven in [19].

The current perspective of the statistical mechanics of 2D turbulent flows is to develop a non-equilibrium statistical mechanics theory. As a major progress in this direction, we discuss in section IV the application of large deviation theory to the 2D stochastically forced Navier-Stokes equations. In this situation, we consider, as an example, the large deviation approach to the stationary probability P_s of observing a state ω. In this case, we can derive a large deviation result which describe the probability of large energy states. The energy E is then the large deviation parameter

$$\lim_{E\to\infty} -\frac{1}{E}\log(P_s) = \alpha \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \omega_1^2. \tag{3}$$

The right-hand side of Eq. (3) is proportional to the enstrophy of the final state, and is analogous to the rate function $I(x)$.

The article is laid out as follows: In section II, we state the equations of motion and discuss the basic properties associated to them. In section III, we construct microcanonical invariant measures for the 2D Euler equations and discuss the entropy maximization problem in predicting the most probably steady states on the 2D Euler equation. In section IV, we discuss large deviations for non-equilibrium problems and illustrate this using a simple academic example followed by the application to the 2D Navier-Stokes equations.

II. THE 2D EULER AND STOCHASTIC NAVIER-STOKES EQUATIONS

Equations of motion

The aim of this section is to 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 can be used to predict the most probable macrostate in which the flow will self-organize for the 2D Euler equations. This form of equilibrium statistical mechanics is known as the RSM theory [13, 15]. Unfortunately, this theory cannot be applied for non-equilibrium systems where forcing and dissipation are present. Instead, we plan on utilizing large deviation 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:

$$\frac{\partial\omega}{\partial t} + \mathbf{v}\cdot\nabla\omega = -\alpha\omega + \nu\Delta\omega + \sqrt{2\alpha}\eta, \tag{4a}$$

$$\mathbf{v} = \mathbf{e}_z \times \nabla\psi, \quad \omega = \Delta\psi, \tag{4b}$$

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 [2]) 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. (4) with forcing and dissipation set to zero, i.e. when $\alpha = \nu = 0$. The kinetic energy of the flow is given by

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

where the last equality is obtained with an integration by parts. 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 equations also conserve an infinite number of functionals, named 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 [20]. These functionals are of the form

$$\mathscr{C}_s[\omega] = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, s(\omega), \tag{5}$$

where s is any sufficiently regular function. We note that on a doubly-periodic domain the total circulation is zero:

$$\Gamma = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \omega = 0. \tag{6}$$

These infinite number of conserved quantities are responsible for the equations having an infinite (continuous) set of steady states (see section 2 in [2]). 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

$$\mathbf{v}\cdot\nabla\omega = 0.$$

For instance, there is a functional relation between the vorticity and the streamfunction, i.e. $\omega = \Delta\psi = f(\psi)$, where f is any continuous function then $\mathbf{v}\cdot\nabla\omega = 0$. The specific function f that is reached after a complex evolution can be predicted in certain situation using equilibrium statistical mechanical arguments presented in the next section (see [2] for more details).

III. EQUILIBRIUM STATISTICAL MECHANICS AND THE MEAN FIELD VARIATIONAL PROBLEM AS A LARGE DEVIATION RESULT

In this section, we define precisely the macrocanonical measure for the 2D Euler equations and prove that the entropy $S[p, E_0]$ is a large deviation rate function for p. This justifies the mean field variational problem (2b).

The conservation of the vorticity distribution

Due to the infinite number of conserved Casimirs, the 2D Euler equations conserve the distribution of vorticity, i.e. the total area of a specific vorticity level set is conserved. We will begin by showing that this is indeed the case by considering a special class of Casimir (5):

$$C(\sigma) = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, H(-\omega + \sigma), \tag{7}$$

where $H(\cdot)$ is the Heaviside step function. The function $C(\sigma)$ returns the area occupied by all vorticity levels smaller or equal to σ. $C(\sigma)$ is an invariant for any σ and therefore any derivative of $C(\sigma)$ is also conserved. Therefore, the distribution of vorticity, defined as $D(\sigma) = C'(\sigma)$, where the prime denotes a derivation with respect to σ, is also conserved by the dynamics. The expression $D(\sigma)d\sigma$ is the area occupied by the vorticity levels in the range $\sigma \leq \omega \leq \sigma + d\sigma$.

Moreover, any Casimir can be written in the form

$$\mathcal{C}_f[\omega] = \int_{\mathscr{D}} \mathrm{d}\sigma\, f(\sigma)\, D(\sigma).$$

The conservation of all Casimirs, Eq. (5), is therefore equivalent to the conservation of $D(\sigma)$.

The conservation of the distribution of vorticity levels, as proven above, can also be understood from the equations of motion. We find that $D\omega/Dt = 0$, showing that the values of the vorticity field are Lagrangian tracers. This means that the values of ω are transported through the non-divergent velocity field, thus keeping the distribution unchanged.

From now on, we restrict ourselves to a K-level vorticity distribution. We make this choice for pedagogical reasons, but generalization to a continuous vorticity distribution is straightforward. The K-level vorticity distribution is defined as

$$D(\sigma) = \sum_{k=1}^{K} A_k \delta(\sigma - \sigma_k), \tag{8}$$

where A_k denotes the area occupied by the vorticity value σ_k. The areas A_k are not arbitrary, their sum is the total area $\sum_{k=1}^{K} A_k = |\mathscr{D}|$. Moreover, the constraint (6), imposes the constraint $\sum_{k=1}^{K} A_k \sigma_k = 0$.

Microcanonical measure

In order to properly construct a microcanonical measure, we discretize the vorticity field on a uniform grid, define a measure on the corresponding finite-dimensional space and take the limit $N \to \infty$. A uniform grid has to be chosen in order to comply with a formal Liouville theorem for the 2D Euler equations [21, 22].

We denote the lattice points by $\mathbf{x}_{ij} = \left(\frac{i}{N}, \frac{j}{N}\right)$, with $0 \leq i, j \leq N-1$ and denote $\omega_{ij} \equiv \omega(\mathbf{x}_{ij})$ to be the vorticity value at point $\mathbf{x}_{ij}$. The total number of points is N^2.

As discussed in the previous section, we assume $D(\sigma) = \sum_{k=1}^{K} A_k \delta(\sigma - \sigma_k)$. For this finite-$N$ approximation, our set of microstates (configuration space) is then

$$X_N = \left\{\omega^N = (\omega_{ij})_{0 \leq i,j \leq N-1} \mid \forall i, j\ \omega_{ij} \in \{\sigma_1, \ldots, \sigma_K\}, \text{ and } \forall k\ \#\{\omega_{ij} \mid \omega_{ij} = \sigma_k\} = N^2 A_k\right\}.$$

Here, $\#(A)$ is the cardinal of set A. We note that X_N depends on $D(\sigma)$ through A_k and σ_k (see (8)).

Using the above expression we define the energy shell $\Gamma_N(E, \Delta E)$ as

$$\Gamma_N(E, \Delta E) = \left\{\omega^N \in X_N \mid E_0 \leq \mathscr{E}_N\left[\omega^N\right] \leq E_0 + \Delta E\right\},$$

where

$$\mathscr{E}_N = \frac{1}{2N^2} \sum_{i,j=0}^{N-1} \mathbf{v}_{ij}^2 = -\frac{1}{2N^2} \sum_{i,j=0}^{N-1} \omega_{ij} \psi_{ij},$$

is the finite-N approximation of the system energy, with $\mathbf{v}_{ij} = \mathbf{v}(\mathbf{x}_{ij})$ and $\psi_{ij} = \psi(\mathbf{x}_{ij})$ being the discretized velocity field and streamfunction field, respectively. ΔE is the width of the energy shell. Such a finite width is necessary for our discrete approximation, as the cardinal of X_N is finite. Then the set of accessible energies on X_N is also finite. Let $\Delta_N E$ be the typical difference between two successive achievable energies. We then assume that $\Delta_N E \ll \Delta E \ll E_0$. The limit measure defined below is expected to be independent on ΔE in the limit $N \to \infty$.

The fundamental assumption of statistical mechanics states that each microstate in the configuration space is equi-probable. By virtue of this assumption, the probability to observe any microstate is $\Omega_N^{-1}(E_0, \Delta E)$, where $\Omega_N(E_0, \Delta E)$ is the number of accessible microstates, is the cardinal of the set $\Gamma_N(E_0, \Delta E)$. The finite-N specific Boltzmann entropy is defined as

$$S_N(E_0, \Delta E) = \frac{1}{N^2} \log\, \Omega_N(E_0, \Delta E). \tag{9}$$

The microcanonical measure is then defined through the expectation values of any observables A. For any observable $A[\omega]$ (for instance a smooth functional of the vorticity field), we define its finite-dimensional approximation by $A_N\left[\omega^N\right]$. The expectation value of A_N for the microcanonical measure reads

$$\left\langle \mu_N(E_0, \Delta E),\, A_N\left[\omega^N\right]\right\rangle_N \equiv \left\langle A_N\left[\omega^N\right]\right\rangle_N \equiv \frac{1}{\Omega_N(E_0, \Delta E)} \sum_{\omega^N \in \Gamma_N(E_0, \Delta E)} A_N\left[\omega^N\right].$$

The microcanonical measure μ for the 2D Euler equation is defined as a limit of the finite-N measure:

$$\langle \mu(E_0),\, A[\omega]\rangle \equiv \lim_{N\to\infty} \left\langle \mu_N(E_0, \Delta E),\, A_N\left[\omega^N\right]\right\rangle_N.$$

The specific Boltzmann entropy is then defined as

$$S(E_0) = \lim_{N\to\infty} S_N(E_0, \Delta E). \tag{10}$$

The mean field variational problem as a large deviation result

Computing the Boltzmann entropy by direct evaluation of Eq. (10) is usually an intractable problem. However, we shall proceed in a different way and show that this alternative computation yields the same entropy in the limit $N \to \infty$. We give heuristic arguments in order to prove that the computation of the Boltzmann entropy Eq. (10) is equivalent to the maximization of the constrained variational problem (2b) (called a mean field variational problem). This variational problem is the foundation of the RSM approach to the equilibrium statistical mechanics for the 2D Euler equations. The essential message is that the entropy computed from the mean field variational problem (2b) and from Boltzmann's entropy definition (10) are the equal in the limit $N \to \infty$. The ability to compute the Boltzmann entropy through this type of variational problems is one of the cornerstones of statistical mechanics.

Our heuristic derivation is based on the same type of combinatorics arguments as the ones used by Boltzmann for the interpretation of its H function in the theory of relaxation to equilibrium of a dilute gas. This derivation doesn't use the technicalities of large deviation theory. The aim is to actually obtain the large deviation interpretation of the entropy and to provide a heuristic understanding using basic mathematics only. The modern mathematical proof of the relationship between the Boltzmann entropy and the mean field variational problem involves Sanov theorem.

Macrostates are set of microscopic configurations sharing similar macroscopic behaviors. Our aim is to properly identify macrostates that fully describe the main features of the largest scales of 2D turbulent flow, and then to compute their probability or entropy.

Let us first define macrostate through local coarse-graining. We divide the $N \times N$ lattice into $(N/n) \times (N/n)$ non-overlapping boxes each containing n^2 grid points (n is an even number, and N is a multiple of n). These boxes are centered on sites $(i,j) = (In, Jn)$, where integers I and J verify $0 \le I, J \le N/n - 1$. The indices (I,J) label the boxes.

For any microstate $\omega^N \in \Gamma_N$, let f_{IJ}^k be the frequency to find the value σ_k in the box (I,J)

$$F_{IJ}^k(\omega^N) = \frac{1}{n^2} \sum_{i=I-n/2+1}^{I+n/2} \sum_{j=J-n/2+1}^{J+n/2} \delta_{\mathrm{d}}(\omega_{ij} - \sigma_k),$$

where $\delta_{\mathrm{d}}(x)$ is equal to one whenever $x = 0$, and zero otherwise. We note that for all (I,J), $\sum_{k=1}^{K} F_{IJ}^k(\omega^N) = 1$.

A macrostate $p_N = \{p_{IJ}^k\}_{0 \le I,J \le N/n-1; 1 \le k \le K}$, is the set of all microstates of $\omega^N \in X_N$ such that $F_{IJ}^k(\omega^N) = p_{IJ}^k$ for all I, J, and k (by abuse of notation, and for simplicity, $p_N = \{p_{IJ}^k\}_{0 \le I,J \le N/n-1; 1 \le k \le K}$ refers to both the set of values and to the set of microstates having the corresponding frequencies). The entropy of the macrostate is defined as the logarithm of the number of microstates in the macrostate

$$S_N[p_N] = \frac{1}{N^2} \log \left(\# \left\{ \omega^N \in X_N \mid \text{ for all } I, J, \text{ and } k, \; F_{IJ}^k(\omega^N) = p_{IJ}^k \right\}\right). \tag{11}$$

Following an argument by Boltzmann, it is a classical exercise in statistical mechanics, using combinatorics and the Stirling formula, to prove that in the limit $N \gg n \gg 1$, without taking into account of the area constraints A_k, the entropy of the macrostate would converge to

$$S_N[p_N] \underset{N \gg n \gg 1}{\sim} \begin{cases} \mathscr{S}_N[p_N] = -\frac{n^2}{N^2} \sum_{I,J=0}^{N/n-1} \sum_{k=1}^{K} p_{IJ}^k \log p_{IJ}^k & \text{if } \forall I, J, \; \mathcal{N}[p_{IJ}] = 1 \\ -\infty & \text{otherwise,} \end{cases}$$

where $\mathcal{N}[p_{IJ}] \equiv \sum_k p_{IJ}^k$. The area constraints are easily expressed as constraints over p_N: $A_N\left[p_N^k\right] \equiv \frac{n^2}{N^2} \sum_{I,J=0}^{N/n-1} p_{IJ}^k = A_k$ and $\forall I, J$, $\mathcal{N}[p_{IJ}] = 1$. An easy generalization of the above formula gives

$$S_N[p_N] \underset{N \gg n \gg 1}{\sim} \begin{cases} \mathscr{S}_N[p_N] & \text{if } \forall k \; A_N\left[p_N^k\right] = A_k \\ -\infty & \text{otherwise.} \end{cases}$$

In the theory of large deviation, this result could have been obtained using Sanov's theorem. We now consider a new macrostate (p_N, E_0) which is the set of microstates ω^N with energy $\mathscr{E}_N\left[\omega^N\right]$ verifying $E_0 \le \mathscr{E}_N\left[\omega^N\right] \le E_0 + \Delta E$ (the intersection of $\Gamma_N(E, \Delta E)$ and p_N). For a given macrostate p_N, not all microstates have the same energy. The constraint on the energy thus can not be recast as a simple constraint on the macrostate p_N. Then one has to treat the energy constraint in a more subtle way. The energy is

$$\mathscr{E}_N\left[\omega^N\right] = -\frac{1}{2N^2} \sum_{i,j=0}^{N-1} \omega_{ij}^N \psi_{ij}^N.$$

The streamfunction ψ_{ij}^N is related to ω^N through

$$\psi_{ij} = \frac{1}{N^2} \sum_{i',j'=0}^{N-1} G_{ij,i'j'} \omega_{i'j'}^N,$$

where $G_{ij,i'j'}$ is the Laplacian Green function in the domain $\mathscr{D}$. In the limit $N \gg n \gg 1$, the variations of $G_{ij,i'j'}$ for (i',j') running over the small box (I,J) are vanishingly small. Then $G_{ij,i'j'}$ can be well approximated by their average value over the boxes $G_{IJ,I'J'}$. Then

$$\psi_{ij} \simeq \psi_{IJ} \equiv \frac{1}{N^2} \sum_{I',J'=0}^{N/n-1} G_{IJ,I'J'} \sum_{i'=I-n/2+1}^{I+n/2} \sum_{j'=J-n/2+1}^{J+n/2} \omega_{i'j'}^N = \frac{n^2}{N^2} \sum_{I',J'=0}^{N-1} G_{IJ,I'J'} \overline{\omega_{IJ}^N},$$

where the coarse-grained vorticity is defined as

$$\overline{\omega_{IJ}^{N}} = \frac{1}{n^2} \sum_{i'=I-n/2+1}^{I+n/2} \sum_{j'=J-n/2+1}^{J+n/2} \omega_{i'j'}^{N}.$$

We note that, over the macrostate p_N, the coarse-grained vorticity depends on p_N only:

$$\overline{\omega_{IJ}^{N}} = \sum_{k=1}^{K} p_{IJ}^{k} \sigma_k \text{ for } \omega^N \in p^N.$$

Using similar arguments, it is easy to conclude that in the limit $N \gg n \gg 1$ the energy of any microsate of the macrosate p_N is well approximated by the energy of the coarse-grained vorticity

$$\mathscr{E}_N\left[\omega^N\right] \underset{N \gg n \gg 1}{\sim} \mathscr{E}_N\left[\overline{\omega_{IJ}^{N}}\right] = -\frac{n^2}{2N^2} \sum_{I,J=0}^{N/n-1} \overline{\omega_{IJ}^{N}} \psi_{IJ}^{N}.$$

Then the Boltzmann entropy of the macrostate is

$$S_N[p_N, E_0] \underset{N \gg n \gg 1}{\sim} \begin{cases} \mathscr{S}_N[p_N] & \text{if } \forall k \, \mathcal{N}[p_N^k] = 1 \text{ , } A_N\left[p_N^k\right] = A_k \text{ and } \mathscr{E}_N\left[\overline{\omega_{IJ}^{N}}\right] = E_0 \\ -\infty & \text{otherwise.} \end{cases} \quad (12)$$

Consider $P_{N,E_0}(p_N)$ to be the probability density to observe the macrostate p_N in the finite-N microcanonical ensemble with energy E_0. By definition of the microcanonical ensemble of the entropy $S_N(E_0)$ (see Eq. (9) and the preceding paragraph), we have

$$P_{N,E_0}(p_N) = \exp\left\{N^2\left[S_N[p_N, E_0] - S_N(E_0)\right]\right\}. \quad (13)$$

From the general definition of a large deviation result given by Eq. (1), we clearly see that formula (12) is a large deviation result for the macrostate p_N in the macrocanonical ensemble. The large deviation parameter is N^2 and the large deviation rate function is $-S_N[p_N, E_0] + S_N(E_0)$.

We now consider the continuous limit. The macrostates p_N^k are now seen as the finite-N approximation of p_k, the local probability to observe $\omega(\mathbf{x}) = \sigma_k$: $p_k(\mathbf{x}) = \langle \delta(\omega(\mathbf{x}) - \sigma_k) \rangle$. The macrostate is then characterized by $p = \{p_1, \ldots, p_K\}$. Taking the limit $N \gg n \gg 1$ allows us to define the entropy of the macrostate (p, E) as

$$S[p, E_0] = \begin{cases} \mathscr{S}[p] \equiv \sum_k \int_{\mathscr{D}} \mathrm{dx}\, p_k \log p_k & \text{if } \forall k \, \mathcal{N}[p_k] = 1 \text{ , } A\left[p_k\right] = A_k \text{ and } \mathscr{E}[\overline{\omega}] = E_0 \\ -\infty & \text{otherwise.} \end{cases} \quad (14)$$

In the same limit, it is clearly seen from definition (11) and result (14) that there is a concentration of microstates close to the most probable macrostate. The exponential concentration close to this most probable state is a large deviation result, where the entropy appears as the opposite of a large deviation rate function (up to an irrelevant constant).

The exponential convergence towards this most probable state also justifies the approximation of the entropy with the entropy of the most probable macrostate. Thus, in the limit $N \to \infty$ we can express the Boltzmann entropy, Eq. (10), as

$$S(E_0) = \sup_{\{p \,|\, \mathcal{N}[p]=1\}} \left\{\mathscr{S}[p] \;|\; \mathscr{E}[\bar{\omega}] = E_0, \forall k \; A[p_k] = A_k\right\}, \quad (15)$$

where $p = \{p_1, \ldots, p_K\}$ and $\forall$ $\mathbf{x}$, $\mathcal{N}[p](\mathbf{x}) = \sum_{k=1}^{K} p_k(\mathbf{x}) = 1$ is the local normalization. Furthermore, $A[p^k]$ is the area of the domain corresponding to the vorticity value $\omega = \sigma_k$. The fact that the Boltzmann entropy $S(E_0)$ Eq. (10) can be computed from the variational problem (15) is a powerful non-trivial result of large deviation theory.

IV. NON-EQUILIBRIUM PHASE TRANSITIONS

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 occur relatively rapidly. Such systems include magnetic field reversals in the Earth or in MHD experiments (e.g. the von Kármán Sodium (VKS) turbulent dynamo in Fig. 2) [1], Rayleigh-Bénard convection cells [24–27], 2D turbulence [23, 28, 29] (see Fig. 3), 3D flows [30] and for ocean and atmospheric flows [31, 32]. 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.

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 RMS theory allows for the prediction set of attractors for the dynamics. Those attractors are a subsets 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 [23]. Interestingly, the same simulation showed sporadic non-equilibrium phase transitions, where the system spontaneously switched 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 section we will discuss how large deviation theory can explain these non-equilibrium phase transitions. With large deviation theory, we can compute the transition probability of observing such a rare transition and furthermore compute 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. Moreover, most rare transitions are situated around the same transition path, which can be computed using large deviation theory.

The main objective of this section is to present the initial applications of large deviation theory to non-equilibrium phase transitions in the 2D Navier-Stokes equations, where we wish to predict the transition probability and instanton 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 [23]. Fig. 3 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 [23]. 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 large deviation theory.

As preliminary results, we prove that there is no large deviation result in the weak forcing-dissipation limit for the 2D Navier-Stokes equations with non-degenerate noise. In this case, the transition between two types of equilibria is not a rare event – a consequence of the fact that there are no two well-defined sets of attractors in the 2D Navier-Stokes equations. Independently of this transition problem, we can derive a non-trivial large deviation result for transitions to high energy steady states of 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 $E \to \infty$.

Large deviation theory

The application of large deviation theory to non-equilibrium problems has been extensively studied in gradient dynamics of Brownian particles in a potential and in weakly perturbed Hamiltonian systems with weak forcing and dissipation. The large deviation properties of both of these systems can be solved either by

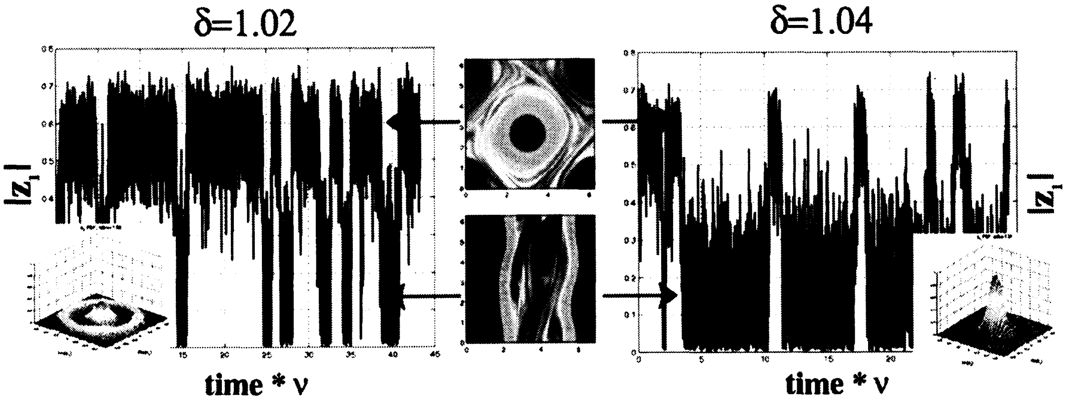

FIG. 3. Figure taken from [23] showing rare transitions (illustrated by the Fourier component of the largest y mode) between two large scale attractors of the periodic 2D Navier-Stokes equations. The system spends the majority of its time close to the vortex dipole and parallel flows configurations.

using saddle-point approximations to path integrals or more rigorously, from a mathematical point of view, using the theory developed by Freidlin and Wentzell [33]. Both cases consider a diffusion process described by an Itô stochastic differential equation (SDE)

$$\dot{x}_i = -F_i(\mathbf{x}) + \sqrt{2\alpha}\eta_i, \tag{16}$$

where η_i, $1 \leq i \leq n$ 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, $\mathbf{x}(0) = \mathbf{x}_0$ and $\mathbf{x}(T) = \mathbf{x}_T$, in time T as

$$P(\mathbf{x}_T, T; \mathbf{x}_0, 0) \;=\; \int \mathscr{D}[\mathbf{x}]\, e^{-\frac{1}{2\alpha}\mathcal{A}[\mathbf{x}]}. \tag{17}$$

Formula (17) is a path integral for the transition probability of observing a trajectory from state $\mathbf{x}_0$ at time $t = 0$ to state $\mathbf{x}_T$ 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 (16) is given by $\mathcal{A}[\mathbf{x}] = (1/2)\int_0^T \mathrm{d}t\, [\dot{\mathbf{x}} + \mathbf{F}(\mathbf{x})]^2$. 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 $\mathcal{A}(\mathbf{x})$. This leads to the large deviation principle

$$\lim_{\alpha\to 0} -\alpha \log(P) = \frac{1}{2} A[\mathbf{x}_0, \mathbf{x}_T, T], \tag{18}$$

where $A[\mathbf{x}_0, \mathbf{x}_T, T] = \mathcal{A}[\mathbf{x}^*]$ is the minimum of the action $\mathcal{A}[\mathbf{x}]$ with $\mathbf{x}$ satisfying the boundary conditions $\mathbf{x}(0) = \mathbf{x}_0$ and $\mathbf{x}(T) = \mathbf{x}_T$. The minimizer $\mathbf{x}^*$ in known as the instanton. In systems that contain disjoint well-defined attractors, formula (18) coincides with the large deviation result obtained by Freidlin and Wentzell [33]. However, as it will be shown later, this is not the case for the stochastically forced 2D Navier-Stokes equations in the weak forcing-dissipation limit.

The double-well potential

We wish to give a pedagogical description of large deviation theory to non-equilibrium systems. Therefore, we will begin by applying large deviation theory to a simple academic example of an over-damped particle in a double-well potential where a large deviation result exists. We will show that we can compute the transition probability for the transition of a particle from one well to the other and that it is proportional to the exponential of the energy barrier height between the two wells. In fact, this is a large deviation result and is precisely the Arrhenius formula for the reaction rate in a chemical reaction described by a double-well potential.

We consider a single over-damped particle in a 1D double-well potential $V(x)$. The motion of a particle can be defined in terms of its position $x(t)$ by the SDE

$$\dot{x} = -\frac{\mathrm{d}V}{\mathrm{d}x} + \sqrt{2\alpha}\eta,$$

where η is a Gaussian white noise defined by $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$, $V(x) = (x^2-1)^2/4$ (see Fig. 4), and α is a parameter for the amplitude of the noise. In the deterministic situation, when $\alpha = 0$, the particle relaxes to one of the two stable steady states of the potential V, i.e. it goes to either $x = -1$ or $x = 1$. In the presence of forcing, the particle may gain enough momentum to jump the potential barrier at $x = 0$ and settle in the other potential well. If the forcing is weak, i.e. $\alpha \ll \Delta V$, then the jump between wells will be a rare event and one can apply the theory of large deviations.

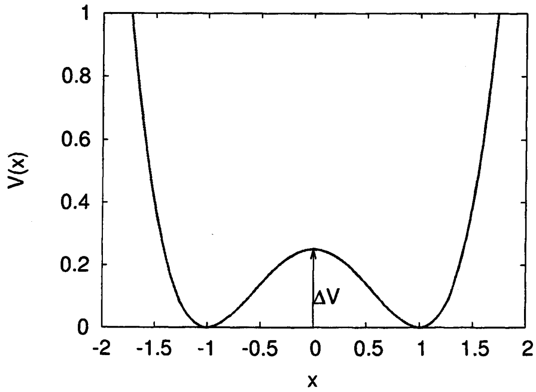

FIG. 4. Graph of the double well potential $V(x) = (x^2-1)^2/4$. We observe two stable steady states at $x = \pm 1$ and a saddle at $x = 0$ with height $\Delta V = 1/4$.

In the case of the double-well potential, one can derive the action $\mathcal{A}$, which can be written as the time integral of a Lagrangian $\mathcal{L}$, as

$$\mathcal{A}[x] = \int_0^T \mathrm{d}t\ \mathcal{L}[x,\dot{x}] = \frac{1}{2}\int_0^T \mathrm{d}t\ \left(\dot{x} + \frac{\mathrm{d}V}{\mathrm{d}x}\right)^2. \tag{19}$$

We observe from the definition of the action (19) that the deterministic motion of the particle, defined by $\dot{x} = -\mathrm{d}V/\mathrm{d}x$, gives $\mathcal{A} = 0$ - an intrinsic property of the action. This is because the deterministic motion does not require any input from the forcing. However, a deterministic trajectory cannot connect the two attractors. This is because the particle must gain momentum (from the forcing) to pass the potential barrier at $x = 0$.

The dynamics of the instanton is a solution to the Euler-Lagrange equations derived from the Lagrangian $\mathcal{L}$ given in Eq. (19). One can then solve the boundary value problem associated to the minimization of the action $\mathcal{A}$ with $x(0) = -1$ and $x(T) = 1$.

Moreover, we observe that there exists no explicit time-dependence in the Lagrangian, and therefore, one can apply Noether's theorem [34] to derive the formula for the instanton energy H, an energy conserved by the dynamics of the instanton trajectory. For the double-well potential this gives

$$H = \frac{\dot{x}^2}{2} - \frac{1}{2}\left(\frac{\mathrm{d}V}{\mathrm{d}x}\right)^2. \tag{20}$$

For a transition that occurs within an infinitely long time ($T \to \infty$), the instanton has zero energy $H = 0$. This is because at the end points $\dot{x} = 0$ and $\mathrm{d}V/\mathrm{d}x = 0$. In this case, we observe from (20) that the trajectory must satisfy $\dot{x} = \pm \mathrm{d}V/\mathrm{d}x$. Here, the negative signed solution ($\dot{x} = -\mathrm{d}V/\mathrm{d}x$) corresponds to the deterministic trajectory, and simply implies that the particle rolls down the from the top of the potential barrier at $x = 0$ to the bottom of one of the wells, which produces a zero contribution to the action. The other solution, with the positive sign ($\dot{x} = \mathrm{d}V/\mathrm{d}x$) corresponds to the optimum trajectory escaping from the initial well and traveling to the top of the potential barrier at $x = 0$. It is this part of the trajectory that leads to a contribution to the action. This contribution can be computed by substituting $\dot{x} = \mathrm{d}V/\mathrm{d}x$ into Eq. (19):

$$A_\infty = 2\int_0^\infty \mathrm{d}t\, \dot{x}\frac{\mathrm{d}V}{\mathrm{d}x} = 2\Delta V.$$

The resulting large deviation principle (18) is

$$\lim_{\alpha \to 0} -\alpha \log(P_s) = \Delta V. \tag{21}$$

Formula (21) states that the transition probability for observing the rare transition between the two potential wells, in the limit of the weak noise limit, is proportional to the exponential of the barrier height ΔV. This is precisely the Arrhenius formula $k = A\exp(\Delta E/k_B T)$, where k is transition rate of a chemical reaction ($\sim 1/P_s$), ΔE is the energy barrier height and $k_B T$ is the noise amplitude due to thermal excitations.

We have shown in this section how the large deviation theory can be applied to a the simple example of an over-damped particle in 1D double-well potential, and how the large deviation result (21) coincides precisely with the Arrhenius formula for the rate of transition of a chemical reaction. We now proceed onto the application of large deviation theory to the 2D stochastically forced Navier-Stokes equations.

The 2D Navier-Stokes action

In this subsection, we discuss the application of large deviation theory to the 2D Navier-Stokes equations (4). We extend the description outlined for the double-well potential to the vorticity field of the 2D Navier-Stokes equations. The initial step is the construction of the action functional associated to Eqs. (4). The action functional is given by

$$\begin{aligned}\mathcal{A}[\omega] &= \frac{1}{2}\int_0^T \mathrm{d}t \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{x}'\ [\dot{\omega} + \mathbf{v}\cdot\nabla\omega + \alpha\omega - \nu\Delta\omega](\mathbf{x}) C(\mathbf{x}-\mathbf{x}') [\dot{\omega} + \mathbf{v}\cdot\nabla\omega + \alpha\omega - \nu\Delta\omega](\mathbf{x}') \\ &= \frac{1}{2}\int_{\mathscr{D}} \mathrm{d}t\, \mathcal{L}[\omega, \dot{\omega}],\end{aligned} \tag{22}$$

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 (22). Specifically, this instanton trajectory is a solution of

$$\dot{q} + \mathbf{v}\cdot\nabla q = \Delta^{-1}(\mathbf{e}_z\cdot[\nabla\omega \times \nabla q]) + \alpha q - \nu\Delta q, \tag{23a}$$

$$q(\mathbf{x}) = \int_{\mathscr{D}} \mathrm{d}\mathbf{x}'\, p(\mathbf{x}')C(\mathbf{x}-\mathbf{x}'), \tag{23b}$$

$$p = \dot{\omega} + \mathbf{v}\cdot\nabla\omega + \alpha\omega - \nu\Delta\omega, \tag{23c}$$

subject to the boundary conditions $\omega(0) = \omega_0$ and $\omega(T) = \omega_T$. The Euler-Lagrange equations (23) 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.

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. 3 and [23]). We present in the following subsections several simplified cases of transitions in the 2D Navier-Stokes equations that can be treated analytically [35].

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 not present a simple example to illustrate this.

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 $\mathbf{v}_T \cdot \nabla\omega_T = 0$. This example is one of the simplest and most important to be considered as it corresponds to considering a large deviation result for the stationary probability P_s, defined as the infinite transition time limit ($T \to \infty$) of the transition probability P: $P_s = \lim_{T\to\infty} P$. More precisely, for the 2D Navier-Stokes equations (with finite non-zero dissipation), any instanton with a transition time larger than the dissipation timescale ($T \gg 1/\alpha$), from an arbitrary steady state ω_0, will (deterministically) relax to zero before transitioning to ω_T. Therefore, as we shall see, the stationary probability will only depend on the final state ω_T and not the initial state ω_0, so for simplicity it is sufficient to consider $\omega_0 = 0$.

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 [36]. For Gaussian white noise, the Euler-Lagrange equations (23) simplify to

$$\dot{p} + \mathbf{v} \cdot \nabla p = \Delta^{-1}(\mathbf{e}_z \cdot [\nabla\omega \times \nabla p]) + \alpha p, \tag{24a}$$

$$p = \dot{\omega} + \mathbf{v} \cdot \nabla\omega + \alpha\omega. \tag{24b}$$

We make an ansatz for the instanton trajectory, and show that this satisfies the Euler-Lagrange equations (24). We consider the ansatz:

$$\omega(\mathbf{x}, t) = \gamma(t)\omega_T(\mathbf{x}), \quad \text{then} \quad p(\mathbf{x}, t) = [\dot{\gamma}(t) + \alpha\gamma(t)]\,\omega_T(\mathbf{x}), \tag{25}$$

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 (25) into the Euler-Lagrange equations (24), we find that Eq. (25) is an instanton (solution to the Euler-Lagrange equation) if

$$\ddot{\gamma} = \alpha^2\gamma, \quad \text{with} \quad \gamma(0) = 0,\ \gamma(T) = 1. \tag{26}$$

We can solve the evolution equation (26) subject to the boundary conditions to determine the instanton trajectory. The instanton trajectory is then given by

$$\omega^*(\mathbf{x}, t) = \frac{\sinh(\alpha t)}{\sinh(\alpha T)}\omega_T(\mathbf{x}). \tag{27}$$

We remark, that by showing the instanton solves the Euler-Lagrange equation, we have only proved that the trajectory (27) is a critical point of the action, and not the global minimizer.

Now that we have the formula for the instanton, Eq. (27), we can compute the action corresponding to the instanton trajectory (27)

$$A[\omega_T, T] = \mathcal{A}[\omega^*] = \frac{\alpha e^{\alpha T}}{2\sinh(\alpha T)} \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \omega_T^2. \tag{28}$$

In the limit of any infinitely long transition time ($T \to \infty$), which corresponds to the minimum of (28) over all $T \in (0, \infty)$, the action equals

$$\lim_{T\to\infty} A[\omega_T, T] = A_\infty[\omega_T] = \alpha \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \omega_T^2. \tag{29}$$

We observe that the action is proportional to the enstrophy of the final steady state ω_T, and moreover, that it is proportional to α. The fact that the action is proportional to α implies that there is no large deviation result in the limit of vanishing forcing-dissipation ($\alpha \to 0$) as $\mathcal{A}[\omega^*]$ will be everywhere zero. 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 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 (i.e. zero forcing on these modes), 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 transition trajectory that isn't simply described by an Ornstein–Uhlenbeck process through a continuous set of steady states. Subsequently, a large deviation result consistent with formula (18) should exist.

Large deviations for 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. (29), then for an instanton trajectory starting at zero, one can derive a large deviation result for transitions to final states with $E \to \infty$, i.e.

$$\lim_{E\to\infty} -\frac{1}{E}\log(P_s) = \alpha \int_{\mathscr{D}} \mathrm{d}\mathbf{x}\, \omega_1^2, \tag{30}$$

for finite α. Eq. (30) 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 attractors which have minimum enstrophy. The above result can be generalized to a force defined by an arbitrary correlation $C(\mathbf{x}-\mathbf{x}')$ for several types of transitions, i.e. the rare transitions between two parallel flows or between two vortex steady states with the same eigenmodes in both spatial dimensions [35].

V. ACKNOWLEDGMENTS

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