# Statistical Ensemble Inequivalence and Bicritical Points for Two-Dimensional Flows and Geophysical Flows

Antoine Venaille and Freddy Bouchet

*LEGI, UJF, INPG, CNRS, BP 53, 38041 Grenoble, France*
*and INLN, CNRS, UNSA, 1361 route des lucioles, 06 560 Valbonne–Sophia Antipolis, France*
(Received 30 October 2007; revised manuscript received 13 October 2008; published 12 March 2009)

A theoretical description for the equilibrium states of a large class of models of two-dimensional and geophysical flows is presented. A statistical ensemble equivalence is found to exist generically in these models, related to the occurrence of peculiar phase transitions in the flow topology. The first example of a bicritical point (a bifurcation from a first toward two second order phase transitions) in the context of systems with long-range interactions is reported. Academic ocean models, the Fofonoff flows, are studied in the perspective of these results.

DOI: 10.1103/PhysRevLett.102.104501 PACS numbers: 47.10.−g, 05.20.−y, 05.70.Fh, 47.20.−k

In many physical systems, the dynamics of particles or fields is not governed by local interactions. For instance, stellar systems in astrophysics [1], vortices in two-dimensional and geophysical flows [2], unscreened plasma, or models describing interactions between waves have interaction potentials which are not integrable [3].

One of the striking features of systems with long-range interactions is the generic existence of negative heat capacity. This means that the temperature decreases as the energy is increased. This very strange phenomenon is possible as a consequence of the lack of additivity of the energy [3] and is related to the fact that equilibrium states for the microcanonical ensemble of statistical mechanics may not be equilibrium states for the canonical ensemble (ensemble inequivalence). This was first predicted in the context of astrophysics [4]. For two-dimensional flows, the existence of such an inequivalence has been mathematically proved for point vortices [5] (without explicit computation), and numerically observed in a Monte Carlo study of point vortices in a disk [6] and in a particular situation of a one layer quasigeostrophic (QG) model [7]. The one layer QG model is the simplest model of large scale (two-dimensional) geophysical flows [8]. One of the novelties of the current work is the prediction of ensemble inequivalence, with analytical computation of the associated phase transitions, for a very large class of models including Euler equations or QG models. In systems with long-range interactions, as in usual thermodynamics, one observes transition phenomena such as critical points when changing external parameters. Phase transitions are extremely important as they induce huge physical changes in the system considered. For instance, such phase transitions lead to drastic changes in the flow structure, as illustrated by streamline modifications in Fig. 1. In systems with long-range interactions, some of those transitions can be associated with the appearance of inequivalence between statistical ensembles [9]. As a generalization of Landau's classification, all theoretically possible routes to ensemble inequivalence and their relations to phase transitions in the different statistical ensembles have been classified and linked together [10]. Astonishingly, some of the transitions theoretically predicted have never been observed, either in models nor in real physical systems. This is, for instance, the case of the ensemble inequivalence associated with bicritical points (a bifurcation from a first towards two second order phase transitions) and for second order azeotropy (the simultaneous outbreak, from nothing, of two second order phase transitions). For the first time, we exhibit bicritical points and azeotropy in systems with long-range interactions and their associated ensemble inequivalence. Interestingly, from a physical point of view, the bifurcations associated with bicritical points are governed mainly by the domain geometry.

The statistical prediction of large scale geophysical flows is a promising application field for the statistical mechanics of systems with long-range interactions. For instance, the structure of Jupiter's troposphere has been successfully explained using the Robert-Sommeria-Miller (RSM) equilibrium theory [11]. One of the major scopes of

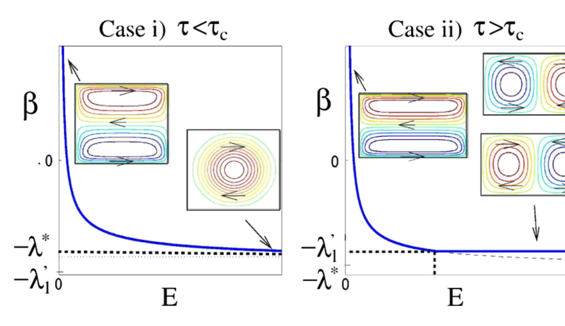


FIG. 1 (color online). Evolution of Fofonoff flows (statistical equilibrium of the one layer QG model) and their inverse temperature $\beta$, when the energy $E$ is varied, for a given, nonzero circulation. Insets are isolines of the stream function $\psi$ in a rectangular domain. For higher domain aspect ratio $\tau$ (right-hand panel) there is a discontinuity of $\partial\beta/\partial E$. This corresponds to a second order phase transition, above which two equilibrium states coexist.

 

this field is to go towards applications to Earth's oceans. All textbooks in oceanography present the Fofonoff flows, which have played an important historical role [8,12]. They are particular steady states of the one layer QG model, corresponding to the low energy solution depicted in Fig. 1. In this Letter, we propose a theoretical description of Fofonoff flows and obtain a new type of solutions and of phase transitions (the high energy solutions in Fig. 1), which relates for the first time these models with properties associated with ensemble inequivalence.

Some of the phase transitions analyzed here have already been described in a similar context [13]. In particular, they report a transition from a monopole to a dipole when the aspect ratio of the domain increases above a critical value. However, the present theoretical treatment is different as we use directly general relations between constrained and unconstrained variational problems, and provide then the first ensemble inequivalence results for these phase transitions.

To simplify, we present in the following the computations for the Euler equations, but our results generalize easily to a large class of geophysical models.

*Euler equations and variational problems.*—The 2D Euler equations describe a perfect flow. They can be expressed as a transport equation for the vorticity $\omega$ by a nondivergent velocity field $\mathbf{u}$: $\partial_t\omega + \boldsymbol{u}\cdot\boldsymbol{\nabla}\omega = 0$. The velocity and the vorticity fields are related by a stream function $\psi$: $u_x = -\partial_y\psi$, $u_y = \partial_x\psi$, and $\omega = \partial_x u_y - \partial_y u_x = \Delta\psi$. We study here the case of a closed domain $\mathcal{D}$. The flow evolution is fully determined by the knowledge of an initial vorticity field. The 2D Laplacian may be inverted with boundary condition $\psi = 0$ (there is no normal flow across the boundary). Because the Green function of the Laplacian diverges logarithmically in 2D, the interactions between vorticity patches is long ranged [3].

The 2D Euler equations are known to develop complex vorticity filaments at finer and finer scales. This makes almost impossible any attempt to a deterministic approach to those systems. Rather than describing the fine-grained structures, equilibrium statistical theories of two-dimensional turbulent flows, assuming ergodicity, predict final organization of the flow on a coarse-grained level [2]: a mixing entropy is maximized by taking into account the constraints, namely, all the flow invariants, which are the energy $\mathcal{E} = \langle \mathbf{u}^2\rangle/2 = -\langle\omega\psi\rangle/2$, and the Casimirs $\mathcal{C}_g = \langle g(\omega)\rangle$, where $g$ is any continuous function. The brackets $\langle\cdot\rangle$ stand for a spatial average over the whole domain $\mathcal{D}$. This theory predicts for the statistical equilibrium state a functional relation $\omega = f(\psi)$, which characterizes a steady state of the Euler equation. The theory is predictive, but it requires the knowledge of all the flow invariants that can be computed from any initial vorticity field. In practice, the analytic computation of RSM equilibrium states is a difficult task: one has to solve a variational problem involving an infinite number of constraints. It has been proposed to study simpler variational problems, with only a few constraints, to compute RSM statistical equilibria [14]. In particular, it has been shown that any maximizer of

$$S(E,\Gamma) = \max_{\omega}\{\mathcal{S}[\omega] = -\frac{1}{2}\langle\omega^2\rangle|\mathcal{C}_1[\omega] = \Gamma \text{ and } \mathcal{E}[\omega] = E\},$$

where $\mathcal{S}$ is sometimes referred to as generalized entropy, is also a RSM equilibrium state (it maximizes a mixing entropy), but the converse is wrong. The particular choice of a quadratic functional for $\mathcal{S}$ will be discussed later.

We have kept only the constraints on the energy and on the circulation $\mathcal{C}_1[\omega] = \langle\omega\rangle$. Let us introduce the Lagrange parameters $\beta$ (inverse temperature) and $\gamma$ (fugacity) associated with these constraints, in order to compute the critical points of the variational problem: $\delta\mathcal{S} - \beta\delta\mathcal{E} - \gamma\delta\mathcal{C} = 0$, where $\delta$ refers to the first variations of the functional with respect to $\omega$. Then $\omega = \beta\psi - \gamma$, where $\beta, \gamma$ are eventually computed by using the constraints on $E, \Gamma$. To conclude, the study of this variational problem provides any RSM equilibrium state associated with a linear $\omega - \psi$ relation, and makes possible a classification of those states in a phase diagram $(\Gamma, E)$.

*Statistical ensembles.*—The problem introduced in the previous paragraph involves two constraints $E$ and $\Gamma$. The corresponding statistical ensemble will be referred to as microcanonical, by analogy with usual thermodynamic, with the equilibrium entropy $S(E, \Gamma)$. Dealing with unconstrained variational problems is much easier than dealing with constrained ones. Moreover, solutions for a variational problem are necessarily solutions for a more constrained dual problem [9]. In order to solve the microcanonical problem, it is convenient to consider the grand-canonical ensemble with the thermodynamical potential $J(\beta, \gamma) = \min_\omega\{\mathcal{J}[\omega] = -\mathcal{S} + \beta\mathcal{E} + \gamma\mathcal{C}\}$ and the canonical ensemble, by keeping only the constraint on the circulation, with the free energy $F(\beta, \Gamma) = \min_\omega\{\mathcal{F}[\omega] = -\mathcal{S} + \beta\mathcal{E}|\mathcal{C}[\omega] = \Gamma\}$. Each solution for the grand-canonical problem is also a canonical solution, and each solution of the canonical problem is also a microcanonical solution, but the converse is wrong in general [9]. For given values of $E$ and $\Gamma$, the microcanonical ensemble is said to be equivalent to the (grand)canonical ensemble, when a (grand)canonical solution having the energy $E$ and the circulation $\Gamma$ exists. Otherwise there is inequivalence between microcanonical and (grand)canonical ensembles.

*Laplacian eigenmodes.*—The vorticity can be decomposed on the complete, orthonormal basis $\{e_i(x, y)\}_{i\in\mathbb{N}}$ of Laplacian eigenmodes: $\omega = \sum_i \omega_i e_i$, where $\Delta e_i = -\lambda_i e_i$, with the $\lambda_i > 0$ in increasing order. Then

$$\mathcal{S} = -\sum_i \frac{\omega_i^2}{2}, \qquad \mathcal{E} = \sum_i \frac{\omega_i^2}{2\lambda_i}, \qquad \mathcal{C} = \sum_i \langle e_i\rangle\omega_i.$$

The grand-canonical problem is to find the minimum of a quadratic functional $\mathcal{J}[\omega]$. The canonical problem can be transformed also into a quadratic unconstrained variational problem: the constraint on the circulation is used to express one coordinate as a linear combination of the others: $\omega_1 = (\Gamma - \sum_{i\geq 2}\omega_i\langle e_i\rangle)/\langle e_1\rangle$ ($\langle e_1\rangle \neq 0$ for a closed domain).

*Solution of quadratic variational problems.*—We look for the minimum of quadratic functionals, with linear parts. Let $Q$ and $L$ be the purely quadratic and linear parts, respectively. Then we have three cases. (1) The smallest eigenvalue of $Q$ is positive: the minimum exists and is achieved by a unique minimizer. (2) At least one eigenvalue of $Q$ is strictly negative. There is no minimum. (3) The smallest eigenvalue of $Q$ is zero (with eigenfunction $e_0$). A minimum exists only if $L[e_0] = 0$. The neutral direction $\{\alpha e_0\}_{\alpha\in\mathbb{R}}$ is the ensemble of minimizers.

*Grand-canonical ensemble.*—Computations are not difficult; their details will be provided in a companion paper [15]. We start with the easiest, grand-canonical problem. We look for the range of parameters $\beta, \gamma$ such that a grand-canonical solution exists (positive quadratic part): it gives the condition $\beta > -\lambda_1$, whatever $\gamma$. The corresponding equilibria are written $\omega(\beta, \gamma)$. We then compute $\mathcal{E}[\omega(\beta, \gamma)]$ and $\mathcal{C}[\omega(\beta, \gamma)]$: it appears that those states fill the area below a parabola $E_{\lambda_1}(\Gamma) = \Gamma^2/(2\lambda_1\langle e_1\rangle^2)$ in the plane $(\Gamma, E)$ (represented as a solid blue parabola in Figs. 2(b-i) and 2(b-ii)].

*Ensemble inequivalence area.*—We thus conclude that $E$ and $\Gamma$ values above this parabola do not correspond to any grand-canonical solution. This is a situation of ensemble inequivalence. In order to find equilibria with $(\Gamma, E)$ values above the parabola, we have to consider a more constrained variational problem.

*Canonical and microcanonical ensembles.*—For a given value of the constraint $\Gamma$, we look for the range of parameters $\beta$ such that a canonical solution $\omega(\beta, \Gamma)$ exists: it gives the condition $\beta \geq -\min\{\lambda_1', \lambda^*\}$, where $\lambda_1'$ is the smallest of the $\lambda_i$ with the condition $\langle e_i\rangle = 0$ and where $\lambda^*$ is the smallest zero of $f(x) = 1 - x\sum_{i\geq 1}\langle e_i\rangle^2/(x - \lambda_i)$ (see Eq. 3.8 in [13] for a different interpretation of this function). We then compute $\mathcal{E}[\omega(\beta, \Gamma)]$ and check that all possible values of $E$ correspond to a canonical solution.

In principle, we could eventually have to solve the microcanonical problem, but it is not necessary since the whole range of admissible values of $E$ and $\Gamma$ are covered by canonical solutions. To conclude, there is inequivalence between grand-canonical and canonical ensembles and equivalence between canonical and microcanonical ensembles. Now that states with all values of $(\Gamma, E)$ are found, we can compute and plot the entropy $S(\Gamma, E)$ [see Figs. 2(a-i) and 2(a-ii)]. In this figure, the ensemble inequivalence area is clearly recognized as it is known to be characterized by regions where the entropy $S(E, \Gamma)$ does not coincide with its concave envelope [9].

*Geometry governed criterion.*—We deduce from the previous analysis a criterion that provides two classes of phase diagrams, referred as case (i) ($\min\{\lambda^*, \lambda_1'\} = \lambda^*$) and case (ii) ($\min\{\lambda^*, \lambda_1'\} = \lambda_1'$) (see [13] for a discussion independent of ensemble inequivalence). It depends only on the Laplacian eigenvalues and eigenmodes, which depend themselves only on the domain geometry. Note that if the domain does not admit any symmetry axis, there is generically no zero-mean Laplacian eigenmodes, so $\lambda_1'$ does not exist and then only case (i) is possible. By contrast, if the domain admits a symmetry axis, the sign of $\lambda_1' - \lambda^*$ must be computed. In the case of a rectangular domain, there is a critical aspect ratio $\tau_c \simeq 1.12$, as reported in [13]; case (i) and case (ii) correspond, respectively, to $\tau < \tau_c$ and $\tau > \tau_c$. It is expected that any domain geometry sufficiently stretched in a direction perpendicular to its symmetry axis is in case (ii).

*Description of phase transitions.*—Let us consider first the phase diagram in case (i) [see Figs. 2(a-i), 2(b-i), and 2(c-i)]. When the line $\Gamma = 0$ is crossed, the flow structure changes from a monopole of a given sign to a similar monopole with the opposite sign, with coexistence of both states on the line $\Gamma = 0$ [Fig. 2(b-i)] [13]. The

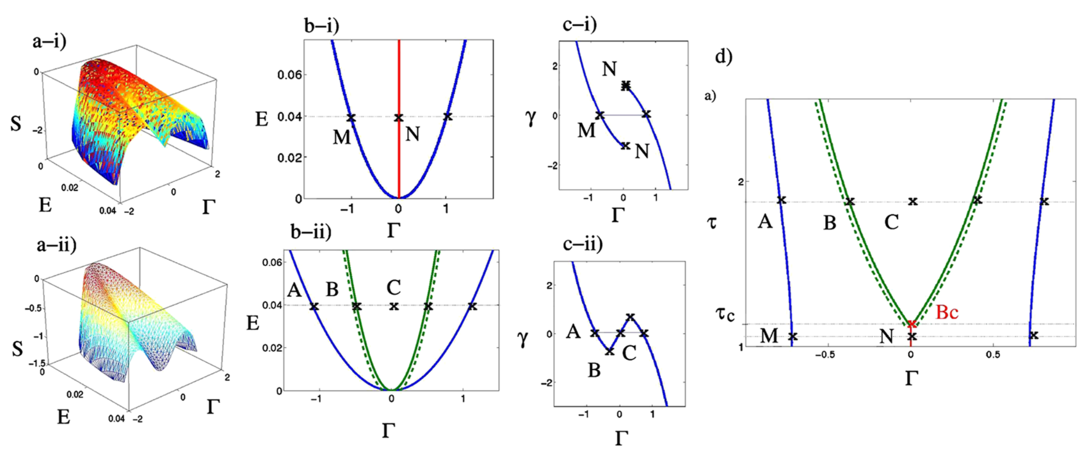


FIG. 2 (color online). (a) Equilibrium entropy $S(E, \Gamma)$. (b) Lines of microcanonical phase transition. Red straight line: first order; dashed, green parabola: second order; solid blue parabola: ensemble inequivalence boundary. (c) $\gamma = \partial S/\partial\Gamma$ vs $\Gamma$ at fixed $E$. (d) Transition from a first to two second order phase transitions (bicritical point $Bc$), when the aspect ratio $\tau$ is varied and $E$ is held fixed.

discontinuity of $\gamma(\Gamma) = \partial S/\partial\Gamma$ [see Fig. 2(c-i)] indicates that this corresponds to a first order transition. Let us then consider the phase diagrams in case (ii) [Figs. 2(a-ii), 2(b-ii), and 2(c-ii)]. Whatever the values of $E, \Gamma$ located below a second parabola $E_{\lambda_1'}(\Gamma)$, represented as a green dashed line, one can show that there exits a single canonical solution. When the parabola is crossed, there is a discontinuity of $\partial^2 S/\partial\Gamma^2$ [see Fig. 2(c-ii)]. It corresponds thus to a microcanonical second order transition line. Above this parabola, $\beta = -\lambda_1'$ everywhere, each point corresponds to two equilibrium states, differing only by the value of their projection on the zero-mean Laplacian eigenmode $e_1'(x, y)$ associated with $\lambda_1'$ (a dipole). The choice of one state among the two possibilities breaks the system symmetry. At high energy, this contribution dominates: the flow is then a dipole.

The phase transitions described all take place in the ensemble inequivalence area. They have unusual thermodynamic properties: a positive jump of $\gamma$ in Fig. 2(c-i) and positive values of $\partial^2 S/\partial\Gamma^2$ in Fig. 2(c-ii). This last peculiarity is equivalent for $\Gamma$ of what would be negative heat capacity $c = \partial^2 S/\partial E^2$ for the energy $E$.

*Bicritical point.*—Finding critical points or triple point requires the tuning of two external parameters (codimension 2). Other examples of codimension 2 phase transition associated with symmetry breaking are bicritical points and second order azeotropy (see [10] and references therein for examples). Before this Letter, none of these have either been observed in systems with long-range interaction or been associated with ensemble inequivalence. Let us apply our previous general analysis to the case of a rectangle with aspect ratio $\tau$ and fixed energy. Changing $\tau$ modifies the eigenvalues $\{\lambda_i\}$. As illustrated in Fig. 2(d), we then predict a bifurcation from a microcanonical first order transition line to two second order transition lines (a bicritical point) at the point $\tau_c = 1.12$, $\Gamma = 0$ ($Bc$), corresponding to the shift from case (i) to case (ii) phase diagrams.

*Nonquadratic entropy functionals.*—In the preceding discussion, we have treated the case of a quadratic generalized entropy $\mathcal{S}[\omega]$. It corresponds to the choice of a Gaussian prior distribution, when the Casimir functionals are treated canonically [9]. It is thus a very natural first choice. Moreover, we argue that the scope of our results is much wider because phase transitions are generally very robust phenomena. We will assess this general idea more precisely in our longer companion paper [15] by studying the limit of small energy of the generalized entropy maximization of $\mathcal{S}[\omega] = \langle s(\omega)\rangle$ with any concave $s$. In this limit, we recover at leading order a problem with a quadratic entropy.

*Generalization to geophysical flows.*—The previous theoretical analysis is exclusively based on the minimization of quadratic functionals. Then it is clear that similar results exist for a whole class of models having linear and quadratic invariants and such that the equilibrium RSM theory applies. We thus predict similar phase transitions and ensemble inequivalence for the whole class of QG models [8] (with one or more layers, with or without topography, etc.). The one layer QG equations on a beta plane is one example: the advected quantity ($\partial_t q + \mathbf{u}\nabla q = 0$) is now the potential vorticity ($q = \Delta\psi - by = \beta\psi - \gamma$). Its lowest energy equilibria are the celebrated Fofonoff flows, that can be computed explicitly by a boundary layer approximation in the limit $\beta \to +\infty$ [12]. As in the Euler case, all the steady states can be formally computed in terms of the Laplacian eigenmodes. The previous analysis of the quadratic variational problems allows us to select the values of $\beta$ and $\gamma$ corresponding to statistical equilibria, and then to compute their energy, circulation, and entropy. Standard numerical procedures can then be applied to compute Laplacian eigenmodes (for any domain geometry) and to draw the flow structure for different values of the parameters, as done Fig. 1. The previous analysis relates for the first time the properties of these flows with phase transitions and ensemble inequivalence. Among other interesting properties not described here, the phase diagram of such academic ocean models can present second order azeotropy. This will be discussed in a companion paper [15], with detailed computations.

[1] P. H. Chavanis, Int. J. Mod. Phys. B **20**, 3113 (2006).
[2] J. Miller, Phys. Rev. Lett. **65**, 2137 (1990); R. Robert, J. Stat. Phys. **65**, 531 (1991); J. Sommeria and R. Robert, J. Fluid Mech. **229**, 291 (1991).
[3] T. Dauxois, S. Ruffo, E. Arimondo, and M. Wilkens, *Dynamics and Thermodynamics of Systems with Long-Range Interactions*, Vol. 602 Lecture Notes in Physics (Springer-Verlag, Berlin, 2002).
[4] D. Lynden-Bell and R. Wood, Mon. Not. R. Astron. Soc. **138**, 495 (1968).
[5] E. Caglioti, P. L. Lions, C. Marchioro, and M. Pulvirenti, Commun. Math. Phys. **174**, 229 (1995).
[6] R. A. Smith and T. M. O'Neil, Phys. Fluids B **2**, 2961 (1990).
[7] R. S. Ellis, K. Haven, and B. Turkington, Nonlinearity **15**, 239 (2002).
[8] J. Pedlosky, *Ocean Circulation Theory* (Springer-Verlag, New York, 1998).
[9] R. S. Ellis, K. Haven, and B. Turkington, J. Stat. Phys. **101**, 999 (2000).
[10] F. Bouchet and J. Barré, J. Stat. Phys. **118**, 1073 (2005).
[11] F. Bouchet and J. Sommeria, J. Fluid Mech. **464**, 165 (2002); B. Turkington, A. Majda, K. Haven, and M. Dibattista, Proc. Natl. Acad. Sci. U.S.A. **98**, 12 346 (2001).
[12] N. P. Fofonoff, J. Mar. Res. **13**, 254 (1954).
[13] P. H. Chavanis and J. Sommeria, J. Fluid Mech. **314**, 267 (1996).
[14] F. Bouchet, Physica (Amsterdam) **237D**, 1976 (2008).
[15] A. Venaille and F. Bouchet, "Thermodynamics of Two-Dimensional and Geophysical Flows" (unpublished).