Ensemble inequivalence, bicritical points and azeotropy for generalized Fofonoff flows

Antoine Venaille and Freddy Bouchet*

Laboratoire des Écoulements Géophysiques et Industriels, UJF, INPG, CNRS ; BP 53, 38041 Grenoble, France and Institut Non Linéaire de Nice , CNRS, UNSA, 1361 route des lucioles, 06 560 Valbonne - Sophia Antipolis, France

(Dated: 30th October 2007)

We present a theoretical description for the equilibrium states of a large class of models of two-dimensional and geophysical flows, in arbitrary domains. We account for the existence of ensemble inequivalence and negative specific heat in those models, for the first time using explicit computations. We give exact theoretical computation of a criteria to determine phase transition location and type. Strikingly, this criteria does not depend on the model, but only on the domain geometry. We report the first example of bicritical points and second order azeotropy in the context of systems with long range interactions.

PACS numbers: 05.20.-y, 05.70.Fh, 47.32.-y.

In many fields of physics, the particle or fields dynamics is not governed by local interactions. For instance for self gravitating stars in astrophysics [1, 2], for vortices in two dimensional and geophysical flows [3, 4, 5], for unscreened plasma or models describing interactions between waves and particles [6], the interaction potential is not integrable [7]. Recently, a new light was shed on the equilibrium statistical mechanics of such systems with long range interactions : there has been a mathematical characterization of ensemble inequivalence [8], a study of several simple models [9, 10], and a full classification of phase transitions and of ensemble inequivalence [11] .

One of the promising field of application for the statistical mechanics of systems with long range interactions, is the statistical prediction of large scale geophysical flows. For instance, the structure of Jupiter's troposphere has been successfully explained using the Robert-Sommeria-Miller (RSM) equilibrium theory [12] [13]. One of the major scope of this field is to go towards earth ocean applications. All textbook in oceanography present the Fofonoff flows which have played an important historical role in that field [14]. In this letter, we propose a theoretical description of such flows in the context of the statistical theories which, for the first time, relates its properties to phase transitions (see Fig. 1), negative specific heat and ensemble inequivalence.

One of the striking features of the equilibrium theory of systems with long range interactions is the generic existence of negative specific heat. This strange phenomena is possible as a consequence of the lack of additivity of the energy and is related to the inequivalence between the microcanonical and canonical ensemble of statistical physics. This was first predicted in the context of astrophysics [15]. For two dimensional flows, existence of such inequivalence has been matematically proven for point vortices [16] (without explicit computation), and numerically observed in a particular situation of a Quasi-Geostrophic (QG) model [17], and in a Monte Carlo study of points vortices in a disk [18]. One of the novelty and achievement of the current work, is that we predict such ensemble inequivalence, with exact theoretical computation of the associated phase transitions, for a very large class of models including the Euler equation or QG models.

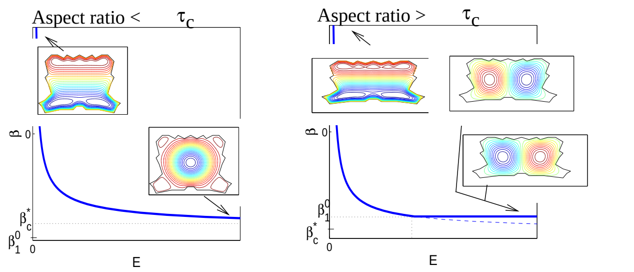

Figure 1: Geometry governed phase transition : second order phase transition from Fofonoff modes in a domain with axial symmetry to dipole solutions, breaking the symmetry, only when the domain is sufficiently stretched ($\tau > \tau_C$) .

In the context of systems with long range interactions, a classification of phase transitions associated to ensemble inequivalence has been proposed [11]. Some of the transitions predicted have never been observed, neither in models, nor in real physical systems. One of the main interest of the current work, is the finding of two examples of such unobserved phase transitions : bicritical points (a bifurcation from a first order phase transition towards two second order phase transitions) and second order azeotropy (the simultaneous appearance of two second order phase transitions at a bifurcation). We prove that those phase transitions are governed by the geometry of the domain in which the flow takes place. We explain how to easily compute the transition point for any domain geometry.

Euler and QG equations This letter describes phase transitions existing in a broad ensemble of models : 2D Euler flows, one layer QG models in a closed domain $\mathcal{D}$. The common character of all of those models comes from the fact that they can all be expressed as a quasi-

2D transport equation $\partial_t q + \boldsymbol{u} \cdot \boldsymbol{\nabla} q = 0$. For the one layer QG model, the potential vorticity (PV) $q = \Delta\psi - \psi/R^2 + h$ is a scalar ; $h(x,y)$ is the topography and R is the Rossby radius of deformation. The velocity field is related to q via ψ : $\mathbf{u} = \mathbf{e}_z \times \boldsymbol{\nabla}\psi$. The case $h = 0$, $R = +\infty$ corresponds to the Euler equation.

For all of these models we use an impermeability condition at the boundaries. The energy of such systems can always be written $\mathcal{E}[q] = -\frac{1}{2}\langle \mathcal{O}[q-h], q-h\rangle$ where $\mathcal{O}$ is a symmetric linear operator.For instance, $\mathcal{E} = \frac{1}{2}\langle (\nabla\psi)^2 + \psi^2/R^2\rangle$ in the 1-1/2 layer QG model, which corresponds to $\mathcal{O} = (\Delta - R^{-2})^{-1}$. In all these models, both energy and circulation $\mathcal{C}[q] = \langle q\rangle$ are conserved quantities.

Variational problem In the following we consider the solutions of the variational problem :

$$S(E,\Gamma) = \max_q \{\mathcal{S}[q] \mid \mathcal{E}[q] = E \;\&\; \mathcal{C}[q] = \Gamma\}, \qquad (1)$$

where $\mathcal{S}$ is the entropy of the PV field q : $\mathcal{S}[q] = \langle s(q)\rangle$, with s a concave function, and $S(E,\Gamma)$ is the equilibrium entropy. Such a variational problem may be interpreted in two ways. First, in the Robert-Sommeria-Miller statistical mechanics of the Euler equation, one obtain a much more complex variational problem which involves the usual Maxwell-Boltzmann entropy and which is constrained on the whole initial vorticity distribution. One can prove that if this vorticity distribution is treated canonically, then the statistical equilibrium verify the variational problem (1) [19]. Moreover any solution to (1) is a RSM equilibrium [19]. An alternative interpretation is to assume directly that, in some physical situations, one has to consider the most probable state with respect to a prior vorticity distribution, which can be related to the shape of s [8].

To compute critical points of the variational problem (1), we introduce two Lagrange parameters β and γ associated respectively with the energy and the circulation conservation. These critical points are stationary solutions for the initial transport equation : $q = f(\psi)$, with $f(\psi) = s'^{-1}(-\beta\psi + \gamma)$. In all of the following, we study the case of a quadratic entropy $\mathcal{S}[q] = \langle -q^2/2\rangle$. This leads to a linear vorticity-stream function relationship ($f(\psi) = \beta\psi - \gamma$). The original Fofonoff solution corresponds to the particular case $\beta \gg 1$ and $h(x,y) = y$. Among the states we study, only the ones with β lower than the phase transition value have already been described as Fofonoff flows or in the context of the Kraichnan statistical mechanics [20, 21]. In the context of the RSM statistical mechanics, in the case of Euler equation, Chavanis and Sommeria [22] found a criteria for the existence of a transition from a monopole to a dipole when increasing the energy (as in figure 1). By using a different method (by solving directly the variational problem), we generalize these results to a wide class of model, analyze for the first time ensemble inequivalence, find unobserved phase transitions and establish the relations of these to Fofonoff flows.

Dual variational problems Our problem is to find the minimum of a quadratic functional (1), taking into account the constraints on circulation (linear) and energy (quadratic with possibly a linear contribution). This will be referred as the microcanonical problem. Dealing with unconstrained variational problems is much easier than dealing with constrained ones: solutions for a variational problem are necessarily solutions for a more constrained dual problem [8]. Moreover, when all the possible constraint values are achieved in the less constraint ensemble, we are in a situation of ensemble equivalence. The study of the unconstrained variational problems is then sufficient [11]. We will thus consider, by relaxing one or both constraints, two dual problems : a) canonical, by relaxing the energy constraint, with the free energy $F(\beta,\Gamma) = \min_q \{-\mathcal{S}[q] + \beta\,\mathcal{E}[q] \mid \mathcal{C}[q] = \Gamma\}$; b) grand canonical, by relaxing both energy and circulation constraints, with the thermodynamical potential $J(\beta,\gamma) = \min_q \{-\mathcal{S}[q] + \beta\,\mathcal{E}[q] + \gamma\mathcal{C}[q]\}$. It is natural to consider first the grand canonical ensemble. If ensemble inequivalence does exist, we will then study a more constrained variational problem, and so on, until the whole range of E and Γ has been covered. Notice that in our case, the ensemble of accessible values for $(\mathcal{E}, \mathcal{C})$ is the half plane $E \geq 0$.

Solutions of quadratic variational problems For all variational problem to be considered in the following, we will look for the minimum of a quadratic functional, with a linear part. Let us call Q the purely quadratic part and L the linear part of this functionnal. Then we have three cases

1. The smallest eigenvalue of Q is strictly 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 (the infimum is $-\infty$).
3. The smallest eigenvalue of Q is zero (with eigenfunction e_0). If $Le_0 = 0$ (case 3a), the maximum exists and each state of the neutral direction $\{\alpha e_0\}$ is a minimizer. If $Le_0 \neq 0$, (case 3b) then no minimum exist.

The grand canonical ensemble We consider in this part $h = 0$, so the energy is purely quadratic. We look for the minimum of $\mathcal{J} = -\mathcal{S} + \beta\,\mathcal{E} + \gamma\mathcal{C}$. We introduce the projections q_i of the PV q on a complete orthonormal basis of eigenfunctions $e_i(x,y)$ of the operator $\mathcal{O}$ ($\mathcal{O}[e_i] = e_i/\lambda_i$) (see the definition of the energy) and find:

$$\mathcal{J}[q] = \sum_{i,j\geq 1} \delta_{ij}\,(1-\beta/\lambda_i)\,q_i q_j + \sum_{i\geq 1} \gamma\langle e_i\rangle q_i$$

where δ_{ij} is the Kronecker symbol, and where the λ_i (all negative) are in decreasing order. One can see that the quadratic part is diagonal, and that all eigenvalues are strictly positive if and only if $\beta > \lambda_1$(case 1. above) . If $\beta = \lambda_1$(case 3), a neutral direction exists if and only if $\gamma = 0$ (case 3a). Thus, grand canonical solutions exist only for $\beta > \lambda_1$ or ($\beta = \lambda_1$ and $\gamma = 0$). By computing the energy and circulation of all those states, we prove that it exists a unique solution at each point in the diagram (E, Γ), below a parabola $\mathcal{P}$ of equation $E = -\Gamma^2 \lambda_1 / \left(2 \langle e_1 \rangle^2\right)$. Because the values of energies above the parabola $\mathcal{P}$ are not reached, we conclude that there is ensemble inequivalence for parameters in this area. As explained previously, we have to consider a more constrained variational problem to find solutions in this area.

The canonical ensemble We now look for the minimum of $-\mathcal{S} + \beta\,\mathcal{E}$ for a fixed circulation Γ. In order to take into account this constraint, we express one coordinate in term of the others : $q_1 = \left(\Gamma - \sum_i q_i \langle e_i \rangle\right) / \langle e_1 \rangle$. Then, we have to minimize

$$\mathcal{F}[q] = \sum_{i,j \geq 2} \left(\delta_{ij} \left(1 - \frac{\beta}{\lambda_i}\right) + \left(1 - \frac{\beta}{\lambda_1}\right) \frac{\langle e_i \rangle \langle e_j \rangle}{\langle e_1 \rangle^2} \right) q_i q_j - \sum_{i \geq 2} \Gamma \frac{\langle e_i \rangle}{\langle e_1 \rangle^2} \left(1 - \frac{\beta}{\lambda_1}\right) q_i,$$

without constraint.

The linear operator Q, associated to the quadratic part of $\mathcal{F}$, is not diagonal in the basis $\{e_i\}$. We first notice that if the domain geometry admits one or more symmetries, it generically exists eigenfunctions having the property $\langle e_i \rangle = 0$. In the subspace spanned by all those eigenfunctions, Q is diagonal, and its smallest eigenvalue is positive as long as $\beta > \beta_1^0$, where β_1^0 is the greatest λ_i on this subspace. Then we look for the value of β such that the smallest eigenvalue of Q is zero in the subspace spanned by eigenfunctions with $\langle e_i \rangle \neq 0$. Let us call β_c^* this value, and q_c^* the corresponding eigenfunction : $Q[q_c^*] = 0$. Using this last equation, we prove that β_c^* is the greatest zero of the function $f(x) = 1 - x \sum_{i \geq 1} \langle e_i \rangle^2 / (x - \lambda_i)$. We conclude that there is a single solution to the variational problem for $\beta > \max\left(\beta_1^0,\ \beta_c^*\right)$ (case 1) and no solution for $\beta < \max\left(\beta_1^0,\ \beta_c^*\right)$ (case 2). When $\beta = \max\left(\beta_1^0,\ \beta_c^*\right)$, to discuss the existence of a neutral direction, we distinguish two cases according to the sign of $\beta_1^0 - \beta_c^*$:

i) $\beta_1^0 < \beta_c^*$ we then consider $\beta = \beta_c^*$. We are in case 3a for $\Gamma = 0$ and in case 3b for $\Gamma \neq 0$.

ii) $\beta_1^0 > \beta_c^*$ we then consider $\beta = \beta_1^0$. We are in case 3a whatever the value of Γ.

In case i), if $\Gamma \neq 0$, all energy value are reached in the canonical ensemble. If $\Gamma = 0$, the solutions of the neutral directions are αq_c^*. Thus, varying α, all energy values are reached ; there is two canonical solutions corresponding to each energy E, depending on the sign of α. In case ii), $\lim_{\beta \to \beta_1^0} E(\beta) = E_{\mathcal{P}_0}(\Gamma) \propto \Gamma^2$. This defines a parabola $\mathcal{P}_0$. Then, whatever the value of Γ, there is a unique canonical solution $q(\beta, \Gamma)$ for each point of the diagram (E, Γ) below $\mathcal{P}_0$. The canonical solutions of the neutral directions is $q = \alpha e_1^0 + \lim_{\beta \to \beta_1^0} q(\beta, \Gamma)$ where e_1^0 is the eigenfunction associated with β_1^0. Varying α, all energy larger than $E_{\mathcal{P}_0}(\Gamma)$ are reached. For each energy above the parabola $\mathcal{P}_0$, it exists two canonical solutions, depending on the sign of α. In both cases we find that all circulation and energy values have been reached by canonical solutions. We conclude that microcanonical and canonical ensembles are equivalent.

Description of phase transitions. In case i), at fixed energy, we can show by a direct computation that $\gamma(\Gamma) = \frac{\partial S}{\partial \Gamma}$ is discontinuous in $\Gamma = 0$. This means that there is a microcanonical first order transition (see point G figure 2-c). In case ii), one can show that $\frac{\partial \gamma}{\partial \Gamma}$ is discontinuous when (E, Γ) belongs to $\mathcal{P}_0$ (see points B and D, figure 2-b). The ensemble inequivalence area is associated with the existence of a first order transition in the ensemble with only one constraint on the energy (see the corresponding Maxwell constructions on figure 2-b,c). Similarly, if we now fix the circulation, there is a discontinuity of $\frac{\partial \beta}{\partial E}$ when (E, Γ) belongs to $\mathcal{P}_0$. It means that $\mathcal{P}_0$ is a line of second order phase transition for canonical and microcanonical ensembles.

General criteria. The main interest of the abstract previous analysis is to conclude that all of the models considered will behave according to only two types of phase diagram structures. The difference between the two classes of systems is the existence of either first or second order phase transitions, corresponding respectively to case i) and ii). If the domain has no symmetry, only case i) is possible (generically). If there is a symmetry, both cases are possible. The criteria for class i) or class ii) systems is the sign of $\beta_1^0 - \beta_c^*$, that can be easily computed for a system at hand. The same criteria was obtained in [22] for the Euler equation, using a different method. Very interestingly, this criteria does not depend on the model considered (it does not depend on the Rossby radius of deformation R), but only on the domain shape. For some classes of domain geometries, as ellipses for instance, we are always in case ii). More generally, any domain geometry sufficiently stretched in a direction perpendicular to its symmetry axis is in case ii). This is for instance the case of a rectangular domain The transition from systems of type i) to systems of type ii), when the geometry is modified, leads to very interesting phenomena that are described now.

The bicritical point On figure 2, we consider a fixed energy, and present the phase diagram in the (Γ, τ) plane, where τ is a parameter characterizing the aspect ratio of the domain (horizontal over vertical width). In the microcanonical ensemble, there is a bifurcation from a first order transition line to two second order transition lines at a critical value $\tau = \tau_c$. Such a bifurcation is

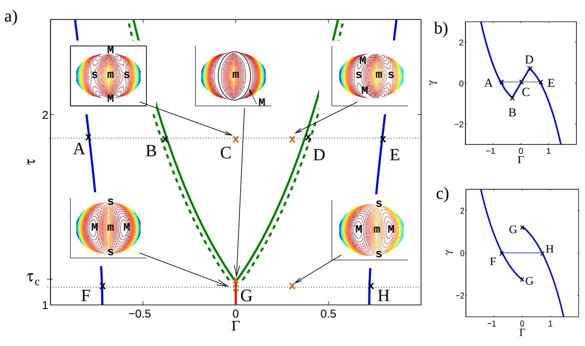

Figure 2: First observation of a bicritical point (change from a first order to two second order phase transitions) in a system with long range interactions. Euler equation in a rectangular domain of aspect ratio τ. Green line : second order phase transition (discontinuity of $\partial\gamma/\partial\Gamma$ in b). Red line : 1st order phase transition (discontinuity of γ in c). Insets are projection of the Entropy $\mathcal{S}[q]$ in a plane (q_1^0, q_1) for fixed energy and circulation.

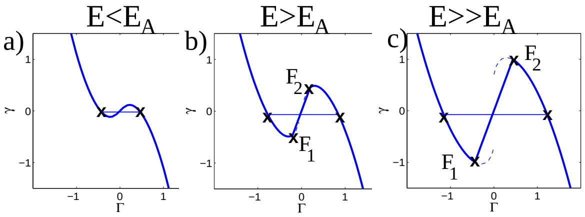

Figure 3: First observation of second order azeotropy (at energy E_A there is simultaneous appearance of two second order phase transitions). a) $\partial\gamma/\partial\Gamma$ is continuous ; b and c) $\partial\gamma/\partial\Gamma$ is not continuous in F_1 and F_2.

referred as a bicritical point (see [11]).

With a topography We now give the main striking features arising when adding the term h, especially the new unobserved phase transitions. Concerning the existence of first and second order phase transitions in the microcanonical ensemble, there is now three possibilities. If $\beta_1^0 - \beta_c^* < 0$, the phase diagram is similar to the one of case i). If $\beta_1^0 - \beta_c^* > 0$ and $\langle h, e_1^0 \rangle = 0$, then we are in the case ii), except that the minima of $\mathcal{P}$ and $\mathcal{P}_0$ are no more at the same place in the diagram (E, Γ). If $\beta_1^0 - \beta_c^* > 0$ and $\langle h, e_1^0 \rangle \neq 0$, there is neither second nor first order transition.

Second order Azeotropy In case ii) with topography, if we consider the energy as an external parameter, there is the simultaneous appearance of two second order phase transitions in the microcanonical ensemble (see figure 3 and the corresponding flows figure 1), which is the signature of second order azeotropy.

Conclusion We report the generic existence of ensemble inequivalence and of new phase transitions in a large class of 2D flows. All phase transitions presented here appear in the inequivalence ensemble area. They are in that respect a signature of such an inequivalence in a long range interacting system, which has never been observed experimentally. The observation of those transitions could be carried in laboratory experiments on quasi 2D flows. This could be done by using either magnetized electron columns [23] or three dimensionnal tanks with small height compared to the horizontal scale, with a further ordering (strong rotation or a transverse magnetic field). The interest for ocean applications will be described in a companion paper, as well as the detailed complete computations, generalization to multi level QG equations and analysis of the ensemble inequivalence associated to the bicritical points.

We thank J. Barré, P.H. Chavanis and J. Sommeria for interesting discussions. This work was supported by the ANR program STATFLOW (ANR-06-JCJC-0037-01).

* Freddy.Bouchet@inln.cnrs.fr

[1] P.-H. Chavanis, Phys. Rev. E **65**, 056123 (2002).
[2] I. Ispolatov and E. G. D. Cohen, Phys. Rev. E **64**, 056103 (2001).
[3] J. Miller, Phys. Rev. Lett. **65**, 2137 (1990).
[4] R. Robert, J. Stat. Phys. (1991).
[5] J. Sommeria and R. Robert, J. Fluid Mech. **229**, 291 (1991).
[6] A. Macor, F. Doveil, and Y. Elskens, Phys. Rev. Lett. **95**, 264102 (2005).
[7] T. Dauxois, S. Ruffo, E. Arimondo, and M. Wilkens, eds., *Dynamics and Thermodynamics of Systems With Long Range Interactions* (2002).
[8] R. S. Ellis, K. Haven, and B. Turkington, J. Stat. Phy. **101** (2000), math/0012081.
[9] J. Barré, D. Mukamel, and S. Ruffo, Phys. Rev. Lett. **87**, 030601 (2001).
[10] M. Costeniuc, R. S. Ellis, and H. Touchette, J. Math. Phys. **46**, 063301 (2005), cond-mat/0410744.
[11] F. Bouchet and J. Barré, J. Stat. Phys. **118 5/6**, 1073 (2005).
[12] F. Bouchet and J. Sommeria, J. Fluid. Mech. **464**, 465 (2002).
[13] B. Turkington, A. Majda, K. Haven, and M. Dibattista, PNAS **98**, 12346 (2001).
[14] N. P. Fofonoff, J. Mar. Res. **13**, 254 (1954).
[15] D. Lynden-Bell and R. Wood, mnras **138**, 495 (1968).
[16] E. Caglioti, P. L. Lions, C. Marchioro, and M. Pulvirenti, Com.Math. Phys. **174**, 229 (1995).
[17] R. S. Ellis, K. Haven, and B. Turkington, Nonlinearity **15**, 239 (2002).
[18] R. A. Smith and T. M. O'Neil, Physics of Fluids B **2**, 2961 (1990).
[19] F. Bouchet, sub. to Physica D (2007), arXiv:0710.5094v1.
[20] R. H. Kraichnan, Journal of Fluid Mechanics **67**, 155 (1975).
[21] R. Salmon, G. Holloway, and M. C. Hendershott, Journal of Fluid Mechanics **75**, 691 (1976).
[22] P. H. Chavanis and J. Sommeria, J. Fluid Mech. **314**, 267 (1996).
[23] D. A. Schecter, D. H. E. Dubin, K. S. Fine, and C. F. Driscoll, Physics of Fluids **11**, 905 (1999).