

Statistical mechanics of non-extensive systems/Mécanique statistique des systèmes non-extensifs

## Statistical mechanics and long range interactions

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### Abstract

We briefly review the classical approach to equilibrium and out of equilibrium statistical mechanics of long range interacting systems, for which the energy is not additive, and emphasize some new results.

At equilibrium, we explain the thermodynamic consequences of the lack of additivity, like the generic occurrence of statistical ensemble inequivalence and negative specific heat. We then present a recent new classification of phase transitions and ensemble inequivalence in systems with long range interactions, and note a number of generic situations that have not yet been observed in any physical systems.

Out of equilibrium, we show that algebraic temporal correlations or anomalous diffusion may occur in these systems, and can be explained using usual statistical mechanics and kinetic theory. *To cite this article: J. Barré, F. Bouchet, C. R. Physique 7 (2006).* © 2006 Académie des sciences. Published by Elsevier SAS. All rights reserved.

### Résumé

**Mécanique statistique et interactions à longue portée.** Nous résumons d'abord brièvement les approches classiques de la mécanique statistique d'équilibre et hors équilibre des systèmes avec interactions à longue portée, pour lesquels l'énergie n'est pas additive, puis nous développons quelques résultats nouveaux.

À l'équilibre, la non additivité a des conséquences thermodynamiques inattendues, comme la possibilité générique d'inéquivalence d'ensemble et de chaleur spécifique négative. Nous présentons une classification récente des transitions de phase et situations d'inéquivalence d'ensemble pour les systèmes à longue portée; cette classification met en lumière plusieurs situations génériques qui n'ont pas encore été observées sur un système physique particulier.

Hors d'équilibre, nous montrons que des corrélations temporelles algébriques, ou de la diffusion anormale, peuvent être présentes dans ces systèmes, et s'expliquent à l'aide d'outils de la mécanique statistique usuelle et de théorie cinétique. *Pour citer cet article: J. Barré, F. Bouchet, C. R. Physique 7 (2006).*

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## 1. Introduction

The methods of statistical mechanics are most commonly applied to large systems with short range interactions between the components, that is with an interaction range much smaller than the size of the system. In this case, many convenient properties hold: energy is additive, see Fig. 1, the thermodynamic limit is usually appropriate, different statistical ensembles (like canonical and microcanonical) are equivalent. . . .

However, for many systems the interaction range is not negligible with respect to the total size, the main example being self-gravitating stars. All the nice properties cited above are then questionable, and indeed are wrong, as we shall see: energy is not additive any more; thermodynamic limit has to be replaced by another procedure to study large systems, different statistical ensembles may generically be inequivalent, specific heat may be negative. . . . These peculiarities of long range interacting systems have been studied for a long time in many different contexts, starting in astrophysics [1,2]. Besides astrophysical self gravitating systems [3–13], the main physical examples of non-additive systems with long range interactions are two-dimensional or geophysical fluid dynamics [14–19] and a large class of plasma effective models [20–24]. Spin systems [25] and toy models with long range interactions [26–28] have also been widely studied. The links between these different subjects have been emphasized recently [28]. Although we will restrict here to large systems with long range interactions, let us note that these share some phenomenology with small systems, that are also non additive [29].

In Section 2, we discuss the usual assumptions of equilibrium statistical mechanics, their interpretation in systems with long range interactions and we explain how large deviation techniques may be used in this context. The aim of this section, which contains mainly classical results, is to introduce Section 3, where new results are presented. In particular, we show how the description of microcanonical and canonical ensembles may be reduced to two dual variational problems. Such variational problems lead to possible generic ensemble inequivalence, and to a richer zoology of phase transitions than in usual systems. A natural question then arises: do we know all possible behaviors stemming from long range interactions, and, if not, what are the possible phenomenologies? In Section 3, we answer this question by discussing a *classification* of all microcanonical and canonical phase transitions, in long range interacting systems, with emphasis on situations of ensemble inequivalence [30].

Because systems with long range interactions relax very slowly towards equilibrium, the study of out of equilibrium situations is physically essential. Obviously, it is much more difficult to reach general conclusions in this context. In Section 4, we briefly present the standard tools of kinetic theory, that have been developed since a long time to study the dynamics of long range interacting systems. We present also some recent results in this field, and show on a toy model how kinetic theory can explain long range temporal correlations and anomalous diffusions in such systems [31].

## 2. Scaling limit and large deviation results

### 2.1. Scaling limit

The first surprising fact when studying statistical mechanics of nonadditive systems is the inadequacy of the thermodynamic limit ( $N \rightarrow \infty$ ,  $V \rightarrow \infty - V$  is the volume—with  $N/V$  kept constant). Indeed, what is physically important in order to understand the behavior of large systems, is not really to study the large  $N$  limit, but rather to obtain properties that do not depend much on  $N$  for large  $N$  (the equivalent of intensive variable).<sup>1</sup> For short range interacting

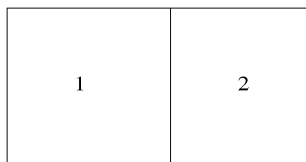


Fig. 1. Let us consider a macroscopic system composed of two subsystems 1 and 2. The energy is additive if the interface energy is negligible so that  $E_{\text{tot}} = E_1 + E_2$ .

<sup>1</sup> Comment by Robert MacKay.

systems, this is achieved through the thermodynamic limit; for nonadditive systems, the scaling limit to be considered is different and depends on the problem. Let us consider  $N$  particles which dynamics is described by the Hamiltonian

$$H_N = \frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{c}{2} \sum_{i,j=1}^N V(r_i - r_j) \quad (1)$$

where  $c$  is a coupling constant. The thermodynamic limit in this case amounts to send  $N$  and the volume to infinity, keeping density and  $c$  constant. If  $V(r)$  decreases fast enough so that interactions for a particle come mainly from the first neighbors, then increasing  $N$  at constant density has almost no effect on the bulk, and physical properties are almost independent of  $N$ : the thermodynamic limit is appropriate. This is wrong, of course, if the potential for a particle is dominated by the influence of far away particles. The appropriate scaling in this case may be as follows: fixed volume,  $c \propto 1/N^2$ , and  $N \rightarrow \infty$  (others equivalent combinations are possible, as the one given below for self gravitating particles).

The best known example of such a special scaling concerns self gravitating stars, for which the ration  $M/R$  is usually kept constant, where  $M$  is the total mass and  $R$  is the system's radius (thermodynamic limit would be  $M/R^3$  constant). Another toy example is given and studied for instance in [32]. This type of scaling is also the relevant one for point vortices in two dimensional and geophysical turbulence, where the total volume and total vorticity have to be kept fixed, but divided in smaller and smaller units. Let us note for completeness that in some cases, the thermodynamic limit is appropriate in presence of long range interactions, for instance when some screening is involved [33]; we shall exclude these cases in the following.

## 2.2. The microcanonical and canonical ensembles

In Sections 2.3 and 3, we will consider equilibrium properties of systems with long range interactions. We suppose that the energy  $E$  of our system is known. We consider the microcanonical ensemble. In this statistical ensemble all phase space configurations with energy  $E$  have the same probability. We thus consider the microcanonical measure

$$\mu_N = \frac{1}{\Omega_N(E)} \prod_{i=1}^N dr_i dp_i \delta(H_N(\{r_i, p_i\}) - E) \quad (2)$$

where  $\Omega_N(E)$  is the volume of the energy shell in the phase space  $\Omega_N(E) \equiv \int \prod dr_i dp_i \delta(H_N(\{r_i, p_i\}) - E)$ . We consider here the energy as the only parameter, however generalization of the following discussion to other quantities conserved by the dynamics is straightforward.

The only hypothesis of equilibrium statistical mechanics is that averages with respect to  $\mu_N$  will correctly describe the macroscopic behavior of our system. This hypothesis is usually verified after a sufficiently long time, when the systems has 'relaxed' to equilibrium.

The Boltzmann entropy per particle is defined as

$$S_N(E) \equiv \frac{1}{N} \log \Omega_N(E) \quad (3)$$

In the following, we will justify that in the long range scaling limit, the entropy per particle  $S_N(E)$  has a limit:

$$S_N(E) \xrightarrow{N \rightarrow \infty} S(E) \quad (4)$$

The canonical ensemble is defined similarly, using the canonical measure

$$\mu_{c,N} = \frac{1}{Z_N(E)} \prod_{i=1}^N dr_i dp_i \exp[-\beta H_N(\{r_i, p_i\})] \quad (5)$$

with the associated partition function  $Z_N(\beta) \equiv \int \prod dr_i dp_i \exp[-\beta H_N(\{r_i, p_i\})]$  and free energies  $F_N(\beta) \equiv \frac{1}{N} \log Z_N(\beta)$  and  $F_N(\beta) \xrightarrow{N \rightarrow \infty} F(\beta)$ .

### 2.3. Large deviation results

Large deviation theory provides a very efficient tool to compute the entropy per particle and the free energy per particle in the large  $N$  limit, with the appropriate scaling. Although the following explanations are schematic, we stress that results obtained this way are often mathematically rigorous: essentially, large deviation theory is in this case a way to justify a mean-field like approach to the statistical mechanics in the large  $N$  limit. We refer for more details to the book of Ellis and the very interesting contributions of Ellis and coworkers [34–37]. We also refer to [38] for a detailed explanation of many large deviations results in the context of long range interacting systems.

Starting from the definitions of entropy and free energy given in Section 2.2, we now sketch the different steps that reduce the evaluation of entropies and free energies to variational problems.

- In a first step one describes the system at hand by a macroscopic variable; this may be a coarse-grained density profile  $f$ , a density of charges in plasma physics, a magnetization profile for a magnetic model. In the following, we will generically call this macroscopic variable  $m$ ; it may be a scalar, a finite or infinite dimensional variable.

One then associates a probability to each macrostate  $m$ . Large deviation theory comes into play to estimate  $\Omega(m)$ , the number of microstates corresponding to the macrostate  $m$ :

$$\log(\Omega_N(m)) \underset{N \rightarrow \infty}{\sim} Ns(m) \tag{6}$$

This defines the entropy  $s(m)$ .

For instance the macroscopic variable  $m$  may be the  $\mu$ -space particle distribution  $f(r, p)$  ( $f(r, p) dr dp$  is the probability to observe a particle with position  $r$  and momentum  $p$ ). Many microscopic states correspond to a given  $f$ . It is a classical result to show that the logarithm of the number of these microscopic states is given by

$$s[f] = - \int dr dp f \log f \tag{7}$$

where  $s$  is sometimes called the Boltzmann–Gibbs entropy. It is the Boltzmann entropy associated to the macrostate  $f$ , in the sense that it counts the number of microstates corresponding to  $f$ . We stress that *no other functional has this probabilistic meaning*, and that this property is independent of the Hamiltonian.

- In a second step, one has to express the constraints (energy or other dynamical invariants) as functions of the macroscopic variable  $m$ . In general, it is not possible to express exactly the Hamiltonian  $H_N$  as a function of  $m$ ; however, for long range interacting systems, one can very often define a suitable approximating mean field functional  $h(m)$ , as in (Eq. (8)).

For instance, using Hamiltonian (Eq. (1)) and the  $\mu$ -space density  $f$  as macroscopic variable, the energy functional is of the form

$$h[f] \underset{N \rightarrow \infty}{\sim} \int dr_1 dp_1 dr_2 dp_2 f(r_1, p_1) f(r_2, p_2) V(r_1 - r_2) \tag{8}$$

Having now at hand the entropy and energy functionals, one can compute the microcanonical density of states  $\Omega(E)$  [35]: the microcanonical solution is simply given by the variational problem

$$\log(\Omega_N(E)) \underset{N \rightarrow \infty}{\sim} NS(E) \quad \text{with } S(E) = \sup_m \{s(m) \mid h(m) = E\} \tag{9}$$

In the canonical ensemble, similar considerations lead to the conclusion that the free energy and the canonical equilibrium are given by the variational problem

$$\log(Z_N(\beta)) \underset{N \rightarrow \infty}{\sim} NF(\beta) \quad \text{with } F(\beta) = \inf_m \{-s(m) + \beta h(m)\} \tag{10}$$

The variational problems (Eqs. (9) and (10)) are dual to each other; however, a one-to-one relation between  $E$  and its Lagrange multiplier  $\beta$  is not guaranteed: this is at the root of the ensemble inequivalence phenomenon.

We insist that this reduction of the microcanonical and canonical calculations to the variational problems (Eqs. (9) and (10)) is in many cases rigorously justified. The first result assumes a smooth interaction potential  $V$  between particles and has been proved by Messer and Spohn [39]; see also the works by Hertel and Thirring on the self gravitating fermions [40].

### 3. Classification

The thermodynamics of long range interacting systems in the microcanonical and canonical ensembles is now reduced to the dual variational problems (Eqs. (9) and (10)). The precise form of the solution obviously depends on the problem at hand through the functions  $s(m)$  and  $h(m)$ . However, many qualitative features of the thermodynamics depend only on the *structure* of the variational problem. Thus, it is possible to *classify* all the different possible phenomenologies that one may find in the study of a particular long range interacting system. The questions in that respect are, increasing complexity at each step:

- what are the different possible types of generic points on an entropy curve  $S(E)$  (these correspond to different phases)?
- what are the possible singular points of a generic  $S(E)$  curve (these correspond to phase transitions)?
- what are the possible singular points on the  $S(E)$  curve, when an external parameter is varied in addition to the energy (that is how phase transitions evolve when a parameter is varied)?

We address these different levels in the following paragraphs, using results from [35,30]. These results are obtained by adapting to the dual variational problems (Eqs. (9) and (10)) ideas that lead to the Landau classification of phase transitions. In the long range case however, there is no approximation involved, so the classification does not suffer from the problems of standard Landau theory (wrong critical exponents for instance).

#### 3.1. Generic points of an entropy curve

There are three types of generic points on the entropy curve, see Fig. 2:

- Concave points (that is  $C_v > 0$ ) where canonical and microcanonical ensembles are equivalent.
- Concave points where ensembles are inequivalent.
- Convex points ( $C_v < 0$ ), where ensembles are always inequivalent.

#### 3.2. Singular points of a generic entropy curve: phase transitions

Generic points as described above define segments of entropy curves, separated by singular points, that can be of several types. These points for systems without symmetry are classified in Fig. 3.

#### 3.3. Singular points on a singular entropy curve

When an external parameter is varied, the entropy curve is modified. Some special values of the parameter correspond to qualitative changes for the phase transitions. All these possible qualitative changes are classified on Fig. 4,

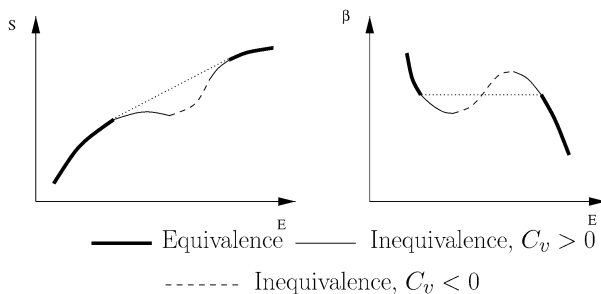


Fig. 2. The three types of generic points; on the left: entropy  $S(E)$  curve, on the right: caloric  $\beta(E)$  curve. Thick, thin and dashed lines correspond respectively to the three types of points. The dotted lines shows the Maxwell construction giving the canonical solution in the inequivalence range.

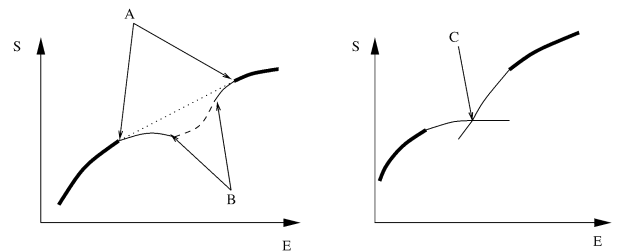


Fig. 3. The three types of phase transitions (codimension 0 singularities), for a system with no symmetry. A: canonical 1st order transition. B: canonical destabilization. C: microcanonical 1st order, temperature jump.

	Singularities	Canonical	S(E)			$\beta(E)$		
<b>Maximization singularities</b>	Critical point	invisible						
	Triple point	invisible						
	Azeotropy	<b>Azeotropy</b>						
<b>Convexity</b>	Convexity modification	<b>Critical point</b>						
	First order and cano. destab.	invisible						
<b>Concavification</b>		<b>Triple point</b>						

Fig. 4. Classification of singularities, when one external parameter is varied (codimension 1 singularities). The first two columns give the singularity origin and name; the third one gives its status in the canonical ensemble: invisible means it has no consequence on the canonical solution; the six following plots are entropic and caloric curves showing the crossing of the singularity when the external parameter is varied. One recovers the usual phase transitions (triple point, azeotropy, critical point) in both ensembles. What is new is the list of the possible links between the behaviors in each ensembles, and the associated appearance of ensemble inequivalence. Please see [30] for a more detailed explanation, and singularities associated with symmetry breaking.

from [30]. Most interesting are the changes leading to the appearance of ensemble inequivalence. Besides the known critical point, the classification shows for instance the possibility of a new route to ensemble inequivalence, through azeotropy; this one is not necessarily associated with a negative  $C_v$ , and has not been found yet on a specific model.

#### 4. Out of equilibrium statistical mechanics and kinetic theory

After a rapid violent relaxation, systems with long range interactions relax towards quasi-stationary (virialized) states [41]. These states are often out of equilibrium. They then relax very slowly towards equilibrium on a time scale  $t_R$  diverging with the number of particle (for instance  $t_R \sim \log(N)/N$  for self gravitating systems or  $t_R \sim N$  for smooth potentials or  $t_R \gg N$  for one dimensional systems [31]). In this relaxation regime, thanks to the separation of time scale between the evolution of fluctuations and the evolution of the quasi-stationary density  $f$ , a kinetic approach of the relaxation towards equilibrium is justified. This gives the classical Lenard–Balescu equation for plasma physics, or the kinetic equations for self-gravitating systems [8,42]. We note a peculiarity for one dimensional systems where the Lenard–Balescu operator vanishes [31]. We also stress, that the Boltzmann–Gibbs entropy is still the correct entropy to measure the relative probability of an out of equilibrium state, in such systems.<sup>2</sup>

We want to emphasize some recent results, in the old and long history of kinetic theory for systems with long range interactions. Let us consider the Hamiltonian Mean Field model [26] with Hamiltonian (Eq. (1)), with a cosine (thus regular) interaction. Fig. 5 shows the numerically computed diffusion of angles compared with an asymptotic

<sup>2</sup> This property is not valid in general, out of equilibrium. It may be valid when the two-point correlations between particles can be neglected. This is the case for systems with long range interaction in the kinetic regime. This is also the case for a dilute gas, as shown by the celebrated works of Boltzmann more than one century ago.

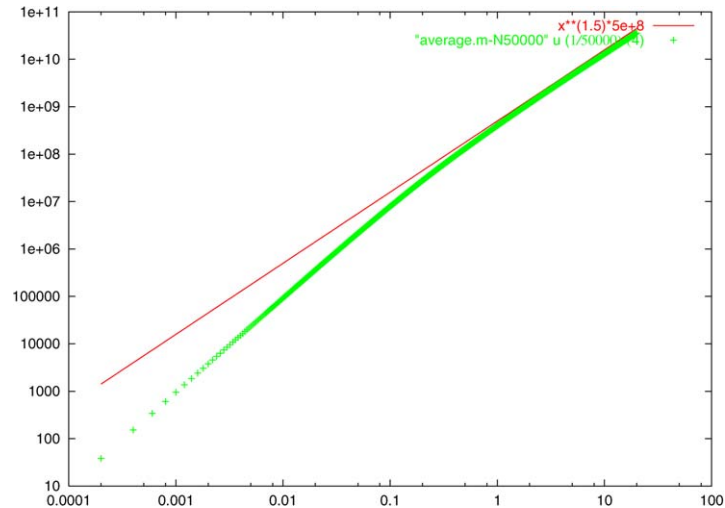


Fig. 5. Angles diffusion ( $\langle (\theta(t) - \theta(0))^2 \rangle$ ) as a function of time in the HMF model, for a quasi-stationary state. Points are from a  $N$  body numerical simulation, the straight line is the analytic prediction by the kinetic theory [31]. For large times  $\langle (\theta(t) - \theta(0))^2 \rangle \sim t^\nu$  with  $\nu \neq 1$ . Such an unexpected anomalous diffusion is also observed at equilibrium (see [31] for more details).

behavior predicted using kinetic theory. This figure illustrates some unexpected behavior of systems with long range interactions.

Because of a very small diffusion in the momentum space, some very long temporal correlations do exist. This is illustrated by the algebraic tails in the autocorrelation function [43]. This behavior can be predicted using kinetic theory [31] and is directly linked to the anomalous diffusion. This shows that usual kinetic theory can explain unusual behavior of the dynamics of systems with long range interactions (we note that we disagree with an other interpretation using Tsallis statistics [44]. We refer to [31] and references therein for a complete discussion). Some recent related results have also been reported in [45]. Thanks to kinetic theory, the index for anomalous diffusion can thus be predicted from first principles.

## 5. Conclusion

In conclusion, it seems to us that equilibrium statistical mechanics of nonadditive systems, briefly reviewed in Sections 2 and 3, is very well understood. Out of equilibrium, the classical tools of kinetic theory are able to explain some unexpected phenomena (Section 4), and there is at present no obvious need for an alternative theory.

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