OUT–OF–EQUILIBRIUM PHASE TRANSITIONS
IN MEAN–FIELD HAMILTONIAN DYNAMICS

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Systems with long-range interactions display a short-time relaxation towards
Quasi-Stationary States (QSSs), whose lifetime increases with system size.
With reference to the Hamiltonian Mean Field (HMF) model, we here review
Lynden-Bell’s theory of “violent relaxation”. The latter results in a maximum
entropy scheme for a water-bag initial profile which predicts the presence of
out–of–equilibrium phase transitions separating homogeneous (zero magneti-
zation) from inhomogeneous (non–zero magnetization) QSSs. Two different
parametric representations of the initial condition are analyzed and the fea-
tures of the phase diagram are discussed. In both representations we find a
second order and a first order line of phase transitions that merge at a tri-
critical point. Particular attention is payed to the condition of existence and
stability of the homogenous phase.

Keywords: Quasi-stationary states, Hamiltonian Mean-Field model, Out–of–
equilibrium phase transitions
1. Introduction

Hamiltonian systems arise in many branches of applied and fundamental physics and, in this respect, constitute a universal framework of extraordinary conceptual importance. Spectacular examples are undoubtely found in the astrophysical context. The process of hierarchical clustering via gravitational instability, which gives birth to the galaxies,\(^1\) can in fact be cast in a Hamiltonian setting. Surprisingly enough, the galaxies that we observe have not yet relaxed to thermodynamic equilibrium and possibly correspond to intermediate Quasi–Stationary States (QSSs). The latter are in a long-lasting dynamical regime, whose lifetime diverges with the size of the system. The emergence of such states has been reported in several different domains, ranging from charged cold plasmas\(^2\) to Free Electron Lasers (FELs),\(^3\) and long-range forces have been hypothesized to be intimately connected to those peculiar phenomena.

Long-range interactions are such that the two-body interaction potential decays at large distances with a power–law exponent which is smaller than the space dimension. The dynamical and thermodynamical properties of physical systems subject to long-range couplings were poorly understood until a few years ago, and their study was essentially restricted to astrophysics (e.g., self-gravitating systems). Later, it was recognized that long–range systems exhibit universal, albeit unconventional, equilibrium and out–of–equilibrium features.\(^4\) Besides slow relaxation to equilibrium, these include ensemble inequivalence (negative specific heat, temperature jumps), violations of ergodicity and disconnection of the energy surface, subtleties in the relation of the fluid (i.e. continuum) picture and the particle (granular) picture, new macroscopic quantum effects, etc..

While progress has been made in understanding such phenomena, an overall interpretative framework is, however, still lacking. In particular, even though the ubiquity of QSSs has been accepted as an important general concept in non-equilibrium statistical mechanics, different, contrasting, attempts to explain their emergence have catalysed a vigorous discussion in the literature.\(^5\)

To shed light onto this fascinating field, one can resort to toy models which have the merit of capturing basic physical modalities, while allowing for a dramatic reduction in complexity. This is the case of the so-called Hamiltonian Mean Field (HMF) model which describes the evolution of N rotators, coupled through an equal strength, attractive or repulsive, cosine
interaction. The Hamiltonian, in the attractive case, reads

$$H = \frac{1}{2} \sum_{j=1}^{N} p_j^2 + \frac{1}{2N} \sum_{i,j=1}^{N} \left[ 1 - \cos(\theta_j - \theta_i) \right] ,$$

(1)

where $\theta_j$ represents the orientation of the $j$-th rotator and $p_j$ stands for the conjugated momentum. To monitor the evolution of the system, it is customary to introduce the magnetization, an order parameter defined as $M = |\mathbf{M}| = |\sum \mathbf{m}_i|/N$, where $\mathbf{m}_i = (\cos \theta_i, \sin \theta_i)$ is the magnetization vector. The HMF model shares many similarities with gravitational and charged sheet models and has been extensively studied as a paradigmatic representative of the broad class of systems with long-range interactions. The equilibrium solution is straightforwardly worked out and reveals the existence of a second-order phase transition at the critical energy density $U_c = 3/4$: below this threshold value the Boltzmann-Gibbs equilibrium state is inhomogeneous (magnetized).

In the following, we shall discuss the appearence of QSSs in the HMF setting and review a maximum entropy principle aimed at explaining the behaviour of out-of-equilibrium macroscopic observables. The proposed approach is founded on the observation that in the continuum limit (for an infinite number of particles) the discrete HMF equations converge towards the Vlasov equation, which governs the evolution of the single–particle distribution function (DF). Within this scenario, the QSSs correspond to statistical equilibria of the continuous Vlasov model. As we shall see, the theory allows us to accurately predict out-of-equilibrium phase transitions separating the homogeneous (non-magnetized) and inhomogeneous (magnetized) phases. Special attention is here devoted to characterizing analytically the basin of existence of the homogeneous zone. Concerning the structure of the phase diagram, a bridge between the two possible formal settings, respectively and, is here established.

The paper is organized as follows. In Section 2 we present the continuous Vlasov picture and discuss the maximum entropy scheme. The properties of the homogeneous solution are highlighted in Section 3, where conditions of existence are also derived. Section 4 is devoted to analyze the stability of the homogeneous phase. A detailed account of the phase diagram is provided in Sections 5 and 6, where the case of a “rectangular” and generic water–bag initial distribution are respectively considered. Finally, in Section 7 we sum up and draw our conclusions.
2. On the emergence of quasi-stationary states: Predictions from the Lynden-Bell theory within the Vlasov picture

As previously mentioned, long-range systems can be trapped in long-lasting Quasi-Stationary-States (QSSs), before relaxing to Boltzmann thermal equilibrium. The existence of QSSs was firstly recognized with reference to galactic and cosmological applications (see and references therein) and then, more recently, re-discovered in other fields, e.g. two-dimensional turbulence and plasma-wave interactions. Interestingly, when performing the infinite size limit \( N \to \infty \) before the infinite time limit, \( t \to \infty \), the system remains indefinitely confined in the QSSs. For this reason, QSSs are expected to play a relevant role in systems composed by a large number of particles subject to long-range couplings, where they are likely to constitute the solely experimentally accessible dynamical regimes.

QSSs are also found in the HMF model, as clearly testified in Fig. 1. Here, the magnetization is monitored as a function of time, for two different values of \( N \). The larger the system the longer the intermediate phase where it remains confined before reaching the final equilibrium. In a recent series of papers, an approximate analytical theory based on the Vlasov equation has been proposed which stems from the seminal work of Lynden-Bell. This is a fully predictive approach, justified from first principles, which captures most of the peculiar traits of the HMF out-of-equilibrium dynamics. The philosophy of the proposed approach, as well as the main predictions derived within this framework, are reviewed in the following.

In the limit of \( N \to \infty \), the HMF system can be formally replaced by the following Vlasov equation

\[
\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial \theta} - (M_x[f] \sin \theta - M_y[f] \cos \theta) \frac{\partial f}{\partial p} = 0,
\]

where \( f(\theta, p, t) \) is the one-body microscopic distribution function normalized such that \( M[f] \equiv \int f d\theta dp = 1 \), and the two components of the complex magnetization are respectively given by

\[
M_x[f] = \int f \cos \theta d\theta dp,
\]
\[
M_y[f] = \int f \sin \theta d\theta dp.
\]

The mean field energy can be expressed as

\[
U = \frac{1}{2} \int f p^2 d\theta dp - \frac{M_x^2}{2} + \frac{M_y^2}{2} + \frac{1}{2}.
\]
Fig. 1. Magnetization $M(t)$ as function of time $t$. In both cases, an initial “violent” relaxation toward the QSS regime is displayed. The time series relative to $N = 1000$ (thick full line) converges more rapidly to the Boltzmann equilibrium solution (dashed horizontal line). When the number of simulated particles is increased, $N = 10000$ (thin full line), the relaxation to equilibrium gets slower (the convergence towards the Boltzmann plateau is outside the frame of the figure). Simulations are carried on for a rectangular water–bag initial distribution, see Eq. (13).

Working in this setting, it can be then hypothesized that QSSs correspond to stationary equilibria of the Vlasov equation and hence resort to the pioneering Lynden-Bell’s violent relaxation theory\textsuperscript{17}. The latter was initially devised to investigate the process of galaxy formation via gravitational instability and later on applied to the two-dimensional Euler equation.\textsuperscript{18} The main idea goes as follows. The Vlasov dynamics induces a progressive filamentation of the initial single particle distribution profile, i.e. the continuous counterpart of the discrete N-body distribution, which proceeds at smaller and smaller scales without reaching an equilibrium. Conversely, at a coarse grained level the process comes to an end, and the distribution function $f(\theta, p, t)$, averaged over a finite grid, eventually converges to an asymptotic form. The time evolution of a rectangular water–bag initial distribution is shown in Fig. 2

Following Lynden-Bell, one can associate a mixing entropy to this pro-
cess and calculate the statistical equilibrium by maximizing the entropy, while imposing the conservation of the Vlasov dynamical invariants. More specifically, the above procedure implicitly requires that the system mixes well, in which case, assuming ergodicity (efficient mixing), the QSS predicted by Lynden-Bell, \( \bar{f}_{QSS}(\theta, p, t) \), is obtained by maximizing the mixing entropy. As a side remark, it is also worth emphasising that the prediction of the QSS depends on the details of the initial condition, not only on the value of the mass \( M \) and energy \( U \) as for the Boltzmann statistical equilibrium state. This is due to the fact that the Vlasov equation admits an infinite number of invariants, the Casimirs or, equivalently, the moments \( M_n = \int f^n d\theta dp \) of the fine-grained distribution function. In the following, we shall consider a very simple initial condition where the distribution function takes only two values \( f_0 \) and 0. In that case, the invariants reduce to \( M \) and \( U \) since the moments \( M_{n \geq 1} \) can all be expressed in terms of \( M \) and \( f_0 \) as \( M_n = \int f^n d\theta dp = \int \left( f_0^{n-1} \times f \right) d\theta dp = \int f_0^{n-1} f d\theta dp = f_0^{n-1} M \).

For the specific case at hand, the Lynden-Bell entropy is then explicitly constructed from the coarse-grained DF \( \bar{f} \) and reads...
\[ S[f] = -\int dp d\theta \left[ \frac{\bar{f}}{f_0} \ln \frac{\bar{f}}{f_0} + \left( 1 - \frac{\bar{f}}{f_0} \right) \ln \left( 1 - \frac{\bar{f}}{f_0} \right) \right]. \]  

We thus have to solve the optimization problem

\[ \max_T \{ S[T] \mid U[T] = U, M[T] = 1 \}. \]  

The maximization problem (6) is also a condition of formal nonlinear dynamical stability with respect to the Vlasov equation, according to the refined stability criterion of Ellis \textit{et al.} \cite{Ellis20} (see also Chavanis \cite{Chavanis21}). Therefore, the maximization of \( S \) at fixed \( U \) and \( M \) guarantees (i) that the statistical equilibrium macrostate is stable with respect to the perturbation on the microscopic scale (Lynden-Bell thermodynamical stability) and (ii) that the coarse-grained DF \( \bar{f} \) is stable for the Vlasov equation with respect to macroscopic perturbations (refined formal nonlinear dynamical stability).

We again emphasize that it is only when the initial DF takes two values \( f_0 \) and 0 that the Lynden-Bell entropy can be expressed in terms of the coarse-grained DF \( \bar{f} \), as in Eq. (5). In general, the Lynden-Bell entropy is a functional of the probability distribution of phase levels. \cite{Footnote19} From Eq. (5), we write the first order variations as

\[ \delta S - \beta \delta U - \alpha \delta M = 0, \]

where the inverse temperature \( \beta = 1/T \) and \( \alpha \) are Lagrange multipliers associated with the conservation of energy and mass. Requiring that this entropy is stationary, one obtains the following distribution \cite{Footnote10,Footnote11}

\[ \bar{f}_{QSS}(\theta, p) = \frac{f_0}{1 + e^{\beta (p^2/2 - M_\theta \bar{f}_{QSS} \cos \theta - M_\theta \bar{f}_{QSS} \sin \theta) + \alpha}}. \]

As a general remark, it should be emphasized that the above distribution differs from the Boltzmann-Gibbs one because of the “fermionic” denominator, which in turn arises because of the form of the entropy. Morphologically, this distribution function is similar to the Fermi-Dirac statistics so that several analogies with the quantum mechanics setting are to be expected. Notice also that the magnetization is related to the distribution function by Eq. (3) and the problem hence amounts to solving an integro-differential system. In doing so, we have also to make sure that the critical

\[ \text{The momentum } P = \int f pd\theta dp \text{ is also a conserved quantity but since we look for solutions where the total momentum is zero, the corresponding Lagrange multiplier } \gamma \text{ vanishes trivially}\]  

\cite{Footnote11} so that, for convenience, we can ignore this constraint right from the beginning.
point corresponds to an entropy maximum, not to a minimum or a saddle point. Let us now insert expression (8) into the energy and normalization constraints and use the definition of magnetization (3). Further, defining \( \lambda = e^\alpha \) and \( m = (\cos \theta, \sin \theta) \) yields:

\[
\begin{align*}
\frac{f_0}{\sqrt{2}} \int d\theta I_{-1/2} (\lambda e^{-\beta M} m) & = 1, \\
\frac{f_0}{2} \left( \frac{2}{\beta} \right)^{3/2} \int d\theta I_{1/2} (\lambda e^{-\beta M} m) & = U + \frac{M^2 - 1}{2}, \\
\frac{f_0}{\sqrt{2}} \int d\theta \cos \theta I_{-1/2} (\lambda e^{-\beta M} m) & = M_x, \\
\frac{f_0}{\sqrt{2}} \int d\theta \sin \theta I_{-1/2} (\lambda e^{-\beta M} m) & = M_y,
\end{align*}
\]

where we have defined the Fermi integrals

\[
I_n(t) = \int_0^{+\infty} \frac{x^n}{1+te^x} dx.
\]

We have the asymptotic behaviours for \( t \to 0 \):

\[
I_n(t) \sim \frac{(-\ln t)^{n+1}}{n+1}, \quad (n > -1),
\]

and for \( t \to +\infty \)

\[
I_n(t) \sim \frac{\Gamma(n+1)}{t}, \quad (n > -1).
\]

The magnetization in the QSS, \( M_{\text{QSS}} = M[\bar{f}_{\text{QSS}}] \), and the values of the multipliers are hence obtained by numerically solving the above coupled implicit equations. It should be stressed that multiple local maxima of the entropy are in principle present when solving the variational problem, thus resulting in a rich zoology of phase transitions. This issue has been addressed in\(^{10,11}\) and more recently in,\(^{12}\) to which the following discussion refers to.

It is important to note that, in the two-levels approximation, the Lynden-Bell equilibrium state depends only on two control parameters \((U, f_0)\)\(^b\). This is valid for any initial condition with \( f(\theta, p, t = 0) \in \{0, f_0\} \). This general case will be studied in Section 6 where we describe the phase

\(^b\)These parameters are related to those introduced in\(^{10}\) by \( U = \epsilon/4 + 1/2, \beta = 2\eta, f_0 = \eta_0/N = \mu/(2\pi), k = 2\pi/N, x = \Delta \theta, y = (2/\pi)\Delta p \) and the functions \( F \) in\(^{11}\) are related to the Fermi integrals by \( F_k(1/y) = 2^{(k+1)/2}yI(k-1)/2(y) \).
diagram in the \((f_0, U)\) plane. Now, many numerical simulations of the \(N\)-body system or of the Vlasov equation have been performed starting from a family of rectangular water–bag distributions. The latter correspond to assuming a constant value \(f_0\) inside the phase-space domain \(D\):

\[
D = \{(\theta, p) \in [-\pi, \pi] \times [-\infty, \infty] \mid |\theta| < \Delta \theta, |p| < \Delta p\},
\]

where \(0 \leq \Delta \theta \leq \pi\) and \(\Delta p \geq 0\). The normalization condition results in \(f_0 = 1/(4\Delta \theta \Delta p)\). Notice that, for this specific choice, the initial magnetization \(M_0\) and the energy density \(U\) can be expressed as functions of \(\Delta \theta\) and \(\Delta p\) as

\[
M_0 = \frac{\sin(\Delta \theta)}{\Delta \theta}, \quad U = \frac{(\Delta p)^2}{6} + \frac{1 - (M_0)^2}{2}.
\]

For the case under scrutiny, \(0 \leq M_0 \leq 1\) and \(U \geq U_{MIN}(M_0) \equiv (1-M_0^2)/2\). The variables \((M_0, U)\) are therefore used to specify the initial configuration and hereafter assumed to define the relevant parameters space. This particular but important case will be studied specifically in Section 5 where we illustrate the phase diagram in the \((M_0, U)\) plane for the rectangular water–bag initial condition. Before that, we analytically study the stability of the Lynden-Bell homogeneous phase: two important limits, namely the non degenerate and the completely degenerate ones, are considered. We also discuss the condition for the existence of a homogeneous, non–equilibrium phase.

3. Properties of the homogeneous Lynden-Bell distribution

If we consider spatially homogeneous configurations \((M_QSS = 0)\), the Lynden-Bell distribution becomes

\[
\bar{f}_{QSS}(p) = \frac{f_0}{1 + \lambda e^{\beta p^2/2}}.
\]

Using Eqs. (9), the relation between the inverse temperature \(\beta\) and the energy \(U\) is given in parametric form by

\[
U - \frac{1}{2} = \frac{1}{8\pi^2} \frac{I_{1/2}(\lambda)}{f_0^2 I_{-1/2}(\lambda)^3}, \quad \beta = 8\pi^2 f_0^2 I_{-1/2}(\lambda)^2.
\]

This defines the series of equilibria \(T(U)\) for fixed \(f_0\) parametrized by \(\lambda\) (see Fig. 3 in\(^{10}\)). The stable part of the series of equilibria is the caloric curve. Note that the temperature \(T\) is a Lagrange multiplier associated with the conservation of energy in the variational problem (7). It also has the interpretation of a kinetic temperature in the Fermi-Dirac distribution.
(15). If we start from a water–bag initial condition, recalling that \( f_0 = 1/(4\Delta \theta \Delta p) \) and \( (\Delta p)^2 = 6[U - (1 - M_0^2)/2] \), we can express \( f_0 \) as a function of \( M_0 \) and \( U \) by

\[
f_0^2 = \frac{1}{48[(2U - 1)(\Delta \theta)^2 + \sin^2 \Delta \theta]},
\]

where \( \Delta \theta \) is related to \( M_0 \) by Eq. (14). Inserting this expression in Eqs. (16), we obtain after some algebra the caloric curve \( T(U) \) for fixed \( M_0 \) parametrized by \( \lambda \):

\[
U - \frac{1}{2} = \frac{\sin^2 \Delta \theta}{\frac{\pi^2}{6} I_{-1/2}(\lambda)^3} - 2(\Delta \theta)^2,
\]

\[
\beta = \frac{1}{\sin^2 \Delta \theta} \left( \frac{\pi^2}{6} I_{-1/2}(\lambda)^2 - 2(\Delta \theta)^2 \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)} \right).
\]

Eqs. (16) can be rewritten

\[
(U - \frac{1}{2})8\pi^2 f_0^2 = G(\lambda) \equiv \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)^3},
\]

where \( G(\lambda) \) is a universal function monotonically increasing with \( \lambda \) (see Fig. 2 of\(^{10}\)). A solution of the above equation certainly exists provided:

\[
(U - \frac{1}{2})8\pi^2 f_0^2 \geq G(0).
\]

To compute \( G(0) \) we use the asymptotic expansions (11) and (12) of the Fermi integrals. This yields \( G(0) = 1/12 \). Therefore, the homogeneous Lynden-Bell distribution with fixed \( f_0 \) exists only for:\(^{10}\)

\[
U \geq U_{\text{min}}(f_0) \equiv \frac{1}{96\pi^2 f_0^2} + \frac{1}{2}.
\]

For the rectangular water–bag initial condition, using Eqs. (17) and (21), we here find that the homogeneous Lynden-Bell distribution with fixed \( M_0 \) exists only for:

\[
U \geq U_{\text{min}}(M_0) \equiv \frac{1}{2} \left( \frac{\sin^2 \Delta \theta}{\pi^2 - (\Delta \theta)^2} + 1 \right).
\]

This result can also be obtained from Eq. (18) by taking the limit \( \lambda \to 0 \).

Let us now describe more precisely the asymptotic limits of the Fermi-Dirac distribution (see Fig. 3):

**Non degenerate limit:** In the limit \( \lambda \to +\infty \), the Lynden-Bell distribution reduces to the Maxwell-Boltzmann distribution

\[
\mathcal{f}_{QSS}(p) = \left( \frac{\beta}{2\pi} \right)^{1/2} e^{-\beta p^2/2}.
\]
Fig. 3. Spatially homogeneous Lynden-Bell distribution function for increasing values of $\lambda$ (top to bottom). For $\lambda = 0$, the distribution reduces to a step function (completely degenerate) and for $\lambda \to +\infty$, it becomes equivalent to the Maxwell-Boltzmann distribution (non degenerate). In the figure, we have taken $f_0 = 0.13$ and $\beta$ has been calculated from Eq. (16).

Since $f \ll f_0$, this corresponds to a dilute limit (or to a non degenerate limit if we use the terminology of quantum mechanics). The non degenerate limit corresponds, for a given value of $f_0$, to $\lambda \to +\infty$, $\beta \to 0$ and $U \to +\infty$. For $f_0 \to +\infty$, we are always in the non degenerate limit, for any $\beta$ and $U$. In that case, the caloric curve takes the “classical” expression

$$ U = \frac{1}{2\beta} + \frac{1}{2}, \quad (24) $$

a relation that can be directly obtained from Eq. (23). For the water–bag initial condition, the non degenerate limit $\lambda \to +\infty$ corresponds, for a given $M_0$, to $U \to +\infty$. The non degenerate limit $f_0 \to +\infty$ corresponds to $\Delta \theta = 0$ leading to $M_0 = 1$ for any $U^c$. In the non degenerate limit, the

\footnote{It also corresponds to $\Delta \rho = 0$ leading to $U = U_{MIN}(M_0)$ for any $M_0$. However, in that case the homogeneous phase does not exist since $U_{MIN}(M_0) \leq U_{min}(M_0)$ so this case will not be considered here.}
Lynden-Bell statistical equilibrium state describing the QSS has the same structure as the Boltzmann distribution describing the collisional statistical equilibrium state (but with, of course, a completely different interpretation).

**Completely degenerate limit:** In the limit \( \lambda \to 0 \), the Lynden-Bell distribution (15) reduces to the Heaviside function

\[
\mathcal{f}_{QSS}(p) = \begin{cases} 
  f_0 & (p < p_F), \\
  0 & (p \geq p_F),
\end{cases}
\]  

(25)

where

\[ p_F = \frac{1}{4\pi f_0}, \]  

(26)

is a maximum velocity. The distribution (25) is similar to the Fermi distribution in quantum mechanics and \( p_F \) is similar to the Fermi velocity. Thus, the limit \( \lambda \to 0 \) corresponds to a completely degenerate limit in the quantum mechanics terminology. The completely degenerate limit corresponds to \( \lambda \to 0, \beta \to +\infty \) and \( U \to U_{\text{min}}(f_0) \) given by (21). This result can be directly obtained from Eq. (25). This is the minimum energy of the homogeneous Lynden-Bell distribution for a fixed \( f_0 \). This is also the minimum energy of any homogeneous distribution with \( f \in \{0, f_0\} \). It corresponds to a water–bag initial condition with zero magnetization \( M_0 = 0 \). If we start from a water bag initial condition, the completely degenerate limit corresponds to \( M_0 = 0 \) for any \( U \) and to \( U = U_{\text{min}}(M_0) \) for any \( M_0 \). A stable water–bag initial condition with \( M_0 = 0 \) is a maximum Lynden-Bell entropy state, so it does not mix at all.

In conclusion, we have in the general case, using the \((U, f_0)\) variables:

- **non degenerate limit**
  - \( U \to +\infty \) for any \( f_0 \)
  - \( f_0 \to +\infty \) for any \( U \)

- **completely degenerate limit**
  - \( U = U_{\text{min}}(f_0) \) for any \( f_0 \)

For the water–bag initial condition, using the \((U, M_0)\) variables, we have:

- **non degenerate limit**
  - \( U \to +\infty \) for any \( M_0 \)
  - \( M_0 = 1 \) for any \( U \)

- **completely degenerate limit**
\( - \ M_0 = 0 \) for any \( U \)
\( - \ U = U_{\text{min}}(M_0) \) for any \( M_0 \)

4. Stability of the Lynden-Bell homogeneous phase

We have seen that the maximization problem (6) provides a condition of thermodynamical stability (in Lynden-Bell’s sense) and a condition of nonlinear dynamical stability with respect to the Vlasov equation. We thus have to select the maximum of \( S \) at fixed \( U, \ M \). Indeed, a saddle point of \( S \) is unstable and cannot be obtained as a result of a violent relaxation. Let us consider the minimization problem

\[
\min \{ F[\mathcal{f}] = U[\mathcal{f}] - T S[\mathcal{f}] \mid \mathcal{M}[\mathcal{f}] = 1 \}. \tag{27}
\]

The criterion (6) can be viewed as a criterion of microcanonical stability and the criterion (27) as a criterion of canonical stability where \( F \) is interpreted as a free energy. Quite generally, the solutions of (27) are solutions of (6) but the reciprocal is wrong in case of ensemble inequivalence. Therefore, in the general case, criterion (27) forms a sufficient (but not necessary) condition of thermodynamical and formal nonlinear dynamical stability. In the present case, it can be shown that, if we restrict ourselves to spatially homogeneous solutions \(^d\), the ensembles are equivalent so that the set of solutions of (27) coincides with the set of solutions of (6). Therefore, considering homogeneous states, criterion (27) forms a necessary and sufficient condition of thermodynamical and formal nonlinear dynamical stability. We shall therefore consider in the following the minimization problem (27), which has been studied in\(^9,22\) for general functionals of the form

\[
S[f] = - \int C(f) d\theta dp
\]
where \( C \) is a convex function. A simple stability criterion has been obtained in the case where the steady state is spatially homogeneous, which can be expressed in terms of the distribution function as:

\[
1 + \pi \int_{-\infty}^{+\infty} \frac{f'(p)}{p} dp \geq 0. \tag{28}
\]

It was shown in\(^9\) that the same criterion can be expressed simply in terms of the density as

\[
c_s^2 \geq \frac{1}{2}, \tag{29}
\]

\(^d\)Concerning spatially inhomogeneous solutions, the microcanonical and canonical ensembles are not equivalent in the region of first order phase transition. This important point will be further developed in a future contribution.
where $c_s^2 = p'(\rho)$ is the velocity of sound in the corresponding barotropic gas. The equivalence between the criteria (28) and (29) is proven in. In this Section, we apply these criteria to the Lynden-Bell distribution (15). It is shown in that the criteria (28) and (29) can be rewritten:

$$I - \frac{1}{2} \left( \lambda I' - \frac{1}{2} \left( \lambda \right) \right) | \leq \frac{1}{(2\pi f_0)^2}. \quad (30)$$

If the DF satisfies $(30) \leftrightarrow (28) \leftrightarrow (29)$, then it is (i) Lynden-Bell thermodynamically stable (ii) formally nonlinearly dynamically stable. Otherwise, it is (i) Lynden-Bell thermodynamically unstable (ii) linearly dynamically unstable. For given $f_0$, the relation (30) determines the range of $\lambda$ for which the homogeneous distribution is stable/unstable. Then, using Eqs. (16), we can determine the range of corresponding energies. Specifically, the critical curve $U_c(f_0)$ separating stable and unstable homogeneous Lynden-Bell distributions is given by the parametric equations:

$$I - \frac{1}{2} \left( \lambda I' - \frac{1}{2} \left( \lambda \right) \right) = \frac{1}{(2\pi f_0)^2}, \quad U - \frac{1}{2} = \frac{1}{8\pi^2 f_0^2} \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)^{3}} \quad (31)$$

where $\lambda$ goes from 0 (completely degenerate) to $+\infty$ (non degenerate). This leads to the phase diagram reported in Fig. 6. In fact, the criteria (28) and (29) only prove that $f$ is a local entropy maximum at fixed mass and energy. If several local entropy maxima are found, we must compare their entropies to determine the stable state (global entropy maximum) and the metastable states (secondary entropy maxima). For systems with long-range interactions, metastable states have in general very long lifetimes, scaling like $e^N$, so that they are stable in practice and must absolutely be taken into account.

For $f_0 \to +\infty$, we are in the non degenerate limit $\lambda \to +\infty$ and the stability criterion (30) for the homogeneous phase becomes

$$U \geq U_c = \frac{3}{4}. \quad (32)$$

This returns the well-known nonlinear dynamical stability criterion (with respect to the Vlasov equation) of a homogeneous system with Maxwellian distribution function (see, e.g., [9,22]). This also coincides with the ordinary thermodynamical stability criterion applying to the collisional regime, for $t \to +\infty$, where the statistical equilibrium state is the Boltzmann distribution for $f$ (without the bar!). On the curve $U = U_{\text{min}}(f_0)$, we are in the completely degenerate limit
\[ \lambda \to 0 \text{ and the stability criterion (30) for the homogeneous phase becomes} \]

\[ f_0 \leq (f_0)_c = \frac{1}{2\pi \sqrt{2}}, \quad i.e. \quad U \geq U_c = \frac{7}{12}. \quad (33) \]

This is the well-known nonlinear dynamical stability criterion (with respect to the Vlasov equation) of the water–bag distribution (see, e.g., \cite{9,22}).

If we start from a rectangular water–bag initial condition and use the \((U, M_0)\) variables, we must express \(f_0\) in terms of \(U\) and \(M_0\) using Eq. (17). Then, the critical curve \(U_c(M_0)\) separating stable and unstable homogeneous Lynden-Bell distributions is given by the parametric equations

\[ I_{-1/2}(\lambda) |I_{-1/2}^L(\lambda)| = \frac{1}{(2f_0)^2}, \quad U - \frac{1}{2} = \frac{1}{8\pi^2 f_0^2} \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)^3}, \quad (34) \]

\[ f_0^2 = \frac{1}{48[(2U-1)(\Delta \theta)^2 + \sin^2 \Delta \theta]}, \quad M_0 = \frac{\sin(\Delta \theta)}{\Delta \theta}, \quad (35) \]

where \(\lambda\) goes from 0 (completely degenerate) to \(+\infty\) (non degenerate). This leads to the phase diagram reported in Fig. 4. For \(M_0 = 1\), we get \(\lambda \to +\infty\) so we are in the non degenerate limit and the critical energy is \(U_c = 3/4\). For \(M_0 = 0\), we get \(\lambda = 0\) so we are in the completely degenerate limit and the critical energy is \(U_c = 7/12\).

5. The rectangular water–bag initial condition: phase diagram in the \((M_0, U)\) plane

We first comment on the structure of the phase diagram in the \((M_0, U)\) plane when we start from a water–bag initial condition. In Fig. 4 the transition line \(U_c(M_0)\) divides the region of the plane where a homogeneous \((M_{QSS} = 0)\) state is predicted to occur (upper area), from that (lower area) associated to a non-homogeneous phase \((M_{QSS} \neq 0)\). Along the transition line two distinct segments can be isolated: the dashed line corresponds to a second order phase transition, the full line refers to a first order phase transition. First and second transition lines merge together at a tricritical point, approximately located at \((M_0, U) = (0.17, 0.61)\). The lateral edges of the metastability region associated to the first order transition line are also reported in the inset of Fig. 4.

The correctness of the above analysis is assessed in \cite{12} where numerical simulations of the HMF model (1) are performed for different values of the system size \(N\). The transition predicted in the realm of Lynden Bell’s theory are indeed numerically observed, thus confirming the adequacy of the
Fig. 4. Theoretical phase diagram in the control parameter plane \((M_0, U)\) for a rectangular water–bag initial profile. The dashed line \(U_c(M_0)\) stands for the second order phase transition, while its continuation as a full line refers to the first order phase transition. The full dot is the tricritical point. The region below the thick full line \(U_{MIN}(M_0)\) corresponds to the forbidden domain of the parameter space. The region of existence of the homogeneous solution is delimited from below by the thin full line \(U_{min}(M_0)\) (see Eq. (22)). Inset: zoom of the first order transition region. Dash-dotted lines represent the limits of the metastability region. In region (II), delimited from above by the upper dash-dotted line and from below by the full line, the homogeneous phase is fully stable and the inhomogeneous phase is metastable. In region (III), located below the full line and above the lower dash-dotted line, the homogeneous phase is metastable and the inhomogeneous phase is fully stable. These labels will appear again in Fig. 8, in connection with the discussion of the general case.

proposed interpretative scenario. Moreover, the coexistence of homogeneous and inhomogeneous phases, corresponding to different local maxima of the entropy, is also reported in\(^{12}\) where the probability distribution function of \(\hat{M}\) is reconstructed.

For all values of the energy larger than \(U_c(M_0)\) (where the homogeneous phase is stable), the systems can potentially encounter a homogeneous quasi-stationary phase which slows down the approach to the thermodynamic equilibrium. Notice that above \(U_c = 0.75\), the equilibrium value of the magnetization is also zero: there is hence no macroscopic transition
for \( M(t) \) of the type displayed in Fig. 1. One has therefore to rely on other, quantitative, indicators to monitor the dynamical state of the system,\(^{25}\) and eventually assess the presence of a QSS. This explains why in the past QSSs regimes where believed to be localized only in specific energy windows below the critical threshold \( U_c \). Significant deviations from equilibrium are instead detected even for \( U > U_c \), as reported in Fig. 5. Single particle velocity distributions reconstructed from direct \( N \)--body simulations at \( U = 0.85 \) display a bumpy profile, analogous to the one discussed in\(^{11}\) for the reference energy \( U = 0.69 < U_c \). Interestingly, for specific choices of the initial magnetization, the two bumps are even more pronounced than those analyzed in.\(^{11}\) The presence of these bumps shows that relaxation is incomplete. These bumps correspond to the “vortices” (or phase space clumps) visible in Fig. 2. This state is stationary for the Vlasov equation, but Quasi-Stationary for the \( N \)-body simulation. Hence, in the long run, the two “vortices” will merge, due to finite \( N \) effects, as the HMF system proceeds towards Boltzmann-Gibbs equilibrium.

![Probability distribution function of velocities](image)

Fig. 5. Probability distribution function of velocities \( f(p) \), for \( U=0.85 \) and different initial magnetization, as reported in the legend of each panel.
6. The general case: phase diagram in the \((f_0, U)\) plane

In the two-levels approximation, the Lynden-Bell equilibrium state depends only on two control parameters \((U, f_0)\). This is valid for any initial condition with \(f(\theta, p, t = 0) \in \{0, f_0\}\), whatever the number of patches and their shape. The variables \((U, M_0)\) used in the previous section are valid only for a rectangular water–bag configuration. Furthermore, we note that two configurations with different values of \((U, M_0)\) in a rectangular water–bag configuration can correspond to the same values of \((U, f_0)\), hence to the same Lynden-Bell equilibrium state. To avoid any redundancy, it is preferable to use the general variables \((U, f_0)\). Therefore, in the following, we shall discuss the general phase diagram in the \((U, f_0)\) plane and compare it with the one in the \((U, M_0)\) plane for the rectangular water–bag assumption.\(^{12}\)

The stability diagram of the homogeneous Lynden-Bell distribution \((15)\) is plotted in Fig. 6 in the \((f_0, U)\) plane. The representative curve \(U_c(f_0)\) marks the separation between the stable (maximum entropy states) and the unstable (saddle points of entropy) regions. We have also plotted the minimum accessible energy for the homogeneous phase \(U_{\text{min}}(f_0)\). Here, the term “unstable” means that the homogeneous Lynden-Bell distribution is not a maximum entropy state, i.e. (i) it is not the most mixed state (ii) it is dynamically unstable with respect to the Vlasov equation. Hence, it should not be reached as a result of violent relaxation. One possibility is that the system converges to the spatially inhomogeneous Lynden-Bell distribution \((15)\) with \(M_{\text{QSS}} \neq 0\) which is the maximum entropy state (most mixed) in that case. Another possibility, always to consider, is that the system does not converge towards the maximum entropy state, i.e. the relaxation is incomplete.\(^{26}\)

Let us enumerate some properties of the \((f_0, U)\) phase diagram of Fig. 6. For \(U > U_c = 3/4\) (supercritical energies), the homogeneous phase is always stable (maximum entropy state) for any \(f_0\) (recall that the curve \(U_c(f_0) \to 3/4\) for \(f_0 \to +\infty\)). On the other hand, there exists a critical point (we shall see later that it corresponds to the tricritical point of Fig. 4) located at

\[
(f_0)_* = 0.10947..., \quad U_* = 0.608...
\]  

(36)

For \(f_0 < (f_0)_*\), the homogeneous phase is always stable (maximum entropy state) for any \(U \geq U_{\text{min}}(f_0)\). For \(f_0 > (f_0)_c\), the homogeneous phase is stable for \(U > U_c(f_0)\) and unstable for \(U_{\text{min}}(f_0) \leq U < U_c(f_0)\). This range of parameters corresponds to a second order phase transition. For \((f_0)_* < f_0 < (f_0)_c\), there is an interesting regime with a “re-entrant” phase\(^{27}\).
The homogeneous phase is stable for $U > U_c^{(2)}(f_0)$, unstable for $U_c^{(2)}(f_0) > U > U_c^{(1)}(f_0)$ and stable again for $U_c^{(1)}(f_0) > U \geq U_{\text{min}}(f_0)$. This range of parameters corresponds to a first order phase transition.

To make the connection between the phase diagram $(f_0, U)$ obtained in\(^{10}\) and the phase diagram $(M_0, U)$ obtained in\(^{12}\) we can plot the iso-$M_0$ lines in the $(f_0, U)$ phase diagram. If we fix the initial magnetization $M_0$, or equivalently if we fix the parameter $\Delta \theta$, the relation between the energy $U$ and $f_0$ is

$$U_{\Delta \theta}(f_0) = \frac{1}{6(4\Delta \theta f_0)^2} - \frac{1}{2} \left( \frac{\sin \Delta \theta}{\Delta \theta} \right)^2 + \frac{1}{2}.$$  \hspace{1cm} (37)

Therefore, the iso-$M_0$ lines are of the form

$$U_{\Delta \theta}(f_0) = \frac{A(\Delta \theta)}{f_0^2} - B(\Delta \theta),$$  \hspace{1cm} (38)
Fig. 7. Iso-$M_0$ lines in the $(f_0, U)$ phase diagram. This graphical construction allows one to make the connection between the $(f_0, U)$ phase diagram of Fig. 6 and the $(M_0, U)$ phase diagram of Fig. 4. We can vary the energy at fixed initial magnetization by following a dashed line. The intersection between the dashed line and the curve $U_{\text{min}}(f_0)$ determines the minimum energy $U_{\text{min}}(M_0)$ of the homogeneous phase. The intersection between the dashed line and the curve $U_c(f_0)$ determines the energy $U_c(M_0)$ below which the homogeneous phase becomes unstable.

with $A(\Delta \theta) = \frac{1}{6(4\Delta \theta)^2}$ and $B(\Delta \theta) = \frac{1}{2} \left( \frac{\sin \Delta \theta}{\Delta \theta} \right)^2 - \frac{1}{2}$, which are easily represented in the $(f_0, U)$ phase diagram (see Fig. 7). As an immediate consequence of this geometrical construction, we can recover the minimum energy of the homogeneous phase for a fixed initial magnetization $M_0$ (or $\Delta \theta$). Indeed, for a given $\Delta \theta$, the homogeneous phase exists iff $U_{\Delta \theta}(f_0) \geq U_{\text{min}}(f_0)$ leading to

$$f_0^2 \leq (f_0^2)^2_{\Delta \theta} = \frac{\pi^2 - (\Delta \theta)^2}{48\pi^2 \sin^2 \Delta \theta}.$$  \hspace{1cm} (39)

This corresponds to $U \geq U_{\text{min}}(M_0) = U_{\Delta \theta}(f_0)_{\Delta \theta}$ leading to

$$U \geq U_{\text{min}}(M_0) = \frac{1}{2} \left( \frac{\sin^2 \Delta \theta}{\pi^2 - (\Delta \theta)^2} + 1 \right),$$ \hspace{1cm} (40)
Fig. 8. Zones of metastability in the \((f_0, U)\) phase diagram. In region (I), the homogeneous phase is fully stable and the inhomogeneous phase is inexist. In region (II) the homogeneous phase is fully stable and the inhomogeneous phase is metastable. In region (III) the homogeneous phase is metastable and the inhomogeneous phase is stable. In region (IV) the homogeneous phase is unstable and the inhomogeneous phase is fully stable. The three curves separating these regions connect themselves at the tricritical point. In region (V) the homogeneous phase is nonexistent. The corresponding caloric curves as well as the absolute minimum energy \(U_{MIN}(f_0)\) of the inhomogeneous phase will be determined in a future contribution.

which is identical to (22). Note again that \(\Delta \theta\) is related to \(M_0\) by Eq. (14). Figure 7 is in good agreement with the structure of the phase diagram in the \((U, M_0)\) plane. Indeed, along an iso-\(M_0\) line, we find that for large energies \(U > U_c(M_0)\) the homogeneous phase is stable and for low energies \(U < U_c(M_0)\) the homogeneous phase becomes unstable. In that case, there is no re-entrant phase.

In,\(^{10}\) only the stability of the homogeneous phase has been studied, i.e. whether it is an entropy maximum at fixed mass and energy or not. The question of its metastability, i.e. whether it is a local entropy maximum with respect to the inhomogeneous phase, has not been considered. However, considering Fig. 7 and comparing with the results of,\(^{12}\) we conclude that
there must exist zones of metastability in the \((f_0, U)\) phase diagram. They have been represented in Fig. 8. In region (I) the inhomogeneous phase does not exist while the homogeneous phase is fully stable. In region (II), the inhomogeneous phase appears but is metastable while the homogeneous phase is fully stable. In region (III), the inhomogeneous phase becomes fully stable while the homogeneous phase becomes metastable. In region (IV), the homogeneous phase becomes unstable while the inhomogeneous phase is fully stable. The three curves separating these regions connect themselves at a tricritical point. This is clearly the same as in Fig. 4. Using Eqs. (36), (37), (14) we find that it corresponds to

\[
U_* = 0.608..., \quad (M_0)_* = 0.1757...
\]

with \(\Delta \theta_* = 2.656\). Therefore, the phase diagrams in \((f_0, U)\) and \((M_0, U)\) planes are fully consistent. Note, however, that the physics is different whether we vary the energy at fixed \(f_0\) or at fixed \(M_0\). In particular, there is no “re-entrant” phase when we vary the energy at fixed \(M_0\) while a “re-entrant” phase appears when we vary the energy at fixed \(f_0\).

7. Conclusions

In this paper, we have discussed the emergence of out-of-equilibrium Quasi Stationary States (QSSs) in the Hamiltonian Mean Field (HMF) model, a paradigmatic representative of systems with long-range interactions. The analysis refers to a special class of initial conditions in which particles are uniformly occupying a finite portion of phase space and the distribution function takes only two values, respectively 0 and \(f_0\). The energy can be independently fixed to the value \(U\).

The Lynden-Bell maximum entropy principle is here reviewed and shown to result in a rich out-of-equilibrium phase diagram, which is conveniently depicted in the reference plane \((f_0, U)\). When considering a rectangular water–bag distribution the concept of initial magnetization, \(M_0\), naturally arises as a control parameter and the different QSSs phases can be represented in the alternative space \((M_0, U)\). In both settings first and second order phase transitions are found, which merge together in a tricritical point. These findings have been tested versus numerical simulation in, where the adequacy of Lynden-Bell theory was confirmed.

A formal correspondence between the two above scenarios is here drawn and their equivalence discussed. It is worth mentioning that swapping from one parametric representation to the other allows us to put the focus on intriguingly different physical mechanisms, as it is the case of the “re-entrant”
phases discussed in Section 6.

Further, in this paper, we have provided an analytical characterization of the domain of existence of the Lynden-Bell spatially homogenous phase and investigated its stability. Homogeneous QSS are also expected to occur for $U > U_c = 3/4$, a claim here supported by dedicated numerical simulations.

Despite the fact that Lynden-Bell’s theory results in an accurate tool to explain the peculiar traits of QSSs in HMF dynamics, one should be aware of the limitations which are intrinsic to this approach. Most importantly, Lynden-Bell’s recipe assumes that the system mixes well so that the hypothesis of **ergodicity**, which motivates the statistical theory (maximization of the entropy), applies. Unfortunately, this is not true in general. Several example of **incomplete** violent relaxation have been identified in stellar dynamics and 2D turbulence (see some references in\(^{26}\)) for which the QSSs cannot be exactly described in term of a Lynden-Bell distribution. Also in this case, however, the QSSs are stable stationary solution of the Vlasov equation and novel analytical strategies are to be eventually devised which make contact with the underlying Vlasov framework.

**Acknowledgements:**

D.F. and S.R. wish to thank A. Antoniazzi, F. Califano and Y. Yamaguchi for useful discussions and long-lasting collaboration. This work is funded by the PRIN05 grant *Dynamics and thermodynamics of systems with long-range interactions*.

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