Out-of-equilibrium phase re-entrance(s) in long-range interacting systems

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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. The application of Lynden-Bell’s theory of “violent relaxation” to the Hamiltonian Mean Field model leads to the prediction of out-of-equilibrium first and second order phase transitions between homogeneous (zero magnetization) and inhomogeneous (non-zero magnetization) QSSs, as well as an interesting phenomenon of phase re-entrances. We compare these theoretical predictions with direct $N$-body numerical simulations.

We confirm the existence of phase re-entrance in the typical parameter range predicted from Lynden-Bell’s theory, but also show that the picture is more complicated than initially thought. In particular, we exhibit the existence of secondary re-entrant phases: we find un-magnetized states in the theoretically magnetized region as well as persisting magnetized states in the theoretically unmagnetized region.

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I. INTRODUCTION

In statistical physics, phase re-entrance is a quite typical phenomenon occurring in many physical systems, such as spin-glasses, colloids and polymers, in which there is a competition between different entropic terms \[1, 2, 3, 4, 5, 6\]. A phase re-entrance is normally associated with inverse melting, a counterintuitive phenomenon in which isobaric addition of heat causes a disordered (e.g., liquid) phase to crystallize, the reverse of the usual situation. Phase re-entrance occurs when, providing additional heating to the system, the latter undergoes a new transition, from the ordered to the disordered phase. The phenomenon of phase re-entrance has been widely studied at thermodynamic equilibrium in systems whose constituents interact through short-range forces.

In this paper we give evidence to the existence of phase re-entrance also in the case of long-range interacting systems in out-of-equilibrium dynamical conditions.

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 these systems were poorly understood until a few years ago, and their study was essentially restricted to astrophysics (stellar systems) and two-dimensional turbulence (large-scale vortices) \[5\]. Later, it was recognized that long-range systems exhibit universal, albeit unconventional, equilibrium and out-of-equilibrium features \[6\]. It is for instance well known that such systems get trapped in long-lasting Quasi-Stationary States (QSS) \[5, 10, 11, 12, 13, 14, 15, 16\], before relaxing to thermal equilibrium. The duration of a QSS increases with the number of particles $N$ in the system. Remarkably, when the thermodynamic limit ($N \to \infty$) is performed before the infinite time limit ($t \to +\infty$), the system remains permanently trapped in QSSs. As a consequence, QSSs represent the only accessible experimental dynamical regimes for systems composed by a large number of long-range interacting particles. This includes systems of paramount importance, such as non-neutral plasmas confined by a strong magnetic field \[17, 18\], free-electron lasers \[19\] and ion particle beams \[20\]. The ubiquity of QSSs has originated an intense debate \[21\] about the mechanisms responsible for their emergence, their persistence, and their eventual evolution towards statistical equilibrium. In fact, QSSs keep memory of the initial condition and, as a consequence, they cannot be interpreted by making use of the classical Boltzmann-Gibbs approach.

In a series of recent papers \[22, 23, 24, 25, 26\], an approximate analytical theory based on the Vlasov equation and inspired by a seminal work of Lynden-Bell \[27\] in astrophysics has been proposed. This is a fully predictive approach, enabling one to explain the emergence and the
The Hamiltonian reads
\[ H = \frac{1}{2} \sum_{j=1}^{N} p_j^2 + \frac{1}{2N} \sum_{i,j=1}^{N} (1 - \cos(\theta_j - \theta_i)) \]
(1)
where \( \theta_j \) represents the orientation of the \( j \)-th rotator and \( p_j \) stands for its conjugated momentum. To monitor the evolution of the systems it is customary to introduce the magnetization, an order parameter defined as
\[ M = \frac{1}{N} \sum_i m_i \] where \( m_i = (\cos \theta_i, \sin \theta_i) \).
(2)

The infinite-range coupling between rotators, provides the system with all typical characteristics of a long-range system, as clearly displayed in Fig. 1. Here, the magnetization is monitored as a function of time: after an initial "violent" relaxation, the system reaches a QSS, which is followed by a slow relaxation towards Boltzmann equilibrium (thick line). Simulations are performed starting from a two-body distribution with energy \( U = 0.6400 \), and averaging over different system realizations with the same initial distribution (50, 100, 200, 500 and 1000, respectively).

In this paper we utilize a well-known hamiltonian toy model, the so-called Hamiltonian Mean Field (HMF) model\(^\text{[28]}\), to demonstrate that phase re-entrance(s) may also occur in a long-range interacting system, dynamically trapped in a QSS. The HMF describes the motion of \( N \) rotators, coupled through an equal strength cosine interaction. The Hamiltonian reads

\[ H = \frac{1}{2} \sum_{j=1}^{N} p_j^2 + \frac{1}{2N} \sum_{i,j=1}^{N} [1 - \cos(\theta_j - \theta_i)] \]
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In the limit of \( N \to \infty \), the HMF dynamics can be formally described using the Vlasov equation
\[ \frac{\partial f}{\partial t} + p \frac{\partial f}{\partial \theta} - (M_x[f] \sin \theta - M_y[f] \cos \theta) \frac{\partial f}{\partial p} = 0, \]
(3)
where \( f(\theta, p, t) \) is the one-body microscopic distribution function (DF), and the two components of the magnetization are respectively given by
\[ M_x[f] = \int f \cos \theta d\theta dp, \]
(4)
\[ M_y[f] = \int f \sin \theta d\theta dp. \]
(5)

The mean field energy can be expressed as
\[ U = \frac{1}{2} \int f p^2 d\theta dp - \frac{M_x^2 + M_y^2}{2} + \frac{1}{2}. \]

Working in this setting, it can be then hypothesized that QSSs correspond to stable stationary equilibria of the Vlasov equation on a coarse-grained scale. Lynden-Bell’s 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 \( f_{QSS}(\theta, p, t) \), averaged over a finite grid, eventually converges to an asymptotic form. Following Lynden-Bell, one can then associate a mixing entropy to this process. Assuming ergodicity (i.e., efficient mixing), \( f_{QSS}(\theta, p) \), is obtained by maximizing the mixing entropy, while imposing the conservation of
Vlasov dynamical invariants. It is worth emphasizing that the prediction of the QSS depends on the details of the initial condition \[30\], not only on the values of energy and mass as for the Boltzmann statistical equilibrium state. This is due to the fact that the Vlasov equation admits an infinite number of invariants, i.e. the Casimirs or, equivalently, the moments \( \mathcal{M}_n = \int \! f d\theta dp \) of the fine-grained distribution function. The first moment \( \mathcal{M}_1 = \mathcal{M} \) is just the normalization of the distribution function, and we can refer to it as the conservation of the total mass.

In the case of a two-levels initial condition, where the fine-grained DF takes only two values \( f = f_0 \) and \( f = 0 \), the invariants reduce to \( \mathcal{M} \) and \( f_0 \), since the moments \( \mathcal{M}_n > 1 \) can all be expressed in terms of \( \mathcal{M} \) and \( f_0 \) as \( \mathcal{M}_n = \int \! f^{n-1} \! d\theta dp = \int \! f_0^{n-1} \! d\theta dp = f_0^{n-1} \mathcal{M} \). For the specific case at hand, the Lynden-Bell entropy is then explicitly constructed from the coarse-grained distribution function \( \bar{f} \) and reads \[22, 31\]:

\[
S[\bar{f}] = - \int \! dpd\theta \left[ \frac{\bar{f}}{f_0} \ln \frac{\bar{f}}{f_0} + \left( 1 - \frac{\bar{f}}{f_0} \right) \ln \left( 1 - \frac{\bar{f}}{f_0} \right) \right].
\]

We thus have to solve the maximization problem

\[
\max_{\bar{f}} \{ S[\bar{f}] \mid U[\bar{f}] = U, \mathcal{M}[\bar{f}] = 1 \}. \tag{6}
\]

This maximization problem assures that the distribution function is thermodynamically stable (most probable macrostate) in the sense of Lynden-Bell \[22\]. The maximization problem \[7\], for an arbitrary functional of the form \( S[\bar{f}] = - \int \! C(\bar{f}) \! d\theta dp \) where \( C \) is convex, also forms a criterion of formal nonlinear dynamical stability with respect to the Vlasov equation \[32\]. In the two levels approximation, where the Lynden-Bell entropy is a functional of \( \bar{f} \), the criteria of dynamical and Lynden-Bell thermodynamical stability coincide. From Eq. \[6\], we write the first order variations as

\[
\delta S - \beta \delta U - \alpha \delta \mathcal{M} = 0, \tag{8}
\]

where the inverse temperature \( \beta = 1/T \) and the “chemical potential” \( \alpha \) are Lagrange multipliers associated to the conservation of energy and mass. Requiring that this functional is stationary, one obtains the following distribution \[22, 24\]:

\[
\bar{f}_{\text{QSS}}(\theta, p) = \frac{f_0}{1 + e^{\beta(p^2/2 - M_x[\bar{f}_{\text{QSS}}] \cos \theta - M_y[\bar{f}_{\text{QSS}}] \sin \theta)}} + \alpha. \tag{9}
\]

As a general remark, it should be emphasized the “fermionic” form of the distribution, which arises because of the form of the entropy. Notice also that the magnetization is related self-consistently to the distribution function by Eq. \[14\], and the problem hence amounts to solving an integro-differential equation. In doing so, we have also to make sure that the critical point corresponds to an entropy maximum, not to a minimum or a saddle point. Let us now insert expression \[9\] into the energy and normalization constraints and use the definition of magnetization \[4\]. Further, defining \( \lambda = e^\alpha \) and \( \mathbf{m} = (\cos \theta, \sin \theta) \) yields \[38\]:

\[
\begin{align*}
 f_0 \sqrt{\frac{2}{\beta}} \int \! d\theta I_{-1/2}(\lambda e^{-\beta M_\mathbf{m}}) &= 1, \quad (10) \\
 f_0 \frac{1}{2} \left( \frac{2}{\beta} \right)^{3/2} \int \! d\theta I_{1/2}(\lambda e^{-\beta M_\mathbf{m}}) &= U + \frac{M^2 - 1}{2}, \\
 f_0 \sqrt{\frac{2}{\beta}} \int \! d\theta \cos \theta I_{-1/2}(\lambda e^{-\beta M_\mathbf{m}}) &= M_x, \\
 f_0 \sqrt{\frac{2}{\beta}} \int \! d\theta \sin \theta I_{-1/2}(\lambda e^{-\beta M_\mathbf{m}}) &= M_y,
\end{align*}
\]

where we have defined the Fermi integrals

\[
I_n(t) = \int_0^{\infty} \frac{x^n}{1 + e^{\beta x}} \! dx. \tag{11}
\]

Its asymptotic limits are recalled in \[22\].

If we consider spatially homogeneous configurations \( \mathcal{M}_{\text{QSS}} = 0 \), the Lynden-Bell distribution becomes

\[
\bar{f}_{\text{QSS}}(p) = \frac{f_0}{1 + e^{\beta p^2/2}}. \tag{12}
\]

In the non degenerate limit \( \lambda \to +\infty \), the latter reduces to the Boltzmann distribution \( \bar{f} = (\beta/2\pi)^{1/2}e^{-\beta p^2/2} \) and in the completely degenerate limit \( \lambda \to 0 \), it becomes a step function: \( \bar{f} = f_0 \) for \( p < 1/(4\pi f_0) \) and \( \bar{f} = 0 \) otherwise. If we make use of Eqs. \[10\], we get the following parametric relation, with parameter \( \lambda \), between the inverse temperature \( \beta \) and the energy \( U \) (for a fixed value of \( f_0 \) \[22\]):

\[
\begin{align*}
(U - \frac{1}{2}) 8\pi^2 f_0^2 &= \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)} \equiv G(\lambda), \quad (13) \\
\frac{\beta}{8\pi^2 f_0^2} &= I_{-1/2}(\lambda)^2,
\end{align*}
\]

where \( G(\lambda) \) is a universal function monotonically increasing with \( \lambda \). A solution of the above equation certainly exists provided that

\[
(U - \frac{1}{2}) 8\pi^2 f_0^2 \geq G(0). \tag{14}
\]

To compute \( G(0) \) one can use the asymptotic expansions of the Fermi integrals. This yields \( G(0) = 1/12 \). Therefore, the homogeneous Lynden-Bell distribution with fixed \( f_0 \) exists only for \[22\]:

\[
U \geq U_{\text{min}}(f_0) = \frac{1}{96\pi^2 f_0^2} + \frac{1}{2}. \tag{15}
\]

The completely degenerate limit \( (\lambda = 0) \) of the homogeneous distribution corresponds to:
(i) $U = U_{\text{min}}(f_0)$ and $\beta \to +\infty$ for any $f_0$. The non-degenerate limit ($\lambda \to +\infty$) of the homogeneous distribution corresponds to:

(ii) $U \to +\infty$ and $\beta \to 0$ for any $f_0$. In this limit, the caloric curve takes the classical form $U \simeq 1/(2\beta) + 1/2$.

(ii) $f_0 \to +\infty$ for any $U$.

Let us now address the problem of stability of the homogeneous Lynden-Bell distribution. In [22], it has been shown that the homogeneous Lynden-Bell distribution is stable if, and only if:

$$I_{-1/2}(\lambda)|I'_{-1/2}(\lambda)| \leq \frac{1}{(2\pi f_0)^2}.$$  \hspace{1cm} (16)

If the distribution function satisfies then it is both Lynden-Bell thermodynamically stable (entropy maximum) and formally non-linearly dynamically stable. Otherwise, it is Lynden-Bell thermodynamically unstable (saddle point of entropy) and linearly dynamically unstable. For a given $f_0$, the relation determines the range of $\lambda$ for which the homogeneous distribution is stable/unstable. Then, using Eqs. (18), 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:

$$I_{-1/2}(\lambda)|I'_{-1/2}(\lambda)| \leq \frac{1}{(2\pi f_0)^2},$$  \hspace{1cm} (17)

$$U - \frac{1}{2} = \frac{1}{8\pi^2 f_0^2} I_{1/2}(\lambda)$$

where $\lambda$ goes from 0 (completely degenerate) to $+\infty$ (non-degenerate). In fact, the criterion only proves that $f$ is a local entropy maximum at fixed mass and energy. If several local entropy maxima are found (for example, homogeneous and inhomogeneous Lynden-Bell distributions), 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 this reason, (out-of-equilibrium) stability diagrams do not coincide with phase diagrams. In fact, the latter require a careful investigation of metastable states.

B. Phase diagram in the $(f_0, U)$ plane

The phase diagram of the Lynden-Bell distribution in the $(f_0, U)$ plane is shown in Fig. 2. We have also plotted the stability curve $U_c(f_0)$ of the homogeneous phase (split in two parts, $U'(f_0)$ and $U''(f_0)$) defined by Eqs. (17) and parameterized by $\lambda$. On the left of this curve, the homogeneous phase is stable (maximum entropy state) and on the right of this curve it is unstable.
FIG. 2: Phase diagram in the \((f_0, U)\) plane. The homogeneous phase only exists above the line \(U_{\text{min}}(f_0)\). The stability curve \(U_{\ast}(f_0)\) is parameterized by \(\lambda\). For \(\lambda \to 0\) (completely degenerate limit), we get \(f_0 = (f_0)_\ast = 1/(2\pi \sqrt{2})\) and \(U_{\ast} = 7/12\). For \(\lambda \to +\infty\) (non-degenerate limit), we get \(f_0 \to +\infty\) and \(U_{\ast} = 3/4\). On the left of this curve, the homogeneous phase is stable and on the right of this curve it is unstable. The stability curve is divided in two parts, i.e. \(U'_{\ast}(f_0)\) and \(U''_{\ast}(f_0)\), by the tricritical point (full round dot) located at \((f_0)_\ast, U_{\ast}\). The continuous line corresponds to the second-order transition line while the dotted lines correspond to the borders of the metastable region. The thick line represents the first-order transition line. All these lines divide the diagram in four regions. In region (I), the homogeneous phase is stable and the inhomogeneous phase does not exist; in (II), the homogeneous phase is stable and the inhomogeneous phase metastable; in (III), the homogeneous phase is metastable and the inhomogeneous phase stable; in (IV) the homogeneous phase is unstable and the inhomogeneous phase stable. \(U_{\text{min}}(f_0)\) is the line below which the homogeneous phase does not exist, and \(U_{\text{MIN}}(f_0)\) is the lowest accessible value of energy for a rectangular water-bag initial condition (see Sec. II E). The square dot is \((f_0)_\ast, U_{\ast}\) (Sec. II E), and the empty round dot is \((f_0)_0, U_{\ast}(f_0)_0\)). For \(f_0 \in [(f_0)_0, (f_0)_\ast]\) there is a re-entrant phase.

Now, many numerical simulations of the N-body system \([25]\), of the Vlasov equation \([24]\), 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 \(D\):

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

and zero outside. Here \(0 \leq \Delta \theta \leq \pi\) and \(\Delta p \geq 0\). The normalization condition results in

\[
f_0 = \frac{1}{4\Delta \theta \Delta p}
\]

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

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

\[
M_0 = \frac{\sin(\Delta \theta)}{\Delta \theta}.
\]

For the case under scrutiny, \(0 \leq M_0 \leq 1\) and \(U \geq U_{\text{MIN}}(M_0) \equiv (1 - M_0^2)/2\). The energy \(U_{\text{MIN}}(M_0)\) represents the absolute minimum accessible energy for a rectangular water-bag distribution with magnetization \(M_0\). The initial configuration is completely specified by the variables \((\Delta \theta, \Delta p)\) or, equivalently, by the variables \((M_0, U)\). On the other hand, for the determination of the Lynden-Bell equilibrium state, only the variables \((f_0, U)\) matter. Now, we note that different values of \((M_0, U)\) can correspond to the same \((f_0, U)\) and, consequently, to the same Lynden-Bell equilibrium (see Sec. II D). Therefore, the use of these variables leads to some redundances. Nevertheless, their advantage is that they are more directly related to physically accessible parameters. In any case, it is of interest to compare the two phase diagrams in \((f_0, U)\) and \((M_0, U)\) planes to see their similarities and differences.

For the rectangular water-bag initial condition, using Eqs. (19) and (21), 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. (21). Inserting this expression in Eqs. (19), we obtain after some algebra the caloric curve \(T(U)\) for fixed \(M_0\) parameterized by \(\lambda\):

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

\[
\beta = \frac{1}{\sin^2 \Delta \theta} \left( \frac{\pi^2}{6} I_{-1/2}(\lambda)^2 - 2(\Delta \theta)^2 \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)} \right).
\]
Using Eqs. [15] and [22], we find that the homogeneous Lynden-Bell distribution with fixed \( M_0 \) exists if and only if

\[
U \geq U_{\text{min}}(M_0) = \frac{1}{2} \left( \frac{\sin^2 \Delta \theta}{\pi^2 - (\Delta \theta)^2} + 1 \right). \tag{24}
\]

This result can also be obtained from Eq. [20] by considering the limit \( \lambda \to 0 \).

The completely degenerate limit (\( \lambda = 0 \)) of the homogeneous distribution corresponds to:

(i) \( U = U_{\text{min}}(M_0) \) and \( \beta \to +\infty \) for any \( M_0 \).
(ii) \( M_0 = 0 \) for any \( U \).

The non degenerate limit (\( \lambda \to +\infty \)) of the homogeneous distribution corresponds to:

(i) \( U \to +\infty \) and \( \beta \to 0 \) for any \( M_0 \). In that case \( U \simeq 1/(2\beta) + 1/2 \).
(ii) \( M_0 = 1 \) for any \( U \). In that case \( f_0 \to +\infty \).

On the other hand, regrouping all the preceding results, the critical curve \( U_c(M_0) \) separating stable and unstable homogeneous Lynden-Bell distributions is given by the parametric equations

\[
L_{-1/2}(\lambda)|I'_{-1/2}(\lambda)| = \frac{1}{(2\pi f_0)^2}, \tag{25}
\]

\[
U - \frac{1}{2} = \frac{1}{8\pi^2 f_0^2} \frac{I_{1/2}(\lambda)}{I_{-1/2}(\lambda)^3}, \tag{26}
\]

\[
f_0^2 = \frac{1}{48[(2U - 1)(\Delta \theta)^2 + \sin^2 \Delta \theta]}, \tag{27}
\]

\[
M_0 = \frac{\sin(\Delta \theta)}{\Delta \theta}, \tag{28}
\]

where \( \lambda \) goes from 0 (completely degenerate) to \( +\infty \) (non degenerate).

The phase diagram of the Lynden-Bell distribution in the \((M_0, U)\) plane is represented in Fig. 3. We have first plotted the minimum accessible energy of the homogeneous phase \( U_{\text{min}}(M_0) \) defined by Eq. [24]. We have also plotted the stability curve \( U_c(M_0) \) of the homogeneous phase defined by Eqs. [20]-[22] and parameterized by \( \lambda \).

Above this curve the homogeneous \((M_{QSS} = 0)\) phase is stable (maximum entropy state) and below this curve it is unstable (saddle point of entropy). For \( M_0 = 1 \), we are in the non degenerate limit \( \lambda \to +\infty \) (because \( f_0 \to +\infty \)) and the critical energy is \( U_c = 3/4 \) (Maxwell distribution). For \( M_0 = 0 \), we are in the completely degenerate limit \( \lambda = 0 \) and the critical energy is \( U_c = 7/12 \) (spatially homogeneous water bag).

If we now take into account Lynden-Bell’s inhomogeneous states, solving numerically Eqs. [11], we find that the phase diagram displays first-order and second-order phase transitions. The second order phase transition corresponds to the branch \( U''_c(M_0) \) and the first order phase transition to the branch \( U'_c(M_0) \).

D. Connection between the two phase diagrams

To make the connection between the phase diagram \((f_0, U)\) of Sec. [11B] and the phase diagram \((M_0, U)\) of Sec. [11C] we can plot the iso-\( M_0 \) lines in the \((f_0, U)\)
phase diagram or the iso-$f_0$ lines in the $(M_0, U)$ phase diagram.

Let us first consider 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

$$U_{\Delta \theta}(f_0) = \frac{1}{6(4\Delta \theta f_0)^2} - \frac{1}{2} \left( \frac{\sin \Delta \theta}{\Delta \theta} \right)^2 + \frac{1}{2}. \quad (29)$$

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

$$U_{\Delta \theta}(f_0) = \frac{A(\Delta \theta)}{f_0^2} - B(\Delta \theta), \quad (30)$$

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. 4). 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 if $U_{\Delta \theta}(f_0) \geq U_{\min}(f_0)$ leading to

$$f_0^2 \leq \left( \frac{\Delta \theta}{\pi} \right)^2 = \frac{\pi^2 - (\Delta \theta)^2}{48\pi^2 \sin^2 \Delta \theta}. \quad (31)$$

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

$$U \geq U_{\min}(M_0) = \frac{1}{2} \left( \frac{\sin^2 \Delta \theta}{\pi^2 - (\Delta \theta)^2} + 1 \right), \quad (32)$$

which is identical to Eq. (24). Figure 4 is in good agreement with the structure of the phase diagram in the $(M_0, U)$ 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. We also note that for $M_0 < (M_0)_c$, the phase transition goes from second order to first order. This corresponds to the case where the iso-$M_0$ line crosses the tricritical point.

Remark: we see on Fig. 4 that different iso-$M_0$ lines can cross each other. This means that different initial conditions $(M_0', U)$ and $(M_0'', U)$ can correspond to the same $(f_0, U)$ hence to the same Lynden-Bell distribution. In other words, in Lynden-Bell’s theory the couples $(M_0', U)$ and $(M_0'', U)$ are equivalent. There is therefore some redundance in using the variables $(M_0, U)$ instead of the variables $(f_0, U)$. Note, however, that the Lynden-Bell prediction does not always work so that, in case of incomplete relaxation, the couples $(M_0', U)$ and $(M_0'', U)$ may lead to different QSS. However, this happens for $f_0 \geq 0.11053\ldots$, i.e. in a parameter range which is only marginally interesting for our analysis.

Let us now consider the iso-$f_0$ lines in the $(M_0, U)$ phase diagram. If we fix the phase level $f_0$, the relation between the energy $U$ and $M_0$, or equivalently $\Delta \theta$, is

$$U_{f_0}(\Delta \theta) = \frac{1}{6(4\Delta \theta f_0)^2} - \frac{1}{2} \left( \frac{\sin \Delta \theta}{\Delta \theta} \right)^2 + \frac{1}{2}. \quad (33)$$

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

$$U \geq U_{\min}(f_0) = \frac{C(f_0)}{(\Delta \theta)^2} - \frac{1}{2} \left( \frac{\sin \Delta \theta}{\Delta \theta} \right)^2 + \frac{1}{2}, \quad (34)$$

with $C(f_0) = \frac{1}{6(4f_0)^2}$, which are easily represented in the $(f_0, U)$ phase diagram (see Fig. 4). Recall that $\Delta \theta$ is related to $M_0$ by Eq. (21). Figure 5 is in good agreement with the structure of the phase diagram in the $(f_0, U)$ plane. In particular, we can see that for a set of values of $f_0 \in \{(f_0)_1, (f_0)_2\}$, it intersects the curve $U_c(M_0)$ twice leading to re-entrant phases. We also note that the iso-$f_0$ lines cannot cross each other contrary to the iso-$M_0$ lines.

**E. Determination of the absolute minimum energy in the $(f_0, U)$ plane for a rectangular water-bag initial condition**

We recall that homogeneous Lynden-Bell distributions exist only for $U > U_{\min}(f_0)$. However, there can exist inhomogeneous Lynden-Bell distributions for $U < U_{\min}(f_0)$. Let us determine the minimum accessible energy $U_{\text{MIN}}(f_0)$ when we start from a rectangular water-bag initial condition. For fixed $f_0$ the energy of the initial condition is a function of $\Delta \theta$ (or initial magnetization $M_0$) given by

$$U_{f_0}(\Delta \theta) = \frac{1}{6(4\Delta \theta f_0)^2} - \frac{1}{2} \left( \frac{\sin \Delta \theta}{\Delta \theta} \right)^2 + \frac{1}{2}. \quad (35)$$

FIG. 4: 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. 2 and the $(M_0, U)$ phase diagram of Fig. 3. We can vary the energy at fixed initial magnetization by following a dashed line. The intersection between the dashed line and the curve $U_{\min}(f_0)$ determines the minimum energy $U_{\min}(M_0)$ 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.
We thus have to determine the minimum of this function for \( 0 \leq \Delta \theta \leq \pi \). First of all, the condition \( U'_0(\Delta \theta) = 0 \) is equivalent to

\[
f_0 = \frac{1}{\sqrt{48 \sin(\Delta \theta) (\sin(\Delta \theta) - \Delta \theta \cos(\Delta \theta))}}.
\] (36)

This function is represented in Fig. 4. For \( f_0 < 0.11053 \ldots \) there is no solution and for \( f_0 > 0.11053 \ldots \) there are two solutions \( \Delta \theta_1 \) and \( \Delta \theta_2 \) corresponding to one local minimum and one local maximum (see Fig. 7). For \( f_0 = 0.11053 \ldots \), we have \( \Delta \theta_1 = \Delta \theta_2 = 2.2467 \ldots \). Then, we find that the local minimum is the absolute minimum iff \( U_{0\text{MIN}}(\Delta \theta_1) < U_f(\pi) \). This is the case if \( f_0 > (f_0)_m = 0.12135 \ldots \) corresponding to an energy \( U_m = 0.57167 \ldots \) (see Fig. 7). For \( f_0 < (f_0)_m \), the absolute minimum correspond to \( \Delta \theta = \pi \).

In conclusion, for \( f_0 < (f_0)_m \), we find that

\[ U_{MIN}(f_0) = U_{0\text{MIN}}(f_0) = 0 = \frac{1}{96 \pi^2 f_0^2} + \frac{1}{2}. \] (37)

For \( f_0 > (f_0)_m \), we find that

\[ U_{MIN}(f_0) = U_{0\text{MIN}}(f_0) = \Delta \theta_1 \]

where \( \Delta \theta_1 \) is the smallest root of Eq. (36). Combining these equations, we find that the absolute minimum energy \( U_{MIN}(f_0) \) is given in parametric form by

\[
U_{MIN} = \frac{1}{2} \left( 1 - \frac{\sin(2 \Delta \theta_1)}{2 \Delta \theta_1} \right),
\]

\[
f_0 = \frac{1}{\sqrt{48 \sin(\Delta \theta_1) (\sin(\Delta \theta_1) - \Delta \theta_1 \cos(\Delta \theta_1))}}.
\] (39)

with \( 0 \leq \Delta \theta_1 \leq 1.85063 \ldots \). For \( f_0 \to +\infty \) (non degenerate limit), we get \( \Delta \theta_1 \to 0 \) and \( U_{MIN}(f_0) \to 0 \). This is the energy corresponding to an initial condition \( f(\theta, p, t = 0) = \delta(p) \delta(\theta) \).

**Remark:** for \( f_0 > 0.11053 \), we confirm on Fig. 7 that there can exists several initial conditions with the same \( f_0 \) and \( U \) but a different initial magnetization \( M_0 \). They lead to the same Lynden-Bell prediction.

### III. NUMERICAL RESULTS

To assess the correctness of the above theoretical prediction about the existence of a phase re-entrance, we have performed direct numerical simulations of the HMF model \( \Pi \) for finite \( N \). For that, we have chosen \( f_0 \) in the interval \((f_0)_c < f_0 < (f_0)_m\) and ran simulations at different energies. Results, for \( f_0 = 0.1096 \), are shown in Fig. 8 where both the theoretical and numerical values of magnetization at the QSS, \( M_{QSS} \), are plotted as a function of energy.

Simulations (dashed line) confirm the existence of a regime of phase re-entrance. However, the agreement with theory (continuous line) is mainly qualitative, as there is a systematic shift between the two curves, although the magnetization value of the main bump is consistent with the one predicted from Lynden-Bell’s approach. Moreover, simulations show the existence of two zones of magnetization revival at both sides of the central magnetized region. If we move at \( f_0 = 0.1100 \) (Fig. 9), we find that one of the two bumps has grown; this confirms that the structure of the phase diagram is more

![Figure 5: Stability diagram in the \((M_0, U)\) plane, with \(f_0\) lines. The thick lines are the two parts of the stability curve, the dotted line is the iso-\(f_0\) line with \(f_0 = 0.1096\) and the dash-dotted line is the iso-\(f_0\) line with \(f_0 = 0.1100\).](image1)

![Figure 6: Graphical construction determining the solutions of the equation \( U_{0\text{MIN}}'(\Delta \theta) = 0 \).](image2)

![Figure 7: Energy of the initial condition as a function of \( \Delta \theta \) for different values of \( f_0 \). From top to bottom: \( f_0 = 0.10, f = (f_0)_m = 0.12135, f_0 = 0.14 \).](image3)
the continuous line correspond to N = 10^6, are performed using a symplectic integration algorithm, and averaging the magnetization over the time window 40 < t < 140, and over 50 different realizations. For this f_0, U_{min} = 0.5878, U_c = 0.5955, U'_c = 0.6026 and U''_c = 0.6131.

A possible explanation for the discrepancies between the theoretical and numerical one may easily lead: a) to a further numerical phase re-entrance, if the iso-f_0 line crosses the numerical phase-transitions curves without crossing the theoretical one; b) to a larger numerical value of M_{QSS}, if the iso-f_0 separates from the numerical curve, while staying close to the theoretical one.

We also compared theory and simulations for higher f_0 (> (f_0)_c). As shown in Fig. 10, here theoretical and numerical results are close. This is in agreement with what is reported in [25]. In Fig. 11 we plotted our numerical results for a f_0 lower than (f_0)_c. For f_0 = 0.1085, close to the critical line U_c(f_0), we observe a magnetized phase although Lynden-Bell’s approach predicts a non-magnetized phase. For lower values of f_0, homogeneous QSS are observed in agreement with the theoretical prediction (data not shown).

To provide a complete picture of the whole phase diagram, we carried out simulations on a grid in the (f_0, U) plane and plotted the numerically obtained values of M_{QSS} in color scale, see Fig. 12. At first order, we observe a fair agreement between theory and simulations. In particular, the predicted re-entrant phase phenomenon is clearly observed. This can be considered as a success of the Lynden-Bell theory. We also note that the region (III) of the phase diagram appears to be non-magnetized. It corresponds therefore to a local Lynden-Bell entropy maximum. This confirms our claim about the robustness of metastable states. Note, however, that starting from different initial conditions (with identical values of U and f_0), we could have found that the QSSs in this region are magnetized. Indeed, in the metastability region, the selection between between local (metastable) or global (state) entropy maxima depends on a complicated notion of basin of attraction. Furthermore, we also find some unpredicted phenomena, as the additional phase re-entrance, for U ≃ 0.605 (see also Fig. 9) and a persisting complex than predicted by the theory, as we find the existence of additional phase re-entrances. Simulations performed using different numbers of particles show that the magnetization values of the central magnetized region and of the two bumps do not depend on the system size. Instead, as expected, the curve offset goes to zero when the system size is increased, see Fig. 9.

A possible explanation for the discrepancies between theory and simulations can be found by considering that the energy range in which phase-reentrance is observed is quite narrow. In fact, the iso-f_0 lines, in the interval (f_0)_* < f_0 < (f_0)_c, are very close to the theoretical phase-transition curve, see Fig. 5. This means that any possible (i.e., even small) disagreement between the theoretical and numerical one may easily lead: a) to a further numerical phase re-entrance, if the iso-f_0 line crosses the numerical phase-transitions curves without crossing the theoretical one; b) to a larger numerical value of M_{QSS}, if the iso-f_0 separates from the numerical curve, while staying close to the theoretical one.

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FIG. 11: Magnetization value, $M_{QSS}$, versus energy for $f_0 = 0.1085 < (f_0)_*$. For $f_0 < (f_0)_*$, the Lynden-Bell approach predicts that the QSS should be non-magnetized so there is a disagreement with theory when $f_0$ is close to the tricritical point.

FIG. 12: Stability diagram in the $f_0$-$U$ space with numerically calculated mean magnetizations. The dashed line is the stability curve. The theoretical re-entrant phase is clearly visible as well as the second (unexpected) re-entrant phase. In addition to this interesting new re-entrance phase, the other main discrepancy is the persisting magnetized phase for low $f_0$.

We also studied the order of phase transitions, by plotting the probability histogram of $M_{QSS}$ sampled with 300 different realizations. We show the results for two of the transitions occurring in Fig. 9. In Fig. 13, one can see that for the transition at $U \simeq 0.5980$, distributions are characterized by a double peak, which is a clear signature of a first-order phase transition. For the one at $U \simeq 0.6230$, see Fig. 14, the distributions are instead characterized by a single peak, which validates the prediction of a second-order phase transition. The two transitions at the boundaries of the smaller phase re-entrance, occurring around $U \simeq 0.605$, not predicted by the theory, are found to be of first (at low energy) and second (at high energy) order (data not shown).

Finally, we compared the analytical and numerical caloric curves $\beta(U)$ for a given value of $f_0$. In the simulations, the temperature has been calculated from the usual expression

$$\frac{1}{\beta_{kin}} = \langle p^2 \rangle = \int d\theta dp f_{QSS}(\theta, p) p^2.$$  \hspace{1cm} (40)

We note that the “kinetic” temperature defined by Eq. (40) does not coincide with the Lagrange multiplier $\beta$ associated to the energy conservation in the Lynden-Bell distribution. This is due to the fermionic nature of this distribution. Therefore, in order to make the comparison between simulations and theory relevant, we have calculated the theoretical temperature from the mean square momentum (40) averaged with the Lynden-Bell distribution given by Eq. (9). The results are reported in Fig. 15. In continuity with the results of Fig. 8, the range of energies where the inhomogeneous phase appears is shifted with respect to the theoretical prediction. As a further point, we also notice the presence of a region with negative specific heat, both in the numerical and an-
FIG. 15: Comparison between theoretical (continuous line) and numerical (dashed line) caloric curves, for $f_0 = 0.1096$.

alytical curves. To the best of our knowledge, this is the first time negative specific heat is observed out of equilibrium. Surprisingly, this phenomenon is here observed in correspondence of a second order transition line.

IV. CONCLUSION

In this paper, we have confronted the predictions of a theory based on Lynden-Bell’s statistical mechanics of violent relaxation to the results of numerical experiments. The application of Lynden-Bell’s theory to the HMF model predicts a re-entrant phase in the $(f_0, U)$ plane, and, indeed, we observe it. It occurs for a narrow range of parameters which would have been difficult to find without such a theoretical prediction. In this sense, this is a great success of Lynden-Bell’s approach. The theory also predicts the correct value of the magnetization in the inhomogeneous phase and the correct order of the phase transition. This is again remarkable because the phase diagram displays first and second order phase transitions in a very narrow range of parameters $(f_0, U)$. All these predictions are confirmed by direct N-body experiments. We have also numerically observed that metastable states (local Lynden-Bell entropy maxima) can be very robust, so that they are stable in practice. This is a specificity of systems with long-range interactions.

However, we have also found some discrepancies with respect to Lynden-Bell’s theory. In particular, numerical simulations have demonstrated the existence of second re-entrant phases: a band of un-magnetized states in the theoretically magnetized region, as well as persisting magnetized states in the theoretically un-magnetized region. As a matter of fact, there is a systematic shift of the transition line with respect to theory. We must emphasize, however, the very small selected region of parameters in Figs. 8 and 12. This gives the impression of a big discrepancy although the discrepancy is in fact very small.

Therefore, from these numerical experiments, we can conclude that the Lynden-Bell statistical theory gives a fair first order description of QSSs in the HMF model. However, for some initial conditions, there can be more or less severe discrepancies with respect to the prediction. This is a well-known fact in stellar dynamics and vortex dynamics to which this theory was initially applied (see a detailed discussion in [22]). Discrepancies with the Lynden-Bell theory have also been reported for the HMF model in [22] and [36]. These discrepancies are usually the result of an incomplete relaxation, i.e. a lack of efficient mixing in the system phase space. Indeed, the Lynden-Bell theory is based on a hypothesis of ergodicity and the prediction fails (by definition) if the evolution is not ergodic. A detailed understanding of incomplete violent relaxation is still lacking and appears to be very difficult.

Another cause of discrepancy may be related to the proximity of the numerically considered parameters $(f_0, U)$ to the critical line and to the tricritical point. Indeed, it is well-known in equilibrium statistical mechanics that strong fluctuations are present close to a critical point, and that the mean field results cease to be valid in the vicinity of a critical point. In the present case, we are studying out-of-equilibrium phase transitions and it is not clear if we can directly extend equilibrium results to that situation. Nevertheless, it is not unreasonable to expect that the theoretical results may be altered close to the critical line and this is indeed what we observe numerically. Further away from the critical line (i.e. for larger or smaller values of $f_0$), we find a very good agreement with the Lynden-Bell prediction (see also [22]). These different observations concerning the success or the failure of the Lynden-Bell theory are consistent with the discussion given in [22].

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[38] These parameters are related to those introduced in [22] 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 [24] are related to the Fermi integrals by $F_k(1/y) = 2^{(k+1)/2}y I_{k-1/2}(y)$.
[39] 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, and (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 (9) with $M_{QSS} \neq 0$ 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 [22].