The quasilinear theory in the approach of long-range systems to quasi-stationary states

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Abstract. We develop a quasilinear theory of the Vlasov equation in order to describe the approach of systems with long-range interactions to quasi-stationary states. The quasilinear theory is based on the assumption that, although the initial distribution is not Vlasov stable, nevertheless its evolution towards a Vlasov stable stationary state is such that it is always only slightly inhomogeneous. We derive a diffusion equation governing the evolution of the velocity distribution of the system towards a steady state. This steady state is expected to correspond to the space-averaged quasi-stationary distribution function reached by the Vlasov equation as a result of a collisionless relaxation. We compare the prediction of the quasilinear theory to direct numerical simulations of the Hamiltonian mean field model, starting from an unstable spatially homogeneous distribution, either Gaussian or semi-elliptical. In the Gaussian case, we find that the quasilinear theory works reasonably well for weakly unstable initial conditions (i.e. close to the critical energy $\epsilon_c = 3/4 = 0.75$) and that it is able to predict the energy $\epsilon_t \simeq 0.735$ marking the effective out-of-equilibrium phase transition between unmagnetized and magnetized quasi-stationary states found in the numerical simulations. Similarly, the quasilinear theory works well for energies close to the instability threshold of the semi-elliptical case $\epsilon^*_c = 5/8 = 0.625$, and it predicts an effective out-of-equilibrium transition at $\epsilon_t \simeq 0.619$. In both situations, the quasilinear theory works less well at energies lower than the out-of-equilibrium
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transition, the disagreement with the numerical simulations increasing with 
decreasing energy. In that case, we observe, in agreement with our previous 
numerical study (Campa and Chavanis 2013 *Eur. Phys. J.* B 86 170), that the 
quasi-stationary states are remarkably well fitted by polytropic distributions 
(Tsallis distributions) with index \( n = 2 \) (Gaussian case) or \( n = 1 \) (semi-elliptical 

case). In particular, these polytropic distributions are able to account for the 
region of negative specific heats in the out-of-equilibrium caloric curve, unlike 
the Boltzmann and Lynden-Bell distributions.

**Keywords:** classical phase transitions, dynamical processes, kinetic theory of 
gases and liquids, transport properties

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1. Introduction

Systems with long-range interactions exhibit peculiar properties both at equilibrium and out of equilibrium. Among the equilibrium features that are not present in short-range systems, probably the most striking ones are the ensemble inequivalence and the negative specific heat in the microcanonical ensemble. Even richer is the phenomenology one observes out of equilibrium: long-lived quasi-stationary states (QSSs), non-mixing behavior, phase transitions between non-Boltzmannian distributions, etc [1–6]. Many results have been established, or illustrated, in the context of a toy model called the Hamiltonian mean field (HMF) model [7]. Although progress has constantly been made in the last couple of decades, there are still points very poorly understood. One of these issues concerns the approach to QSSs.

In the statistical dynamics study of long-range systems, one of the main tools is the Vlasov equation that represents the interaction through a mean-field. For this reason the Vlasov equation describes a ‘collisionless’ dynamics. It can be shown that this is a very good approximation, that improves more and more when the number of components increases (the Vlasov equation becomes essentially exact when the number of particles $N \to +\infty$)\(^3\). More precisely, the larger the system the larger the time range for which the true dynamics can be studied with the Vlasov equation. Eventually, ‘collisional’ effects, i.e. finite $N$ effects, will take over, driving the system towards Boltzmann–Gibbs equilibrium. However, in some cases, especially in the astrophysical context, the time scale of these ‘collisional’ effects can be orders of magnitude larger than the age of the Universe [9, 10]. It is therefore important to characterize the various stages of the Vlasov dynamics. This equation admits both an infinite number of conserved quantitites (the Casimirs) and an infinite number of stationary states. The QSS reached by the system after an initial transient is just one of these stationary states, obviously one which is stable with respect to perturbations. The infinite number of stationary states of the Vlasov equation makes the prediction of which one will be selected by the system very difficult [11, 12]. Actually, it is fair to say that, theoretically, this is still a completely unsolved problem.

\(^3\)For neutral plasmas, the Vlasov equation becomes exact when the number of particles within the Debye sphere (plasma parameter) $\Lambda \to +\infty$ [8].
The initial state is in general a non-stationary, or unstable stationary, state of the Vlasov equation. In that case, the system evolves very rapidly, with the dynamics governed by the Vlasov equation, towards a QSS. Simulations show that, as one could argue on the basis of the existence of an infinite number of stationary states, the selected QSS strongly depends on the initial state of the system. A predictive theory was built by Lynden-Bell [13] in an astrophysical context. According to this theory, the QSS reached by the system is the one that maximizes an entropy functional while preserving the energy and all the Casimirs. Although perfectly defined, this problem is amenable to a computable solution only when the distribution of the initial state has a small number of phase levels, i.e. it is piecewise constant. However, even when the computation is possible, the comparison with the simulations shows that the prediction of the Lynden-Bell theory works only in some cases. The explanation of its failure has to be sought in the absence of a complete mixing of the dynamics (under given constraints) [12], a property that is implicitly assumed in the theory [13]. Even worse, in self-gravitating systems, e.g. elliptical galaxies, the Lynden-Bell distribution has infinite mass, thus it cannot represent the actual QSS of the system.

In the attempt to find alternatives, we have proposed [16] to compare the QSS found in numerical simulations of the HMF model with polytropic distributions (sometimes called Tsallis distributions [17]). These distributions are critical points of functionals of the one-particle distribution function that generalize the usual Boltzmann entropy. This by itself does not give a privileged status to polytropes with respect to other possible stationary states of the Vlasov equation. The reasons to employ them can be summarized as follows. They have been introduced long ago in astrophysics, where they are called stellar polytropes, in the attempt to describe the non-Boltzmannian distributions observed [10]. Being the critical points (at fixed particle number and energy) of functionals of the form \( S[f] = - \int dx dp C(f) \), where \( C(f) \) is a convex function, they determine distributions of the form \( f(e) \), where \( e \) is the individual energy, with \( f'(e) < 0 \) [18]. The stability of these Vlasov stationary states has to be determined in each case (see, e.g. the comments in this respect in [19, 20]). The function \( C(f) \) corresponding to the Boltzmann entropy is \( C(f) = f \ln f \). Under suitable assumptions the function \( C(f) = f^q/(q - 1) \) that gives rise to polytropic distributions can be obtained from a modification of the Lynden-Bell theory that takes into account the absence of complete mixing [12, 20]. A nice feature of polytropic distributions is that they can drop to zero at a finite value of the individual energy \( e \), accounting heuristically for the phenomenon of incomplete mixing. In a numerical study [16], we have shown that in some cases in which the prediction of the Lynden-Bell theory fails to obtain the distribution of the QSSs reached by the system after the violent relaxation, polytropic distributions are a good approximation of the QSSs. However, we have found that the quality of the approximation deteriorates when the initial distribution is only weakly unstable.

In the case of weak instability of initially homogeneous distributions, another type of approximation could be more suitable, viz. the quasilinear (QL) approximation. This approach is based on the assumption that, although the initial distribution is not

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4 Although we shall focus in this paper on situations where the Lynden-Bell theory does not provide a good description of the QSSs, we would like to emphasize that there exist situations where the Lynden-Bell theory works remarkably well and is able to predict the existence of out-of-equilibrium phase transitions and re-entrant phases that would not have been detected without the help of this theory; see in particular [14, 15] and figure 36 of [16] for successful predictions of the Lynden-Bell theory.
Vlasov stable, nevertheless its evolution towards a Vlasov stable stationary state is such that it is always only slightly inhomogeneous. The assumption will be made more precise below.

The QL theory is well-known in plasma physics for the Coulombian interaction \cite{8}. In fact, there are many works in the literature concerning this subject, starting from the early works in \cite{27–29}. A thorough study of the QL theory and the issues raised by its application is found in \cite{30}. We stress that the framework in which we here use the QL approximation, applying it to the HMF model, is quite different. This model has a purely attractive potential, with a functional expression very different from the Coulombian case, and the structure of the Vlasov stable states differs correspondingly greatly. The HMF model has many (actually, infinitely many) Vlasov stable states, which can be homogeneous or inhomogeneous (inhomogeneous steady states are the counterpart of the BGK modes \cite{8} in plasma physics). Each such state is a possible QSS. As we have emphasized above, the solution of the problem of predicting the QSS reached by the system initially found in a Vlasov unstable state is still far off, and few alternatives to the Lynden-Bell theory have been proposed \cite{5}. Although based on some analytical considerations, these alternative procedures are mostly empirical.

We point out that the main difficulty is exactly the prediction of the QSS reached by the system. As it will be clear in the following, we are not interested in the dynamical details of the approach of the system to the QSS, but in the properties of the selected QSS itself. In particular, for our model, we focus on the magnetization and on the velocity distribution function of the QSS. From the operative point of view, our study is empirical since we compare these properties with those emerging from a full \(N\)-body simulation. Therefore in this work our aim is to test the predictive power of the QL approximation, through comparison with simulations, as far as the selection of QSSs is concerned. The main reason to analyze the QL approximation is that the approaches already investigated have shown to be numerically good in their predictive performance only in some cases, depending on the degree of Vlasov instability of the initial state.

The derivation of the expressions of the QL approximation can be found in textbooks like, e.g. \cite{8}. However, to make the paper self-contained, we have described its derivation in appendix A, focusing on one-dimensional systems on a circle, since we apply the theory to the HMF model. The main text contains only the final expressions.

From the technical point of view, the characteristics of the system studied in this paper is the presence of a single unstable mode, due to the particular form of the interaction. In the QL theory, this is reflected in the structure of the diffusion coefficient that in the general case has contributions from all the unstable modes. The case of a single unstable mode has received particular attention in plasma physics (see, e.g., a related form of QL theory, called the Stochastic Structural Stability Theory (SSST), has been developed in the context of the stochastically forced 2D Navier–Stokes equations \cite{21–24}. On the other hand, we should not confuse the QL theory considered in this paper with the QL theory used to derive the Landau and Lenard–Balescu equations in plasma physics \cite{25}. There are crucial physical differences. We are considering here the collisionless evolution \((N \to +\infty)\) of a Vlasov unstable distribution function, while the Landau and Lenard–Balescu kinetic theories are concerned with the collisional evolution (induced by finite \(N\) effects) of a Vlasov stable distribution. Thus, our QL kinetic theory is based on the Vlasov equation instead of the Klimontovich equation. Our kinetic theory is also different from the kinetic theory developed by Kadomtsev and Pogutse \cite{26}, leading to a coarse-grained Vlasov equation, that relaxes towards the Lynden-Bell distribution \cite{13}. This kinetic theory implicitly assumes an efficient mixing while our theory, as we shall see, assumes a weak mixing.
The quasilinear theory in the approach of long-range systems to quasi-stationary states [31–36]). For our empirical approach the presence of just a single unstable mode is only something that simplifies the structure of the diffusion coefficient.

In this paper we have tested the validity of the QL theory in the HMF model, motivated by the fact that the simulations performed in [16] to study the polytropic approximation have shown that, when the initial distribution is only weakly unstable and the polytropic approximation is not good, the QSS is only weakly inhomogeneous. Therefore, we make the hypothesis that the distribution is only slightly inhomogeneous all the time and compare the prediction of the QL theory to the results of numerical simulations.

The paper is organized as follows. In section 2 we give the main expressions of the QL approximation for a generic mean field system composed of particles moving on a circle, and we apply the theory to the HMF model, where the particular form of the interaction allows a simplification of the expressions. In sections 3 and 4 we show the results for a Gaussian initial condition and determine the domain of validity of the QL theory and the polytropic fit. The case of a semi-elliptical initial condition that presents similarities and differences with the Gaussian case is treated in appendix B.

2. The QL approximation and its application to the HMF model

2.1. The general diffusion equation

We describe here the QL approximation for the evolution of the one-particle distribution function as determined from the Vlasov equation. In view of the application to the HMF model, we consider a generic one dimensional system on the circle, i.e. a system with Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i}{2} + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(\theta_i - \theta_j), \quad (1)$$

where $\theta \in [0, 2\pi]$, and the potential $V(\theta)$, which has $2\pi$ periodicity, is supposed to be continuous (the mass of the particles has been put equal to 1 without loss of generality). The Vlasov equation for the one-particle distribution function $f(\theta, p, t)$ is

$$\frac{\partial f(\theta, p, t)}{\partial t} + p \frac{\partial f(\theta, p, t)}{\partial \theta} - \frac{\partial \Phi(\theta, t; f)}{\partial \theta} \frac{\partial f(\theta, p, t)}{\partial p} = 0, \quad (2)$$

where the mean field potential is given by

$$\Phi(\theta, t; f) = \int dp' \int_0^{2\pi} d\theta' V(\theta - \theta') f(\theta', p', t). \quad (3)$$

For large long-range systems with $N \gg 1$ the Vlasov equation is a very good approximation for times of order $N [1–6]$. Functions $f_0(p)$ that depend only on $p$ are particular stationary solutions of the Vlasov equation. The stability of these stationary solutions is studied by putting $f(\theta, p, t) = f_0(p) + f_1(\theta, p, t)$ and linearizing the Vlasov

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6 It is easy to see that the mean field potential $\Phi$ is constant in $\theta$ for a uniform distribution, i.e. a function $f$ that does not depend on $\theta$. 

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equation around $f_0(p)$, i.e. keeping only the terms at most linear in $f$. We then obtain the following linear equation for $f_1(\theta, p, t)$:

$$\frac{\partial f_1(\theta, p, t)}{\partial t} + p\frac{\partial f_1(\theta, p, t)}{\partial \theta} - \frac{\partial \Phi(\theta, t; f_1)}{\partial \theta} \frac{\partial f_0(p)}{\partial p} = 0 ,$$

(4)

which is valid as long as $f_1(\theta, p, t) \ll f_0(p)$. This is the linearized Vlasov equation. The proper frequencies $\omega$ of the dynamics determined by this equation can be studied by inserting solutions where the time dependence is of the form $e^{-i\omega t}$. The function $f_0(p)$ is stable if all the solutions for $\omega$ have a non-positive imaginary part. In that case, the distribution function $f_0(p)$ can change only because of the effects of ‘collisions’ (finite $N$ effects) that are not considered in the Vlasov equation [4]. We recall that in the case of one dimensional systems the time range of validity of the Vlasov equation grows like $N$ (for inhomogeneous systems) or with a higher power of $N$ (for homogeneous systems) [4]. If, on the contrary, some of the frequencies have a positive imaginary part, $f_0(p)$ is Vlasov unstable, and the distribution $f(\theta, p, t)$ will depart from $f_0(p)$ rapidly, so that $f_1$ will no longer be much smaller than $f_0$. In this case there is an approximation that can work if the positive imaginary parts of the proper frequencies are small enough (the scale with which to measure this smallness will be specified later): the so-called QL approximation [8]. In appendix A we derive the corresponding equations. The QL approximation gives an evolution equation for the angle average of the distribution $f(\theta, p, t)$:

$$f_0(\theta, p, t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta f(\theta, p, t) .$$

(5)

The angle-averaged distribution is then used to define $f_1(\theta, p, t)$ by

$$f(\theta, p, t) = f_0(p, t) + f_1(\theta, p, t) .$$

(6)

Clearly the angle average of $f_1$ is zero. As shown in appendix A, under the assumption that $f_1(\theta, p, t) \ll f_0(p, t)$ all the time (and other assumptions discussed in section 2.2), one obtains an equation for the evolution of $f_0(p,t)$:

$$\frac{\partial f_0(p,t)}{\partial t} = \frac{\partial}{\partial p} \left( D(p,t) \frac{\partial f_0(p,t)}{\partial p} \right) ,$$

(7)

which is of the form of a diffusion equation. The time and velocity dependent diffusion coefficient $D(p,t)$ is given by

$$D(p,t) = \sum_{k>0} \frac{2\chi_k(t)\omega_1(k,t)}{(pk - \omega_R(k,t))^2 + \omega_I^2(k,t)}$$

(8)

with

$$\frac{\partial \chi_k(t)}{\partial t} = 2\omega_1(k,t)\chi_k(t) .$$

(9)

In equation (8), $\omega_R(k,t)$ and $\omega_I(k,t)$ are the real and imaginary parts of the frequencies associated with the unstable mode of wavenumber $k$ ($k$ takes on only integer values since our system is on a circle). As explained in appendix A, in equation (8) we assume that for each $k$ there is only one unstable mode (this is what happens in the HMF model, as

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shown below). In the general case, for each \( k \) one has to sum over all the unstable modes of the Vlasov operator linearized around \( f_0 \), or retain the most unstable one.

### 2.2. The assumptions of our approach

Let us clearly state the approximations that are done in order to obtain the diffusion equation for \( f_0(p,t) \) in the QL theory (see appendix A for more details):

(i) The first assumption, which is at the heart of the QL theory, is the smallness of \( f_1(\theta, p, t) \) with respect to \( f_0(p,t) \). This is the necessary assumption to neglect the higher order terms in \( f_1(\theta, p, t) \).

(ii) The second assumption is that the timescale of variation of \( f_0(p,t) \) determined by the diffusion equation is large compared to the timescale of \( f_1(\theta, p, t) \) determined by the linearized Vlasov equation (more precisely, the assumption that the time derivatives of the coefficients \( a_k(p,t) \) and \( b_k(p,t) \) in equations (A.30) and (A.31) of appendix A can be neglected). Although this adiabatic approximation is not fully under control, it is reasonable. Indeed, the approximation is clearly correct if the function \( f_0 \) is stable, since in that case \( f_1(\theta, p, t) \) has no exponential growth, and its time variation is described by the linearized Vlasov equation. We can expect that when the instability of \( f_0 \) is weak, the approximation is still good, with the time variation of \( f_1(\theta, p, t) \) captured essentially by the growth due to the weakly unstable modes, while its validity worsens for stronger instabilities. In fact, for weak instabilities the time variation of \( f_0(p,t) \) will be small (see equations (7) and (8) where \( \omega_1(k,t) \) is small for weak instabilities) and, in turn, this means that neglecting the time variation of \( a_k(p,t) \) and \( b_k(p,t) \) is a reasonable approximation. We can thus conclude that the approximation is expected to be good close to criticality. In addition, we recall that we are interested in the angle-averaged distribution \( f_0(p,t) \), for which one might assume a sort of averaging over \( \theta \) of the possible fast variation of \( f_1(\theta, p, t) \). It would be interesting to determine whether it is possible to relax this assumption and whether the sole use of the QL approximation would result in much better results.

Let us discuss when we expect that the first assumption (QL approximation) is good, i.e. when \( f_1(\theta, p, t) \ll f_0(p, t) \) is satisfied throughout the time evolution of the system. If we assume that \( f_0(p,t) \) is of order 1, we can argue that the approximation is good as long as \( \chi_k^{1/2}(t) \ll 1 \) for each \( k \) (see appendix A). This defines the smallness of \( \omega_1(k) \) also in relation to the initial values \( \chi_k(0) \). We note that, in general, we expect that \( \omega_1(k) \) decreases in time since the dynamics drives the function \( f_0(p,t) \) towards a Vlasov (marginally) stable distribution (see below). Therefore, the approximation should be better and better.

In practice, it is difficult to determine \( \chi(0) \) precisely because it is physically related to how far the velocity distribution of the \( N \)-body system at time \( t = 0 \) is away from the stationary but unstable Vlasov state \( f_0(p, 0) \). In section 3.2, we shall argue that \( \chi(0) \) is determined by finite \( N \) effects and scales as \( N^{-1} \). This estimate is confirmed by the results of \( N \)-body numerical simulations.

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2.3. Application to the HMF model

The expressions simplify for the HMF model where the potential is $V(\theta) = 1 - \cos \theta$. Its Fourier coefficients $V_k$ are given by

$$V_k = 2\pi \delta_{k,0} - \pi (\delta_{k,1} + \delta_{k,-1}).$$  \hspace{1cm} (10)

As a consequence, the dielectric function $D(k, \omega)$ defined by equation (A.18) has a structure only for $k = \pm 1$, and there is a collective dynamics only for these wavenumbers:

$$D(k, \omega) = 1 + \pi k (\delta_{k,1} + \delta_{k,-1}) \int dp \frac{\partial f_0}{pk - \omega}.$$  \hspace{1cm} (11)

The diffusion coefficient of the QL approximation is then

$$D(p, t) = \frac{2\chi(t)\omega_1(t)}{(p - \omega_R(t))^2 + \omega_1^2(t)},$$  \hspace{1cm} (12)

where the evolution of $\chi(t)$ is given by equation (9). It is sufficient to study the dispersion relation $D(k, \omega) = 0$ only for $k = 1$. It is given by

$$1 + \pi \int dp \frac{\partial f_0(p, t)}{p - \omega} = 0.$$  \hspace{1cm} (13)

Things simplify further if we consider a function $f_0(p)$ that is initially even in $p$ and has only a single maximum at $p = 0$. These properties are conserved by the diffusion equation for $f_0(p, t)$ (we will prove this below). It is then easy to show that if there is a proper frequency with a positive imaginary part (unstable case), its real part must be zero. Indeed, we can write the dispersion relation as

$$1 + \pi \int dp \frac{f_0'(p, t)(p - \omega_R(t))}{(p - \omega_R(t))^2 + \omega_1^2(t)} + i\pi\omega_1 \int dp \frac{f_0'(p, t)}{(p - \omega_R(t))^2 + \omega_1^2(t)} = 0.$$  \hspace{1cm} (14)

The real and imaginary parts must be separately equal to zero. However, the last integral is negative (positive) definite if $\omega_R(t) > 0 (< 0)$, and is zero when $\omega_R(t) = 0$. This can be seen as follows: (i) for $\omega_R(t) = 0$ it vanishes since $f_0'(p, t)$ is odd; (ii) for $\omega_R(t) > 0$, exploiting that $f_0'(p, t)$ is odd and that it is negative (positive) for $p > 0 (< 0)$, the sum of the values of the integrand for $p$ and $-p$ is negative; (iii) analogously, for $\omega_R(t) < 0$ this sum is positive. To be more explicit, consider for example the case $\omega_R(t) > 0$. Then, for any $p > 0$, we have $|p - \omega_R(t)| < |p - \omega_R(t)|$, i.e. $(p - \omega_R(t))^2 + \omega_1^2(t) < (-p - \omega_R(t))^2 + \omega_1^2(t)$. Thus, since for $p > 0$ one has $f_0'(p, t) = -f_0'(-p, t) < 0$, the sum of the contributions of $p$ and $-p$ to the last integral in equation (14) is negative. In conclusion, since we must have $\omega_R(t) = 0$, the dispersion relation becomes\(^7\)

$$1 + \pi \int dp \frac{p f_0'(p, t)}{p^2 + \omega_1^2(t)} = 0,$$  \hspace{1cm} (15)

and the diffusion coefficient

\(^7\) Another proof of this result is given in section 2.8 of [37]. Considering an unstable single humped symmetric distribution $f_0(p)$, and using the Nyquist theorem, one can show that the dispersion relation (14) has a unique solution with $\omega > 0$; it is such that $\omega_R = 0$. 

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\[ D(p, t) = \frac{2\chi(t)\omega_I(t)}{p^2 + \omega_I^2(t)}. \]  \hspace{1cm} (16)

Summarizing, for the HMF model, the integration of the diffusion equation (7) is performed with \( D(p, t) \) given by equation (16), where \( \omega_I(t) \) is the unique positive solution of equation (15), with \( f_0(p, t) \) single humped and even, and where the evolution equation for \( \chi(t) \) is

\[ \frac{d\chi(t)}{dt} = 2\omega_I(t)\chi(t). \]  \hspace{1cm} (17)

We remark that equation (7) is a diffusion equation with a time (and velocity) dependent diffusion coefficient given, for the HMF model, by equation (16), which is different from 0 as long as \( \omega_I(t) \) does not vanish. If it happens that \( \omega_I \) vanishes at a certain time, then the solution of the diffusion equation reaches a stationary state. Actually, as already noted, we expect that the diffusion equation will drive the function \( f_0(p, t) \) towards a stationary state by monotonically decreasing \( \omega_I(t) \) to 0 (this is what we observe numerically). We do not have a general proof of this, but we can show that, if at time \( t = 0 \) the imaginary pulsation \( \omega_I(t) \) is positive, it has to tend to 0 for increasing time (see equation (28) below). We cannot prove that \( \omega_I(t) \) decreases monotonically. However, we can give an approximate argument, described in appendix C, to show that this is likely to be the case. The argument is based on the result presented below in equation (25), and on the fact, found in the numerical integration of the diffusion equation and shown in the next section, that the function \( f_0(p, t) \) keeps approximately the same functional form while it varies as driven by the diffusion equation.

2.4. Properties of the diffusion equation

It is useful to make the following evaluation. If we suppose that, at a given time \( t \), \( f_0(p, t) \) is a Gaussian

\[ f_0(p, t) = \frac{1}{2\pi} \sqrt{\frac{\beta(t)}{2\pi}} e^{-\frac{1}{2} \beta(t)p^2}, \]  \hspace{1cm} (18)

which is normalized such that \( \int_{-\infty}^{\infty} f_0(p, t) \, dp = 1/2\pi \), then the dispersion relation (15) becomes

\[ 1 - \sqrt{\frac{\beta^3}{8\pi}} \int dp \frac{p^2 e^{-\frac{1}{2} \beta p^2}}{p^2 + \omega_I^2} = 0, \]  \hspace{1cm} (19)

where we have not indicated the time dependence of \( \beta \) and \( \omega_I \). The integral in the last expression can be expressed in term of the error function

\[ \text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dy \, e^{-y^2}. \]  \hspace{1cm} (20)

We have

\[ 1 - \frac{1}{2} \beta + \omega_I \sqrt{\frac{\pi \beta^3}{8} e^{\frac{1}{2} \beta \omega_I^2}} \left[ 1 - \text{erf} \left( \sqrt{\frac{\beta}{2} \omega_I} \right) \right] = 0. \]  \hspace{1cm} (21)
For a general distribution function $f_0(p,t)$, we define the kinetic temperature $T(t)$ by
\[ T(t) = \langle p^2 \rangle = 2\pi \int_{-\infty}^{+\infty} dp \, p^2 f_0(p,t). \] (22)

This is the variance of the distribution. The kinetic energy of the system is exactly given by $\epsilon_{\text{kin}}(t) \equiv \int d\theta dp \, \frac{p^2}{2} f(p,\theta,t) = 2\pi \int dp \, p^2 f_0(p,t) = \frac{1}{2} T(t)$ since $\int d\theta \, f_1(p,\theta,t) = 0$. For the Gaussian distribution (18), we have $\beta = 1/T$. Therefore, equation (21) relates the growth rate $\omega_I$ to the temperature $T$ for the Gaussian distribution (18). Let us suppose that at time $t = 0$ the function $f_0$ is a Gaussian. Its evolution, as determined by equation (7) together with equations (16) and (17), will not maintain this structure, i.e. we cannot hope that there will simply be a change with time of the parameter $\beta$. However, in our simulations we will see that the actual evolution does not depart very much from a Gaussian, at least for the cases considered.

We now prove that an initial $f_0(p)$ which is even in $p$ and with only a single maximum at $p = 0$ will keep these properties during the dynamics determined by equation (7). We have seen that, as long as $f_0(p,t)$ is of this form, then $\omega_I(t) = 0$, and the diffusion coefficient is given by equation (16). This is an even function of $p$, with a single maximum at $p = 0$. Therefore, the right-hand side of equation (7) is even in $p$. Furthermore, taking the derivative of equation (7) with respect to $p$ we have
\[ \frac{\partial}{\partial t} \frac{\partial f_0}{\partial p} = \frac{\partial^2 D}{\partial p^2} \frac{\partial f_0}{\partial p} + 2 \frac{\partial D}{\partial p} \frac{\partial^2 f_0}{\partial p^2} + D \frac{\partial^3 f_0}{\partial p^3}. \] (23)

If $f_0(p,t)$ develops a point $p > 0$ with $\frac{\partial f_0}{\partial p} = 0$, at that moment, by continuity, we will have $\frac{\partial^2 f_0}{\partial p^2} = 0$ and $\frac{\partial^3 f_0}{\partial p^3} < 0$. Then, we will have $\frac{\partial}{\partial t} \frac{\partial f_0}{\partial p} < 0$. This proves that the function $f_0(p,t)$ will remain with a single maximum at $p = 0$.

We also prove that the average kinetic energy increases with time. In fact, we have
\[ \frac{\partial}{\partial t} \int dp \, \frac{p^2}{2} f_0(p,t) = \int dp \, \frac{p^2}{2} \frac{\partial f_0(p,t)}{\partial t} = \int dp \, \frac{p^2}{2} \frac{\partial}{\partial p} \left(D(p,t) \frac{\partial f_0(p,t)}{\partial p} \right) = - \int dp \, p D(p,t) \frac{\partial f_0(p,t)}{\partial p}. \] (24)

Substituting the expression of the diffusion coefficient (16) into equation (24), and using the dispersion relation (15), we obtain
\[ \frac{\partial}{\partial t} \int dp \, \frac{p^2}{2} f_0(p,t) = -2\chi(t) \omega_I(t) \int dp \, p \frac{\frac{\partial f_0(p,t)}{\partial p}}{p^2 + \omega_I^2(t)} = \frac{2\chi(t) \omega_I(t)}{\pi} > 0. \] (25)

Since
\[ \epsilon_{\text{kin}}(t) = 2\pi \int dp \, \frac{p^2}{2} f_0(p,t) = \frac{1}{2} T(t), \] (26)
we find that
\[ \frac{dT}{dt} = 8\chi(t) \omega_I(t) > 0, \] (27)
and we conclude that the kinetic temperature $T(t)$ increases with time. Therefore, the velocity distribution has the tendency to spread. The increase of the kinetic temperature also qualitatively confirms that the system tends to be less unstable as time goes on.

As anticipated, we can prove that $\omega_I(t)$ must necessarily tend to 0. In fact, the relation

$$\frac{\partial}{\partial t} \int dp f_0(p,t)^2 = 2 \int dp f_0(p,t) \frac{\partial f_0(p,t)}{\partial t}$$

$$= 2 \int dp f_0(p,t) \frac{\partial}{\partial p} \left( D(p,t) \frac{\partial f_0(p,t)}{\partial p} \right) = -2 \int dp D(p,t) \left( \frac{\partial f_0(p,t)}{\partial p} \right)^2 \leq 0$$

is a sort of $H$-theorem for the functional $\Gamma_2 = \int dp f_0(p,t)^2$ similar to the enstrophy in two-dimensional turbulence. Since $\Gamma_2 \leq 0$ and since $\Gamma_2$ is bounded from below by 0, we conclude that $\Gamma_2 \to 0$ for $t \to +\infty$. According to the last equality in equation (28), this implies that $D(p,t) \to 0$ for $t \to +\infty$ at least for some values of $p$ (note that $f_0(p,t)$ cannot become independent on $p$ otherwise it would not be normalizable). Considering the expression (16) of $D(p,t)$ this in turn implies that $\omega_I(t)$ must necessarily tend to 0.

Finally, we derive the approximate expression of the dispersion relation that holds when $\omega_I(t)$ is very small. This can be useful in the numerical computations. In fact, as emphasized previously, we expect that during the dynamics $\omega_I(t)$ decreases towards zero, so that $f_0(p,t)$ becomes (marginally) Vlasov stable. It is not difficult to see that at first order in $\omega_I(t)$ the dispersion relation (15) (we recall that this expression is valid for an even $f_0(p,t)$ with a single maximum at $p = 0$) becomes for $\omega_I(t) \geq 0$:

$$1 + \pi \int dp \frac{f_0'(p,t)}{p} - \pi^2 \omega_I(t) f_0''(0,t) = 0.$$  \hfill (29)

Specializing to the case of the Gaussian (18), equation (29) becomes

$$1 - \frac{1}{2} \beta + \sqrt{\frac{\pi \beta^3}{8}} \omega_I(t) = 0.$$  \hfill (30)

This relation can also be obtained by a power expansion of equation (21). From equation (29) we get

$$\omega_I(t) = \frac{1}{\pi^2 f_0''(0,t)} \left[ 1 + \pi \int dp \frac{f_0'(p,t)}{p} \right].$$  \hfill (31)

We recall that the term in square brackets is exactly the expression that one obtains from the Nyquist criterion for the Vlasov stability of a normalized distribution function $f_0(p)$ which is even in $p$ and has a single maximum at $p = 0$ [37]. Such a function is stable if, and only if, that expression is positive:

---

8 This inequality is actually true for any $H$-function [18] of the form $H = -\int C(f) \, dp$ where $C(f)$ is convex ($C'' \geq 0$) since $H = \int dp D(p,t) C''(f_0(p,t)) \left( \frac{\partial f_0(p,t)}{\partial p} \right)^2 \geq 0$.

9 For $\omega_I(t) < 0$, in the last term of the left-hand side of equation (29), $\omega_I(t)$ must be substituted by $|\omega_I(t)|$. This is consistent with the fact that the expression in equation (15) is even in $\omega_I(t)$ (but not differentiable at $\omega_I(t) = 0$). Equation (29) is obtained from a straightforward adaptation to the HMF model of the method developed in section 3.7 of [38] for self-gravitating systems. Another, more direct, proof of equation (29) is given in appendix D.
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\[ f_0(p) \text{ stable } \Leftrightarrow 1 + \pi \int dp \frac{f_0'(p, t)}{p} > 0. \]  \tag{32}

Thus, we expect to have a positive \(\omega_I(t)\) if that expression is negative. Since \(f_0''(0, t) < 0\) we therefore have a consistent expression.

Remark: We note that the stability criterion \((32)\) can be rewritten as

\[ T_{\text{eff}} = \frac{-1}{2\pi} \int dp \frac{f_0'(p, t)}{p} > \frac{1}{2}, \]  \tag{33}

where \(T_{\text{eff}}\) is an effective temperature (it coincides with the ordinary temperature when \(f_0(p)\) is the Gaussian distribution). This formula shows that stability is achieved when the width of the distribution function is sufficiently large, except that the width is not measured by the kinetic temperature \((22)\) but by the effective temperature \((33)\).

3. Results for a homogeneous Gaussian initial condition

At statistical equilibrium, the HMF model exhibits a second order phase transition between a homogeneous unmagnetized phase and a magnetized phase at the critical temperature \(T_c = 1/2\), corresponding to the critical energy \(\epsilon_c = 3/4 = 0.75\) (we denote by \(\epsilon\) the energy per particle) [4]. The homogeneous phase is thermodynamically stable if, and only if, \(T \geq T_c\). The critical temperature \(T_c = 1/2\) also coincides with the dynamical stability threshold of the homogeneous Gaussian distribution

\[ f_0(p) = \frac{1}{2\pi} \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2} p^2}. \]  \tag{34}

Indeed, one finds that in this case the expression in the right-hand side of equation \((32)\) vanishes for \(\beta = \beta_c = 2\), while it is positive (resp. negative) for \(\beta < 2\) (resp. \(\beta > 2\)). Therefore, a Gaussian distribution at temperature smaller than 1/2, i.e. at energy smaller than 0.75, is Vlasov unstable.

Other forms of homogeneous distribution functions have other (dynamical) stability thresholds. In appendix B, we consider a semi-elliptical distribution given by

\[ f_0(p) = \frac{1}{2\pi^2 b} \sqrt{2b - p^2} \Theta(2b - p^2), \]  \tag{35}

where \(\Theta(\cdot)\) is the Heaviside step function, and where the parameter \(b\) is related to the energy \(\epsilon\) by \(b = 4\epsilon - 2\). A semi-elliptical distribution is a polytrope of index \(n = 1\) [16, 20]. The stability threshold for this function is \(\epsilon^*_c = \epsilon_{n=1} = 5/8 = 0.625\); therefore, we will study the dynamics when \(\epsilon\) is somewhat smaller than this value.

We have performed simulations of both the diffusion equation and the full \(N\)-body dynamics of the HMF model at several energies smaller than the critical energy, for both the case in which the initial homogeneous distribution is a Gaussian and that in which it is a semi-ellipse. The analysis and comparison of the results have been as follows. Starting from a Vlasov unstable state, the \(N\)-body system has a violent relaxation that ends at a QSS, a Vlasov stationary and stable state. Afterwards, the system
The quasilinear theory in the approach of long-range systems to quasi-stationary states evolves slowly, driven by finite-size effects, a phase of the dynamics in which we are not interested in this work. The QSS is characterized by a single particle distribution function that in general will not be homogeneous, depending on both \( \theta \) and \( p \). On the other hand, the diffusion equation concerns the evolution of the angle-averaged distribution function \( f_0(p,t) \), and this evolution stops when \( f_0(p,t) \) reaches a marginally Vlasov stable state for which \( \omega_1 = 0 \). Therefore, we have compared the angle-averaged distribution function of the \( N \)-body QSS with the function \( f_0(p) \) obtained when the evolution of the diffusion equation reaches an end. To characterize this comparison with a single parameter, we have considered the temperature associated to these distributions, i.e. the expected value of \( p^2/2 \) (since we consider only distributions that are even in \( p \), the expected value of \( p \) is zero). We note that for the HMF model the kinetic temperature \( T \) and the magnetization \( m \) of the system, for a given energy, are uniquely related. In fact we have

\[
\epsilon = \frac{1}{2} T + \frac{1}{2} (1 - m^2)
\]

Therefore, the analysis of the temperature is equivalent to that of the magnetization, i.e. the order parameter. From equation (36) we note that the smallest possible energy for a homogeneous initial condition \( (m = 0) \) is \( \epsilon = 1/2 \).

3.1. Integration of the diffusion equation

For convenience we rewrite here the diffusion equation

\[
\frac{\partial f_0(p,t)}{\partial t} = \frac{\partial}{\partial p} \left( D(p,t) \frac{\partial f_0(p,t)}{\partial p} \right),
\]

and the diffusion coefficient for the case of the HMF model with an even and single humped distribution function

\[
D(p,t) = \frac{2 \chi(t) \omega_1(t)}{p^2 + \omega_1^2(t)}.
\]

Equation (15) determines the value of \( \omega_1(t) \), while \( \chi(t) \) evolves according to equation (17). It follows that the time scale of the dynamics of the diffusion equation depends on the chosen initial value \( \chi(0) \). We want to be sure that, independently from this value, provided that it is sufficiently small for the QL approximation to be valid, the final distribution is practically the same. We provide details about this by showing the diffusion equation results for the initial Gaussian distribution. Before proceeding with the results, let us clarify the following point. We have already remarked that when \( \omega_1(t) \) reaches the value 0 the diffusion equation stops, in the sense that \( f_0(p,t) \) does not evolve any more in time, as can be easily seen from equations (37) and (38)\(^\text{10} \). In our numerical integrations of the diffusion equation we have therefore stopped the integration when, within machine precision, \( \omega_1(t) \) vanishes and \( f_0(p,t) \), for all \( p \) values where

\(^{10} \text{Although the diffusion coefficient } D(p,t) \text{ is not uniformly small for } p \sim 0 \text{ when } \omega_1(t) \text{ tends to 0, the quantity } D(p,t) \left( \frac{\partial f_0(p,t)}{\partial p} \right) \text{ is uniformly bounded, actually tending to 0 for } p \to 0, \text{ since, as we have proved above, the equality } \frac{\partial f_0(p,t)}{\partial p} \big|_{p=0} = 0 \text{ is conserved by the diffusion equation.} \)
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it is not negligible, does not change any more. The obtained function $f_0$ would then be the final distribution of the diffusion equation.

In figure 1 we show the evolution of $\omega_I(t)$ and of $\chi(t)$ as determined by the diffusion equation (37) together with equations (38), (15) and (17), for two different initial values of $\chi(0)$. The initial distribution function is the Gaussian (34) at $T = 1/\beta = 0.38$. Left panel: $\chi(0) = 10^{-6}$; right panel: $\chi(0) = 10^{-2}$. For graphical convenience, in both cases a multiple of $\chi(t)$ is plotted.

Figure 1. Evolution of $\omega_I(t)$ and of $\chi(t)$ as determined by the diffusion equation (37) together with equations (38), (15) and (17), for two different initial values of $\chi(0)$. The initial distribution function is the Gaussian (34) at $T = 1/\beta = 0.38$. Left panel: $\chi(0) = 10^{-6}$; right panel: $\chi(0) = 10^{-2}$. For graphical convenience, in both cases a multiple of $\chi(t)$ is plotted.

Figure 2. Left panel: the final distribution functions $f_0(p)$, obtained when $\omega_I(t)$ vanishes, for the two cases plotted in figure 1. They are indistinguishable. Right panel: the initial ($f_{in}$) and the final ($f_0$) distributions. We have also added an intermediate distribution (dashed line) to illustrate the progressive formation of the plateau. The distribution function is normalized such that $\int f(\theta, p) d\theta dp = 1$ and $2\pi \int f(p) dp = 1$.

Figure 2. Left panel: the final distribution functions $f_0(p)$, obtained when $\omega_I(t)$ vanishes, for the two cases plotted in figure 1. They are indistinguishable. Right panel: the initial ($f_{in}$) and the final ($f_0$) distributions. We have also added an intermediate distribution (dashed line) to illustrate the progressive formation of the plateau. The distribution function is normalized such that $\int f(\theta, p) d\theta dp = 1$ and $2\pi \int f(p) dp = 1$.

it is not negligible, does not change any more. The obtained function $f_0$ would then be the final distribution of the diffusion equation.

In figure 1 we show the evolution of $\omega_I(t)$ and of $\chi(t)$, according to the diffusion equation, starting from an initial $f_0(p,0)$ given by the Gaussian (34) at temperature $T = 1/\beta = 0.38$, corresponding, for $m = 0$, to $\epsilon = 0.69 < \epsilon_c$. The left and right panels refer to the integration with initial values $\chi(0) = 10^{-6}$ and $\chi(0) = 10^{-2}$ respectively.

We see that the evolutions are qualitatively different. In particular, the convergence towards a stationary solution ($\omega_I = 0$) is more rapid when $\chi(0)$ is large. However, the distribution $f_0(p)$ obtained at the end of the evolution does not depend on $\chi(0)$. In the left panel of figure 2 we plot this distribution for both cases. It is evident that the two final distributions actually plotted are virtually indistinguishable\textsuperscript{11}. In the right panel we plot the initial and the final distributions. This figure suggests that the form of the final distribution is not very different from a Gaussian, except in the central

\textsuperscript{11} We note that the final values of $\chi$ are different in the two cases (by a factor 10) even if this difference has been reduced with respect to the initial condition.
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region, where a sort of flat region seems to have developed. This can be understood as follows. In the core of the distribution $p \ll 1$, the diffusion coefficient can be approximated by $D(p, t) \approx 2\chi(t)/\omega_I(t)$. Since $\omega_I(t)$ decreases to 0, the diffusion coefficient in the core becomes very large and this implies $\partial f_0(p, t)/\partial p \approx 0$, so that the distribution function in the core forms a plateau (we may note that the formation of this plateau is consistent with the fact that the diffusion equation conserves the property that $\partial f_0(p, t)/\partial p|_{p=0} = 0$ strictly). On the other hand, in the tail of the distribution $p \gg 1$, the diffusion coefficient can be approximated by $D(p, t) \approx 2\chi(t)\omega_I(t)/p^2$. Since $\omega_I(t)$ decreases to 0, and since $p \gg 1$, the diffusion coefficient in the tail is very small and this implies $\partial f_0(p, t)/\partial t \approx 0$, so that the distribution function in the tail does not evolve substantially. As a matter of fact, under the assumption that the final distribution has a Gaussian structure apart from a central region, which is flat, it is possible to obtain its parameters exactly. Such an assumption is equivalent to assuming that the diffusion equation gradually develops a flat portion in the central part of the distribution, while maintaining the Gaussian form outside that portion. The possibility to derive this distribution exactly stems from the fact that there are as many equations to satisfy as parameters characterizing the distribution. In fact, the assumed form can be written as

$$f_{mG}(p) = \begin{cases} C & |p| \leq p_1, \\ Ae^{-\beta \frac{p^2}{2}} & |p| \geq p_1, \end{cases}$$

(39)

where the subscript denotes a ‘modified Gaussian’, and where $p_1 \geq 0$. Continuity implies that $C = Ae^{-\beta \frac{p_1^2}{2}}$. Therefore, there are three parameters to be determined, i.e. $A$, $\beta$ and $p_1$. On the other hand, there are also three equations to satisfy. They are the normalization, the marginal stability of the distribution, and the relation expressing the average kinetic energy:

$$2\pi \int dp f_{mG}(p) = 1,$$

(40)

$$1 + \pi \int dp \frac{f'_{mG}(p)}{p} = 0,$$

(41)

$$2\pi \int dp \frac{p^2}{2} f_{mG}(p) = \epsilon_{kin},$$

(42)

where $\epsilon_{kin}$ is the final average kinetic energy, determined numerically from the distribution at the end of the integration. In appendix E we show how to solve this system of equations for $A$, $\beta$ and $p_1$.

In figure 3 we show the comparison, for the energies $\epsilon = 0.69$ and $\epsilon = 0.65$, between the final distribution of the diffusion equation and the approximation with a modified Gaussian. It is evident that for the larger energy the approximation with a modified Gaussian is rather good, while for the smaller energy there is a clear difference in the region of the plateau.
3.2. The N-body simulations and the comparison with the results of the diffusion equation

In this section, we compare the results of the QL theory with the results of \( N \)-body simulations. We begin the analysis by showing the evolution of the magnetization for both the diffusion equation and the \( N \)-body simulations. These simulations have been performed with \( N = 2^{18} \) particles. As remarked above, for the diffusion equation the magnetization can be computed using equation (36), obtaining the kinetic temperature at time \( t \) from the variance of \( f_0(p, t) \) using equation (22).

Let us first comment on the comparison between the time scales in the two dynamical evolutions. As explained above, and as evidenced in figure 1, the time scale of the dynamics of the diffusion equation depends strongly on the initial value \( \chi(0) \). This is of course reflected in the temporal evolution of the magnetization.

In figure 4, we plot the dynamics of the magnetization as obtained from the diffusion equation for the Gaussian initial condition with energy \( \epsilon = 0.69 \) for the two cases of figure 1, i.e. \( \chi(0) = 10^{-6} \) and \( \chi(0) = 10^{-2} \). We see that the final magnetization is the same in both cases, as expected from the fact that the final distributions are the same, although the time scale is different. In the diffusion equation, \( \chi(0) \) is related to the initial perturbation to the stationary but Vlasov unstable distribution \( f_0(p, 0) \). It therefore depends on the order of magnitude of \( f_1^2(\theta, p, 0) \) in equation (6). In the \( N \)-body simulation, this role is played by the finite size effects in the initial conditions determined according to \( f_0(p, 0) \). From the definition of \( \chi(t) \), given implicitly by the comparison of equations (A.33)–(A.35), it is clear that the order of magnitude of \( \chi(0) \) is that of \( f_1^2(\theta, p, 0) \). In turn, in the \( N \)-body simulations we expect that the order of magnitude of \( f_1(\theta, p, 0) \), due to finite size effects, is \( N^{-\frac{3}{2}} \). Therefore, we expect that the simulations performed with \( N = 2^{18} = 0.262144 \times 10^6 \) particles should evolve, as far as the relaxation to the stationary state is concerned, on a time scale similar to that of the diffusion equation with a value of \( \chi(0) \) of the order \( 10^{-6} \). In figure 5 we show that this is indeed the case. We stress, however, that the \( N \) dependence of this time scale which is due to the dynamical instability of the initial state is expected to behave like \( \log N \), contrary to the power law dependence occurring for the slow evolution in the QSS due to collisional effects [4, 39].
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The analysis of figure 5 puts in evidence several important things. Firstly, there is no perfect agreement on the final value of the magnetization, which is about 0.057 for the diffusion equation and about 0.10 for the \( N \)-body simulation. However, these magnetization values are comparable, and they are substantially different from that of the BG equilibrium state corresponding to \( \epsilon = 0 \), which is about 0.31. On the other hand, the left panel shows that in the state reached by the \( N \)-body system at the end of the fast relaxation the magnetization has relevant oscillations. Therefore the system is not in a proper QSS, although one could extend the definition of such a state also to cases that present these oscillations. The QL theory does not account for these oscillations because they appear in the regime where the system is dynamically stable. They may correspond to small perturbations about a stable steady state of the Vlasov equation. A possibility is that these oscillations will decay by Landau damping. Another possibility considered in [16] is that these oscillations will survive during the whole collisionless regime, like in the simulations performed by Morita and Kaneko [40]. Apart from the presence of the oscillations, we conclude that, at the level of the final magnetization value, there is a reasonable but not a perfect agreement between the full \( N \)-body simulation and the approximation represented by the QL theory since, in relative terms, the difference is large. However, we have to consider that for such small values of the magnetization, a very small change in \( T \) causes a strong variation in \( m \), since the derivative of \( m \) with respect to \( T \), which can be computed from equation (36), diverges as \( \frac{dm}{dT} = \frac{1}{2}(T - 2\epsilon + 1)^{-1/2} \) for \( T \rightarrow 2\epsilon - 1 \). As a matter of fact, while the temperature of the QSS of the \( N \)-body simulation is about 0.390, the temperature of the final state of the diffusion equation is about 0.383. At this energy, \( T \) is about 0.475 at BG equilibrium. Therefore the relative error in the temperature value of the QSS is much smaller than the error in the magnetization.

Let us now compare the velocity distribution functions of the QSS reached in the \( N \)-body simulation and the final distribution function of the diffusion equation\(^{12}\). In figure 6 we show this comparison for the two cases of \( \epsilon = 0.725 \) and \( \epsilon = 0.69 \) for

\( \chi(0) = 10^{-6} \). Right panel: \( \chi(0) = 10^{-2} \).

The analysis of figure 5 puts in evidence several important things. Firstly, there is no perfect agreement on the final value of the magnetization, which is about 0.057 for the diffusion equation and about 0.10 for the \( N \)-body simulation. However, these magnetization values are comparable, and they are substantially different from that of the BG equilibrium state corresponding to \( \epsilon = 0.69 \) which is about 0.31. On the other hand, the left panel shows that in the state reached by the \( N \)-body system at the end of the fast relaxation the magnetization has relevant oscillations. Therefore the system is not in a proper QSS, although one could extend the definition of such a state also to cases that present these oscillations. The QL theory does not account for these oscillations because they appear in the regime where the system is dynamically stable. They may correspond to small perturbations about a stable steady state of the Vlasov equation. A possibility is that these oscillations will decay by Landau damping. Another possibility considered in [16] is that these oscillations will survive during the whole collisionless regime, like in the simulations performed by Morita and Kaneko [40]. Apart from the presence of the oscillations, we conclude that, at the level of the final magnetization value, there is a reasonable but not a perfect agreement between the full \( N \)-body simulation and the approximation represented by the QL theory since, in relative terms, the difference is large. However, we have to consider that for such small values of the magnetization, a very small change in \( T \) causes a strong variation in \( m \), since the derivative of \( m \) with respect to \( T \), which can be computed from equation (36), diverges as \( \frac{dm}{dT} = \frac{1}{2}(T - 2\epsilon + 1)^{-1/2} \) for \( T \rightarrow 2\epsilon - 1 \). As a matter of fact, while the temperature of the QSS of the \( N \)-body simulation is about 0.390, the temperature of the final state of the diffusion equation is about 0.383. At this energy, \( T \) is about 0.475 at BG equilibrium. Therefore the relative error in the temperature value of the QSS is much smaller than the error in the magnetization.

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\(^{12}\) During the oscillations of the magnetization after the fast relaxation, the variations between the velocity distribution functions obtained from the \( N \)-body simulations are much smaller than the difference shown with respect to the distribution function obtained from the QL diffusion equation. Although these variations are very small, in the figures, instead of plotting a snapshot of the \( N \)-body simulation velocity distribution function, an average over a suitable time window is made.

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the initial Gaussian distribution. We observe a very good agreement for the energy \( \epsilon = 0.725 \) which is closer to the instability threshold \( \epsilon_c = 3/4 \). For the case \( \epsilon = 0.69 \), there is a very good agreement in the tail of the distribution but a disagreement concerns the central region of the distribution. The distribution function obtained from the diffusion equation clearly exhibits a central plateau, while there is only the hint of a plateau in the distribution function obtained from the \( N \)-body simulation. We also note that the QL theory predicts that the central distribution function \( f(0, t) \) decreases\(^{13}\)

\[^{13}\text{This is consistent with the notion of ‘coarse-graining’. The maximum value of the coarse-grained distribution can only decrease with phase mixing [13].}\]

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\[\text{Figure 5.} \quad \text{Magnetization as a function of time at energy} \ \epsilon = 0.69 \ \text{for a homogeneous Gaussian velocity initial distribution. Both the} \ N\text{-body simulation with} \ N = 2^{18} \ \text{particles (black) and the diffusion equation (red) curves are shown (we have taken} \ \chi(0) = 10^{-6} \ \text{, which provides the best fit to the data and is consistent with our order of magnitude estimate of} \ \chi(0) \sim 1/N \ \text{based on the value of} \ N \text{). Left panel: plot of the magnetization during the whole duration of the simulation. Right panel: plot of the magnetization during the early times of the simulation. In the diffusion equation, the magnetization remains constant at times larger than those computed since the evolution stops when} \ \omega_I(t), \ \text{and consequently} \ D(p, t), \ \text{reaches the value 0.}\]

\[\text{Figure 6.} \quad \text{The final distribution function} \ f_0(p) \ \text{of the diffusion equation and the velocity distribution} \ f_{Nb}(p) \ \text{of the QSS of the} \ N\text{-body simulation, starting from a Gaussian initial distribution. Left panel:} \ \epsilon = 0.725. \ \text{Right panel:} \ \epsilon = 0.69. \ \text{We have also plotted the initial condition} \ f_{in}(p) \ \text{for comparison. We emphasize that the initial distribution is Vlasov unstable while the final distribution is (marginally) Vlasov stable even when the profile does not seem to have changed a lot (left panel).}\]
with respect to its initial value (see figure 2), in qualitative agreement with the $N$-body simulation, although the decrease is stronger in the $N$-body simulation.

We note that the distribution of the QSS obtained from $N$-body simulations and the distribution predicted by the QL theory have a form very similar to the initial distribution. Actually, the distribution function almost does not change in the tail of the distribution. Nevertheless, the slight change in the central region (core) is crucial because the initial distribution is Vlasov unstable while the QSS and the distribution predicted by the QL theory are Vlasov stable. Therefore, close to the instability threshold, stability can be regained by a very slight modification of the distribution function that essentially affects the core of the distribution (small velocities) while preserving the tail (large velocities).

3.3. The effective nonequilibrium phase transition predicted by the QL theory

In [16] we studied the evolution of several unstable homogeneous initial conditions in situations where the Lynden-Bell theory fails to predict with good approximation the QSS reached by the system. We found that, in most of these cases, the QSS could be well approximated by a polytropic distribution. Furthermore, the index of the polytrope, even if it was not possible to predict if from first principles, happened to be the same for a given class of initial conditions (e.g. Gaussian, semi-elliptical...) for a wide range of energies. However, we remarked that the polytropic approximation was not good for energies close to the instability threshold pertaining to the class of the initial distribution. We have seen here that, in this case, the QL theory provides a better approximation. In fact, we have seen that the final distribution computed by the QL theory is close to the angle-averaged distribution of the QSS obtained in the $N$-body simulations. Furthermore, the values of the kinetic temperature and magnetization predicted by the QL theory are relatively close to those obtained from the direct $N$-body simulations, even if the quality of the agreement deteriorates if we are too far away from the instability threshold.

To give an easily grasped quantitative meaning to this agreement/disagreement, we plot in figure 7 the kinetic temperature and magnetization of the final distribution of the QL theory as a function of the energy for the Gaussian initial distribution. The plots also show the kinetic temperature and the magnetization of the QSS reached in the $N$-body simulation at the same energy. Although the magnetization of the QL theory is different from that of the simulation, they both become virtually indistinguishable from zero at some energy $\epsilon_t$ strictly smaller than $\epsilon_c$. The energy $\epsilon_t$ defines a phase transition from the unmagnetized state ($m = 0$) to the magnetized state ($m \neq 0$). This phase transition is well predicted by the QL theory. We stress that this is to be interpreted as a nonequilibrium phase transition, since it refers to the magnetization of the out-of-equilibrium QSSs. We can conclude that the QL theory is able to localize this phase transition correctly. A more detailed discussion is provided in the following section.

We stress that the abovementioned phase transition is only an empirical phase transition, i.e. a transition from a state in which the magnetization is substantially different from zero to a state in which the magnetization is practically equal to zero. However, rigorously speaking, this is not a mathematical phase transition—because, as argued below,
the magnetization is strictly positive below $\epsilon_c$. We can give two arguments for this. In the framework of the QL theory, equations (27) and (36) imply that the magnetization strictly increases during the evolution of the diffusion equation at any given energy smaller than $\epsilon_c$. Therefore, the magnetization cannot be exactly equal to zero below $\epsilon_c$ even if we find that in the interval $[\epsilon_t, \epsilon_c]$ the magnetization corresponding to the final distribution $f_0(p)$ of the diffusion equation is virtually indistinguishable from zero, in agreement with the results of the N-body simulations. On the other hand, another theory based on amplitude equations (see, e.g. [33, 34]) predicts a nonvanishing but very small magnetization if the initial state is very weakly unstable. In that case, $m$ is nonzero below $\epsilon_c$ but scales as $(\epsilon_c - \epsilon)^2$ for $\epsilon \to \epsilon_c$. This may account for the very small magnetization (smaller than $10^{-4}$), almost indistinguishable from zero, in the interval $[\epsilon_t, \epsilon_c]$. In appendix F we give a few more details on this approach. In the following, we shall interpret our numerical results as exhibiting an effective (empirical) out-of-equilibrium phase transition at $\epsilon_t$, but the reader should be warned that, strictly speaking, this is not a true mathematical transition since the QSSs below $\epsilon_c$ are always magnetized.

4. Comparison of the QSS with the prediction of the QL theory and with the polytropic fit

4.1. Caloric and magnetization curves

In this section, we compare the caloric curve obtained from direct N-body simulations of the HMF model, starting from a homogeneous Gaussian distribution, with the prediction of the QL theory and with the polytropic fit considered in our previous papers [16, 20].

The caloric curve $T(\epsilon)$ is represented in figure 8 and the magnetization curve $m(\epsilon)$ is represented in figure 9. We recall that, for a given energy $\epsilon$, the kinetic temperature $T$ is related to the magnetization by equation (36). Therefore, these two curves are equivalent. The non-magnetized branch $m = 0$ in figure 9 corresponds to the line $T = 2\epsilon - 1$ in figure 8.
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In these curves, the solid line denoted BG corresponds to the Boltzmann–Gibbs caloric curve. It describes the statistical equilibrium state of the system, reached for \( t \to +\infty \), as a result of a collisional evolution (finite \( N \)-effects). Although this curve is not physically relevant to the interpretation of QSSs, which are out-of-equilibrium structures, it is plotted for comparison. It also determines the domain of stability/instability of the initial condition that is a homogeneous Gaussian distribution.

The bullets are the results of direct \( N \)-body simulations. They form the ‘experimental’ caloric curve. It is made of QSSs reached as a result of a violent collisionless relaxation (Vlasov dynamics). This is the curve that we have to explain. This curve presents several striking features that were considered as a ‘surprise’ in the early works on the HMF model [7, 41]: (i) it differs from the BG caloric curve for intermediate energies; (ii) it presents a region of negative specific heats \( C_{\text{kin}} = d\epsilon/dT < 0 \) (unlike the BG caloric curve); (iii) the system remains homogeneous (non-magnetized) slightly below the BG critical energy \( \epsilon_c = 3/4 \). Although many things have been understood on the physics of systems with long-range interactions [1–6] since the original works on the HMF model (in particular the difference between QSSs and true equilibrium states), we believe that the HMF model has still not revealed all its secrets. In particular, the precise nature of the QSSs, the reason for the region of negative specific heats, and the shift of the transition point are still not clearly understood. These are the questions that initiated the topic more than 20 years ago and that still have not found a definitive answer. We stress that the caloric curve of figure 8 cannot be explained by Lynden-Bell’s theory.

Figure 8. Caloric curve of the HMF model for a spatially homogeneous Gaussian initial condition (BG: Boltzmann–Gibbs states; bullets: results of \( N \)-body simulations; dashed line: prediction of the QL theory; \( n = 2 \): polytropic fit).

Figure 9. Magnetization curve of the HMF model for a spatially homogeneous Gaussian initial condition.

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The quasilinear theory in the approach of long-range systems to quasi-stationary states as pointed out in our previous work [16]. We shall interpret this curve in relation to
the QL theory and to polytropic (Tsallis) distributions.

The dashed line corresponds to the prediction of the QL theory. It is obtained
by solving the diffusion equation (37) until its convergence towards a steady state
(expected to represent the angle-averaged QSS). From the obtained velocity distribution $f_0(p)$, we can compute the kinetic temperature $T$ from equation (22) and, using equation (36), we can obtain the corresponding magnetization $m$.

The solid line denoted ‘$n = 2$’ corresponds to the caloric curve obtained by assuming that the QSSs are polytropes of index $n = 2$. This caloric curve exhibits a region of negative specific heats with $C_{\text{kin}} = -5/2$. We emphasize that we do not have any theory to predict why the QSSs should be polytropic (Tsallis) distributions and why their index should be $n = 2$ for a Gaussian initial distribution. However, as shown in [16], and confirmed below, polytropes of index $n = 2$ give a remarkable fit to the QSSs for a wide range of energies.

Let us now describe the curves of figures 8 and 9. For $\epsilon > \epsilon_c = 3/4 = 0.75$, the homogeneous Gaussian distribution is stable (dynamically and thermodynamically), so the system does not evolve (even on a collisional timescale). For $\epsilon < \epsilon_c$, the homogeneous Gaussian distribution is dynamically (Vlasov) unstable and the system rapidly evolves towards a QSS. The $N$-body simulations show that the QSS is homogeneous for $\epsilon_{\text{Nb}} < \epsilon < \epsilon_c$ and that it becomes magnetized for $\epsilon < \epsilon_{\text{Nb}}$ with $\epsilon_{\text{Nb}} \simeq 0.735$ (this is most clearly seen on the magnetization curve of figure 9). The QL theory predicts that the QSS is homogeneous for $\epsilon_{\text{QL}} < \epsilon < \epsilon_c$ and that it becomes magnetized for $\epsilon < \epsilon_{\text{QL}}$ with $\epsilon_{\text{QL}} \simeq 0.735$. We observe that $\epsilon_{\text{QL}} \simeq \epsilon_{\text{Nb}}$ in good approximation so the QL theory correctly predicts the energy threshold $\epsilon_t \simeq \epsilon_{\text{QL}} \simeq \epsilon_{\text{Nb}} \simeq 0.735$ below which the QSSs become magnetized (i.e. depart from the line of homogeneous states). This is a non-trivial prediction of the QL theory. The polytropic caloric curve of index $n = 2$ exhibits a transition energy $\epsilon_{n=2} = 2/3 \simeq 0.666$, but this is not a prediction since we have no way to say a priori why the polytropic index should be $n = 2$ without doing an $N$-body numerical simulation and making a fit by a polytrope [16]. By contrast, the result of the QL theory is a prediction since it does not rely on a direct $N$-body simulation of the HMF model; it is directly obtained from the diffusion equation (37). On the other hand, the transition energy $\epsilon_{\text{QL}} \simeq 0.735$ predicted by the QL theory is in much better agreement with the ‘experimental’ results than the transition energy $\epsilon_{n=2} = 2/3 \simeq 0.666$ corresponding to the $n = 2$ polytropic fit. Indeed, the points of the $N$-body simulation (QSSs) depart from the homogeneous branch ($m = 0$) long before the energy $\epsilon_{n=2}$ (the $N$-body simulation shows that the transition between un-magnetized and magnetized

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states occurs at $\epsilon_{Nt} = 0.735$ which is sensibly larger than $\epsilon_{n=2} = 2/3 \approx 0.666$). In addition, for $\epsilon > \epsilon_{n=2}$ the caloric curve predicted by the QL theory gives a much better agreement with the results of the $N$-body simulation than the caloric curve of an $n = 2$ polytrope that predicts $m = 0$. By contrast, for $\epsilon < \epsilon_{n=2}$ the situation is reversed. In that case, the $n = 2$ polytropes provide a much better agreement with the $N$-body simulation than the QL theory. This is revealed not only by the values of the magnetization and kinetic temperature, which are very close to the numerical ones, but also by the distribution function itself as discussed in section 4.2. Therefore, we conclude that the QL theory works well close to the critical energy $\epsilon_c$ (in particular, it is able to predict the \textit{shift} $\Delta \epsilon = \epsilon_t - \epsilon_c = -0.015$ of the transition energy from un-magnetized to magnetized QSSs) while the polytropic fit works well at lower energies $\epsilon < \epsilon_{n=2}$ (in particular it is able to account for the region of negative specific heats). These results, which were foreseen in \cite{16}, represent an improvement in the understanding of the caloric curve of figure 8. However, everything is still not understood. First, we do not know \textit{why} the QSSs are so well-fitted by polytropic (Tsallis) distributions of index $n = 2$ (this is a property of incomplete mixing but it is not clear how one can predict the efficiency of mixing \cite{12}). Second, even if the QL theory is qualitatively correct close to $\epsilon_c$, it does not give a perfect agreement with the results of the $N$-body simulations.

4.2. Velocity distribution functions

In this section, we compare the velocity distribution functions obtained from the $N$-body simulations, the QL theory, and the $n = 2$ polytropic fit for two different energies.

We first consider an energy $\epsilon = 0.69$ close to the critical point $\epsilon_c = 3/4 = 0.75$. The velocity distributions are plotted in figure 10. As already discussed in section 3.2, we find a relatively good agreement between the QL theory and the $N$-body simulation. This is of course consistent with the discussion of section 4.1 where we showed that the QL theory works well for weakly inhomogeneous systems. We note that the tail of the distribution function has almost not evolved and coincides with the initial Gaussian distribution (see figure 6). Only the core of the distribution has changed in order to make the system dynamically stable. The relatively good agreement between the QL
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theory and the N-body simulation is confirmed by the values of the kinetic temperature and magnetization. We find \( T_{\text{QL}} = 0.383 \) and \( m_{\text{QL}} = 0.057 \) to be compared with \( T_{\text{Nb}} = 0.390 \) and \( m_{\text{Nb}} = 0.1 \). On the other hand, the fit by a polytrope \( n = 2 \) is not good\(^{17} \). The main reason is that the velocity distribution of the polytrope \( n = 2 \) has a compact support that is in contradiction with the infinite extension of the Gaussian tail of the QSS. The disagreement between the \( n = 2 \) polytrope and the \( N \)-body simulation is confirmed by the values of the kinetic temperature and magnetization. We find \( T_{\text{poly}} = 0.38 \) and \( m_{\text{poly}} = 0 \) (homogeneous) to be compared with \( T_{\text{Nb}} = 0.390 \) and \( m_{\text{Nb}} = 0.1 \) (inhomogeneous).

We now consider a lower energy \( \epsilon = 0.6 \). The velocity distributions are plotted in figure 11. In that case, the situation is reversed. We observe a remarkable agreement between the velocity distribution of the QSS reached in the \( N \)-body simulation and the velocity distribution of a polytrope \( n = 2 \).\(^{18} \) The distribution function has substantially evolved from the initial Gaussian distribution and has acquired a compact support, which is a property of polytropic (Tsallis) distribution with index \( n \geq 1/2 \) [16, 20]. As discussed in [16], this ‘confinement’ is a manifestation of an incomplete relaxation (the distribution function predicted by the Lynden-Bell theory, which corresponds to the most mixed state, never has a compact support). The excellent agreement between the \( N \)-body simulation and the \( n = 2 \) polytropic fit is confirmed by the values of the kinetic temperature and magnetization. We find \( T_{\text{poly}} = 0.357 \) and \( m_{\text{poly}} = 0.396 \) to be compared with \( T_{\text{Nb}} = 0.360 \) and \( m_{\text{Nb}} = 0.40 \). On the other hand, the prediction of the QL theory is not good. The main reason is that this distribution has a Gaussian tail, similarly to the initial condition, that is in contradiction with the compact support of the QSS. The disagreement between the QL theory and the \( N \)-body simulation is confirmed by the values of the kinetic temperature and magnetization. We find \( T_{\text{QL}} = 0.265 \) and \( m_{\text{QL}} = 0.255 \) to be compared with \( T_{\text{Nb}} = 0.360 \) and \( m_{\text{Nb}} = 0.40 \).

\(^{17} \) For \( \epsilon = 0.69 > \epsilon_{\text{cr}} = 2/3 \approx 0.666 \) the polytrope \( n = 2 \) is homogeneous, so it is not necessary to average the polytropic distribution function over the angles.

\(^{18} \) For \( \epsilon = 0.6 < \epsilon_{\text{cr}} = 2/3 \approx 0.666 \) the polytrope \( n = 2 \) is inhomogeneous and, in order to obtain the velocity distribution \( f(p) \), we have integrated the polytropic distribution function \( f(\theta, p) \) over the angles using the theoretical results obtained in [16, 20]. As shown in [16], the excellent agreement between the polytrope \( n = 2 \) and the QSS is also valid for the complete distribution function \( f(\theta, p) = f(\epsilon) \).
At even lower energies (typically $\epsilon < 0.55$), our study in [16] shows that the system takes a core–halo structure. The core corresponds to the pure polytrope $n = 2$, but it is now surrounded by a halo of particles. We note that the presence of the halo does not significantly affect the value of the kinetic temperature and magnetization of the QSS, since a pure $n = 2$ polytrope still gives a rather good fit to the caloric curve and magnetization curve at low energies (see figures 8 and 9).

4.3. Summary and discussion

In summary, for a homogeneous Gaussian initial distribution, we have the following results. For $\epsilon > \epsilon_c$, the system remains in the homogeneous Gaussian distribution, which is stable. For $\epsilon_{n=2} < \epsilon < \epsilon_c$, the QL theory works reasonably well. In particular, it is able to predict the energy $\epsilon_t \simeq 0.735$ marking the transition between unmagnetized and magnetized QSSs. More precisely (i) for $\epsilon_t < \epsilon < \epsilon_c$, the system achieves a homogeneous modified Gaussian distribution with a flat core; (ii) for $\epsilon_{n=2} < \epsilon < \epsilon_t$, the system achieves an inhomogeneous modified Gaussian distribution with a flat core. For lower energies, the QL theory does not work. In that case, we observe that the QSSs are remarkably well fitted by polytropic (Tsallis) distributions with index $n = 2$. They have a compact support. For $\epsilon < \epsilon_{n=2}$, the stable polytropic distributions are inhomogeneous. These polytropic distributions are able to account for the region of negative specific heats in the out-of-equilibrium caloric curve, unlike the Boltzmann distribution and (presumably) the Lynden-Bell distribution, and unlike the QL theory. At even lower energies, the system takes a core–halo structure, with a polytropic core and a halo of particles.

The QL theory and the polytropic fit have different, but well-defined, domains of validity. This may be qualitatively understood as follows. The QL theory is based on the assumption that the system remains slightly inhomogeneous during its evolution from the initial condition to the QSS (weak mixing). Therefore, the QL theory is expected to be valid close to the instability threshold $\epsilon_c$. In that case, the distribution function does not substantially change from the initial condition. It just changes a little in such a manner as to become dynamically (Vlasov) stable19. As we have seen, this change only concerns the core of the distribution, which becomes flatter and wider ("hotter"). The tail of the distribution does not change and remains Gaussian, as the initial state. When we depart significantly from the instability threshold, the evolution of the system is expected to be more violent, and the system is expected to be strongly inhomogeneous (strong mixing). In that case, the distribution function is expected to change substantially from the initial condition. This is the regime where the Lynden-Bell [13] theory should apply in principle. However, it turns out that, in many cases, the relaxation to the Lynden-Bell statistical equilibrium state is incomplete [12]. In case of incomplete relaxation, polytropic distributions may provide a good fit of the

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19 This is the stabilization mechanism of the QL theory. The initial condition $f_0(p,t=0)$ is dynamically unstable, meaning that the complex pulsation $\omega_I(t=0)$ is strictly positive. Qualitatively, this is because the velocity dispersion (kinetic temperature) is too low (see equation (33)). The initially positive complex pulsation $\omega_I(t=0) > 0$ causes the distribution function to diffuse (see equations (37) and (38)). By diffusing, the distribution function spreads and its velocity dispersion increases. As a result, the complex pulsation $\omega_I(t)$ decreases (see equation (31)). The diffusion stops when $\omega_I(t)$, hence $D(p,t)$, vanishes, leading the system to a Vlasov stable, or marginally stable, QSS.
QSS because they have a compact support that is typical of an incomplete relaxation (in case of incomplete relaxation, high energy states are less populated than what is predicted from the statistical theory of Lynden-Bell) [16, 20, 42]. This is probably why the polytropic fit works well for low values of the energy. In that case, the distribution function changes from an initial Gaussian to a polytrope with a compact support.

5. Conclusion

In this work, we have considered the QSSs of long-range systems that are reached when the system is initially in a Vlasov unstable spatially homogeneous state, using the paradigmatic HMF model. The Vlasov equation admits an infinity of stable stationary states, each of them representing a possible QSS of the $N$-body system. The prediction of the QSS reached by any given initial unstable state is still practically an unsolved problem although progress has been done lately [1–6]. The Lynden-Bell theory [13] is, in a sense, conceptually satisfying, since it is based—as the equilibrium Boltzmann–Gibbs theory—on the assumption of complete mixing of the dynamics. The differences between the Boltzmann theory and the Lynden-Bell theory come from the difference in the number of integrals of motion between the full $N$-body dynamics (collisional) and the Vlasov dynamics (collisionless). In particular, the Vlasov equation conserves an infinite number of Casimir integrals that must be accounted for in the Lynden-Bell theory. This leads to a great difficulty in the concrete application of the Lynden-Bell theory to generic initial conditions, but—at least in principle—one has the tool to determine the QSS as a function of the initial state. Unfortunately, the basic assumption of the Lynden-Bell theory, i.e. complete mixing, seems very far from being satisfied in general [12]. Without this starting point, the construction of alternative theories is conceptually more difficult, since it is not yet possible to quantify in a sensible way the departure from complete mixing, and even if it were possible, it would still be uncertain how to translate it in a theory of the dynamical behavior of the system. Thus, for the moment one can only resort to semi-empirical approaches. In [16] we have proposed, in the absence of complete mixing, to substitute the Lynden-Bell entropy with other Casimirs of the Vlasov equation, e.g. the Tsallis entropy leading to polytropic QSSs. This is, however, essentially empirical—because we have no way to predict a priori if the QSS will be a polytrope and, if so, what the value of the polytropic index will be. However, the polytropic fit works remarkably well for a wide range of energies, sufficiently far from the instability threshold, and the polytropic index appears to be relatively universal [16] for a given class of initial conditions. Another proposal has been given in [43] where a core–halo structure of the QSS was hypothesized from the start. We showed in [16] that our approach based on polytropic distributions is consistent with this core–halo approach, and generalizes it. At low energies, we find that the QSS has a core–halo structure with a polytropic core surrounded by a halo of equivalence of the initial condition ($n = 2$ for Gaussian, $n = 1$ for semi-elliptical and $n = 1/2$ for waterbag) remains relatively mysterious. Also mysterious is the fact that the collisional evolution of the system can be fitted by a sequence of polytropic distributions with a time-dependent index $n(t)$ both in the homogeneous [39] and in the inhomogeneous [16] phase. These exciting results represent some of the last unsolved mysteries of long-range systems.

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20 The quality of the polytropic fit is impressive, and the universality of the polytropic index for some classes of equivalence of the initial condition ($n = 2$ for Gaussian, $n = 1$ for semi-elliptical and $n = 1/2$ for waterbag) remains relatively mysterious. Also mysterious is the fact that the collisional evolution of the system can be fitted by a sequence of polytropic distributions with a time-dependent index $n(t)$ both in the homogeneous [39] and in the inhomogeneous [16] phase. These exciting results represent some of the last unsolved mysteries of long-range systems.
particles. In the case of waterbag initial conditions (which correspond to polytropes of index \( n = 1/2 \)) we recover the ‘uniform’ core–halo structure found in [43]^{21}. For other initial conditions, we obtain more general ‘polytropic’ core–halo structures. In the present work, we have developed a QL theory that has proven to work with good approximation close to the instability threshold, i.e. in the energy range where the polytropic fit proposed in [16] is not good. Contrary to time-independent approaches that try to predict the form of the distribution of the QSS either by the optimization of a functional or by an assumption about the form of its analytical expression, the QL theory requires solving a dynamical (diffusion) equation that smoothes out the Vlasov equation^{22}. The first approaches are implicitly based on the assumption that the evolution of the system is violent and strongly inhomogeneous, so that a change of structure of the initial distribution function occurs. The QL theory, on the other hand, is based on the assumption that the distribution remains almost homogeneous throughout the transition from the initial distribution to the QSS. The first approaches are expected to work if the instability of the initial distribution is strong, i.e. if the initial condition is far from the instability threshold. The QL theory is expected to work if the instability of the initial distribution is weak, i.e. if the initial condition is close to the instability threshold. These general features have been verified in this work.

We have observed from the results of \( N \)-body simulations, and from the integration of the diffusion equation provided by the QL theory, that below the critical energy \( \epsilon_c \), in a small energy range \( \epsilon_t, \epsilon_c \), the system has a magnetization virtually indistinguishable from zero. On this empirical basis, we considered that the magnetization is equal to zero in this range of energies, and that an out-of-equilibrium phase transition occurs at an energy \( \epsilon_t \) strictly smaller than \( \epsilon_c \). However, we have warned that this is only an effective transition, since the magnetization is strictly positive, although very small. We have seen that in the QL theory the nonvanishing magnetization comes from the strictly positive time derivative of the temperature, see equation (27), and that it is also the consequence of a theory based on amplitude equations in the case of a single mode instability [33, 34]. Thus, the numerical results should not be interpreted as evidencing a rigorous nonequilibrium phase transition, since there should be a very small magnetization in the final state, even close to the critical energy. Clearly, the numerical agreement of the QL theory with the \( N \)-body simulations, for an energy range larger than that in which the magnetization is practically equal to zero, is not affected by this fact. In appendix F we give some details on the approach based on amplitude equations.

Summarizing, the dynamical process leading to a QSS seems to be best described by different approaches depending on the initial state of the system. The Lynden-Bell theory is based on an assumption of efficient mixing (ergodicity) whose validity is hard to establish \textit{a priori}. The polytropic and core–halo fits seem to work well when the Lynden-Bell theory fails. The QL theory is a fully predictive theory that is valid in a perturbative regime close to the instability threshold. These approaches have complementary domains of validity.

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^{21} To some extent, this core–halo structure can be understood from energetic considerations (see figure 34 in [16]).

^{22} Even in the context of the Lynden-Bell theory, it may be necessary to solve a dynamical equation (of a generalized Fokker–Planck form) describing the collisionless coarse-grained dynamics in order to take into account the problem of incomplete relaxation through a space- and time-dependent diffusion coefficient related to the fluctuations of the distribution function, as discussed in [12] and references therein.
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Clearly the QSS reached by the system after the fast relaxation from a Vlasov unstable state could be obtained by numerical integration of the Vlasov equation on a grid, or by numerical integration of the N-body equations of motion that also give the finite N effects. However, this would not reveal anything about the underlying principles determining the dynamics. It was in the search for these principles that the Lynden-Bell theory was introduced (in that case the principle was ‘full mixing’). Alternative, or complementary, approaches follow in the same spirit.

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Appendix A. Derivation of the diffusion equation (7)

In this appendix, we give some technical details concerning the derivation of the diffusion equation (7), starting from equations (2) and (6), and making a QL approximation. We do not aim to be rigorous, nor exhaustive. We refer to the rich plasma physics literature [8, 27–36] for more details, subtleties, and discussions concerning the QL theory.

Substituting equation (6) into the Vlasov equation (2) we get:

\[
\frac{\partial f_0(p,t)}{\partial t} + \frac{\partial f_1(\theta,p,t)}{\partial t} + p \frac{\partial f_1(\theta,p,t)}{\partial \theta} - \frac{\partial \Phi(\theta,t;f_1)}{\partial \theta} \left( \frac{\partial f_0(p,t)}{\partial p} + \frac{\partial f_1(\theta,p,t)}{\partial p} \right) = 0 \quad \text{(A.1)}
\]

We can derive an equation for the time variation of \( f_0 \) by taking the angle average of the last equation. We obtain:

\[
\frac{\partial f_0(p,t)}{\partial t} - \frac{1}{2\pi} \frac{\partial}{\partial p} \int_0^{2\pi} d\theta \frac{\partial \Phi(\theta,t;f_1)}{\partial \theta} f_1(\theta,p,t) = 0 \quad \text{(A.2)}
\]

Using this equation to substitute the time derivative of \( f_0 \) into equation (A.1), we find that:

\[
\frac{\partial f_1(\theta,p,t)}{\partial t} + p \frac{\partial f_1(\theta,p,t)}{\partial \theta} - \frac{\partial \Phi(\theta,t;f_1)}{\partial \theta} \left( \frac{\partial f_0(p,t)}{\partial p} + \frac{\partial f_1(\theta,p,t)}{\partial p} \right)
+ \frac{1}{2\pi} \frac{\partial}{\partial p} \int_0^{2\pi} d\theta \frac{\partial \Phi(\theta,t;f_1)}{\partial \theta} f_1(\theta,p,t) = 0 \quad \text{(A.3)}
\]

Let us now suppose that the following disequality is satisfied during the time evolution:

\[
f_1(\theta,p,t) \ll f_0(p,t) \quad \text{(A.4)}
\]

Then, equation (A.3) can be approximated by keeping only the first order terms in \( f_1 \), i.e.

\[
\frac{\partial f_1(\theta,p,t)}{\partial t} + p \frac{\partial f_1(\theta,p,t)}{\partial \theta} - \frac{\partial \Phi(\theta,t;f_1)}{\partial \theta} \left( \frac{\partial f_0(p,t)}{\partial p} \right) = 0 \quad \text{(A.5)}
\]
The quasilinear theory in the approach of long-range systems to quasi-stationary states which is a linear equation in \( f_1 \) similar to equation (4), but in which \( f_0 \) is not constant in time. The procedure now is to write the solution of this linear equation in \( f_1 \), which depends on \( f_0 \), and to insert it in equation (A.2), to obtain a closed equation for \( f_0 \). We remark the conceptual difference between equation (4) on the one hand, and the pair of equations given by (A.2) and (A.5) on the other hand. In the former case \( f_0(p) \) is a stationary solution of the Vlasov equation (2) and, as such, it is by definition constant in time even if from the proper frequencies of equation (4) we could find that it is unstable. In the latter case, even if solving equation (A.5) we find that \( f_1(\theta, p, t) \) does not have exponential growth, in general \( f_0(p,t) \) defined by equation (A.2) depends on time. To analyze the solution of equation (A.5) we first consider equation (4). Then, we generalize our results to equation (A.5).

The solution of equation (4) is best obtained by decomposing \( f_1(\theta, p, t) \) in Fourier components. To study its \( k \)th Fourier component, we substitute into equation (4) the plane wave expressions

\[
\begin{align*}
  f_1(\theta, p, t) &= a_k(p)e^{i(k\theta - \omega t)}, \\
  \Phi(\theta, t) &= b_k e^{i(k\theta - \omega t)}.
\end{align*}
\]

(A.6)\hspace{1cm} (A.7)

As usual, the physically meaningful solutions are, separately, the real and the imaginary parts of these expressions. The wavenumber \( k \) takes all integer values from \(-\infty\) to \(+\infty\).

Since \( f_1(\theta, p, t) \) and \( \Phi(\theta, t) \) are real, in their Fourier expansion (as in equation (A.24) below) there will be both components with \( k \) and \(-k\). Substituting equation (A.6) and equation (A.7) into equation (4) we get

\[
-i\omega a_k(p) + ipka_k(p) - ikb_k \frac{\partial f_0}{\partial p} = 0.
\]

(A.8)

Obviously \( b_k \) and \( a_k(p) \) are related. Using the Fourier decomposition of the potential \( V(\theta) \):

\[
V(\theta) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} V_ke^{ik\theta},
\]

(A.9)

where

\[
V_k = \int_0^{2\pi} d\theta \, V(\theta)e^{-ik\theta},
\]

(A.10)

we obtain

\[
b_k = V_k \int dp \, a_k(p).
\]

(A.11)

With the natural assumption \( V(-\theta) = V(\theta) \) we have that \( V_k \) is real and that \( V_{-k} = V_k \).

Substituting equation (A.11) into equation (A.8) this equation becomes

\[
(pk - \omega)a_k(p) - kV_k \frac{\partial f_0}{\partial p} \int dp' \, a_k(p') = 0.
\]

(A.12)

We have to look for which values of \( \omega \) this equation admits solutions \( a_k(p) \) that are not identically zero. Since this equation is linear, we can freely impose the normalization condition

\[
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\]
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\[ \int dp' a_k(p') = 1 , \quad (A.13) \]

so that the equation becomes

\[ (pk - \omega)a_k(p) - kV_k \frac{\partial f_0}{\partial p} = 0 . \quad (A.14) \]

As a matter of fact, this equation is satisfied (for \( k \neq 0 \)) for any real value of \( \omega \), which we denote by \( \omega_R \), by putting

\[ a_k(p; \omega_R) = kV_k P \frac{\partial f_0}{pk - \omega_R} + |k|c(k, \omega_R)\delta(pk - \omega_R) , \quad (A.15) \]

where \( P \) denotes that the principal value is taken when integrating over \( p \). The normalization condition for \( a_k(p; \omega_R) \) provided by equation (A.13) implies that

\[ c(k, \omega_R) = 1 - kV_k P \int dp \frac{\partial f_0}{pk - \omega_R} . \quad (A.16) \]

Therefore the real values of \( \omega \) are not solutions of a dispersion relation, and thus they are not proper frequencies of the linear equation (A.14) in the usual sense. These solutions are also present when the Fourier component \( V_k \) is zero; in that case \( a_k(p; \omega_R) \) is a simple delta function and \( c(k, \omega_R) = 1 \). Let us note that \( a_{-k}(p, -\omega_R) = a_k(p, \omega_R) \). For \( k = 0 \) the only solution of equation (A.14) is \( \omega = 0 \).

Another type of solutions of equation (A.14) can be obtained for particular complex values of \( \omega \). They are given by

\[ a_k(p; \omega) = kV_k \frac{\partial f_0}{pk - \omega} , \quad (A.17) \]

provided that the normalization condition (A.13) is satisfied. Integrating both sides with respect to \( p \) we see that the complex value of \( \omega \) is determined by the equation

\[ D(k, \omega) \equiv 1 - kV_k \int dp \frac{\partial f_0}{pk - \omega} = 0 . \quad (A.18) \]

The function \( D(k, \omega) \) is called the response dielectric function. There are isolated complex values of \( \omega \) such that \( D(k, \omega) = 0 \) (dispersion relation). These are the proper frequencies of equation (A.14). There are two important relations to note. Since \( V_k = V_{-k} \) is real, then if \( D(k, \omega) = 0 \) we also have that \( D(k, \omega^*) = 0 \) and \( D(-k, -\omega) = 0 \). Therefore, if for a given wavenumber \( k \) there is a complex proper frequency \( \omega \), there is also the complex conjugate proper frequency \( \omega^* \), while for the wavenumber \(-k\) there will be the proper frequencies \(-\omega\) and \(-\omega^*\). Correspondingly, we have \( a_k(p, \omega^*) = a_k^*(p, \omega) \) and \( a_{-k}(p, -\omega) = a_k(p, \omega) \).

From the Plemelj formula

\[ \lim_{\eta \to 0^+} \frac{1}{x - x_0 \mp i \eta} = P \frac{1}{x - x_0} \pm i \pi \delta(x - x_0) \quad (A.19) \]

we can obtain the value of \( D(k, \omega) \) for real values of \( \omega \). If \( \omega_R \) and \( \omega_I \) are the real and imaginary parts of \( \omega \), we have

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\[
\lim_{\omega \to 0^\pm} D(k, \omega) = 1 - kV_k \int dp \frac{\partial f_0}{\partial p} \frac{pk - \omega_R}{pk - \omega_R} + \frac{i\pi}{k} \frac{\partial f_0}{\partial p} \bigg|_{p = \omega_R/k} = c(k, \omega_R) + \frac{i\pi}{k} \frac{\partial f_0}{\partial p} \bigg|_{p = \omega_R/k}.
\]

(A.20)

The different limits from above and below the real line show that equation (A.18) defines two different analytic functions of \( \omega \), one in the upper plane and one in the lower plane. The two limits coincide only for the particular values of \( \omega_R \) for which the last term in the right-hand side of equation (A.20) is zero, i.e. for \( \omega_R/k \) equal to the values of \( p \) where \( f_0(p) \) is not self-adjoint, and for each solution \( \omega_1 \); \( \omega_2 \). As just mentioned, the sum runs on the discrete values (generally both complex and real) satisfying \( c(k, \omega_R) \equiv 0 \) and \( f_0(\omega_R/k) = 0 \). In this case the normalized \( a_k(p; \omega_R) \) is given by equation (A.17) with \( \omega = \omega_R \) and without the necessity of the principal value.

It is possible to show [44] that, for any given \( k \neq 0 \), the functions \( a_k(p; \omega_R) \) in equation (A.15) and \( a_k(p; \omega) \) in equation (A.17) constitute a complete orthogonal system (with the usual scalar product), when \( \omega_R \) in the former runs over the real axis and \( \omega \) in the latter runs over the discrete solutions of the dispersion relation \( D(k, \omega) = 0 \). Therefore, any function \( h(p) \) can be expanded as

\[
h(p) = \int d\omega_R \alpha(\omega_R; k)a_k(p; \omega_R) + \sum_j \beta_j(k)a_k(p; \omega_j(k))
\]

(A.21)

with proper coefficients \( \alpha(\omega_R; k) \) and \( \beta_j(k) \). As just mentioned, the sum runs on the discrete values (generally both complex and real) satisfying \( D(k, \omega) = 0 \). Therefore, if the initial value of \( f_1(\theta, p, t) \) of equation (4) is \( h(p) \exp(ik\theta) \), the following evolution is given by

\[
f_1(\theta, p, t) = \exp(ik\theta) \left[ \int d\omega_R \alpha(\omega_R; k)a_k(p; \omega_R) e^{-i\omega_R t} + \sum_j \beta_j(k) a_k(p; \omega_j(k)) e^{-i\omega_j(k)t} \right].
\]

(A.22)

The corresponding evolution of \( \partial \Phi(\theta, t) / \partial \theta \) is

\[
\frac{\partial \Phi(\theta, t)}{\partial \theta} = i k V_k e^{ik\theta} \left[ \int d\omega_R \alpha(\omega_R; k) e^{-i\omega_R t} + \sum_j \beta_j(k) e^{-i\omega_j(k)t} \right].
\]

(A.23)

A general initial value of \( f_1 \) can be expanded in Fourier series as

\[
f_1(\theta, p, 0) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} f_k(p) e^{ik\theta},
\]

(A.24)

where the term with \( k = 0 \) can be assumed to be absent (it simply corresponds to a constant in time), and where \( f_k = f_k^* \). Expanding any \( f_\theta(p) \) in the form given by equation (A.21), the evolution of \( f_1 \) is given by

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\( ^{23} \) Equation (4) is not self-adjoint, and for each solution \( a_k(p; \omega_R) \) of \( a_k(p; \omega) \) there is a corresponding solution \( \tilde{a}_k(p; \omega_R) \) or \( \tilde{a}_k(p; \omega) \) of the adjoint equation. The orthogonality of the system is expressed by the fact that each given solution \( a_k \) of equation (4) is orthogonal to all the solutions \( \tilde{a}_k \) of the adjoint equation, except the one corresponding to it [44].
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\[
f_1(\theta, p, t) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} e^{i k \theta} \left[ \int d\omega_R \alpha(\omega_R; k) a_k(p; \omega_R) e^{-i \omega_R t} + \sum_j \beta_j(k) a_k(p; \omega_j(k)) e^{-i \omega_j(k) t} \right].
\]  
(A.25)

The reality of this expression follows from \( \alpha(-\omega_R; -k) = \alpha^*(\omega_R; k) \) and \( \beta_j(-k) = \beta_j^*(k) \) when the proper frequencies for \( k \) and \(-k\) are numbered so that for the same \( j \) we have \( \omega \) for \( k \) and \(-\omega^* \) for \(-k\). Finally, the evolution of \( \partial \Phi(\theta, t)/\partial \theta \) is

\[
\frac{\partial \Phi(\theta, t)}{\partial \theta} = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} i k V_k e^{i k \theta} \left[ \int d\omega_R \alpha(\omega_R; k) e^{-i \omega_R t} + \sum_j \beta_j(k) e^{-i \omega_j(k) t} \right],
\]  
(A.26)

which is also real.

Let us now compute the integral in \( \theta \) of the product of \( \partial \Phi(\theta, t)/\partial \theta \) and \( f_1(\theta, p, t) \), the expression that appears in equation (A.2). Multiplying equations (A.25) and (A.26) and integrating, we obtain

\[
\int_0^{2\pi} d\theta \frac{\partial \Phi(\theta, t)}{\partial \theta} f_1(\theta, p, t) = -\frac{i}{2\pi} \sum_{k=-\infty}^{\infty} k V_k \left[ \int d\omega_R \alpha(\omega_R; -k) e^{-i \omega_R t} + \sum_n \beta_n(-k) e^{-i \omega_n(-k) t} \right]
\times \left[ \int d\omega_R \alpha(\omega_R; k) a_k(p; \omega_R) e^{-i \omega_R t} + \sum_j \beta_j(k) a_k(p; \omega_j(k)) e^{-i \omega_j(k) t} \right].
\]  
(A.27)

When \( f_0(p) \) is stable, there are no complex solutions of equation (A.18). This follows from the fact that its complex solutions come in complex conjugate pairs, and therefore if there are complex solutions there are necessarily unstable modes\(^{24}\). Thus, for a stable \( f_0(p) \), the term with the sum in equations (A.25) and (A.26) is either absent or with only real proper frequencies. Then, \( f_1(\theta, p, t) \), \( \partial \Phi(\theta, t)/\partial \theta \) and the integral of their product, equation (A.27), will not have terms with exponential growth. Actually, the interferences between the real frequencies will give rise to an exponential decay (the Landau damping)\(^{25}\). On the other hand, when there are complex proper frequencies, and then with positive imaginary parts (since they come in complex conjugate pairs), there will be terms with exponential growths. In that case, one could approximate the right-hand side of equation (A.27) by keeping only those terms. With the further assumption that

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\(^{24}\) If \( \omega = \omega_R + i \omega_I \) is a solution of the dispersion relation (A.18), then \( \omega = \omega_R - i \omega_I \) is also a solution. If the first is stable the second is unstable, and vice versa.

\(^{25}\) We remark that, here, we are treating the linearized Vlasov equation à la van Kampen [45], i.e. with the Fourier transform in time. This treatment is the most natural one to find the proper frequencies of a linear problem. However, it is also possible to treat the problem à la Landau [46], i.e. with the Laplace transform in time. The latter procedure is more suitable to the study of an initial value problem and to that of obtaining the collective damped modes that result from the interference effects (in particular the Landau damping). In the treatment with the Laplace transform, the dielectric function is defined by equation (A.18) only in the upper \( \omega \) plane; in the rest of the complex plane, it is defined by the analytic continuation. In the treatment à la Landau one sees how the Landau damping stems from the real frequencies of the treatment à la van Kampen (see, e.g. [8] for mathematical details.)
for each \( k \) there is only one complex proper frequency \( \omega(k) = \omega_R(k) + i\omega_I(k) \) with \( \omega_I(k) > 0 \) (and its complex conjugate) we obtain

\[
\int_0^{2\pi} d\theta \frac{\partial \Phi(\theta,t)}{\partial \theta} f_1(\theta,p,t) \approx -i \frac{1}{2\pi} \sum_{k>0} k V_k |\beta(k)|^2 a_k(p;\omega(k)) e^{-i(\omega(k) - \omega^*(k)) t} .
\]  

(A.28)

Using the expression of \( a_k(p;\omega) \) from equation (A.17) the previous expression can be transformed into

\[
\int_0^{2\pi} d\theta \frac{\partial \Phi(\theta,t)}{\partial \theta} f_1(\theta,p,t) \approx \frac{1}{2\pi} \sum_{k>0} k^2 V_k |\beta(k)|^2 \frac{2\omega_I(k)}{(pk - \omega_R(k))^2 + \omega_I^2(k)} \frac{\partial f_0(p)}{\partial p} e^{2\omega_I(k) t} .
\]  

(A.29)

We now consider equation (A.5). For a linear equation with time dependent coefficients there is no proper frequency in the usual sense, and the solutions are of the same form as in equations (A.6) and (A.7). However, we can try, for a given Fourier component, similar expressions, viz.

\[
f_1(\theta,p,t) = a_k(p,t) e^{ik\theta} e^{-i\int_0^t dt' \omega(t')} ,
\]  

(A.30)

\[
\Phi(\theta,t) = b_k(t) e^{ik\theta} e^{-i\int_0^t dt' \omega(t')} .
\]  

(A.31)

We substitute equations (A.30) and (A.31) into equation (A.5) and neglect the time derivatives of \( a_k(p,t) \) and \( b_k(t) \), so that we obtain an equation similar to (A.8):

\[
-i\omega a_k(p,t) + ipk a_k(p,t) - ikb_k(t) \frac{\partial f_0(p,t)}{\partial p} = 0 .
\]  

(A.32)

With this adiabatic approximation (see section 2.2), in which the time derivatives of \( a_k(p,t) \) and \( b_k(t) \) are neglected, the last equation is solved as before, with the only difference that \( f_0'(p,t) \) and thus \( \omega(t) \) depend on time, and the time dependence of \( a_k(p,t) \) is only through \( \omega(t) \). Without repeating the whole procedure, we write directly the expression for the integral of the product of \( \partial \Phi(\theta,t)/\partial \theta \) and \( f_1(\theta,p,t) \) in the approximation that for each \( k \) there is only one proper frequency with positive imaginary part (see footnote 26):

\[
\int_0^{2\pi} d\theta \frac{\partial \Phi(\theta,t)}{\partial \theta} f_1(\theta,p,t) \approx \frac{1}{2\pi} \sum_{k>0} k^2 V_k |\beta(k)|^2 \frac{2\omega_I(k)}{(pk - \omega_R(k))^2 + \omega_I^2(k)} \frac{\partial f_0(p,t)}{\partial p} e^{2\omega_I(k) t} .
\]  

(A.33)

This equation can be written in a different form by defining a diffusion coefficient

\[
D(p,t) = \sum_{k>0} \frac{2\chi_k(t)\omega_I(k,t)}{(pk - \omega_R(k,t))^2 + \omega_I^2(k,t)}
\]  

(A.34)

with

\[
\frac{\partial \chi_k(t)}{\partial t} = 2\omega_I(k,t)\chi_k(t) .
\]  

(A.35)

---

26 According to the Nyquist theorem [37, 38], for an unstable single humped distribution function \( f_\beta(p) \), there is only one unstable mode. In more general cases, if there are several complex proper frequencies, one selects the largest one, i.e. the one that corresponds to the maximum growth rate.

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where some constants have been incorporated in the definition of $\chi_k(0)$. Therefore, equation (A.33) becomes

$$\int_0^{2\pi} d\theta \frac{\partial \Phi(\theta, t)}{\partial \theta} f_1(\theta, p, t) \approx D(p, t) \frac{\partial f_0(p, t)}{\partial p}. \tag{A.36}$$

Substituting the right-hand side of this expression into equation (A.2) we obtain

$$\frac{\partial f_0(p, t)}{\partial t} = \frac{\partial}{\partial p} \left( D(p, t) \frac{\partial f_0(p, t)}{\partial p} \right), \tag{A.37}$$

which is of the form of a diffusion equation. This is the QL approximation for the evolution of the angle-averaged distribution function $f_0(p, t)$.

**Appendix B. Results for a homogeneous semi-elliptical initial condition**

In this appendix, we show how the results of sections 3 and 4 are modified when we consider a homogeneous semi-elliptical initial condition (homogeneous polytrope of index $n = 1$) instead of a homogeneous Gaussian initial condition.

**B.1. The N-body simulations and the comparison with the results of the diffusion equation**

In figure B1, we plot the temporal evolution of the magnetization obtained from the N-body simulations and by solving the diffusion equation of the QL theory for $\epsilon = 0.61$. The interpretation is similar to that given for the initial Gaussian distribution. For $\epsilon = 0.61$, the final magnetization $m_{QL} = 0.05$ predicted by the QL theory is relatively close to the value $m_{NB} = 0.07$ obtained from the N-body simulation by averaging over the oscillations.

In figure B2, we compare the velocity distribution function of the QSS reached in the N-body simulation and the final distribution function of the diffusion equation. Like the initial distribution function, the final distribution function has a compact
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support (actually, the distribution function keeps a compact support at all times). We consider two energies \( \epsilon = 0.61 \) and \( \epsilon = 0.59 \). For \( \epsilon = 0.61 \), which is close to the instability threshold \( \epsilon^*_c = \epsilon_{n=1} = 5/8 = 0.625 \) of the homogeneous semi-elliptical distribution \( (n = 1 \) polytrope), the agreement between the QL theory and the \( N \)-body simulation is good except in the central region (and to a lesser extent close to the maximum velocity). We note that the distribution function has not changed much as compared to the initial semi-elliptical distribution. Only the core of the distribution and the region close to the maximum velocity have changed in order to make the distribution dynamically stable (without this small change, the distribution would be unstable). In particular, the core of the distribution becomes flatter and wider (‘hotter’). For the lower energy \( \epsilon = 0.59 \), the disagreement is more pronounced everywhere. The distribution function in the \( N \)-body simulation has substantially evolved from the initial semi-elliptical distribution, and has spread (while keeping a compact support) contrary to the distribution of the QL theory. These results are similar to those obtained in the case of a Gaussian initial distribution. We note, however, that in the semi-elliptical case, close to the instability threshold \( \epsilon^*_c \), the distribution function changes from the initial distribution function not only in the core but also in the tail, close to the maximum velocity. By contrast, in the Gaussian case, close to the instability threshold \( \epsilon_c \), the tail of the distribution barely changes from the initial condition.

B.2. Caloric and magnetization curves

In figure B3, we plot the kinetic temperature and the magnetization of the final distribution of the QL theory and of the \( N \)-body simulation as a function of the energy. The two curves approach each other close to the instability threshold. In particular, the QL theory is able to predict the energy of the out-of-equilibrium phase transition from the unmagnetized state \( (m = 0) \) to the magnetized state \( (m \neq 0) \) as discussed below. As for the Gaussian case, this transition is only effective since the magnetization should be strictly positive for any energy smaller than the instability threshold \( \epsilon^*_c \).
In figures B4 and B5, we compare the caloric curve $T(\epsilon)$ and the magnetization curve $m(\epsilon)$ obtained from direct $N$-body simulations of the HMF model, starting from a homogeneous semi-elliptical distribution, with the prediction of the QL theory and with the fit corresponding to a polytrope $n = 1$ considered in our previous papers [16, 20]. The bullets are the results of direct $N$-body simulations. The dashed line corresponds to the prediction of the QL theory. The solid line denoted ‘$n = 1$’ corresponds to the caloric curve obtained by assuming that the QSSs are polytropes of index $n = 1$. This
caloric curve exhibits a region of negative specific heats with $C_{\text{kin}} = -1/2$. As shown in [16], and confirmed below, polytropes of index $n = 1$ give a remarkable fit to the QSSs for a wide range of energies.

The initial condition, which is a spatially homogeneous semi-elliptical distribution, corresponds to a polytrope of index $n = 1$. Therefore, for $\epsilon > \epsilon_c^* = \epsilon_{n=1} = 5/8 = 0.625$, the homogeneous semi-elliptical distribution is dynamically stable, and the system does not evolve on a collisionless timescale. For $\epsilon < \epsilon_c^*$, the homogeneous semi-elliptical distribution is dynamically (Vlasov) unstable, and the system rapidly evolves towards a QSS.

Slightly below $\epsilon_c^*$, the QL theory is in good agreement with $N$-body simulations. It predicts that the QSS remains homogeneous (non magnetized) for $\epsilon_{\text{QL}} \simeq 0.619 < \epsilon < \epsilon_c^*$ and that it becomes inhomogeneous for $\epsilon < \epsilon_{\text{QL}}$ (the value $\epsilon_{\text{QL}} \simeq 0.619$ has been extrapolated from the magnetization curve of figure B3). The transition energy $\epsilon_{\text{QL}} \simeq 0.619$ predicted by the QL theory is in good agreement with the value $\epsilon_{\text{Nb}} \simeq 0.619$ obtained from the $N$-body simulations (also extrapolated from the magnetization curve of figure B3). Therefore, for a homogeneous semi-elliptical initial condition, the out-of-equilibrium transition energy is $\epsilon_1 \simeq \epsilon_{\text{QL}} \simeq \epsilon_{\text{Nb}} \simeq 0.619$ (it can be compared to the value $\epsilon_1 \simeq 0.735$ obtained for a homogeneous Gaussian initial condition). For $\epsilon_1 < \epsilon < \epsilon_c^*$, the distribution is not a homogeneous polytrope of index $n = 1$, since this distribution is unstable. The observed distribution of the QSS is close to the distribution predicted by the QL theory as analyzed in the following section.

For smaller energies, the QL theory does not give a good agreement with the $N$-body simulations anymore. In that case, we observe (in agreement with our earlier paper [16]) that the QSS is well-fitted by an inhomogeneous $n = 1$ polytrope. This is revealed not only by the values of the magnetization and kinetic temperature, which are very close to the numerical ones, but also by the distribution function itself, as discussed in the following section. We have, however, no theory to justify why the $n = 1$ polytropic fit works so well.

In conclusion, the QL theory works well close to the critical energy $\epsilon_c^*$ (in particular it is able to predict the shift $\Delta \epsilon = \epsilon_1 - \epsilon_c^* = -0.006$ of the transition energy from un-magnetized to magnetized QSSs) while the polytropic fit works well at lower energies (in particular it is able to account for the region of negative specific heats). These conclusions are similar to those obtained for a spatially homogeneous Gaussian initial condition. We note, however, that the shift $\Delta \epsilon = \epsilon_1 - \epsilon_c^* = -0.006$ obtained in the semi-elliptical case is smaller than the shift $\Delta \epsilon = \epsilon_1 - \epsilon_c = -0.015$ obtained in the Gaussian case. We also note that, in the semi-elliptical case, the transition energy $\epsilon_1 \simeq 0.619$ predicted by the QL theory is below the transition energy $\epsilon_{c,n=1} = 5/8 = 0.625$ corresponding to $n = 1$ polytropes, while in the Gaussian case the transition energy $\epsilon_1 \simeq 0.735$ predicted by the QL theory is above the transition energy $\epsilon_{n=2} = 2/3 \simeq 0.666$ corresponding to $n = 2$ polytropes. Therefore, the fact that we reach similar conclusions in these two different situations is encouraging.

### B.3. Velocity distribution functions

In this section, we compare the velocity distribution functions obtained from the $N$-body simulations, the QL theory, and the $n = 1$ polytropic fit for two different energies.

We first consider an energy $\epsilon = 0.61$ close to the critical point $\epsilon_c^* = 5/8 = 0.625$. The velocity distributions are plotted in figure B6. As already discussed in the previous
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section, we find a relatively good agreement between the QL theory and the \(N\)-body simulation. This relatively good agreement is confirmed by the values of the kinetic temperature and magnetization. We find \(T_{\text{QL}} = 0.223\) and \(m_{\text{QL}} = 0.05\) to be compared with \(T_{\text{Nb}} = 0.227\) and \(m_{\text{Nb}} = 0.07\). On the other hand, the fit by an inhomogeneous polytropic distribution of index \(n = 1\) is not good. Although it has a compact support, it is more spread than the QSS obtained from the \(N\)-body simulation. The disagreement between the \(n = 1\) polytrope and the \(N\)-body simulation is confirmed by the values of the kinetic temperature and magnetization. We find \(T_{\text{poly}} = 0.28\) and \(m_{\text{poly}} = 0.245\) to be compared with \(T_{\text{Nb}} = 0.227\) and \(m_{\text{Nb}} = 0.07\).

We now consider a lower energy \(\epsilon = 0.59\). The velocity distributions are plotted in figure B7. In that case, the situation is reversed. We observe a remarkable agreement between the velocity distribution of the QSS obtained from the \(N\)-body simulation and the velocity distribution of a polytrope \(n = 1\).\(^{27}\) This is confirmed by the values of the kinetic temperature and magnetization. We find \(T_{\text{poly}} = 0.32\) and \(m_{\text{poly}} = 0.374\)

\(^{27}\) As shown in [16], the excellent agreement between the polytrope \(n = 1\) and the QSS is also valid for the complete distribution function \(f(\theta, p) = f(\epsilon)\).

Figure B6. Velocity distribution of the QSS for \(\epsilon = 0.61\) showing the fairly good quality of the QL theory close to the critical point (black: \(N\)-body simulation; red: QL theory; blue: polytrope \(n = 1\)).

Figure B7. Velocity distribution of the QSS for \(\epsilon = 0.59\) showing the very good quality of the polytropic fit far away from the critical point (black: \(N\)-body simulation; red: QL theory; blue: polytrope \(n = 1\)).
to be compared with $T_{Nb} = 0.324$ and $m_{Nb} = 0.38$. On the other hand, the prediction of the QL theory is not good. This distribution has not spread enough from the initial condition (see figure B2). The disagreement between the QL theory and the $N$-body simulation is confirmed by the values of the kinetic temperature and magnetization. We find $T_{QL} = 0.22$ and $m_{QL} = 0.203$ to be compared with $T_{Nb} = 0.324$ and $m_{Nb} = 0.38$.

At even lower energies (e.g. $\epsilon = 0.55$), our study in [16] shows that the system takes a core–halo structure. The core corresponds to the pure polytrope $n = 1$, but it is now surrounded by a halo of particles.

### B.4. Summary and discussion

In summary, for a homogeneous semi-elliptical initial distribution, we have the following results. For $\epsilon > \epsilon^*_c = \epsilon_{n=1} = 0.625$, the system remains in the homogeneous semi-elliptical distribution which is stable. Close to $\epsilon^*_c$, the QL theory works reasonably well. In particular, it is able to predict the energy, $\epsilon_t \simeq 0.619$, marking the transition between unmagnetized and magnetized QSSs. For lower energies, the QL theory does not work. In that case, we observe that the QSSs are remarkably well fitted by inhomogeneous polytropic distributions (Tsallis distributions) with index $n = 1$. These polytropic distributions are able to account for the region of negative specific heats in the out-of-equilibrium caloric curve, unlike the Boltzmann and Lynden-Bell distributions. At even lower energies, the system takes a core–halo structure with a polytropic core and a halo of particles.

Since the initial condition is a spatially homogeneous polytrope of index $n = 1$, and since it appears that the QSSs are often well-fitted by inhomogeneous polytropes of index $n = 1$, we could expect that the QSS could be fitted by an inhomogeneous polytrope of index $n = 1$ as soon as $\epsilon < \epsilon^*_c = \epsilon_{n=1}$. Actually, this is not the case. There is a small range of energies $[\epsilon_t, \epsilon^*_c]$ where the QSS remains homogeneous. Within this small range of energies, the QL theory works relatively well, unlike the polytropic fit. Therefore, even if the caloric curves differ in the detail, the results obtained for a semi-elliptical initial distribution are relatively similar to those obtained for a Gaussian initial distribution. In consequence, the phenomenology that we have described seems to be relatively general, despite the fact that the nature of the QSS strongly depends on the initial condition.

A striking and mysterious outcome of our study (see also [16, 20]) is the finding that, in many cases, the QSSs are well fitted by polytropic (Tsallis) distributions. The value of the polytropic index depends on the class of initial condition. For the semi-elliptical initial distribution, which is a polytrope of index $n = 1$, the polytrope that fits the QSS has the same index as the initial state, i.e. $n = 1$. Although not considered in the present paper, we found in [16] that for the waterbag initial distribution, which is a polytrope of index $n = 1/2$, the polytrope that fits the QSS also has the same index, i.e. $n = 1/2$. By contrast, for the Gaussian initial distribution, which can be viewed as a polytrope of index $n = \infty$, the polytrope that fits the QSS has a different index, $n = 2$. We have no theory to explain these striking results. However, they confirm that polytropic (Tsallis) distributions can be useful in systems with long-range interaction, as claimed in [42].
Appendix C. The decrease of $\omega_1(t)$ with time

We have seen in the numerical integration of the diffusion equation that the function $f_0(p,t)$ approximately retains its functional form. This can be exploited to give an argument showing that $\omega_1(t)$ decreases monotonically with time. We start from the dispersion relation (15), that for convenience we recall here:

$$1 + \pi \int dp \frac{p f_0(p,t)}{p^2 + \omega_1^2(t)} = 0 .$$

(C.1)

Let us write the function $f_0$ at time $t + dt$ as

$$f_0(p,t + dt) = \alpha f_0(\alpha p,t) + \delta f(p,t),$$

where $\alpha = 1 - \xi$ with $\xi \ll 1$, and where we assume that

$$|\delta f(p,t)| \ll |f_0(p,t) - \alpha f_0(\alpha p,t)|.$$  

(C.3)

By neglecting the term $\delta f$ in equation (C.2) we obtain $\omega_1(t + dt) < \omega_1(t)$ as we show below. The fact that $\alpha < 1$ is obtained from equation (25). Now, writing the dispersion relation (C.1) for $f_0(p,t + dt)$ by using equation (C.2) and neglecting $\delta f$, we have

$$1 + \pi \int dp \frac{p f_0(p,t + dt)}{p^2 + \omega_1^2(t + dt)} = 1 + \pi \int dp \frac{\alpha^2 p f_0(\alpha p,t)}{p^2 + \omega_1^2(t + dt)}$$

$$= 1 + \pi \int dp \frac{p f_0(p,t)}{(p^2/\alpha^2) + \omega_1^2(t + dt)} = 0 ,$$

(C.4)

where the last step has been obtained by a trivial change of variables in the integral. If $\omega_1(t + dt)$ were not smaller than $\omega_1(t)$, then $(p^2/\alpha^2) + \omega_1^2(t + dt) > p^2 + \omega_1^2(t)$ for any $p$. Considering that the integrand in the dispersion relation is negative definite, we infer that the right-hand side of equation (C.4) would be necessarily positive. The only way to make it vanish is to have $\omega_1(t + dt) < \omega_1(t)$.

Appendix D. Proof of equation (29)

We write $p/(p^2 + \omega_1^2(t)) = 1/p - \omega_1^2(t)/[p(p^2 + \omega_1^2(t))]$. Substituting this decomposition into equation (15), the first term gives rise to the integral in equation (29). For the second term we have

$$- \pi \omega_1^2(t) \int dp \frac{f_0'(p,t)}{p(p^2 + \omega_1^2(t))} = - \pi \text{sign}[\omega_1(t)] \int dx \frac{f_0'(\omega_1(t)x,t)}{x(x^2 + 1)}$$

$$= - \pi |\omega_1(t)| \int dx \frac{f_0''(0,t)}{x^2 + 1} + O(\omega_1^2(t)) = - \pi^2 |\omega_1(t)| f_0''(0,t) + O(\omega_1^2(t)).$$

(D.1)

Appendix E. The modified Gaussian

Here, we show how to solve the system of equations (40)-(42) and obtain the values of $A$, $\beta$ and $p_1$ as a function of $\epsilon_{\text{kin}}$. Using the complementary error function $\text{erfc}(x)$ defined by

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt.$$
erfc(x) = 1 - erf(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty dy e^{-y^2}, \quad (E.1)

the three equations become

\begin{align*}
2A p_1 e^{-\frac{\beta p_1^2}{2}} + \sqrt{\frac{2\pi}{\beta}} A \text{erfc}\left(\sqrt{\frac{\beta}{2}} p_1\right) &= \frac{1}{2\pi}, \\
1 - \pi\beta \sqrt{\frac{2\pi}{\beta}} A \text{erfc}\left(\sqrt{\frac{\beta}{2}} p_1\right) &= 0, \\
A p_1 e^{-\frac{\beta p_1^2}{2}} \left(\frac{p_1^2}{3} + \frac{1}{\beta}\right) + \sqrt{\frac{\pi}{2\beta^3}} A \text{erfc}\left(\sqrt{\frac{\beta}{2}} p_1\right) &= \frac{\epsilon_{\text{kin}}}{2\pi}. \quad (E.4)
\end{align*}

We know that for the energy \(\epsilon_{\text{kin}} = 1/4\), corresponding to the critical point of the model for which the Gaussian velocity distribution function is marginally stable, the solution of these three equations is \(\beta = 2\), \(p_1 = 0\) and \(A = 1/2\pi^{3/2}\). Starting from this solution, it is not difficult to find, numerically, the solution for other values of \(\epsilon_{\text{kin}}\). In fact, the system of three equations is of the form

\begin{align*}
F_1(A, \beta, p_1) &= 0, \\
F_2(A, \beta, p_1) &= 0, \\
F_3(A, \beta, p_1; \epsilon_{\text{kin}}) &= 0. \quad (E.7)
\end{align*}

It is then possible to obtain closed expressions for \(\partial A/\partial \epsilon_{\text{kin}}, \partial \beta/\partial \epsilon_{\text{kin}}, \) and \(\partial p_1/\partial \epsilon_{\text{kin}}\). Then, starting from the known solution for \(\epsilon_{\text{kin}} = 1/4\), one can compute the solutions for other values by numerical integration.

Appendix F. Universal trapping scaling on the unstable manifold for a collisionless mode

The case of a single wave instability has been treated, in the literature devoted essentially to plasma physics, within a framework based on amplitude equations that does not entail the approximations used in the QL theory (see, e.g. [33, 34]). This development could also be applied to a different interaction potential, such as that occurring in the HMF model. This approach derives equations for the time evolution of the distribution function that at time \(t = 0\) is a Vlasov stationary but unstable distribution, assuming that the instability is due to a single mode, as in our case. If the initial distribution is only weakly unstable, i.e. if in our case \(\omega_I(0)\) is very small, a power expansion in \(\omega_I(0)\) predicts that the electric field is proportional to \(\omega_I^2(0)\), with a coefficient of proportionality that depends on the initial distribution. In the HMF model the role of the electric field is played by the final magnetization. Then, if the coefficient of proportionality does not vanish, the final magnetization will not be zero below the critical energy, at variance with what we find in \(N\)-body simulations and in the integration of the diffusion
equation. The computation of the coefficient of proportionality would require the integration of a nonlinear equation with coefficients depending on the initial unstable state. This is outside the scope of this work, devoted to the comparison between the $N$-body simulations and the diffusion equation of the QL theory. We can note the following. The smallness of $\omega(I)$ for initial conditions with energy only slightly smaller than $\epsilon_c$ (or $\epsilon_c^*$ for the semi-elliptical case, see appendix B) results in a very small final magnetization. In this respect, the fact that we find a zero magnetization for these initial conditions, both in the $N$-body simulations and in the diffusion equation of the QL theory, does not entail, from the theoretical point of view, a real phase transition, but only the occurrence of a state with a magnetization so small as to be considered equal to zero from a practical point of view. This does not modify the main purpose of this paper, i.e. to show the good numerical agreement between the QL theory and the $N$-body dynamics in a range of energies close to the critical point. We stress that this good agreement also occurs, at the level of the final magnetization and of the final velocity distribution function, for a range of energies where the final magnetization is found to be clearly different from zero.

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28 Actually, even in the context of the QL theory, we have seen in section 3.3 that the magnetization of the QSSs is strictly positive ($m_{QSS} > 0$) below $\epsilon_c$. This is consistent with the theory based on amplitude equations [33, 34].

29 To be specific, let us consider an initial homogeneous Gaussian distribution. From equations (30) and (36), we find $\omega(I) \sim 1/(I + T - T_0) \sim \omega(0)^2 \sim (\epsilon_0 - \epsilon)^2$, with $I = 1/2$ and $\epsilon = 3/4$, implying $m_{QSS} \propto \omega(I)^2 \sim (\epsilon_0 - \epsilon)^2$. If we take $\epsilon = 0.735$ (see section 4.1) and assume that the prefactor is of order one, we get $m_{QSS} \sim 10^{-4}$, which can hardly be distinguished from $m_{QSS} = 0$ in our simulations. This is very different from the magnetization of the inhomogeneous Boltzmann equilibrium state, for which $m_{eq} \sim 2(\epsilon_0 - \epsilon)^1/2 \sim \sqrt{5}/5(\epsilon_0 - \epsilon)^1/2 [4]$, implying $m_{eq} = 0.155$ at $\epsilon = 0.735$. 

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