Exploring the Thermodynamic Limit of Hamiltonian Models: Convergence to the Vlasov Equation

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We here discuss the emergence of quasistationary states (QSS), a universal feature of systems with long-range interactions. With reference to the Hamiltonian mean-field model, numerical simulations are performed based on both the original N-body setting and the continuum Vlasov model which is supposed to hold in the thermodynamic limit. A detailed comparison unambiguously demonstrates that the Vlasov-wave system provides the correct framework to address the study of QSS. Further, analytical calculations based on Lynden-Bell's theory of violent relaxation are shown to result in accurate predictions. Finally, in specific regions of parameters space, Vlasov numerical solutions are shown to be affected by small scale fluctuations, a finding that points to the need for novel schemes able to account for particle correlations.

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The Vlasov equation constitutes a universal theoretical framework and plays a role of paramount importance in many branches of applied and fundamental physics. Structure formation in the Universe is for instance a rich and fascinating problem of classical physics: The fossil radiation that permeates the cosmos is a relic of microfluctuation in the matter created by the big bang, and such a small perturbation is believed to have evolved via gravitational instability to the pronounced agglomerations that we see nowadays on the galaxy cluster scale. Within this scenario, gravity is hence the engine of growth and the Vlasov equation governs the dynamics of the non-baryonic "dark matter" [1]. Furthermore, the continuous Vlasov description is the reference model for several space and laboratory plasma applications, including many interesting regimes, among which the interpretation of coherent electrostatic structures observed in plasmas far from thermodynamic equilibrium. The Vlasov equation is obtained as the mean-field limit of the N-body Liouville equation, assuming that each particle interacts with an average field generated by all plasma particles (i.e., the mean electromagnetic field determined by the Poisson or Maxwell equations where the charge and current densities are calculated from the particle distribution function) while interparticle correlations are completely neglected.

Numerical simulations are presently one of the most powerful resources to address the study of the Vlasov equation. In the plasma context, the Lagrangian particle-in-cell approach is by far the most popular, while Eulerian Vlasov codes are particularly suited for analyzing specific problems, due to the associated low noise level which is secured even in the nonlinear regime [2]. However, any numerical scheme designed to integrate the continuous Vlasov system involves a discretization over a finite mesh. This is indeed an unavoidable step which in turn affects numerical accuracy. A numerical (diffusive and dispersive) characteristic length is in fact introduced, being at best comparable with the grid mesh size: as soon as the latter matches the typical length scale relative to the dynamically generated fluctuations, a violation of the continuous Hamiltonian character of the equations occurs (see Refs. [3]). It is important to emphasize that even if such *non-Vlasov* effects are strongly localized in phase space, the induced large scale topological changes will eventually affect the system globally. Therefore, aiming at clarifying the problem of the validity of Vlasov numerical models, it is crucial to compare a continuous Vlasov, but numerically discretized, approach to a homologous N-body model.

The Vlasov equation has been also invoked as a reference model in many interesting one-dimensional problems, and recurrently applied to the study of wave-particle interacting systems. The Hamiltonian mean-field (HMF) model [4], describing the coupled motion of N rotators, is, in particular, assimilated to a Vlasov dynamics in the mean-field limit on the basis of rigorous results [5]. The HMF model has been historically introduced as representing gravitational and charged sheet models and is quite extensively analyzed as a paradigmatic representative of the broader class of systems with long-range interactions [6]. A peculiar feature of the HMF model, shared also by other long-range interacting systems, is the presence of *quasi-stationary states* (QSS). During time evolution, the system gets trapped in such states, which are characterized by non-Gaussian velocity distributions, before relaxing to the final Boltzmann-Gibbs equilibrium [7]. An attempt has been made [8] to interpret the emergence of QSSs by invoking Tsallis statistics [9]. This approach has been later on criticized in [10], where QSSs were shown to correspond to stationary stable solutions of the Vlasov equation. However, the analysis was limited to a particular choice of the initial condition. More recently, an approximate analytical theory, based on the Vlasov equation, which derives the QSSs of the HMF model using a maximum entropy principle, was developed in [11]. This theory is inspired by the pioneering work of Lynden-Bell [12] and relies on previous work on 2D turbulence by Chavanis [13]. However, the underlying Vlasov ansatz has not been directly examined and it is recently being debated [14].

In this Letter, we shall discuss numerical simulations of the continuous Vlasov model, the kinetic counterpart of the discrete HMF model. By comparing these results to both direct N-body simulations and analytical predictions, we shall reach the following conclusions: (i) the Vlasov formulation is indeed ruling the dynamics of the QSS; (ii) the proposed analytical treatment of the Vlasov equation is surprisingly accurate, despite the approximations involved in the derivation; (iii) Vlasov simulations must be handled with extreme caution when exploring specific regions of the parameters space.

The HMF model is characterized by the following Hamiltonian

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

where θ_j represents the orientation of the jth rotor and p_j is its conjugate momentum. To monitor the evolution of the system, it is customary to introduce the magnetization, a macroscopic order parameter defined as $M = |\mathbf{M}| = |\sum \mathbf{m}_i|/N$, where $\mathbf{m}_i = (\cos\theta_i, \sin\theta_i)$ stands for the microscopic magnetization vector. As previously reported [4], after an initial transient, the system gets trapped into QSSs, i.e., nonequilibrium dynamical regimes whose lifetime diverges when increasing the number of particles N. Importantly, when performing the mean-field limit ($N \to \infty$) *before* the infinite time limit, the system cannot relax towards Boltzmann-Gibbs equilibrium and remains permanently confined in the intermediate QSSs. As mentioned above, this phenomenology is widely observed in systems with long-range interactions, including galaxy dynamics [15], free electron lasers [16], and 2D electron plasmas [17].

In the $N \to \infty$ limit the discrete HMF dynamics reduces to the Vlasov equation

$$\partial f/\partial t + p\partial f/\partial\theta - (dV/d\theta)\partial f/\partial p = 0, \qquad (2)$$

where $f(\theta, p, t)$ is the microscopic one-particle distribution function and

$$V(\theta)[f] = 1 - M_x[f]\cos(\theta) - M_y[f]\sin(\theta), \qquad (3)$$

$$M_x[f] = \int_{-\pi}^{\pi}\int_{-\infty}^{\infty} f(\theta, p, t)\cos\theta d\theta dp, \qquad (4)$$

$$M_y[f] = \int_{-\pi}^{\pi}\int_{\infty}^{\infty} f(\theta, p, t)\sin\theta d\theta dp. \qquad (5)$$

The specific energy $h[f] = \iint (p^2/2) f(\theta, p, t) d\theta dp - (M_x^2 + M_y^2 - 1)/2$ and momentum $P[f] = \iint p f(\theta, p, t) d\theta dp$ functionals are conserved quantities. Homogeneous states are characterized by $M = 0$, while nonhomogeneous states correspond to $M \neq 0$.

Rigorous mathematical results [5] demonstrate that, indeed, the Vlasov framework applies in the continuum description of mean-field type models. This observation corroborates the claim that any theoretical attempt to characterize the QSSs should resort to the above Vlasov based interpretative picture. Despite this, the QSS non-Gaussian velocity distributions have been *fitted* [8] using Tsallis' q exponentials, and the Vlasov formalism assumed valid *only* for the limiting case of homogeneous initial conditions [14,18]. In a recent paper [11], the aforementioned velocity distribution functions were instead reproduced with an analytical expression derived from the Vlasov scenario, with no adjustable parameters and for a large class of initial conditions, including inhomogeneous ones. The key idea dates back to the seminal work by Lynden-Bell [12] (see also [19,20]) and consists in coarse-graining the microscopic one-particle distribution function $f(\theta, p, t)$ by introducing a local average in phase space. It is then possible to associate an entropy to the coarse-grained distribution $\bar{f}$: The corresponding statistical equilibrium is hence determined by maximizing such an entropy, while imposing the conservation of the Vlasov dynamical invariants, namely, energy, momentum and norm of the distribution. We shall here limit our discussion to the case of an initial single particle distribution which takes only two distinct values: $f_0 = 1/(4\Delta_\theta\Delta_p)$, if the angles (momenta) lie within an interval centered around zero and of half-width Δ_θ (Δ_p), and zero otherwise. This choice corresponds to the so-called "water-bag" distribution which is fully specified by energy $h[f] = e$, momentum $P[f] = \sigma$ and the initial magnetization $\mathbf{M}_0 = (M_{x0}, M_{y0})$. The maximum entropy calculation is then performed analytically [11] and results in the following form of the QSS distribution

$$\bar{f}(\theta, p) = f_0 \frac{e^{-\beta(p^2/2 - M_y[\bar{f}]\sin\theta - M_x[\bar{f}]\cos\theta) - \lambda p - \mu}}{1 + e^{-\beta(p^2/2 - M_y[\bar{f}]\sin\theta - M_x[\bar{f}]\cos\theta) - \lambda p - \mu}}, \qquad (6)$$

where β/f_0, λ/f_0, and μ/f_0 are rescaled Lagrange multipliers, respectively, associated with the energy, momentum, and normalization. Inserting expression (6) into the above constraints and recalling the definition of $M_x[\bar{f}]$, $M_y[\bar{f}]$, one obtains an implicit system which can be solved numerically to determine the Lagrange multipliers and the expected magnetization in the QSS. Note that the distribution (6) differs from the usual Boltzmann-Gibbs expression because of the "fermionic" denominator. Numerically computed velocity distributions have been compared in [11] to the above theoretical predictions (where no free parameter is used), obtaining an overall good agreement. However, the central part of the distributions is modulated by the presence of two symmetric bumps, which are the signature of a collective dynamical phenomenon [11]. The presence of these bumps is not explained by our theory. Such discrepancies could be interpreted as an indirect proof of the fact that the Vlasov model holds only approximately. We shall here demonstrate that the deviations between theory and numerical observation are uniquely due to the approximations built in the Lynden-Bell approach.

A detailed analysis of the Lynden-Bell equilibrium (6) in the parameter plane (M_0, e) enabled us to unravel a rich phenomenology, including out of equilibrium phase transitions between homogeneous ($M_{\rm QSS} = 0$) and inhomogeneous ($M_{\rm QSS} \neq 0$) QSS states. Second and first order transition lines are found that separate homogeneous and nonhomogeneous states and merge into a tricritical point approximately located in $(M_0, e) = (0.2, 0.61)$. When the transition is second order two extrema of the Lynden-Bell entropy are identified in the inhomogeneous phase: the solution $M_{\rm QSS} = 0$ corresponds to a saddle point, being therefore unstable; the global maximum is instead associated with $M_{\rm QSS} \neq 0$, which represents the equilibrium predicted by the theory. This argument is important for what will be discussed in the following.

Let us now turn to direct simulations, with the aim of testing the above scenario, and let us first focus on the kinetic model (2)–(5). The algorithm solves the Vlasov equation in phase space and uses the so-called "splitting scheme", a widely adopted strategy in numerical fluid dynamics. Such a scheme, pioneered by Cheng and Knorr [21], was first applied to the study of the Vlasov-Poisson equations in the electrostatic limit and then employed for a wide spectrum of problems [3]. For different values of the pair (M_0, e), which sets the widths of the initial water-bag profile, we have performed a direct integration of the Vlasov system (2)–(5). After a transient, magnetization is shown to eventually attain a constant value, which corresponds to the QSS value observed in the HMF, discrete, framework. The asymptotic magnetizations are hence recorded when varying the initial condition. Results (stars) are reported in Fig. 1(a) where $M_{\rm QSS}$ is plotted as a function of e. A comparison is drawn with the predictions of our theory (solid line) and with the outcome of N-body simulation (squares) based on the Hamiltonian (1), finding an excellent agreement. This observation enables us to conclude that (i) the Vlasov equation governs the HMF dynamics for $N \to \infty$ *both* in the homogeneous and nonhomogeneous case; (ii) Lynden-Bell's violent relaxation theory allows for reliable predictions, including the transition from magnetized to nonmagnetized states.

Deviations from the theory are locally detected when the above transition is progressively approached. To shed light onto this issue, we have performed N-body simulations for N_R random replicas of the initial condition and repeated the numerical experiments for different values of the pair (e, M_0). Quite remarkably, the system attains different QSS

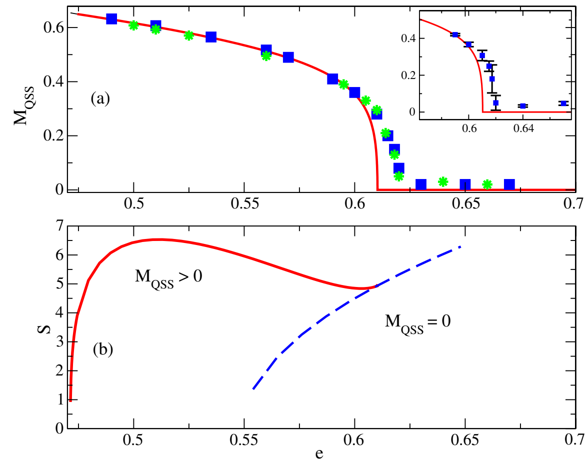

FIG. 1 (color online). Panel (a): The magnetization in the QSS is plotted as a function of energy, e, at $M_0 = 0.24$. The solid line refers to the Lynden-Bell inspired theory. Stars (squares) stand for Vlasov (N-body, $N = 10^6$) simulations. Inset: as in the main frame but for $N = 10^5$. Each point results from averaging over $N_R = 20$ independent realizations. The error bars are calculated as twice the standard deviation. Panel (b): Entropy S at the stationary points, as a function of energy, e: magnetized solution (solid line), and nonmagnetized one (dashed line).

magnetizations. The probability distribution function of $M_{\rm QSS}$ shows a peaked bell-shaped profile. The average value of the magnetization is measured and plotted in the inset of Fig. 1(a) (blue squares), together with the associated error, estimated as twice the standard deviation. The error bars shrink as the number of simulated particles is increased (data not shown). Moreover, at fixed N, more sensible errors are found in proximity of the transition, an observation that can be explained as follows. The coarse-grained entropy is substantially flat in the transition region, which implies that an extended basin of states exists where the system can possibly be trapped. As confirmed by the inspection of Fig. 1(b), close to the transition point, the entropy S of the Lynden-Bell coarse-grained distribution takes almost the same value when evaluated on the global maximum (solid line) or on the saddle point (dashed line). A dedicated campaign of simulations based on the Vlasov code running at different resolutions (grid points) has confirmed this scenario, highlighting a similar degree of variability of $M_{\rm QSS}$. These findings point to the fact that in specific regions of the parameter space, Vlasov numerics needs to be carefully analyzed (see also Refs. [22]). Importantly, it is becoming nowadays crucial to step towards an "extended" Vlasov theoretical model which enables us to account for discrete effects by incorporating at least the two particle correlations interaction term.

Qualitatively, one can track the evolution of the system in phase space, both for the homogeneous and nonhomogeneous cases. Results of the Vlasov integration are displayed in Fig. 2 for $(M_0, e) = (0.5, 0.69)$, where the system is shown to evolve towards a nonmagnetized QSS. The initial water-bag distribution splits into two large reso-

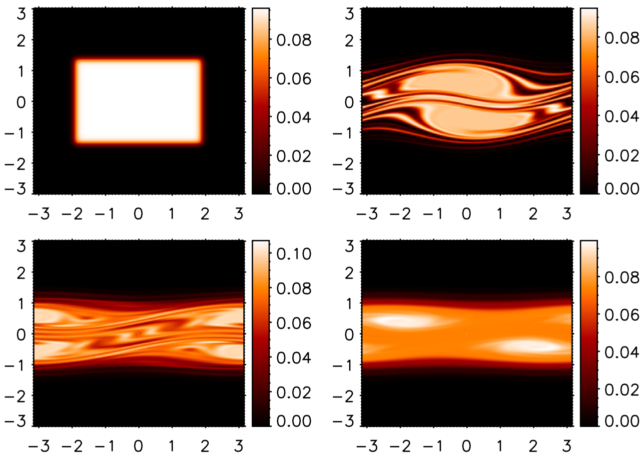

FIG. 2 (color online). Phase space snapshots for $(M_0, e) = (0.5, 0.69)$.

nances, which persist asymptotically: the latter acquire constant opposite velocities which are maintained during the subsequent time evolution, in agreement with the findings of [11]. The two bumps are therefore an emergent property of the model, which is correctly reproduced by the Vlasov dynamics. For larger values of the initial magnetization ($M_0 > 0.89$), while keeping $e = 0.69$, the system evolves towards an asymptotic magnetized state, in agreement with the theory. In this case, several resonances are rapidly developed and eventually coalesce, giving rise to complex patterns in phase space. More quantitatively, one can compare the velocity distributions resulting from, respectively, Vlasov and N-body simulations. The curves are displayed in Figs. 3(a)–3(c) for various choices of the initial conditions in the magnetized region. The agreement

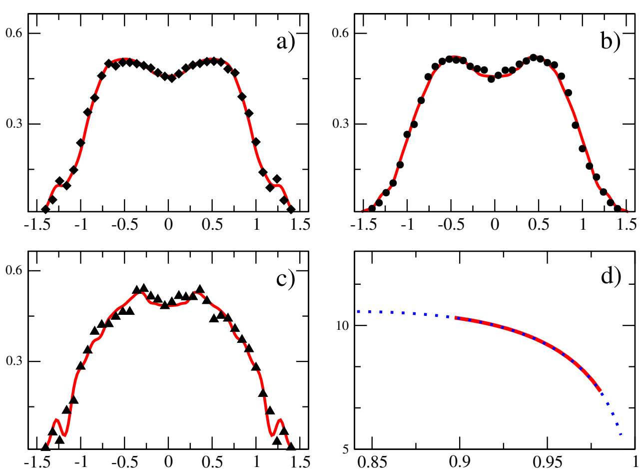

FIG. 3 (color online). Symbols: velocity distributions computed via N-body simulations. Solid line: velocity distributions obtained through a direct integration of the Vlasov equation. Here $e = 0.69$ and $M_0 = 0.3$ (a), $M_0 = 0.5$ (b), $M_0 = 0.7$ (c). Panel (d): Entropy at the stationary points as a function of the initial magnetization: the solid line refers to the global maximum, while the dotted line to the saddle point.

is excellent, thus reinforcing our former conclusion about the validity of the Vlasov model. Finally, let us stress that, when $e = 0.69$, the two solutions (magnetized and nonmagnetized) [11] are associated with a practically indistinguishable entropy level [see Fig. 3(d)]. As previously discussed, the system explores an almost flat entropy landscape and can be therefore stuck in local traps, because of finite size effects. A pronounced variability of the measured M_{QSS} is therefore to be expected. In this Letter, we have analyzed the emergence of QSS, a universal feature that occurs in systems with long-range interactions, for the specific case of the HMF model. By comparing numerical simulations and analytical predictions, we have been able to unambiguously demonstrate that the Vlasov model provides an accurate framework to address the study of the QSS. Working within the Vlasov context one can develop a fully predictive theoretical approach, which is completely justified from first principles. Finally, and most important, results of conventional Vlasov codes are to be critically scrutinized, especially in specific regions of parameters space close to transitions from homogeneous to nonhomogeneous states.

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