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The Vlasov equation and the Hamiltonian mean-field model

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Abstract

We show that the quasi-stationary states of homogeneous (zero magnetization) states observed in the N-particle dynamics of the Hamiltonian mean-field (HMF) model are nothing but Vlasov stable homogeneous states. There is an infinity of Vlasov stable homogeneous states corresponding to different initial momentum distributions. Tsallis q-exponentials in momentum, homogeneous in angle, distribution functions are possible, however, they are not special in any respect, among an infinity of others. All Vlasov stable homogeneous states lose their stability because of finite N effects and, after a relaxation time diverging with a power-law of the number of particles, the system converges to the Boltzmann–Gibbs equilibrium.

Keywords: Hamiltonian dynamics; Long-range interactions; Vlasov equation; Nonlinear stability

1. Intriguing numerical results

The Hamiltonian mean-field model (HMF) [1]

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

describes the motion of globally coupled particles on a circle: θ_i refers to the angle of the ith particle and p_i to its conjugate momentum, while N is the total number of particles. The $1/N$ prefactor, which has been historically introduced to obtain an extensive energy, can be absorbed in a time rescaling (we shall however keep it to compare with previous results).

From the fundamental point of view, this is an ideal toy model. Indeed, although it is simple and the mean-field interaction allows us to perform analytical calculations, it has several features of long-range interactions.

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Moreover, it is a simplification of physical systems like charged or gravitational sheet models. Finally, in some cases, wave-particle Hamiltonians can be reduced to it. In particular, as far as the equilibrium properties are concerned, the Colson–Bonifacio model of the single-pass free electron laser [2] can be mapped onto the HMF Hamiltonian (1).

In this short note, we would like to emphasize that several interesting numerical facts which have been reported in the literature can be accurately explained by considering the limit of infinite number of particles, namely the Vlasov equation corresponding to the HMF model. The first numerical fact is the strong disagreement which was reported in Refs. [1,3] between constant energy molecular dynamics simulations and canonical statistical mechanics calculations. This unexpected and striking result, found for energies slightly below the second-order phase transition energy (see Fig. 1), was first thought to be the fingerprint of inequivalence between microcanonical and canonical ensemble. It was known that such inequivalence might have been present because of the long-range nature of the interaction. However, it has been later proved that inequivalence occurs only if the system has a first-order canonical phase transition; this is not the case for the HMF, which has instead a second-order phase transition. Moreover, the microcanonical entropy of the HMF model has been recently derived using large deviation theory [2], showing that the two ensembles give the same predictions.

It then became clear that the disagreement must have a *dynamical* origin. In order to characterize the dynamical properties of the HMF model, the behaviour of the modulus M of the magnetization

$$\mathbf{M} = \frac{1}{N}\sum_n e^{i\theta_n} \tag{2}$$

has been typically studied. Its time evolution is shown on a logarithmic scale in Fig. 2 for increasing values of N. The initial state is homogeneous in angle (thus the magnetization is zero), with water-bag distribution of momenta (see next section). The figure shows that the system evolves on a fast timescale towards a state which has an almost zero magnetization ($M < 0.05$ in our simulations). Such a state lasts for a long time and its lifetime increases very rapidly with N (note the logarithmic timescale on the abscissa). States with such a property have been called in the literature quasi-stationary states (QSS). It is only in a second stage that the value of M takes off and reaches the Boltzmann–Gibbs value (indicated by BG in Fig. 2) predicted by

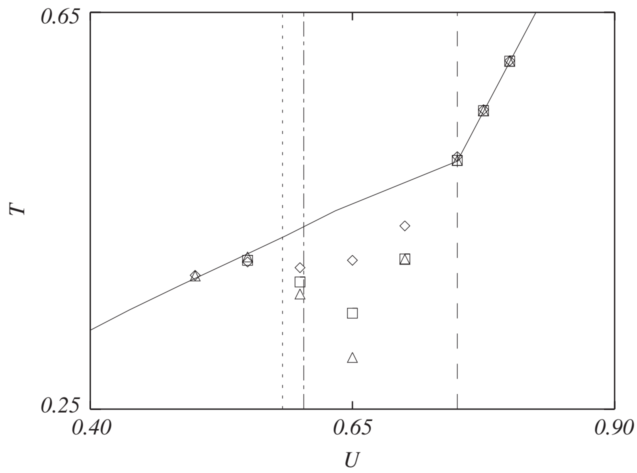

Fig. 1. Caloric curve of the HMF Hamiltonian. The solid line is the equilibrium result in both the canonical and the microcanonical ensemble. The second-order phase transition is revealed by the kink at $U_c = \frac{3}{4}$. The three values of the energy indicated by the vertical lines are the stability thresholds for the homogeneous Gaussian (dashed), power-law of Eq. (7) with $v = 8$ (dash-dotted) and water-bag (dotted) initial momentum distribution. The Gaussian stability threshold coincides with the phase transition energy. The points are the results of constant energy (microcanonical) simulations for the Gaussian (losanges), the power-law (squares) and the water-bag (triangles). Simulations were performed with $N = 5000$. The tendency of the simulation points FOR THE WATER-BAG AND POWER-LAW CASES to lie on the continuation to lower energies of the supercritical branch of the caloric curve would increase when increasing the value of N.

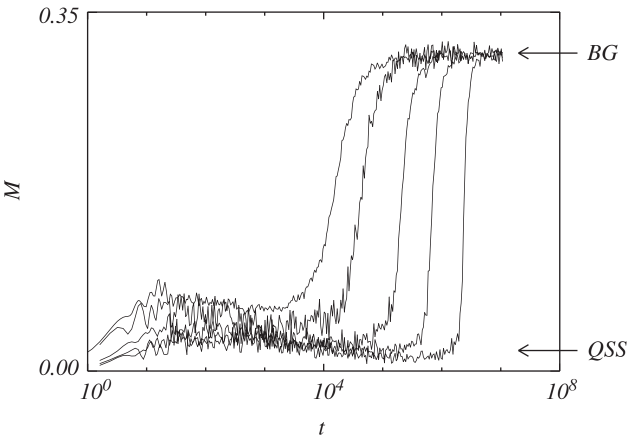

Fig. 2. Time evolution of the modulus of the magnetization $M(t)$ for different particle numbers: $N = 10^3$, 2×10^3, 5×10^3, 10^4 and 2×10^4 from left to right ($U = 0.69$). In all cases, an average over several samples has been taken. Two values of the magnetization, indicated by horizontal arrows, can be identified in this figure: the upper one (labelled BG) corresponds to the expected equilibrium result for the magnetization, while the lower one, labelled QSS, represents the value of M in the quasi-stationary state.

equilibrium statistical mechanics. This numerical result has a profound meaning because it reveals that, for this long-range system, the order in which one performs the $t \to \infty$ with respect to the $N \to \infty$ limit is crucial. Statistical mechanics describes the situation in which the infinite time limit is considered *before* the number of particles tends to infinity. Here, it becomes apparent that reversing the order of the limits leads to a *different equilibrium state*. This aspect has been particularly emphasized in several papers by Tsallis and co-workers (including Ref. [3]), who propose that such a state should be described by Tsallis statistics [4]. However, because of the absence of derivations from first principles and of testable predictions of this theory, this cannot be considered as a satisfactory solution of this puzzling dynamical behaviour.

Let us remark that, although the description at the beginning of last paragraph clarifies the origin of the observed "dynamical" ensemble inequivalence, it does not give any hint on how to characterize the system in the QSS state. In the next section, we will show that a theory based on the Vlasov equation associated to the HMF model provides fully justified arguments and predictions on the behaviour of the QSS state.

Let us finally observe that the slow time evolution towards the Boltzmann–Gibbs equilibrium shown in Fig. 2 also explains why the microcanonical simulations reported in Fig. 1 do not correspond, as expected, to the theoretical results given by microcanonical and canonical statistical mechanics. The simulation time was simply too short and would one have waited longer, the disagreement would have totally disappeared. Moreover, simulation points corresponding to initial velocity distributions which have smaller stability thresholds (see next section) show a stronger disagreement with respect to the canonical caloric curve.

2. The Vlasov equation

For mean-field systems, and Hamiltonian (1) is one example, it has been mathematically proven [5,6] that, for a finite time and in the limit $N \to \infty$, the N-particle dynamics is well described by the Vlasov equation. Let us show how a simple minded kinetic theory allows us to derive the Vlasov equation.

The state of the N-particles system can be exactly described by the *discrete* single particle time-dependent density function, whose dynamics is exactly given by the Klimontovich equation [7]. However, it is far too precise for the description we are interested in, since it is a function of the $2N$ Lagrangian coordinates of the particles, θ_i and p_i.

As we are interested in systems with large number of particles, $1/N$ is a small parameter. This suggests to describe the system with an asymptotic expansion and to approximate the discrete density by a continuous distribution $f_0(t, \theta, p)$, depending on time t and only on the Eulerian coordinates of the phase space, θ and p. These steps are explicitly given in Ref. [8]. However, what is important for the purpose of this paper, is that at the lowest order, one gets the Vlasov equation

$$\frac{\partial f_0}{\partial t} + p\frac{\partial f_0}{\partial \theta} - \frac{\mathrm{d}\langle V\rangle}{\mathrm{d}\theta}\frac{\partial f_0}{\partial p} = 0, \tag{3}$$

where one has introduced the averaged potential

$$\langle V\rangle = -\int_0^{2\pi} \mathrm{d}\alpha \int_{-\infty}^{+\infty} \mathrm{d}p \cos(\theta-\alpha) f_0(t,\alpha,p). \tag{4}$$

The right-hand side of Eq. (3) is zero because of the $N \to \infty$ limit. It would be non-zero only if "collisional" effects were taken into account. It is however important to underline that there are no collisions here: granular effects or finite N corrections would be more appropriate names.

For homogeneous distributions with respect to θ, one gets $\langle V\rangle = 0$. The single particle distribution $f_0(t,p)$ is thus stationary since Eq. (3) can be rewritten as

$$\frac{\partial f_0}{\partial t}(t,p) = 0. \tag{5}$$

This explains the *stationarity* property of any homogeneous distribution $f_0(p)$. However, this does not ensure *stability*. Two different methods were subsequently introduced to determine stability. The first one relies on Lyapunov functional stability analysis using the energy-Casimir method [9], while the second one considers the poles of the dieletric constant of the Hamiltonian (see Refs. [7,10]). In both cases, one obtains that the homogeneous distribution $f_0(p)$ is stable if and only if the quantity

$$I = 1 + \frac{1}{2}\int_{-\infty}^{+\infty} \frac{f_0'(p)}{p}\,\mathrm{d}p \tag{6}$$

is positive. This condition reveals that there can be an infinite number of Vlasov stable distributions. Let us briefly discuss some examples:

- The first one is the Gaussian distributions $f_0(p) \sim \exp(-\beta p^2/2)$ (see Fig. 3) which is expected at equilibrium. With the threshold condition (6), one recovers the statistical mechanics result that the critical inverse temperature is $\beta_c = 2$, and its associated critical energy $U_c = \frac{3}{4}$ as plotted in Fig. 1.
- The second example is the water-bag distribution, also depicted in Fig. 3, which has been often used in the past to numerically test the out-of-equilibrium properties of the HMF model. In that case, one obtains a smaller critical energy $U_c = \frac{7}{12}$.
- Another example would be the q-exponentials of Tsallis statistics: $f_0(p) \sim [1-\alpha(1-q)p^2]^{1/(1-q)}$. In that case, one gets [11] that $U_c = 3/4 + (q-1)/2(5-3q)$, recovering the Gaussian result for $q = 1$ and the water-bag one when q approaches infinity with a cut-off to keep energy finite.
- The last example is a distribution with power-law tails

  $$f_0(p) = \frac{A}{1 + |p/p_0|^{\nu}}, \tag{7}$$

  where $p_0 = \sqrt{(\sin(3\pi/\nu)/\sin(\pi/\nu))(K/N)}$ controls the kinetic energy density K/N and $A = \nu\sin(\pi/\nu)/(2\pi p_0)$ is the normalization factor. The exponent ν must be greater than three to get a finite kinetic energy: we have used $\nu = 8$ (see Fig. 3). Note that the power-law distribution cannot be included in the q-exponential family, although it has similar power-law tails at large $|p|$. Distribution (7) is stable above the critical energy $U_c = 1/2 + \sin(\pi/\nu)/4\sin(3\pi/\nu)$.

All the above distributions are thus stationary solutions of the Vlasov equation (3). They are stable provided the quantity (6) is positive. However, it is important to realize that they are Vlasov stable stationary solutions among *infinitely* many others and there is no reason to emphasize one more than the other.

The existence of an infinite number of Vlasov stable distributions is the key point to explain the out-of-equilibrium QSS observed in the HMF dynamics and is shown in Fig. 2. Although we start initially from such a stable state (the homogeneous water-bag), finite N effects drive the system away from it, through other stable

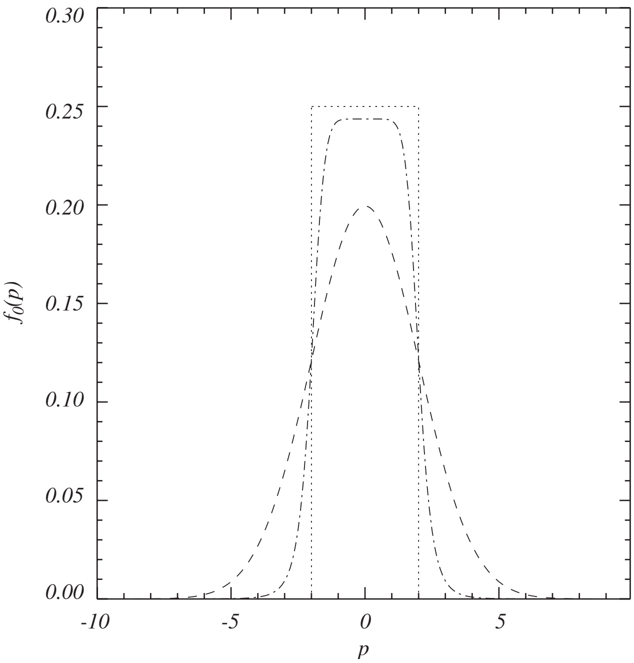

Fig. 3. Three examples of stationary homogeneous solutions of the Vlasov equation. The Gaussian (dashed), the water-bag (dotted) and the power-law (Eq. 7) in the case $v = 8$ (dash-dotted).

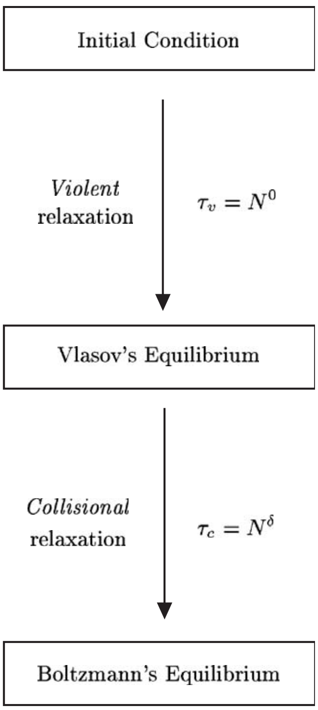

Fig. 4. Schematic description of the typical dynamical evolution of systems with long-range interactions.

stationary states. This slow quasi-stationary evolution across the infinite number of stationary and stable Vlasov states finishes with the ultimate evolution towards the Boltzmann–Gibbs equilibrium state. For the HMF model, it has been proven [7] that Vlasov stable homogeneous distribution functions do not evolve on time scales of order smaller or equal to N. This is in agreement with the $N^{1.7}$ scaling law numerically found [9] for the relaxation towards the Boltzmann–Gibbs equilibrium state.

Let us stress that the above scenario is consistent with what happens generically for systems with long-range interactions [12,13]. In a first stage, called *violent relaxation* the system goes from a generic initial condition, which is not necessarily Vlasov stable, towards a Vlasov stable state. This is a fast process happening usually on a fast timescale, *independent* of the number of particles. In a second stage, named *collisional relaxation*, finite N effects come into play and the Vlasov description is no more valid for the discrete systems. The timescale of this second process is strongly dependent on N. One generally considers that it is a power-law N^{δ}. A typical example is Chandrasekhar relaxation time scale for stellar systems, which is proportional to $N/\ln N$. This scenario of the typical evolution of long-range systems is summarized in Fig. 4.

It is important to remark that, recently, Caglioti and Rousset [14] rigorously proved that for a wide class of potentials, particles starting close to a Vlasov stable distribution remain close to it for times that scale at least like $N^{1/8}$: this result is consistent with the power-law conjectured for collisional relaxation. Unfortunately, apart from a recent progress [15], very few rigorous results exist in the case of singular potentials, which would be of paramount importance for Coulomb and gravitational interactions.

3. Conclusions

We have emphasized that the slow dynamical evolution of the Hamiltonian mean-field model (HMF) can be well understood with the help of the Vlasov equation.

Quasi-stationary states (QSS) observed in the N-particle dynamics of the HMF Hamiltonian are nothing but Vlasov stable stationary states, which lose their stability because of *collisional*, finite N, effects.

There is an *infinity* of Vlasov stable homogeneous (zero magnetization) states corresponding to different initial velocity distributions $f_0(t=0,p)$. Taking three examples (Gaussian, water-bag and power-law), we have shown that their stability domain in energy is different.

Also Tsallis q-exponentials in momentum, homogeneous in angle, distribution functions are Vlasov stable stationary states in a certain energy region where QSS are observed in the HMF model. However, they are not special in any respect, among an *infinity* of others.

In the finite N HMF systems, all of them converge sooner or later to the Boltzmann–Gibbs equilibrium. However, the relaxation time is shown numerically to diverge with a power-law N^{δ}, with $\delta \simeq 1.7$ for the homogeneous water-bag state. Analytically, one can prove that such a divergence must have $\delta > 1$.

On the time scale $\tau = t/N$, the QSS of the HMF model do not evolve. However, one can prove [7] that this is a peculiarity of one-dimensional models. This time scale is the appropriate one to study momentum autocorrelation functions and diffusion in angle. Such issues are discussed in more detail in Ref. [7], where *weak* or *strong anomalous diffusion* for angles is predicted, both at equilibrium and for QSS.

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