J Stat Phys (2013) 150:531–539
DOI 10.1007/s10955-012-0576-9

Non-equilibrium Dynamics of an Infinite Range XY Model in an External Field

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Received: 22 June 2012 / Accepted: 21 August 2012 / Published online: 1 September 2012

Abstract We study the XY model with infinite range interactions in an external magnetic field. The simulations show that in the thermodynamic limit this model does not relax to the thermodynamic equilibrium—instead it becomes trapped in a non-ergodic out-of-equilibrium state. We show how the relaxation towards this non-equilibrium state can be studied using the properties of the collisionless Boltzmann (Vlasov) equation.

Keywords XY model · Vlasov · Long-range

1 Introduction

It is our pleasure to dedicate this paper to Michael Fisher, Ben Widom, and Jerry Percus on the occasion of their 80th birthday. All three are the indisputable giants of the equilibrium statistical mechanics. In this paper, however, we would like to bring their attention to a new and largely unexplored area of physics: statistical mechanics of systems with long-range interactions. We hope that all three can bring their great intellects to bear on this difficult problem.

One of the first thing that we learn in an introductory course on statistical mechanics is that the mean-field approximation becomes exact when the interactions between the particles are infinitely long-ranged. This is a very interesting limit, since it applies both to confined one-component plasmas and to self-gravitating systems. One, might, therefore expect that this problem has been greatly explored by the statistical mechanics community. This, however, is not the case. A possible explanation for this neglect is, perhaps, due to the believe that there is really nothing to study and everything is very well understood—after all long-range systems are supposed to be trivially simple, they should be described exactly by the simple mean-field equations. There are no complicated correlations between the particles, such as the ones studied by Michael, Ben, and Jerry in liquids and magnets. Over

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the last decade, however, it has become very clear that long-range systems are surprisingly complex—much more so, than systems with short-range forces. Exactness of the mean-field limit of the Boltzmann-Gibbs statistical mechanics only applies to long-range systems that are in contact with a thermal bath. In this case, everything that is taught in a basic course on statistical mechanics is perfectly correct—one must take some care to properly define the thermodynamic limit [1–3], but once this is done, there are no great surprises (but see also [4]).

A surprise comes when one tries to study an isolated (microcanonical) system with long-range interactions [5] using molecular dynamics (MD) simulations. What one finds is that instead of relaxing to the thermodynamic equilibrium governed by static mean-field equations, the system becomes trapped in a non-ergodic out-of-equilibrium stationary state, with the one-particle distribution function showing a peculiar core-halo structure [6–11]. In the thermodynamic limit, long-range systems exhibit a strong ensemble inequivalence—while canonically they are perfectly well described by the equilibrium Boltzmann-Gibbs statistical mechanics, when isolated, they fail to relax to the thermodynamic equilibrium [12–15]. It is fairly easy to understand how the ergodicity breaking arises in the microcanonical ensemble. The thermodynamic limit for systems with long-range forces requires that the pairwise interactions between the particles be infinitesimally weak. This is achieved by scaling the two-body interaction potential with the number of particles. The thermodynamic limit, therefore, kills off all the interparticle correlations (collisions), so that the dynamics of each particle is completely controlled by the dynamical mean-field produced by all other particles. Since there are no collisions, the relaxation to equilibrium is controlled by the collective oscillations and the parametric resonances, which result in Landau damping [16]—some particles gain a lot of energy from the collective oscillations (resonances), at the expense of the collective motion. This particles then move to highly energetic regions of the phase space, which are very improbable from the perspective of the Boltzmann-Gibbs statistical mechanics. On the other hand, production of highly energetic particles, in turn, damps out the collective oscillations until the mean-field potential becomes completely static. When this happens, the dynamics of each particle becomes integrable (non-chaotic)—for a radially symmetric system—and the ergodicity is irreversibly broken [11].

The lack of ergodicity requires the development of new methods to study systems with long-range forces, since one can no longer decouple the "equilibrium" from "dynamics". In this paper, we will show how the dynamics determines the phase structure of a paradigmatic infinite range XY spin model in an external magnetic field.

2 The Model

We consider a system of N, XY interacting spins whose dynamics is governed by the Hamiltonian

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

where θ_i is the orientation of the ith spin, p_i is its conjugate momentum, and h is the external magnetic field [17]. The macroscopic behavior of the system is characterized by the order parameters (magnetic moments), $\mathbf{M}_n = (M_{xn}, M_{yn})$, where $M_{xn} \equiv \langle \cos(n\theta) \rangle$, $M_{yn} \equiv \langle \sin(n\theta) \rangle$, $n = 1, 2, \ldots$, and $\langle \cdots \rangle$ stands for the average over all the particles. The order parameters $M_n = |\mathbf{M}_n|$ measure the homogeneity of the distribution of angles: for

$M_n = 0$ we have a disordered paramagnetic state, whereas for finite M_n some degree of inhomogeneity (order) will exist. Using Hamilton's equations of motion, the dynamics of each spin is governed by $\dot{\theta}_i = p_i$, $\dot{p}_i = F(\theta_i)$, where

$$F(\theta_i) = -(h + M_{x1}) \sin\theta_i + M_{y1} \cos\theta_i. \tag{2}$$

The total energy per particle is given by

$$u = \frac{H}{N} = \frac{\langle p^2 \rangle}{2} + \frac{1 - M_1^2}{2} - hM_{x1}. \tag{3}$$

Since the Hamiltonian does not explicitly depend on time t, the total energy per particle u is conserved along the evolution.

We are interested to study how an initially disordered (paramagnetic) state develops order when magnetic field is turned on. We will consider an initial distribution of the waterbag form. Without loss of generality, we choose a frame of reference in which $\langle p \rangle = 0$, so that the initial one-particle distribution function reads

$$f_0(\theta, p) = \frac{1}{4\pi p_0} \Theta\big(p_0 - |p|\big), \tag{4}$$

where p_0 is the maximum modulus of the momentum. The energy per particle for this initial distribution is $u = p_0^2/6 + 1/2$. Because of the symmetry of f_0 and of the force $F(\theta)$ with respect to $\theta = 0$, in the thermodynamic limit the spin distribution $n(\theta)$ must be an even function of θ throughout the evolution, so that $M_{yn}(t) = 0$. Therefore, the macroscopic dynamics is completely determined by $M_{x1}(t)$. Another consequence of the parity of $n(\theta)$ is that the total momentum of the system is conserved, so that $\langle p \rangle = 0$ along the whole dynamics.

3 Nonlinear Equation for the Evolution of Magnetization

For finite h, the initial distribution given by Eq. (4) is not stationary, so that the system will evolve with time. Our aim here is to derive a low dimensional set of equations that can describe the macroscopic dynamics of the system, in particular, the magnetization moments $M_{xn}(t)$. In the thermodynamic limit $N \to \infty$, the dynamical evolution of the one particle distribution function is governed exactly by the collisionless Boltzmann (Vlasov) equation [18]

$$\frac{\partial f}{\partial t} + p \frac{\partial f}{\partial \theta} + F(\theta) \frac{\partial f}{\partial p} = 0. \tag{5}$$

The left-hand side of this equation is just the convective derivative of the one-particle distribution function. Therefore, the system evolves over the phase space as an incompressible fluid. Supposing that the external field h is sufficiently weak to produce only a small change in the phase-space particle distribution,

$$f(\theta, p, t) = \frac{1}{4\pi p_0} \Theta(p_{\max} - p) \Theta(p - p_{\min}), \tag{6}$$

where $p_{\min}(\theta, t)$ and $p_{\max}(\theta, t)$ are assumed to be continuous functions of θ that vary with time as the system evolves. Note that the phase-space density $1/4\pi p_0$ is preserved in accordance with the incompressibility imposed by Eq. (5). Since θ is periodic, we can expand $p_{\min}$ and $p_{\max}$ in a Fourier series. Truncating the series at second order, we write

$$p_l = \sum_{n=0}^{2} \left[A_n^l(t)\cos(n\theta) + B_n^l(t)\sin(n\theta) \right], \tag{7}$$

where $l = \min, \max$ and the coefficients $A_n^l(t)$ and $B_n^l(t)$ will be determined by the spin dynamics.

First, we note that the requirement that the spin distribution $n(\theta, t) = \int f(\theta, p, t)\, dp$ is an even function of θ (and consequently that $\langle p \rangle = 0$) requires that

$$A_n^{\min} = \pm A_n^{\max}, \tag{8}$$

$$B_n^{\min} = B_n^{\max} \equiv B_n, \tag{9}$$

for all n. Next, we observe that the total volume occupied by the distribution (6) in phase space must be preserved, i.e., the norm is conserved, requiring

$$A_0^{\max} = -A_0^{\min} = p_0. \tag{10}$$

Substituting Eqs. (6) and (7) in the definition of the magnetic moments

$$M_{xn} = \left\langle \cos(n\theta) \right\rangle = \int f(\theta, p, t)\cos(n\theta) dp\, d\theta, \tag{11}$$

we readily obtain $M_{xn} = (A_n^{\max} - A_n^{\min})/4p_0$. Therefore, in order to describe states with finite magnetization and to be consistent with the condition expressed by Eq. (8), we must require

$$A_n^{\max} = -A_n^{\min} = 2p_0 M_{xn}, \;\; n = 1, 2. \tag{12}$$

Now, taking the successive derivatives of Eq. (11) we obtain

$$\dot{M}_{xn} = -n \left\langle p \sin(n\theta) \right\rangle, \tag{13}$$

$$\ddot{M}_{xn} = -n^2 \left\langle p^2 \cos(n\theta) \right\rangle - n \left\langle F(\theta)\sin(n\theta) \right\rangle. \tag{14}$$

Note that these equations can also be derived by taking the appropriate moments of the Vlasov equation (5). Substituting Eqs. (6)–(12) into Eq. (13) leads to $\dot{M}_{x1} = [B_1(M_{x2} - 1) - B_2 M_{x1}]/2$ and $\dot{M}_{x2} = -B_2 - B_1 M_{x1}$. Solving these equations with respect to B_1 and B_2 we find

$$B_1 = \frac{2\dot{M}_{x1} - M_{x1}\dot{M}_{x2}}{M_{x1}^2 + M_{x2} - 1}, \tag{15}$$

$$B_2 = -\frac{2M_{x1}\dot{M}_{x1} + (M_{x2} - 1)\dot{M}_{x2}}{M_{x1}^2 + M_{x2} - 1}. \tag{16}$$

Finally, using Eqs. (2) and (6)–(12) in Eq. (14) we obtain

$$\begin{aligned} \ddot{M}_{x1} = {} & \left[h + \left(1 - 2p_0^2\right)M_{x1}\right]/2 - M_{x1}B_1^2/4 \\ & - \left[B_2^2 M_{x1} + B_1 B_2 + M_{x2}(h + M_{x1})\right]/2 \\ & - \left[M_{x1}^2 + 2M_{x2}(M_{x2} + 1)\right]p_0^2 M_{x1}, \end{aligned} \tag{17}$$

$$\begin{aligned} \ddot{M}_{x2} = {} & -4p_0^2\left[M_{x2} + M_{x2}^3 + M_{x1}^2(2M_{x2} + 1)\right] \\ & + B_1^2(1 - 2M_{x2}) - B_2^2 M_{x2} + M_{x1}(h + M_{x1}). \end{aligned} \tag{18}$$

Equations (17) and (18) are a closed set of nonlinear second order differential equations for the evolution of $M_{x1}(t)$ and $M_{x2}(t)$. They provide an approximate description of the macroscopic dynamics of an infinite range XY model with a small external field. The initial distribution given by Eq. (4), provides the initial conditions for the dynamics of magnetic moments, $M_{x1}(0) = \dot{M}_{x1}(0) = M_{x2}(0) = \dot{M}_{x2}(0) = 0$.

4 Linear Analysis

We start by studying the linear regime of Eqs. (17) and (18). For vanishingly small h, we expected that the resulting magnetization of the system will also remain small, i.e., $M_{xn} \sim \mathcal{O}(h)$. Retaining only linear terms in the equations, we obtain

$$\ddot{M}_{x1} + \left(\frac{2p_0^2 - 1}{2}\right) M_{x1} = \frac{h}{2}, \tag{19}$$

$$\ddot{M}_{x2} + 4p_0^2 M_{x2} = 0. \tag{20}$$

Equation (19) shows that M_{x1} will undergo stable oscillations described by

$$M_{x1}(t) = \frac{2h}{2p_0^2 - 1} \sin^2\left(\sqrt{\frac{2p_0^2 - 1}{2}} \frac{t}{2}\right) \tag{21}$$

as long as $p_0^2 > 1/2$. This result is the same as obtained using the linear response theory based on the Vlasov equation (5) [17]. Equation (20) also shows that at the linear order M_{x2}, is not coupled to the external field h, leading to a trivial dynamics, $M_{x2}(t) = 0$. For $p_0^2 < 1/2$, the oscillations of magnetization around $h/(2p_0^2 - 1)$ become unstable. The linear theory, however, is unable to provide any information on the new stable points of oscillation.

5 Nonlinear Macroscopic Oscillations

To investigate the nonlinear dynamics of the magnetic moments, we need to numerically solve Eqs. (17) and (18). In Fig. 1 we show the numerical integration of these equations for $h = 0.1$ and $u = 0.7$ ($p_0 \approx 1.095$). In the panel (a), the theoretically calculated evolution of M_{x1} is compared with the results of MD simulations and with the linear response theory given by Eq. (21). It is clear that the linear response theory rapidly dephases from the results of simulations, while the nonlinear equations (17) and (18) provide a very good description of the dynamics. For longer times, however, there is also a dephasing of the nonlinear equations as well. We expect that inclusion of higher order modes in the Fourier expansion of Eq. (7) should lead to progressively more accurate nonlinear solutions. In Fig. 1(b), we also present the results the evolution of $M_{x2}(t)$. While the linear theory predicts that $M_{x2}(t) = 0$, the figure clearly shows that it undergoes a complicated temporal dynamics, which is well captured by our non-linear equations, as compared to the MD simulations.

In Fig. 2 we present the snapshots of the phase space obtained using the MD simulation for different times along the first oscillating cycle of M_{x1}. The lines correspond to p_{min} and p_{max} of Eq. (7), as obtained from the nonlinear theory. We see that there is a very good agreement between these functions and the borders of the actual particle distribution.

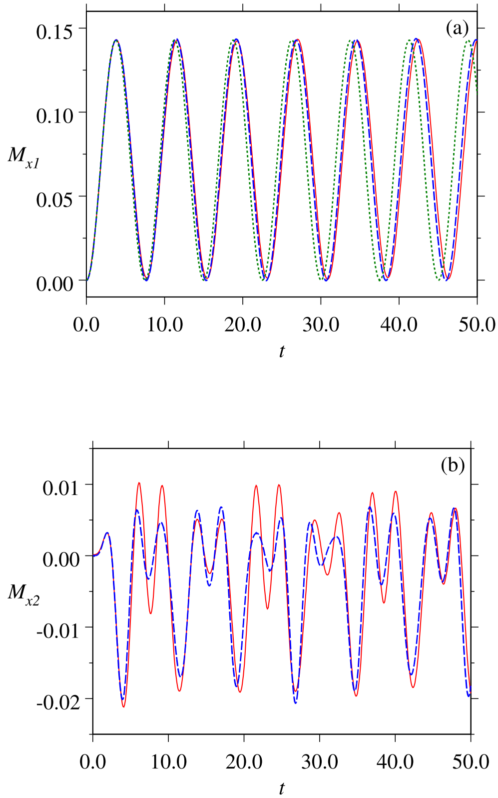

Fig. 1 Evolution of the magnetic moments M_{x1} in (**a**) and M_{x2} in (**b**) for $u = 0.7$ and $h = 0.1$. The *solid red line* is obtained using MD simulation with $N = 10^7$ particles. The *dashed blue line* is the result of the nonlinear evolution equations (17) and (18). In panel (**a**), the *dotted green line* corresponds to the linear response, Eq. (21) (Color figure online)

6 Stationary Solutions

Despite the fact that the Vlasov equation (5) is time reversible and, therefore, the temporal evolution never ceases, in some cases the system may evolve towards a "coarse grained" stationary state. This is possible because in such cases the evolution generates a filamentation of the distribution in the phase-space that occurs at progressively smaller length scales. Upon coarsegraining, it will then appear that the system has reached a stationary state. This is illustrated in Fig. 3. From the point of view of the macroscopic dynamics, the relaxation process may then be seen as an effective damping in the evolution of magnetic moments. The damping is provided by the Landau mechanism in which some spins enter in resonance with the oscillations of $M_{x1}(t)$ gaining large amounts of energy at the expense of the collective motion. The effective damping will then favor the relaxation of M_{x1} and M_{x2} towards the fixed points of Eqs. (17) and (18). In order to test this, we ran MD simulations up to $t = 400$ and computed the time averaged magnetic moment $\bar{M}_{x1}$ over the final interval $\Delta t = 200$. The results are shown in Fig. 4, where, for the sake of comparison, we also plot the prediction from the linear response theory. Although the agreement is not perfect, it is clear that the nonlinear theory of Eqs. (17) and (18) reproduces better the numerical results as compared to the linear theory. In particular, it correctly predicts the increase in the slope of $\bar{M}_{x1}$ as a function of h near $h = 0.03$, followed by a decrease in the slope for $h > 0.05$. We can expect that inclusion of higher order harmonics in Eq. (7) will lead to even a better agreement between the theory and the MD simulations.

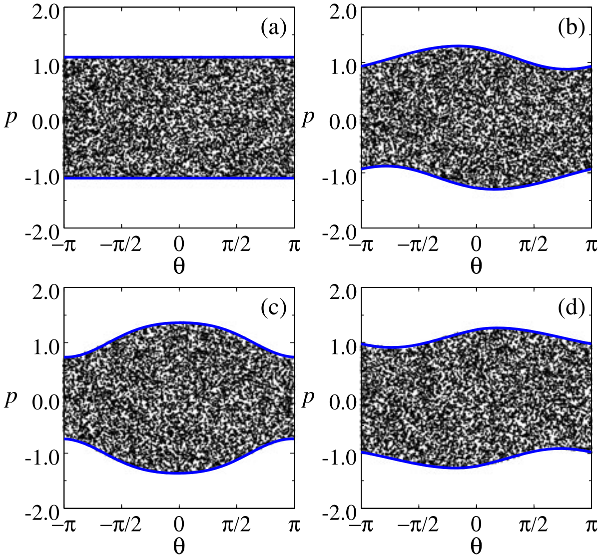

Fig. 2 Snapshots of the phase space obtained using MD simulation with $u = 0.7$ and $h = 0.1$. The snapshots were taken at $t = 0.0$ (**a**), $t = 2.0$ (**b**), $t = 4.0$ (**c**), and $t = 6.0$ (**d**). The *lines* correspond to $p_{\min}$ and $p_{\max}$ of Eq. (7) as obtained from the nonlinear theory (Color figure online)

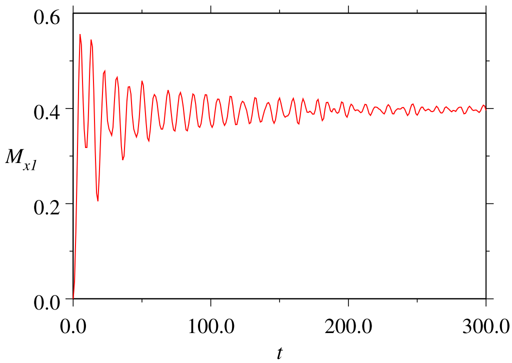

Fig. 3 Evolution of the magnetic moments M_{x1} for $u = 0.6$ and $h = 0.15$ obtained using MD simulations with $N = 10^6$ particles. In this case the system relaxes towards a macroscopic quasi-stationary state. After $t \approx 10^{10}$, the system will crossover to thermodynamic equilibrium state with $M_{x1} = 0.48$ (Color figure online)

7 Conclusions

We have studied the XY model with infinite range interactions, in an external magnetic field. MD simulations show that in the thermodynamic limit this model does not relax to the thermodynamic equilibrium—instead it becomes trapped in a non-ergodic out-of-equilibrium state. Therefore, in the microcanonical ensemble, the Boltzmann-Gibbs statistical mechanics is inapplicable to this model. The model demonstrates the dramatic breakdown of the ensemble equivalence for systems with long-range forces. When put in a contact with a thermal bath, these systems relax to the usual thermodynamic equilibrium. Therefore, in the canonical ensemble they are perfectly well described by the Boltzmann-Gibbs statistical mechanics—there is a well defined entropy and free energy, with the state of thermodynamic equilibrium corresponding to the minimum of free energy. On the other hand, in the microcanonical ensemble, Boltzmann entropy looses all meaning. The stationary state to which an isolated system with long-range interactions will relax does not correspond to the maximum of the Boltzmann entropy. To study the (non-thermodynamic) equilibrium state to which the systems will evolve one must begin with the kinetic theory. The evolution of the one-

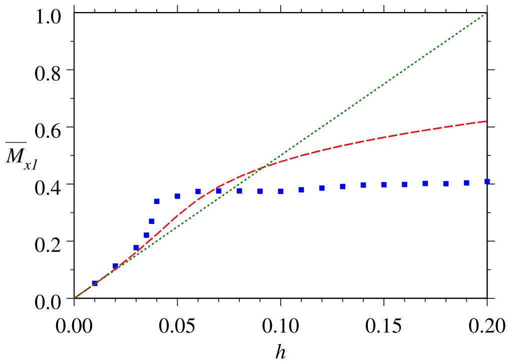

Fig. 4 Values of the time averaged magnetic moment $\bar{M}_{x1}$ as a function of h for $u = 0.6$. The *squares* are results from MD simulations performed up to $t = 400$ and averaged over the last 200 times with $N = 10^6$ particles. The *dashed red* line corresponds to the fixed points of the nonlinear equations (17) and (18), whereas the *dotted green line* is the result from linear response. For $h < 0.03$, the oscillations of $M_{x1}(t)$ do not show any significant damping (as in Fig. 1), while for $h > 0.03$ the oscillations are strongly damped, and the magnetization converges to a stationary value, as is shown in Fig. 3. For the set of parameters presented in the figure, the equilibrium Boltzmann-Gibbs statistics predicts magnetizations in the range $\bar{M}_{x1} = 0.486$–0.478 (Color figure online)

particle distribution function of a system with long-range interactions is governed by the collisionless Boltzmann (Vlasov) equation. The final state to which the system will evolve will not, in general, be described by the Boltzmann distribution—in fact, it will explicitly depend on the initial condition. Therefore, for these systems, dynamics will determine the equilibrium. In this paper, we have shown how the final state can be approximately predicted based on the properties of the Vlasov equation, without having to explicitly solve this complicated PDE. Clearly, long-range interacting systems are much more complicate and interesting than has been supposed only a decade ago. We hope that Michael, Ben, and Jerry might get stimulated by this new challenge.

Acknowledgements This work was partially supported by the CNPq, FAPERGS, INCT-FCx, and by the US-AFOSR under the grant FA9550-09-1-0283.

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