Dynamics of the d-HMF model: Sensitive dependence on size and initial conditions

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Abstract. We characterize the dynamics of systems with type-dipole interactions included in a new Hamiltonian mean field model [proposed by Atenas and Curilef, Phys. Rev. E (2017) 022110]. The sensitivity on the initial conditions is a particular behavior that we try to describe properly using molecular dynamics. We carry out simulations to focus our attention in the primary evolution before reaching the equilibrium. The current anomalies seem to characterize the general behavior of systems with long-range interactions. The dynamics of the system remains in quasi-stationary states before arriving at equilibrium.

1. Introduction
The main motivation in this work is the potential future applications in nanoscience and nanotechnology, where systems of rotors are mounted on surfaces or inside solids of particular interest. Until now, by far most molecular rotors have been studied in solution. After all, the rotor molecules need to be synthesized and their basic characteristics, such as rotational barriers, were established before mounting them on surfaces or examining them inside solids, and such synthesis and characterization are nearly always performed in solution[1]. Besides, to many authors, the investigation of molecular rotors freely floating in a solution is in itself a fascinating concern[1]. A variety of molecular systems have been artificially created, which can exhibit controlled rotational motion [2]. In the development of such systems, the key step is the addition of communication between molecules in a network. Therefore, the total energy of the rotor network, for the observed synchronized rotation mechanism, is analyzed through a model that is described by energy terms composed by: the internal rotational kinetic energy, the dipole energy, the external field energy, the structural energy including the dispersion interactions in the network, and the thermal energy corresponding to a substrate special temperature [2]. In our perspective, we approach the model taking into account just two terms in a Hamiltonian, namely the classical rotational energy and dipole potential in the mean field approximation.

In this regard, families of Hamiltonian mean field models may give a favorable outlook. Such models are related to systems with long-range interactions, which are very common in nature. They are observed from the atomic to the astronomical scale and exhibit some anomalies, such as inequivalence of ensembles, negative heat capacity, ergodicity breaking, non-equilibrium phase transitions, quasi-stationary states and anomalous diffusion [3, 4]. These anomalies are exacerbated when special initial conditions are imposed [4]. This is a topic that we also discuss in the course of the current paper. Canonical ensemble in statistical mechanics does not explain the
molecular dynamics on a short-time scale, though it proves to be correct on a larger time scale; i.e., canonical and microcanonical, whose phase diagrams are overlapped only at equilibrium.

As early concluded by Lynden-Bell statistics[6], a description based on Vlasov dynamics that preserves the hypervolume of phase-space density levels and uses the distribution functions as the solutions of Vlasov equation, that systems with long-range interactions can be trapped in quasi-stationary states (QSS), before going to equilibrium. However, the limitation of this theory is that properties similar to the usual statistical mechanics, as ergodicity and mixing, are required, which are not valid for systems with long-range interactions, where those properties are broken.

The Hamiltonian mean field (HMF) model [4, 5] is axiomatic and useful to characterize general properties of systems with long-range interactions. The existence of quasi-stationary states (QSS) before reaching equilibrium constitutes a fingerprint of this kind of systems, whose behavior of the kinetic energy and other thermodynamic observables are partly used to characterize the QSS [5, 6] in physical models and systems.

Some interesting systems related to charges, spins, rotors and dipoles are previously discussed in literature; for instance, charged particles[7] and noninteracting dipoles[8] in an external magnetic field, long range interactions in a type of Ising model and other generalized models [9, 10].

2. Basic equations
We consider $N$ identical coupled dipole-type particles with a mass equal to 1, whose dynamics evolves in a periodic cell described by a 1D, dipole-type Hamiltonian mean field (d-HMF) model as previously proposed[11], given by

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{\epsilon}{2N} \sum_{i \neq j}^{N} \left[ \cos(\theta_i - \theta_j) - 3 \cos(\theta_i) \cos(\theta_j) - \Delta_{i,j} \right],$$

(1)

where the variable $p_i$ represents the momentum of the particle $i$ and $\theta_i$ represents its corresponding orientation angle. With the integer $i \in [1, N]$, $N$ is the size of the system. In Figure 1 we illustrate two dipoles in a ring, whose angles are defined by the position the ring. Initial condition are defined in $t = 0$ and the illustration in $t \neq 0$ is arbitrary. The parameters $\epsilon$ and $\Delta_{i,j}$ denote the coupling and initial conditions, respectively. The parameter $\Delta_{i,j}$ suitably establishes, as shown[11], the zero of the potential energy.

![Figure 1. Two dipoles are shown in a ring. a) For $t = 0$, initial conditions are represented. b) For $t \neq 0$, an arbitrary state is illustrated.](image)

2.1. Initial distribution
The interaction coupling is rescaled by the number of particles, to make the potential thermodynamically extensive[9, 10, 11, 12]. We take a ferromagnetic system with a coupling,
\( \epsilon \), positive. The application of numerical methods has become an acceptable tool for the study and characterization of anomalies nonequilibrium. Following a previous line of research, some details related to these interactions are shown. Therefore, we can introduce the total spin vector

\[
\vec{M} = \left( \frac{1}{N} \sum_{i=1}^{N} \cos \theta_i, \frac{1}{N} \sum_{i=1}^{N} \sin \theta_i \right)
\]

(2)

\[
= (M_x, M_y)
\]

(3)

\[
= M \exp(i\phi),
\]

(4)

where \((M_x, M_y)\) are the components of the vector \(\vec{M}\), and \(M = |\vec{M}|\). In addition, \(\phi\) denotes the phase of the order parameter. The equation of motion is denoted by the following set of coupled equations given by

\[
\dot{p}_i = -\frac{\epsilon}{2N} (2M_x \sin \theta_i + M_y \cos \theta_i),
\]

(5)

where \(M_x\) and \(M_y\) represent the coupling terms. Then, the potential can be written as

\[
V = -\frac{\epsilon}{2N} (2M_x^2 - M_y^2 - \Delta),
\]

(6)

where \(\Delta = \sum_{i,j} \Delta_{i,j}\) as aforementioned defines the zero of the energy[11]. Moreover, we see that \(M_y \approx 0\) for all time of the evolution. Therefore, \(M \approx M_x\) that it allows us writing the internal energy per particle can be written as:

\[
U = \langle K \rangle - \frac{\epsilon}{2} (2M^2 - \Delta),
\]

(7)

where \(\langle K \rangle\) represents the mean value of the kinetic energy.

3. Discussion of Results
In this section, we introduce and discuss some results that characterize the present model. Numerical simulations in the microcanonical ensemble are carried out through molecular dynamics. The evolution of the system is characterized by two time intervals of QSS.

3.1. Initial distribution
The evolution of thermodynamical properties of the system is discussed by carrying out molecular dynamics simulation using a symplectic integrator[13]. At this stage, the relevant consideration is the choose of the initial distribution that we know as the water bag initial conditions (WBIC). With this respect, let us take the particles uniformly distributed in phase space. Thus, the general definition of the WBIC is related with the probability distribution function, \(f(\theta, p)\), as

\[
f(x, p) d\theta dp = \frac{d\theta dp}{4 \theta_0 p_0},
\]

(8)

where \(-p_0 \leq p \leq p_0\) and \(-\theta_0 \leq \theta \leq \theta_0\), which is properly normalized in all the space. If \(\theta_0 = \pi\) the function \(f(x, p)\) may be called “homogeneous in space” and it is a stationary solution of the Vlasov equation[14]. In the inhomogeneous case, \(0 < \theta_0 < \pi\), it is expected that the dynamics of the system evolves in a self-consistent way to satisfy its pertinent thermodynamic properties. As will see, we mainly discuss in the present contribution, the case where \(\theta_0\) is close to zero and it corresponds to the case where the dipoles are aligned almost in the same direction, preparing the samples with external fields and disconnecting them in \(t = 0\) to make the effort of characterizing the evolution of the properties of the system with this kind of WBIC because the anomalous behavior is exacerbated.
In Figure 2, we represent the average dynamics of the system by the evolution of $\langle K \rangle / N$ in 100 samples with $N = 25,000$ particles. The difference among curves comes from three different initial conditions that we consider. We take the WBIC given by Eq.(8) with a typical value of $\rho_0$ and three different values of $\theta_0$, which typically correspond to the extremely inhomogeneous case, $\theta_0 \approx 0$, an intermediate inhomogeneous case, $\theta_0 = \pi/7$, and the completely homogeneous cases, $\theta_0 = \pi$. In the inset of Figure 2, the first evolution is known as violent relaxation, which is clearly shown when WBIC is inhomogeneous; nevertheless, for the homogeneous case the quantity $\langle K \rangle / N = 0.76$ coincides with its numerical value for the second QSS. While the dynamics of the HMF model does not present evident differences if variations on the WBIC are considered, the d-HMF shows two different plateaus when the WBIC departs from the homogeneous case. Therefore, the results, shown in Figure 2, emphasize the relevance of the initial conditions in the dynamics of the problem. The appearance of two plateaus, before reaching the equilibrium, is due to considering the inhomogeneous WBIC.

3.2. Quasi-stationary states
We remark here some thermodynamic properties that we obtain from the simulations, related to effects of finite size and finite time, where QSS have been observed. In the dynamics of the model, it is important to observe where the kinetic energy is constant. As far as we know, this is relevant for determining the general behavior of other thermodynamic observables.

In Figure 3 (a), the time evolution of $\langle K \rangle / N$ is reported for several sizes of the system, this is $N = 8,000$, $16,000$, $32,000$, $70,000$ and $170,000$. The limiting cases are indicated in the figure, these are $N = 8,000$ and $N = 170,000$. The quantity $\langle K \rangle / N$ shows two plateaus, whose value and duration clearly depend on $N$. If $N$ increases, the value decreases, however, the duration increases. States defined by these plateaus, known as the QSS, are notoriously lower than the canonical temperature. It is known that WBIC stimulates the time that the systems remain in states of non-equilibrium, which are the QSS in the current case. They need times that

![Figure 2](image_url)

*Figure 2.* The evolution of the average over 100 samples of the kinetic energy with $N = 25,000$ as a function of the time. We see the evolution from three different initial condition $\theta_0 = 10^{-4}, \pi/7$ and $\pi$. In the homogeneous case, this is $\theta_0 = \pi$, the behavior is similar to the HMF model. In the extremely inhomogeneous case, $\theta_0 \approx 0$, the anomaly is the greatest and this is the case that we use to characterize the two QSS that are found in this dynamics. In the inset, the first evolution is shown, which is known as violent relaxation in linear scale.
increase with $N$ to transit from the first QSS to the second QSS, finally to relax to the canonical equilibrium. Averages represented in Figure 3(a) are taken in 100 samples for $N = 8,000$ and in 32 samples for $N = 16,000, 32,000, 70,000$ and $170,000$.

As discussed before, the behavior of systems is sensitive to the WBIC, which is remarked in Figure 3(a). In addition, these results evoke the behavior of systems that strongly depend on the size of systems. Properties slowly reach the thermodynamic limit. Results seem to indicate that the difference, between the two plateaus, tends to disappear as $N \to \infty$. Therefore, we indicate the first plateau as a QSS-type, contrary the second plateau that seems to define a true QSS. Hence, it is expected that the dynamics of the system has only one plateau when the thermodynamics limit is reached. Thus, the two plateaus is a peculiar effect induced by applying the inhomogeneous WBIC and by considering finite size of systems.

For simulation with $N = 32,000$ and greater, it is not possible to observe when the mean kinetic energy goes to the equilibrium in the time interval that we have carried out our molecular dynamics simulation, because of the computational limitations. Hence, a detailed characterization of the duration of the second QSS as a function of $N$, the size of the system, is a good challenge for future works. However, it is expected that the behavior becomes similar to the QSS observed for the HMF model. Nevertheless, if we focus our attention in the first plateau, this is the duration of the first QSS as $\tau(N)$, we observe that such a value depends on $N$ according a power law given by $\tau(N) \propto N^{\mu}$. In Figure 3(b) we obtain the approximate slope in log-log scale, that gives $\mu \approx 0.7$. This slope, $\mu$, is less than the $\mu$ known for the unique QSS that is observed in the HMF model[14]. The duration of the second QSS will be studied in the future, but we expect that becomes similar to the unique QSS that shows the HMF model[14].

4. Summary and Concluding Remarks
In summary, the d-HMF model(1) gives a good perspective for studying systems with long-range interactions.

It is generally accepted that two phases appear in the phase diagram that depend on the energy and, consequently, the temperature. At low energy, a phase identified by the presence of a single cluster of particles arises by floating in a diluted homogeneous background. At high energy a homogeneous phase is recovered; the cluster disappears and the particles move (almost) freely. The system is characterized by the microcanonical ensemble with negative specific heat and the resulting instability is extremely relevant[4] because of its strong implications on both experimental and theoretical features. It is expected that the non-equilibrium distribution related to the single cluster evolves into another non-equilibrium distribution, before reaching equilibrium. This behavior corresponds to an apparent thermodynamical inconsistency as explained by Hertel and Thirring[15], who proposed that the canonical and microcanonical ensembles are not equivalent near the transition region. We have successfully confirmed this proposal at least in an interval of time.

To describe the evolution of the model proposed here, we performed molecular dynamics simulations to obtain the QSS before arriving at equilibrium. Due to the non-equilibrium states, we can define two different QSS, as depicted in Figure 3. This observation is novel compared with other models that are known in the literature. We characterize the QSS as a constant value of the average kinetic energy. The second QSS has a value less than the first QSS.

Finally, we remark that the initial conditions and the size of the systems are two relevant considerations that we use in the study of the present topic. Thermodynamic and dynamic properties strongly depend on $N$ the size of systems that we partially characterize for the d-HMF model. We focus the analysis considering three possible initial distributions that correspond to the homogeneous WBIC and two cases of inhomogeneous WBIC. We see that if the homogeneous WBIC is considered, the behavior of the dynamic from the d-HMF model seems to be similar to the standard HMF model. After the process of violent relaxation, the system remains trapped.
Figure 3. The dependence on \( N \), the size of the system, of the twice mean kinetic energy is illustrated. The quantity \( 2\langle K \rangle/N \) is depicted as a function of the time. In (a), several sizes of the systems are considered. The cases indicated in the figure are the limiting ones: \( N = 8,000 \) and \( 170,000 \). Intermediate cases correspond to \( N = 16,000, 32,000, 70,000 \). In (b), we depict \( \tau \), the relaxation time of the first QSS that goes to second QSS, as a function of \( 1/N \) in log-log scale to obtain a power law of the duration of the first QSS in term of the size of the system. Thus, we expect that the lifetime observed in the in the first QSS behaves as \( \tau(N) \propto N^{0.7} \).

In a unique QSS before reaching the equilibrium. However, if the system is prepared in an inhomogeneous WBIC, the dynamics of the system shows two different plateaus before arriving at equilibrium as illustrated in Figure 2. The duration \( \tau \) of the first QSS depend on a power law of \( N \), typically this is \( \tau(N) \propto N^{0.7} \) as depicted in Figure 3. Due to the cost of the computational time, the description of the second QSS will be made in future works.

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