Hard-core collisional dynamics in the Hamiltonian mean-field model

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We consider a modification of the well studied Hamiltonian Mean-Field model by introducing a hard-core point-like repulsive interaction and propose a numerical integration scheme to integrate numerically its dynamics. Our results show that the outcome of the initial violent relaxation is altered, and also that the phase-diagram is modified with a critical temperature at a higher value than in the non-collisional counterpart.

Keywords: long-range systems, collisional HMF model, event-driven

I. INTRODUCTION

When performing molecular dynamics simulations of a classical many-particle system, one is usually concerned with two-particle interactions, where the interaction is characterized by an interaction potential $V(r)$ depending on the distance $r$ between the two particles. A potential in a $D$-dimensional space is considered long-ranged if it decays at large distances as $1/r^α$, with $α < D$, and conversely short-ranged if $α > D$ [1–5]. While systems with short-range interaction reach the thermodynamic equilibrium with a relatively short relaxation time and Gaussian final state depending only on the energy (and possibly other conserved quantities such as linear and angular momentum), systems with long-range interactions have a richer phenomenology. Among unusual properties that are observed in the latter, we may cite non-additivity of the thermodynamic functions, very long relaxation times to equilibrium diverging with the number of particles [6–10], negative heat-capacity [5–11] and non-ergodicity [12–15], although non-additive extensivity can be recovered using Kac’s prescription [16]. Since a negative heat-capacity is impossible in the canonical ensemble, but is observed in many instances of long-range systems, ensemble inequivalence is also possible for such systems. Examples of systems with a long-range interaction potential are: self-gravitating systems [17–19], plasmas [20–22], turbulence in two dimensions, cold Coulomb systems and dipolar systems [1], and different models such as one-dimensional gravity (sheets model) [23–25], the self-gravitating Ring Model [11–26] and the Hamiltonian Mean Field model (HMF) [27]. The latter has been extensively studied in the literature due to its simplicity, for being solvable at equilibrium and allowing much faster molecular dynamics simulations.

The dynamical process in the long-range systems out of equilibrium comprises a short transient violent relaxation into a quasi-stationary state (QSS) [28–29] with a long lifetime diverging with the number of particles $N$. Contrary to the thermodynamic equilibrium, the QSS depends strongly on initial conditions [30–31]. In fact, it depends on an infinite number of conserved quantities (see [32] for a more detailed discussion on this point). In the present work, we are interested in the study of the dynamics of mixed systems, i.e. systems with a long-range potential but also with a strong core interaction at short distances. Previous works on this include the Ising model with neighbor interactions [33–35] and the HMF model modified by adding a short-range term [36–38]. In both cases, the results obtained are similar to the strict long-range case. Here we will consider a hard-core interaction at zero distance. For particles of equal mass, this potential has simply the effect of interchanging the momenta, which is equivalent to a simple label swapping between the two particles involved. As a clear consequence, this has no effect whatsoever on the evolution of the one-particle distribution function, i.e. it does no affect the corresponding kinetic equation. This is no longer the case if one considers the case of particles of an $N$-particle system with different masses.

We consider in the present work a modified version of the HMF model by introducing a zero-distance hard-core potential and considering different masses, and assess its effect on the dynamics of the system, the relaxation to the final thermodynamic equilibrium, and mass segregation in the HMF model [39]. The paper is structured as follows: The model is described in section II, and the simulation algorithm in section III. In section IV presents our results, and we outline perspectives in section V.

II. THE MODEL

The HMF model is composed of $N$ particles on a unit circle with Hamiltonian

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

where $m_i$ is the mass, $\theta_i$ and $p_i$ are the angular position and conjugate momentum of the $i$-th particle, respect-
tively. The prefactor $1/N$ on the potential term is the Kac factor that can be interpreted as a change of time unit valid for any finite $N$ such that the total energy is extensive. The magnetization vector and its components are defined by

$$\mathbf{M} = \frac{1}{N} \sum_{i=1}^{N} (\cos \theta_i, \sin \theta_i) \equiv (M_x, M_y) = (M \cos \varphi, M \sin \varphi).$$

One usually considers the case of identical particles of unit mass. In this case, the total internal energy can be written as

$$e = \frac{H}{N} = \frac{1}{N} \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1 - M^2}{2}.$$  \hspace{1cm} (3)

The motion of particle $i$, generated by the $N$-body self-consistent dynamics of Hamiltonian \([1]\), is also the motion of a test particle generated from the “energy”

$$U_i = \frac{p_i^2}{2} + 1 - M \cos (\theta_i - \varphi).$$ \hspace{1cm} (4)

This single-particle dynamics does not conserve $U_i$, and one easily sees that $\sum_i U_i \neq N e$. This test-particle dynamics provides deep insight in the system evolution \([21, 40]\) because, when $\mathbf{M}$ evolves slowly, one may interpret the motion of each particle as that of a pendulum. Then one may define a separatrix in the single-particle $(p, \theta)$ space, with energy $U_s = 1 + M$, delineating particles with $U_i < U_s$ (which exhibit bounded oscillatory motion in the cat’s eye) from particles with $U_i > U_s$ (which travel over the whole circle). The existence of such a separatrix is the source of instabilities and is related to the chaotic behavior of the system, as discussed in \([40, 42]\).

As discussed above, in order to consider the effect of hard collisions on the dynamics of the system non-trivially, one has to handle the case with particles of different masses, which we consider now.

### III. INTEGRATION ALGORITHM

The particles are ordered in the initial configuration so that

$$\theta_1 < \theta_2 < \cdots < \theta_N.$$ \hspace{1cm} (5)

Due to the hard-core collision term, this ordering is preserved by the dynamics (modulo the crossing at the boundaries at $\theta = 0$ and $\theta = 2\pi$). In usual event-driven simulations, the time for the next collision must be computed and all particles are advanced to this time to implement the collision \([43]\). Of course, for the HMF model, this is not possible as the particle movement between collisions is not integrable. To determine the collision times, we use a simple trick: for a sufficiently small integration time step $\Delta t$, the particles that will eventually collide with each other are very close, and therefore the force on each one due only to the cosine potential is the same up to a small error proportional to $\Delta t^2$. Then the contribution of the force to the computation for the collision time cancels out. This approximation is computed for each particle at position $\theta_i$ and its neighbor particle at $\theta_{i+1}$ (considering that the neighbor of particle $N$ is particle 1). Only the shortest collision times are considered, and since the collision times array is updated at each time step, the induced error is kept very small as the ensuing error is one order of magnitude lower than the error in the integration method. Given the position of particles at a given time $t$, the approximation for the collision time is then

$$t_{i,i+1} = -\frac{\theta_{i,i+1}}{v_{i,i+1}},$$ \hspace{1cm} (6)

with $\theta_{i,i+1} \equiv \theta_i - \theta_{i+1}$, $v_{i,i+1} = v_i - v_{i+1}$ and $v_i = p_i/m_i$ the velocity of particle $i$. All possible collision times $t_{i,i+1}$ are computed at $t = 0$ and stored in the collision times array, which will be updated at each step of our algorithm, in such a way that when the time comes for two particles to collide, the corresponding collision time will be accurate.

Let us illustrate our approach for the second-order synchronized leap-frog scheme. For the HMF model without hard-core collisions, the algorithm has the following steps:

1. $p_i(t + \Delta t/2) = p_i(t) + F_i(\theta(t))\Delta t/2$,
2. $\theta_i(t + \Delta t) = \theta_i(t) + [p_i(t + \Delta t/2)/m_i]\Delta t$,
3. $p_i(t + \Delta t) = p_i(t + \Delta t/2) + F_i(\theta(t + \Delta t))\Delta t/2$,

where $F_i(\theta(t)) \equiv F_i(\theta_1(t), \ldots, \theta_N(t))$ is the force on particle $i$ due to all other particles. Collisions occurring in the time interval $(t, t + \Delta t)$ are implemented by subdividing step (2) above as:

i. Locate the next collision time and the corresponding pair of particles $(i, i+1)$.

ii. Evolve all particles up to time $t_{i,i+1}$ as a free motion with velocity $p_i(t + \Delta t/2)/m_i$.

iii. Update the collision times array for the new positions.

iv. Repeat steps (i) through (iii) until there are no collisions to implement in the time interval $(t, t + \Delta t)$.

The spatial ordering of the particles is kept by the exact dynamics, but small errors in the integration scheme may lead to some particle being in a wrong ordering. As a consequence, after each collision, a fast sequential search, with computer effort proportional to $N$, is performed. This ensures that particles are always ordered according to Eq. (5).
FIG. 1. Left panel: Magnetization as a function of time for the duration of the violent relaxation for $e = 0.5$, $N = 10000$ and averaged over 10 realizations. Right panel: same as the left panel but with $e = 0.8$.

FIG. 2. Left panel: Kinetic energy as a function of time for the duration of the violent relaxation for $e = 0.5$, $N = 10000$ and averaged over 10 realizations. Right panel: same as the left panel but with $e = 0.8$.

IV. RESULTS

As explained in the introduction, hard-core collisions in one dimension for identical particles do not change the time evolution of the system statistics. We thus consider particles with two different masses $m_1 = 1$ and $m_2 = 5$ with a proportion of 90% for particles with mass $m_1$. It is worth noticing that, for the usual HMF model, the dynamics naturally leads to mass segregation [39], while here no mass segregation is possible as the ordering in space of different masses is conserved due to the hard-core collisional force.

Figures 1 and 2 show the total magnetization $M$ and kinetic energy $K$ as a function of time for an interval encompassing the initial violent relaxation, for $N = 10000$ particles and two different initial energies per particle $e = 0.5$ and $e = 0.8$, for both the HMF model with and without collisions. A first important observation is that the QSS resulting from the violent relaxation is different in both cases, having different magnetizations. For the collisional case, the state resulting from the violent relaxation starts to change much more rapidly than for the case without collisions. This can be explained from kinetic theory by the fact that the collisional correction to the Vlasov equation has two contributions in the collisional case: a Balescu-Lenard type and a Boltzmann like integrals. The former is of order $1/N$ or $1/N^2$ for a non-homogeneous or homogeneous state, respectively [44], while the Boltzmann term is $N$-independent [45]. As a consequence, although apparently small, the collisional contributions from the hard-core potential to the kinetic equations dominate the system dynamics. The determination of an explicit kinetic equation for the present case is beyond the scope of the present paper and will be the subject of a forthcoming paper. Figure 3 shows the mag-
FIG. 4. Time evolution of the kinetic energy for $e = 0.8$, $N = 1000$ for the collisional and non-collisional HMF models up to the final equilibrium state.

netization as a function of energy after the violent relaxation at time $t_f = 500$ for a few energy values, where it becomes evident that the QSS after the violent relaxation is changed by the presence of hard-core collisions.

We note also that the existence of a hard-core force at zero distance may also change the final equilibrium state. Figure 4 shows the time evolution of the kinetic energy up to the final simulation time of $t_f = 10000$ for $N = 1000$ for both the collisional and non-collisional cases for $e = 0.8$, where it is evident that the system tends to states with different final temperature ($T = 2K$ taking the Boltzmann constant as unity) for the same energy. This in turn implies that the final magnetization is different. This can be explained physically by the fact that no mass segregation is possible for the collisional case, and the distributions of the two types of particles remain uniform (the initial distribution was chosen this way), while in the non-collisional case mass segregation occurs. This leads to different mean-fields and therefore to different equilibrium states.

V. CONCLUDING REMARKS AND PERSPECTIVES

We implemented collisional effects into the HMF model by considering a hard-core point-like interaction at zero distance, and proposed a numerical approach to simulate the model. The method was implemented using a second-order leap-frog scheme alongside an event-driven method in the spatial evolution part of the leap-frog. The same approach can be straightforwardly generalized to other numerical schemes such as the fourth order Runge-Kutta and symplectic integrators. The extension to higher dimensions is also possible and is the object of ongoing research. We showed that the introduction of a hard collision interaction changes the outcome of the violent relaxation in the HMF model, and also changes strongly the dynamics of the QSS resulting from the violent relaxation. We also presented evidence that the system evolves to a different configuration at equilibrium if the hard-core collision is present or not. This phenomenology may be important in situations where a short distance strong interaction is present, due for instance to a strong repulsive (or attractive) Coulombian interaction, or in a granular medium.

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