

Aging in an infinite-range Hamiltonian system of coupled rotators

Marcelo A. Montemurro,^{1,*} Francisco A. Tamarit,^{1,†} and Celia Anteneodo^{2,‡}¹Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina²Centro Brasileiro de Pesquisas Físicas Rua Xavier Sigaud 150, 22290-180, Rio de Janeiro, Brazil

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We analyze numerically the out-of-equilibrium relaxation dynamics of a long-range Hamiltonian system of N fully coupled rotators. For a particular family of initial conditions, this system is known to enter a particular regime in which the dynamic behavior does not agree with thermodynamic predictions. Moreover, there is evidence that in the thermodynamic limit, when $N \rightarrow \infty$ is taken prior to $t \rightarrow \infty$, the system will never attain true equilibrium. By analyzing the scaling properties of the two-time autocorrelation function we find that, in that regime, a very complex dynamics unfolds, in which *aging* phenomena appear. The scaling law strongly suggests that the system behaves in a complex way, relaxing towards equilibrium through intricate trajectories. The present results are obtained for conservative dynamics, where there is no thermal bath in contact with the system.

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At the very foundations of statistical mechanics, there are still some hypotheses whose validity rests merely on the extrapolation of observational facts and that have to be justified *a posteriori*. Among them, let us mention two assumptions that are intimately related to the issue addressed in this paper. The first one refers to the introduction of a probabilistic description of the evolution of a physical system. The second is related to the mechanical specifications that a system must fulfill so that the results of statistical mechanics can be applied [1]. These two points are closely related to the fundamental problem of establishing a connection between the dynamical behavior of a system, described by the Hamiltonian H , and its thermodynamics. In that sense, statistical mechanics requires the existence of adequate conditions allowing to replace the dynamical temporal predictions by a probabilistic ensemble calculation that yields the correct equilibrium mean value of the relevant quantities.

A very fast relaxation and a high degree of chaos and mixing are usually required in order to guarantee that a system orbit will cover most of its phase space in a short time. These questions have been extensively investigated for low-dimensional systems, whereas, for extended systems, with infinite degrees of freedom, the matter is still far from settled [2].

Due to the analytical and numerical efforts of many authors, it is today a well established fact that even very simple models, when analyzed in the thermodynamical limit $N \rightarrow \infty$, can yield results that bring to surface central questions about the foundations of statistical mechanics. In particular, in this work, we will concentrate on an infinite-range (mean-field) Hamiltonian system that, despite its simplicity, exhibits a very peculiar dynamical behavior: depending on the initial preparation of the system its evolution can get trapped into trajectories that will prevent the system from attaining equilibrium in finite time when the $N \rightarrow \infty$ limit is taken before

the $t \rightarrow \infty$ limit [3–8]. Unlike most models that display complex macroscopic behavior, this infinite-range model includes neither randomness nor frustration in its microscopic interactions. Furthermore, on one hand it can be exactly solved in the canonical ensemble, while on the other hand it can be efficiently integrated in the microcanonical ensemble. In that sense, it is an excellent starting point for analyzing the above mentioned basic questions.

The system consists of N fully coupled rotators whose dynamics is described by the following Hamiltonian:

$$\mathcal{H} = \frac{1}{2} \sum_i L_i^2 + \frac{1}{2N} \sum_{i,j} [1 - \cos(\theta_i - \theta_j)] \equiv K + V. \quad (1)$$

It is worth mentioning that this is a rescaled version of a nonextensive infinite-range Hamiltonian [9]. However, both of them share the same dynamical behavior after appropriate rescaling of the dynamic variables.

In Fig. 1, we display the plot, T vs U , where $T = 2\langle K \rangle / N$ is the temperature and $U = (K + V) / N$ is the total energy per particle. The solid line corresponds to the canonical

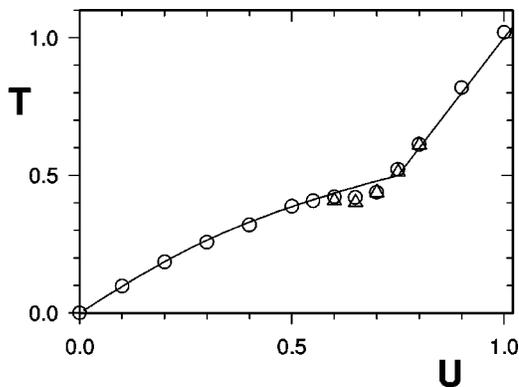


FIG. 1. The full line corresponds to the canonical theoretical caloric curve and the symbols correspond to numerical simulations for systems of size $N=1000$ (circles) and $N=5000$ (triangles), at $t=1000$, averaged over 50 realizations. Initial conditions are “water bag.”

*Email address: mmontemu@famaf.unc.edu.ar

†Email address: tamarit@fis.uncor.edu

‡Email address: celia@cbpf.br

cal calculations [3], which predict a second-order transition at $U_c=0.75$. Above U_c , constant specific heat is found and below U_c the system orders in a clustered phase. The symbols correspond to the numerical results obtained by integrating the equations of motion for $N=1000$, 5000 rotators and until $t=1000$. The system is initially prepared in a “water-bag” configuration, that is, all the angles are set to zero while the momenta are randomly chosen from a uniform distribution such that the system has total energy NU . By measuring the nonequilibrium temperature (or equivalently the magnetization) of a system started in these out-of-equilibrium initial conditions, one observes that, for a range of energy values below the transition, the system enters in a *quasistationary* regime characterized by a mean kinetic energy that varies very slowly. Moreover, the value of this nonequilibrium temperature remains different from that predicted by canonical calculations. Actually, standard equilibrium is attained only after a time which grows with the size of the system, hence an infinite system will never reach true equilibrium [7,8]. In the quasistationary regime preceding equilibrium, trajectories are non-ergodic and the dynamics is weakly chaotic with Lyapunov exponent vanishing in the thermodynamic limit [5].

It is our objective here to show that the discrepancy between the results drawn from the dynamics and those derived from the canonical ensemble is closely associated to the presence of strong long-term memory effects and slow relaxation dynamics, a phenomenon usually named *aging*. Aging is one of the most striking features in the off-equilibrium dynamics of complex systems. It refers to the presence of strong memory effects spanning time lengths that in some cases exceed any available observational time. Although aging has been seen in a wide variety of contexts and systems [10], some of them, actually very simple ones [2,11], it is perhaps in the realm of spin glass dynamics where a systematic study of these phenomena has been carried out (see Ref. [10], and references therein). Systems that *age* can be classified into dynamical universality classes according to the scaling properties of their relaxation function. Moreover, these scaling properties contribute to a quantitative description of complex phenomena, even in cases where a general theory is lacking [10,12].

Aging can be characterized by measuring the two-time autocorrelation function along the system trajectories. If the state of the system in phase space can be completely characterized giving a state vector \vec{x} , then the two-time autocorrelation function is defined as follows:

$$C(t+t_w, t_w) = \frac{\langle \vec{x}(t+t_w) \cdot \vec{x}(t_w) \rangle - \langle \vec{x}(t+t_w) \rangle \cdot \langle \vec{x}(t_w) \rangle}{\sigma_{t+t_w} \sigma_{t_w}}, \quad (2)$$

where $\sigma_{t'}$ are standard deviations and the symbol $\langle \dots \rangle$ stands for average over several realizations of the dynamics. In the case of a Hamiltonian system with N degrees of freedom the state vector is decomposed in coordinates and their conjugate momenta, therefore we establish the following notation: $\vec{x} \equiv (\vec{\theta}, \vec{L})$.

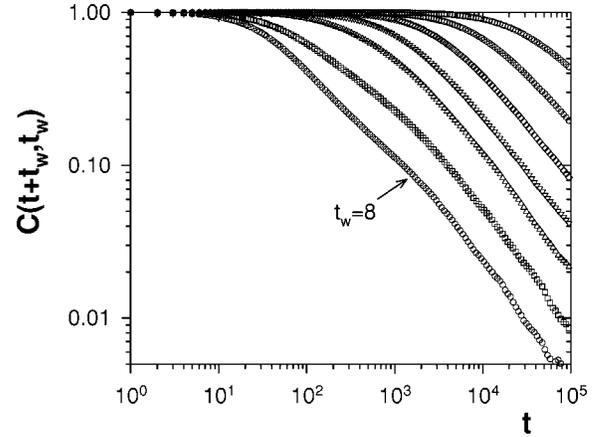


FIG. 2. Two-time autocorrelation function $C(t+t_w, t_w)$ vs t for systems of size $N=1000$ and energy per particle $U=0.69$. The data correspond to an average over 200 trajectories initialized in water-bag configurations. The waiting times are $t_w=8, 32, 128, 512, 2048, 8192, \text{ and } 32768$.

For systems that have attained “true” thermodynamical equilibrium, only time differences make physical sense when calculating relaxation quantities. In this case, it is expected that on an average the system will show only very short memory of past configurations. However, for systems exhibiting *aging*, a complex time dependence is observed in the behavior of $C(t+t_w, t_w)$, indicating long-term memory effects. In such a case, even at macroscopic time scales, the two-time autocorrelation function shows an explicit dependence on both times (t and t_w) together with a slow relaxation regime.

In order to integrate the motion equations numerically, we employed a fourth-order symplectic method [13] with a fixed time step selected so as to keep a constant value of the energy within a relative error $\Delta E/E$ of order 10^{-4} . All the simulations were started from the water-bag initial conditions explained above.

In Fig. 2, we present the results of the numerical calculation of the two-time autocorrelation function (2) for $U=0.69$. This value of the energy, together with the water-bag initial conditions set the system into a particular dynamical regime, in which ensemble discrepancy is more pronounced when finite size results are extrapolated to the thermodynamic limit. In the graph, features characteristic of aging phenomena can be distinguished. For a given t_w the system first enters a quasiequilibrium stage, in the sense that temporal translational invariance holds, with $C(t+t_w, t_w) \approx 1$, up to a time of order t_w . After that, the system enters a second relaxation characterized by a slow power law decay and a strong dependence on both times. This phenomenology can be clearly seen in the curves for the largest t_w 's.

In Fig. 3, we show the best data collapse for the long-time behavior of the autocorrelation function, using the data of Fig. 2 corresponding to the three largest waiting times ($t_w=2048, 8192, \text{ and } 32768$). The resulting scaling law clearly indicates that for the whole range of values of t/t_w considered,

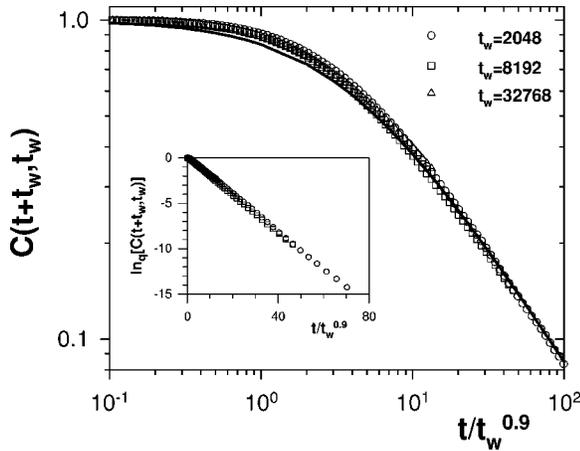


FIG. 3. Data collapse for the long-time behavior of the autocorrelation function $C(t+t_w, t_w)$. The data are the same shown in Fig. 2 for the three largest t_w . The gray solid line corresponds to $e_q(-0.2t/t_w^\beta)$. Inset: \ln_q -linear representation of the same data, with $q \approx 2.35$.

$$C(t+t_w, t_w) = f\left(\frac{t}{t_w^\beta}\right), \quad (3)$$

where $f(t/t_w^\beta) \sim (t/t_w^\beta)^{-\lambda}$. It is worth mentioning that this scaling is the same as observed experimentally in spin glass systems [14]. The values obtained for the scaling parameters are $\beta \approx 0.90$ and $\lambda \approx 0.74$. In the inset, we exhibit an alternative representation of the data which yields a linear plot. It corresponds to $\ln_q[C(t+t_w, t_w)]$ vs t/t_w^β , where the function $\ln_q(x)$, named q logarithm, is defined as follows [15]:

$$\ln_q(x) = \frac{x^{1-q} - 1}{1-q}. \quad (4)$$

In this expression, $q = 1 + 1/\lambda$, which for the data in Fig. 2, yields $q \approx 2.35$. Therefore, we can obtain a complete functional form of the autocorrelation function valid over the whole range of the scaling variable t/t_w^β just by identifying the function $f(x)$ in Eq. (3) with the inverse of $\ln_q(x)$, that is, the q exponential [15]:

$$f(x) \equiv e_q^{-x} = [1 - (1-q)x]^{1/(1-q)}, \quad (5)$$

which naturally arises within the nonextensive statistics introduced by Tsallis inspired by the probabilistic description of multifractal geometries [16]. The same qualitative behavior has been observed for other systems sizes, namely $N = 500, 2000$.

This aging scenario contrasts with the time invariant behavior observed within the high energy phase, where no quasistationary regime is detected. In fact, let us discuss Fig. 4 where we present the results of the calculation of the two-time autocorrelation function (2) for $U = 5.0$, well above the second-order phase transition (i.e., inside the homogeneous phase), with water-bag initial conditions. What we observe here is essentially that the autocorrelation function depends on the two times only through their difference, that is, $C(t$

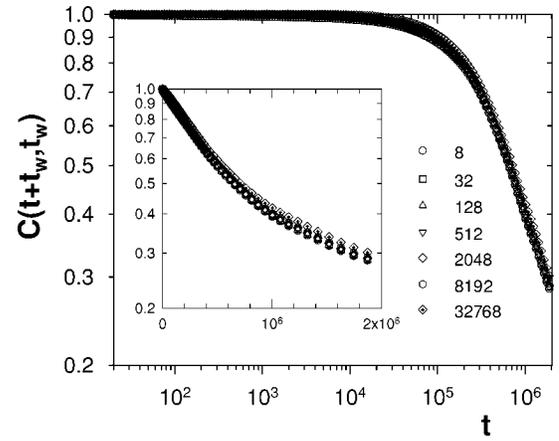


FIG. 4. Two-time autocorrelation function $C(t+t_w, t_w)$ vs t for systems of $N=1000$ and $U=5.0$. The data correspond to an average over 10 trajectories initialized in water-bag configurations. The waiting times are $t_w = 8, 32, 128, 512, 2048, 8192, \text{ and } 32768$. Inset: semilog representation of the same data.

$+t_w, t_w) \approx C(t)$. Therefore, the presence of aging is related to the existence of quasistationary states. It is important to emphasize that, although the dynamics presents temporal translational invariance in the high energy regime, the relaxation of the system is very slow.

There is nowadays growing evidence that aging is a very common dynamical phenomenon, associated to a great variety of physical systems. So far, there are two scenarios within which aging can emerge. On one hand, the onset of aging in many systems derives from the presence of coarsening processes that give place to critical slowing down of the dynamics. In this case the scaling law of the two-time autocorrelation function is ruled by the following expression

$$C(t+t_w, t_w) \sim f(L(t)/L(t_w)), \quad (6)$$

where $L(t)$ is the mean linear size of the domains at time t [17]. On the other hand, aging also appears as a consequence of weak ergodicity breaking [10] and it is related to the complex fractal structure of the region of phase space that the system explores in time. This is the case, for instance, in the Sherrington-Kirkpatrick (SK) model and other spin glass models in which the complexity of the energy landscape is associated to a certain degree of randomness and/or frustration in the Hamiltonian.

What is particularly remarkable in this work is the appearance of a complex aging behavior in a *mean-field* model lacking both randomness and frustration. Since the model we are analyzing in this paper is an infinite-range one, such as the SK model, a coarsening scenario has to be ruled out from the outset. Furthermore, all our results are obtained in a conservative system without any thermal bath in contact with it.

Moreover, it is worth noting that the scaling law found for the two-time autocorrelation functions below the transition, where a quasistationary regime is detected, points to a scenario very similar to that observed in spin glasses [14]. As occurs in spin glasses, there is weak breakdown of ergodicity, which is consistent with the observation of weakly cha-

otic orbits, i.e., with a vanishing Lyapunov exponent in the thermodynamic limit [5]. Drawing the analogy with spin glasses even further, our results seem to confirm that the system visits phase space confined inside very intricate trajectories (presumably nonergodic). This conjecture is also supported by features observed in μ space [6–8]. The fact that the relaxation of the two-time autocorrelation function can be well fitted by a q -exponential decay over the whole range of t/t_w deserves further investigation. Although a possible connection with nonextensive statistics [16] is still not clear, we believe that it would be interesting to examine this possibility.

In summary, in this paper we have characterized the slow relaxation dynamics of a long-range Hamiltonian system

through its aging dynamics. Our observation of the existence of aging in this Hamiltonian system and its characterization by scaling properties reminiscent of spin glass dynamics is a result that can contribute to establish a unified frame for the discussion of the out-of-equilibrium dynamics of systems with many degrees of freedom.

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