Ergodicity Breaking and Parametric Resonances in Systems with Long-Range Interactions

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We explore the mechanism responsible for the ergodicity breaking in systems with long-range forces. In thermodynamic limit such systems do not evolve to the Boltzmann-Gibbs equilibrium, but become trapped in an out-of-equilibrium quasi-stationary-state. Nevertheless, we show that if the initial distribution satisfies a specific constraint—a generalized virial condition—the quasistationary state is very close to ergodic and can be described by Lynden-Bell statistics. On the other hand, if the generalized virial condition is violated, parametric resonances are excited, leading to chaos and ergodicity breaking.

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Statistical mechanics of systems in which particles interact through long-ranged potentials is fundamentally different from the statistical mechanics of systems with short-range forces [1]. In the latter case, starting from an arbitrary initial condition (microcanonical ensemble) systems evolve to a thermodynamic equilibrium in which particle distribution functions are given by the usual Boltzmann-Gibbs statistical mechanics [2]. The state of thermodynamic equilibrium does not depend on the specifics of the initial distribution, but only on the global conserved quantities such as energy, momentum, angular momentum, etc. The situation is very different for systems in which particles interact through long-range potentials, such as gravity or unscreened Coulomb interactions [3–6]. In this case, it has been observed in numerous simulations that these systems do not relax to thermodynamic equilibrium, but become trapped in a quasistationary state (qSS), the lifetime of which diverges with the number of particles [4,6–8]. The distribution functions in this quasistationary state do not obey the Boltzmann-Gibbs statistical mechanics—and, in particular, particle velocities do not follow the Maxwell-Boltzmann distribution, but depend explicitly on the initial condition. It has been an outstanding challenge of statistical mechanics to quantitatively predict the final stationary state reached by systems with unscreened long-range forces, without having to explicitly solve the N-body dynamics or the collisionless Boltzmann (Vlasov) equation.

Some 40 years ago Lynden-Bell (LB) proposed a generalization of the Boltzmann-Gibbs statistical mechanics to treat systems with long-range interactions [9]. Lynden-Bell's construction was based on the Boltzmann counting, but instead of using particles, LB worked directly with the levels of the distribution function. The motivation for this approach was the observation that dynamical evolution of the distribution function for systems with long-range interactions is governed by the Vlasov equation [10]. This equation has an infinite number of conserved quantities, Casimirs—any local functional of the distribution function is a Casimir invariant of the Vlasov dynamics. In particular if the initial distribution function is discretized into levels, the volume of each level must be preserved by the Vlasov flow. For an initially one-level distribution function, Vlasov dynamics requires that the phase-space density does not exceed that of the initial distribution—one-particle distribution function over the reduced phase space (μ-space) evolves as an incompressible fluid. Using this constraint in a combination with the Boltzmann counting, LB was able to derive a coarse-grained entropy, the maximum of which he argued should correspond to the most-probable distribution—the one that should describe the equilibrium state. Numerous simulations, however, showed that, in general, Lynden-Bell statistics was not able to account for the particle distribution in self-gravitating systems, and the theory has been abandoned in the astrophysical context. Recently, however, Lynden-Bell's work has been rediscovered by the statistical mechanics community, which showed that for some systems, specifically the widely studied Hamiltonian mean-field model (HMF), Lynden-Bell's approach could make reasonable predictions about the structure of the phase diagram [11]. The fundamental question that needs to be addressed is: Under what conditions can Lynden-Bell statistics be used to accurately describe systems with long-range interactions? This will be the topic of the present Letter.

To be specific, we will study the HMF model [1], which has become a test bench for theories of systems with long-range forces. However, our results and methods are completely general and can be applied to other systems, such as self-gravitating clusters or confined non-neutral plasmas. The HMF model consists of N particles restricted to move on a circle of radius one. The dynamics is governed by the Hamiltonian

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

where the angle θ_i is the position of ith particle and p_i is its conjugate momentum [11–13]. The *macroscopic* behavior of the system is characterized by the magnetization vector

$\mathbf{M} = (M_x, M_y)$, where $M_x \equiv \langle \cos\theta \rangle$, $M_y \equiv \langle \sin\theta \rangle$, and $\langle \cdots \rangle$ stands for the average over all particles. The Hamilton equations of motion for each particle reduce to

$$\ddot{\theta}_i = -M_x(t)\sin\theta_i(t) + M_y(t)\cos\theta_i(t). \tag{2}$$

Since the Hamiltonian does not have explicit time dependence, the average energy per particle,

$$u = \frac{H}{N} = \frac{\langle p^2 \rangle}{2} + \frac{1 - M(t)^2}{2}, \tag{3}$$

is conserved.

The failure of LB theory in the astrophysical context was attributed to incomplete relaxation, lack of good mixing, or broken ergodicity [14]. The mechanisms behind this failure have not been elucidated. On the other hand, it has been recently observed that if the initial distribution is virialized—satisfies the virial condition—LB's approach was able to quite accurately predict the stationary state of gravitational and Coulomb systems [3–6]. Unfortunately, the virial theorem can be derived only for potentials which are homogeneous functions. This is not the case for the HMF model. Nevertheless, the fact that LB theory seems to apply under some conditions makes one wonder if such conditions can be found for arbitrary long-range potentials, which are not in general homogeneous functions.

To answer the questions posed above, we note that if the initial distribution is virialized, macroscopic oscillations of observables should be diminished. On the other hand, if the system is far from virial, the mean-field potential that each particle feels will undergo strong oscillations. It is then possible for some particles to enter in resonance with the oscillations of the mean-field, gaining large amounts of energy. The parametric resonances will result in the occupation of regions of the phase space which are highly improbable, from the point of view of Boltzmann-Gibbs or LB statistics [15]. Furthermore, resonant particles will take away energy from collective oscillations producing a form of nonlinear Landau damping [16]. After some time, macroscopic oscillations will die out and each particle will feel only the static mean-field potential. From that point on, particle dynamics will become completely regular, with no energy exchange possible between the different particles. The particles which have gained a lot of energy from the parametric resonances will be trapped forever in the highly improbable regions of the phase space, unable to thermalize with the rest of the system.

To see how the theoretical picture advocated above can be applied to the HMF, we first derive a generalized virial condition for this model. For simplicity we will consider initial distributions of the "water-bag" form in (θ, p). Without loss of generality, we choose a frame of reference where $\langle \theta \rangle = 0$ and $\langle p \rangle = 0$. The one-particle initial distribution function then reads

$$f_0(\theta, p) = \frac{1}{4\theta_0 p_0}\Theta(\theta_0 - |\theta|)\Theta(p_0 - |p|), \tag{4}$$

where Θ is the Heaviside step function, and $|\theta_0|$ and $|p_0|$ are the maximum values of angle and momentum, respectively. Note that from symmetry, $M_y(t) = 0$ at all times. When the dynamics starts, the mean-squared particle position will evolve with time. We define the envelope of the particle distribution as $\theta_e(t) = \sqrt{3\langle \theta^2 \rangle}$, so that $\theta_e(0) = \theta_0$. We next differentiate $\theta_e(t)$ twice with respect to time to obtain the envelope equation of motion,

$$\ddot{\theta}_e = \frac{3\langle p^2 \rangle}{\theta_e} + \frac{3\langle \theta\ddot{\theta} \rangle}{\theta_e} - \frac{9\langle \theta p \rangle^2}{\theta_e^3}. \tag{5}$$

Using the conservation of energy, $\langle p^2 \rangle = 2u + M_x^2(t) - 1$. To calculate, $\langle \theta\ddot{\theta} \rangle$, we use the equation of motion for θ. Supposing that the distribution of angles remains close to uniform on the interval $[-\theta_e, \theta_e]$, we obtain

$$\begin{aligned}\langle \theta\ddot{\theta} \rangle &= \frac{-M_x(t)}{2\theta_e}\int_{-\theta_e(t)}^{\theta_e(t)} \theta\sin\theta d\theta \\ &= M_x(t)\cos\theta_e(t) - M_x^2(t),\end{aligned} \tag{6}$$

where the magnetization $M_x(t)$ is

$$M_x(t) = \frac{1}{2\theta_e}\int_{-\theta_e(t)}^{\theta_e(t)} d\theta\cos\theta = \frac{\sin\theta_e(t)}{\theta_e(t)}. \tag{7}$$

Neglecting the correlations between positions and velocities, $\langle \theta p \rangle = 0$, we finally obtain a dynamical equation for the envelope

$$\ddot{\theta}_e = \frac{3}{\theta_e(t)}(2u + M_x(t)\cos\theta_e(t) - 1), \tag{8}$$

where $u = p_0^2/6 + (1 - M_0^2)/2$ and $M_0 = \sin(\theta_0)/\theta_0$. The generalized virial condition is defined by the stationary envelope, $\ddot{\theta}_e = 0$, which means that along the curve

$$(2u - 1)\theta_0 + \sin\theta_0\cos\theta_0 = 0 \tag{9}$$

magnetization remains approximately invariant. In Fig. 1 we plot Eq. (9) in the M_0-u plane and compare it with the full molecular dynamics simulation of the HMF model. As can be seen, agreement between the theory and simulation is excellent.

Along the generalized virial condition curve, Eq. (9), the magnetization—and, therefore, the mean-field potential acting on each particle of the HMF model—has only microscopic oscillations and the parametric resonances are suppressed. Under these conditions, we expect that LB theory will be valid. The coarse-grained entropy within the LB approach is given by

$$s(f) = -\int dpd\theta\left[\frac{f}{\eta_0}\ln\frac{f}{\eta_0} + \left(1 - \frac{f}{\eta_0}\right)\ln\left(1 - \frac{f}{\eta_0}\right)\right], \tag{10}$$

where $\eta_0 = 1/4\theta_0 p_0$ [17]. Maximizing this entropy under the constraints of energy and particle conservation, we obtain the equilibrium distribution function

$$f(p, \theta) = \frac{\eta_0}{e^{\beta[(p^2/2) - M_x\cos\theta - \mu]} + 1}. \tag{11}$$

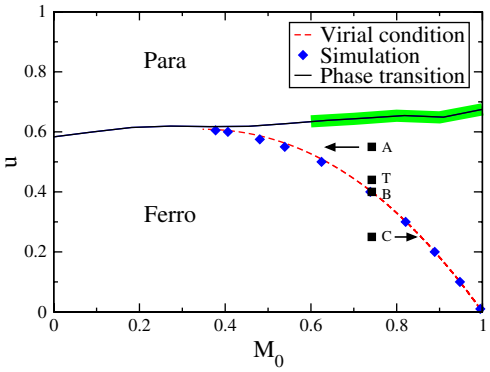

FIG. 1 (color online). Phase diagram of the HMF model obtained using the molecular dynamics simulations. Solid curve is the line of first order phase transitions separating paramagnetic and ferromagnetic phases. This line extends up to $M_0 = 0.6$, after which point the order of the phase transition, shaded region (green line), becomes unclear, with strong dependence on the initial conditions and various reentrant transitions occurring in this region. Dashed curve is the generalized virial condition, Eq. (9). Along this curve oscillations of the envelope are suppressed. Diamonds are the results of simulation. Starting with the initial energy and magnetization along the virial curve, diamonds show the final magnetization to which the system relaxes. For points along this curve, the final magnetization is almost identical to the initial one. Note that the generalized virial curve terminates at $M_0 = 0.34$ slightly below the phase transition line. This small difference, however, is sufficient to invalidate the Lynden-Bell theory, which for $M_0 = 0.4$ predicts a second order phase transition, while the simulations show that the phase transition is of first order [18]. Points (*A*), (*B*), and (*C*) correspond to the initial conditions for the distribution functions shown in Fig. 2. The Poincaré sections of the test particle dynamics for the initial conditions described by the points (B) and (*T*) are shown in Fig. 3. Finally, we note that since the stationary distribution must satisfy the virial condition and the energy is conserved, Eq. (9) allows us to predict the magnetization to which the system will evolve for initial conditions lying inside the ferromagnetic region, see the arrows for points (*A*) and (*C*).

The Lagrange multipliers μ and β are determined by particle and energy conservation,

$$\int dpd\theta f(p,\theta) = 1, \tag{12}$$

$$\int dpd\theta f(p,\theta)\left[\frac{p^2}{2} + \frac{1}{2}(1 - M_x\cos\theta)\right] = u, \tag{13}$$

respectively, and the magnetization by the self-consistency requirement,

$$\int dpd\theta\cos\theta f(p,\theta) = M_x. \tag{14}$$

Solving these equations numerically along the curve Eq. (9), we see that there is an excellent agreement between LB theory and the simulations, Fig. 2. If the macroscopic oscillations are suppressed and the parametric resonances are not excited, the system is able to relax to a quasiergodic equilibrium permitted by the Vlasov dynamics.

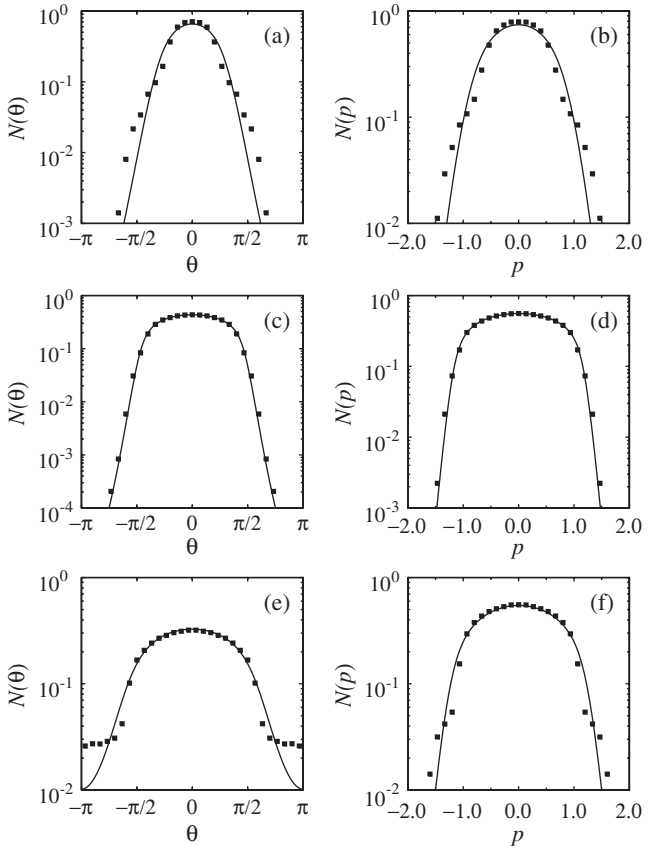

FIG. 2. The angle and velocity distribution functions corresponding to the initial conditions described by points (*A*), (*B*) and (*C*) of Fig. 1, respectively. Symbols are the results of molecular dynamics simulations and solid curves are the predictions of LB theory. The simulated distribution functions for the point (*B*), lying on the generalized virial curve, are in excellent agreement with the predictions of the LB theory [panels (c) and (d)], demonstrating that the dynamics along the generalized virial curve is quasiergodic. On the other hand, the distribution functions for points (*A*) and (*C*) deviate significantly from the predictions of LB theory — showing that away from the generalized virial curve, ergodicity is broken [panels (a),(b) and (e),(f)].

To make clear the role of parametric resonances in ergodicity breaking, in Fig. 3(a) we plot the Poincaré section of a set of noninteracting test particles, which at $t = 0$ are distributed in accordance with Eq. (4). The motion of each particle is governed by Eq. (2) with M_x determined by Eqs. (7) and (8). The position and momentum of each particle are plotted when magnetization is at its minimum. We see that if the energy and the initial magnetization lie on the generalized virial curve—point (B) of Fig. 1—particle trajectories are completely regular. However, when initial conditions do not coincide with the generalized virial curve—point (*T*) of Fig. 1—parametric resonances appear and dynamics becomes chaotic. Particles enter in resonance with the oscillations of the mean-field potential, gaining sufficient energy to move into statistically improbable regions of the phase space.

The Poincaré section of test particle dynamics is remarkably similar to the final stationary distribution obtained using the complete N-body molecular dynamics simulation of the HMF, Fig. 3. Equation (8) can also be used to calculate the period of the first oscillation of $M(t)$. For example, for point (T) of the phase diagram Fig. 1, we find the period to be $T = 5.0$, while the full molecular dynamics simulations gives $T = 5.4$. For point (C) we find $T = 3.85$, while the simulations give $T = 3.82$.

In conclusion, we have studied the mechanism responsible for the ergodicity breaking in systems with long-range interactions. Ergodicity breaking and the parametric resonances are intimately connected. If the macroscopic oscillations—and the resulting resonances—are suppressed, the system is able to relax to a quasiergodic stationary state. However, when the parametric resonances are excited, some particles are ejected to statistically improbable regions of the phase space, at the same time as the oscillations are damped out. The process of continuous particle ejection, and the resulting decrease of macroscopic oscillations of the envelope, leads to the formation of a static mean-field potential and to asymptotically integrable dynamics. Once the integrability of the equations of motion is achieved, the ergodicity becomes irreversibly broken. Unlike for particles with short-range interaction potentials, ergodicity is the exception rather than the rule for systems with long-range forces—it can only be observed if the initial distribution function satisfies the generalized virial condition derived in this Letter. Finally we note, that since the stationary distribution must satisfy the virial condition and the energy must be conserved, Eq. (9) allows us to predict the magnetization to which the system will evolve for initial conditions lying inside the ferromagnetic region. For example, point (A) of Fig. 1 which has initial magnetization and energy $M_0 = 0.74$ and $u = 0.55$, will evolve to a final stationary state with $M = 0.56$; while the point (C) with $M_0 = 0.74$ and $u = 0.25$, will evolve to a final stationary state with $M = 0.86$, which are precisely the values obtained using the molecular dynamics simulations.

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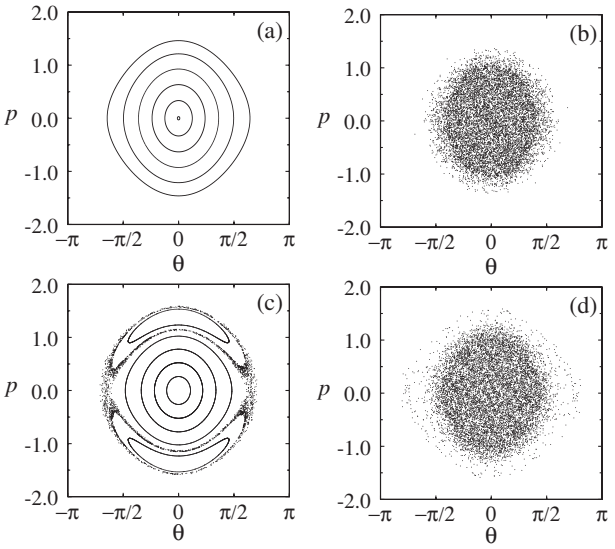

FIG. 3. Poincaré sections of test particles and snapshots of the phase space obtained using molecular dynamics simulation once the system has relaxed to qSS. Panels (a) and (b) correspond to the initial condition lying on the generalized virial curve, point (B) of Fig. 1. In this case the test particle dynamics is completely regular, and the stationary particle distributions are well described by LB theory. Panels (c) and (d) correspond to the initial conditions slightly off the virial curve, point (T) of Fig. 1. Even though we have moved only a little from the virial curve, we see the appearance of resonant islands and the dynamics of some of the test particles becoming chaotic. Such resonances drive some particles of the HMF to statistically improbable—from the point of view of the Boltzmann-Gibbs and LB statistical mechanics—regions of the phase space. Once the envelope oscillations are damped out, particle dynamics becomes completely integrable, and there is no mechanism for the resonant particles to equilibrate with the rest of the distribution. Thus, away from the generalized virial curve, ergodicity becomes broken.

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