Boundary-Induced Instabilities in Coupled Oscillators

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A novel class of nonequilibrium phase transitions at zero temperature is found in chains of nonlinear oscillators. For two paradigmatic systems, the Hamiltonian XY model and the discrete nonlinear Schrödinger equation, we find that the application of boundary forces induces two synchronized phases, separated by a nontrivial interfacial region where the kinetic temperature is finite. Dynamics in such a supercritical state displays anomalous chaotic properties whereby some observables are nonextensive and transport is superdiffusive. At finite temperatures, the transition is smoothed, but the temperature profile is still nonmonotonic.

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The characterization of steady states is a widely investigated problem within nonequilibrium statistical mechanics [1], since it provides the basis for understanding a large variety of phenomena, including transport processes, pattern formation, and the dynamics of living systems. In a nutshell, the simplest setup amounts to determining the currents that emerge as a result of the application of an external force, either across the system, as for electric currents, or at the boundaries, as in heat conduction [2–4]. Anyway, it is quite a nontrivial task to be accomplished, even when the departure from equilibrium is minimal and one can rely on the Green-Kubo formalism for establishing a connection between the microscopic and the hydrodynamic descriptions. For instance, this is testified by the discrepancy that still persists, after many years of careful studies, between the most advanced theories of heat conduction and some numerical simulations. The level of difficulty typically increases when one considers coupled transport [5–11] (i.e., when two or more currents coexist, such as heat and electric ones in thermoelectric effects) or, even worse, far-from equilibrium. This is why most of the theoretical studies concentrate on stochastic models, where fluctuations can be easily controlled, although they lack a truly microscopic justification. This approach proved, nevertheless, very effective, since it has allowed the discovering of nonequilibrium transitions, such as those exhibited by TASEP-like models, that have been used to describe translation of proteins, or traffic flows [12].

In this Letter we describe a novel class of boundary-induced transitions for two models that are typically used as test beds for a wide range of physical phenomena: the so-called Hamiltonian XY (or rotor) model [13–16] subject to an applied mechanical torque and the discrete nonlinear Schrödinger (DNLS) equation [17–19] under a gradient of the chemical potential. This type of qualitative change of the dynamics results from the joint effect of thermal and mechanical forces. It can be interpreted as a desynchronization phenomenon in a spatially extended dynamical system, whereby mutual entrainment of oscillators' phases is abruptly destroyed. As a result of such unlocking, a regime characterized by phase coexistence sets in where, although the chain is attached to two zero-temperature thermostats, an interfacial region is spontaneously created, where the oscillators have a finite kinetic temperature. Such a state can neither be predicted within a linear-response type of theory, nor traced back to some underlying equilibrium transition. Even more remarkably, it constitutes an example of a highly inhomogeneous, unusual chaotic regime. Indeed, we will show that the dynamical invariants have nonstandard dependence on the system size, as the fractal dimension is extensive while the Kolmogorov-Sinai (KS) entropy is not.

Studies of unlocking transitions have been previously performed in purely dissipative chains of phase oscillators [20], where, however, the absence of conservation laws prevents the onset of hydrodynamic regimes such as those herein described. The effect of external forces on the Hamiltonian XY model have been previously addressed only in Ref. [21] (see also Ref. [22]). Boundary-induced transitions are also known to exist for other classes of nonequilibrium models like stochastic lattice gases [23]. In the present case, however, the (zero-temperature) nonequilibrium transition is of purely dynamical origin.

Hamiltonian XY model.—The model consists of a chain of N rotors whose phases q_n evolve according to the equations

$$\dot{p}_n = \sin(q_{n+1} - q_n) - \sin(q_n - q_{n-1}) + (\delta_{1,n} + \delta_{N,n})[\gamma(F_n - p_n) + \sqrt{2\gamma T}\eta_n], \quad (1)$$

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where $p_n = \dot{q}_n$, F_n denotes a torque applied to the chain boundaries, γ is the coupling strength with two external baths, and η_n is a Gaussian white noise with unit variance. Even though the two heat baths are assumed to have the same temperature T, one expects (coupled) momentum and energy currents will flow through the lattice. The momentum (angular velocity) flux is defined as $j_n^p = \langle \sin(q_{n+1} - q_n) \rangle$, while the energy flux is $j_n^e = \langle (p_n + p_{n+1}) \sin(q_{n+1} - q_n) \rangle$ [24] (here and in the following, angular brackets denote a time average). Further useful observables are the average angular frequency $\omega_n = \langle p_n \rangle$ of the nth oscillator and the kinetic temperature $T_n = \langle (p_n - \omega_n)^2 \rangle$ (notice that a correct definition requires subtracting the average drift).

We first discuss the $T = 0$ case. As long as $F \equiv (F_1 - F_N)/2 < F_c = 1/\gamma$, the ground state is a twisted fully synchronized state, whereby each element rotates with the same frequency $\omega_n = (F_1 + F_N)/2$ and constant phase gradient. Here, $T_n = 0$ throughout the whole lattice. For $F > F_c$ the fully synchronized state turns into a chaotic asynchronous dynamics. All numerical simulations hereafter reported have been performed with $\gamma = 1$ and with $F_1 = -F_N = F$ (that amounts to fixed $\omega_n = 0$ below threshold). As shown in Fig. 1(a), the maximum value $\hat{T}$ of T_n along the lattice suddenly jumps to a finite value at $F = F_c$, indicating the presence of a first-order nonequilibrium transition. In fact, although the energy flux j^e vanishes (both heat baths operate at zero temperature), the momentum current j^p is different from zero and undergoes a substantial drop above the transition point [see Fig. 1(b)].

A more detailed characterization of the supercritical phase is reported in Figs. 2 and 3. The temperature profiles

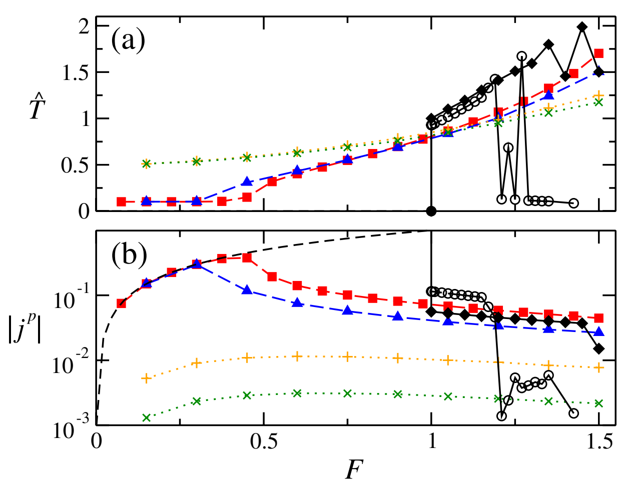

FIG. 1 (color online). Phase diagrams of the XY model. (a) Maximal kinetic temperature $\hat{T}$ vs F; $T = 0$: open circles ($N = 200$) and diamonds ($N = 6400$); $T = 0.1$: squares ($N = 200$) and triangles ($N = 800$); $T = 0.5$: plusses ($N = 200$) and crosses ($N = 800$). (b) Momentum flux j^p vs F for the same temperatures and symbols of panel (a); the black dashed line corresponds to $j^p = F$ for $F < F_c = 1$.

above threshold ($F = 1.05$) are shown in Fig. 2(a) for different values of N, after shifting the origin in the middle of the chain and rescaling the spatial position by $\sqrt{N}$. The nice overlap has two implications: (i) the maximal temperature $\hat{T}$ remains finite even in the thermodynamic limit and can, accordingly, be considered as an appropriate order parameter for this nonequilibrium transition; (ii) T_n is significantly different from zero only in a small central region, whose relative width scales as $N^{-1/2}$. Since the temperature is a macroscopic concept, it is legitimate to ask whether one can truly interpret T_n as a genuine thermodynamic temperature. A preliminary positive answer can be given by noticing that T_n does not vary significantly over a diverging number ($\approx\sqrt{N}$) of sites.

Additional information can be obtained by looking at the profile of the average angular frequency ω_n for $F = 1.05$. In Fig. 2(b) one can appreciate that the profile becomes increasingly kink-shaped, so that, in the thermodynamic limit, the chain is split into two symmetric regions, each one characterized by a rotation frequency equal to the value imposed at the boundary (F_1 and F_N, respectively). The two regions are separated by a localized interfacial area, where T_n is finite and ω_n changes from F_1 to F_N.

The supercritical phase is, however, more complex than revealed by this average characterization. In Fig. 2(c) we plot a space-time representation of the "instantaneous"

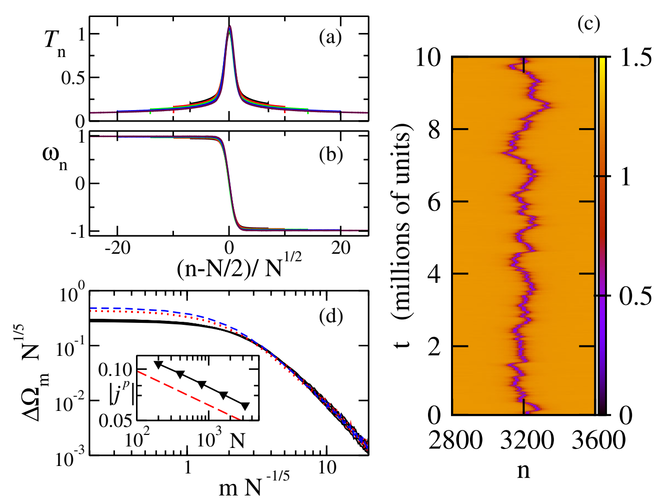

FIG. 2 (color online). Stationary behavior of the rotors chain for $T = 0$. Time averaged spatial profiles of temperature (a) and frequency (b) for $F = 1.05$ and $N = 200$, 400, 800, 1600, and 3200 (the averaging time is $t = 10^7$). The spatial direction is rescaled in order to obtain a data collapse in the central region. (c) Spatiotemporal profile of $|\Omega_n|$ for $F = 1.3$ and $N = 6400$ (see text for details). (d) Local frequency difference $\Delta\Omega_m$. Both axes are suitably rescaled to obtain a data collapse for different system sizes: $F = 1.05$ and $N = 400$, 800, 1600, and 3200 (black lines); $F = 1.2$ and $N = 1600$, 3200, and 6400 (dotted red lines); same parameters of panel (c) (dashed blue line). The inset shows the dependence on N the momentum flux j^p for $F = 1.05$ (black triangles): the red dashed line has slope $-1/5$.

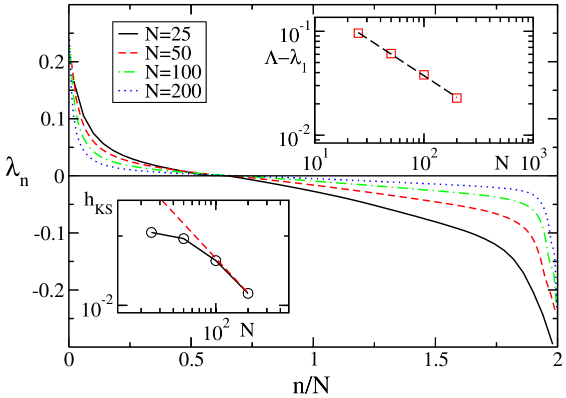

FIG. 3 (color online). Lyapunov spectra of the rotors chain for $F = 1.05$ and increasing sizes N. Upper inset: dependence of the maximal Lyapunov exponent λ_1 on N: the dashed line corresponds to the fit $\lambda_1 = \Lambda + aN^{-0.66\pm0.04}$ with $\Lambda = 0.262$. Lower inset: Kolmogorov-Sinai entropy vs N; the dashed line is the power-law $N^{-1/2}$. Total integration time $t = 2 \times 10^6$, time step 0.01 time units, Gram-Schmidt orthogonalization is applied every 20 time steps.

frequency profile $\Omega_n = \langle p_n \rangle_\tau$, where the average is performed over a time $\tau = 10^4$, that is much longer than the microscopic time scale and significantly shorter than the slow hydrodynamic scales. This representation reveals that the transition region is quite thin and fluctuates. Data have been reported for $F = 1.3$ and $N = 6400$ to show that this behavior is robust also for large values of the torque and for long chains. A more quantitative analysis can be performed by studying the shape of the instantaneous frequency profile. In practice, we study $\Delta\Omega_m = \langle \Omega_{m+\hat{n}(t)+1} - \Omega_{m+\hat{n}(t)} \rangle$, where m is the distance from the instantaneous position $\hat{n}(t)$ of the temperature peak. The data in Fig. 2(d) correspond to different values of F and is plotted after rescaling $\Delta\Omega_m$ and m by $N^{1/5}$ and $N^{-1/5}$, respectively. The good data collapse of the curves corresponding to various system sizes reveals the presence of a second scaling exponent.

The overall scenario can be described in the following way. On the one hand, the $N^{-1/2}$ scaling of the average profiles is related to the decay rate of the strength of the effective force which pins the interfacial region in the middle of the chain. On the other hand, the $N^{-1/5}$ scaling of the width of the instantaneous active region is related to the maintenance of the momentum flux, which, in fact, scales with the same exponent, $j^p \sim N^{-1/5}$ (see the inset in Fig. 2).

In order to further refine our understanding of the supercritical regime, we have computed the spectra of Lyapunov exponents λ_n ($n = 1, \ldots, 2N$). As a first check we have verified that the sum of all λ_n is equal to the dissipation -2γ, as it should. The spectra obtained for different system sizes reveal substantial differences from the standard (extensive) chaotic regime [25,26]. For increasing N, most exponents decrease and approach zero, indicating a weakly chaotic behaviour, consistently with the zero-temperature imposed at the boundaries. The spectrum does not, however, uniformly shrink to zero as λ_1 and λ_{2N} remain finite. In the upper inset of Fig. 3, one can see that the largest exponent $\lambda_1(N)$ approaches a constant $\Lambda = 0.262$ up to corrections of order $N^{-2/3}$. The existence of finite exponents is consistent with the observation of a finite temperature in the central region of the lattice where some chaotic dynamics persists in the thermodynamic limit.

A further inspection of Fig. 3 also reveals that the Lyapunov spectra cross the zero axis at a finite value $n_u/N \approx 0.6$, indicating that the dimension density of the unstable manifold is finite; i.e., this observable is extensive. The same is true also for the Kaplan-Yorke (KY) dimension, that increases with N and possibly converges to 2, meaning that the nonequilibrium invariant measure extends along (almost) all directions. Surprisingly, a qualitatively different behavior is observed for KS entropy-density h_{KS}, estimated as the area under the positive part of the Lyapunov spectrum. The results for different system sizes are reported in the lower inset of Fig. 3. There, we see that h_{KS} vanishes, revealing a nonextensive nature of the chaotic dynamics. By extrapolating from the largest simulations, one can conjecture a decay as $N^{-1/2}$. A yet more detailed analysis could be performed by investigating the convergence of the bulk of the Lyapunov spectrum, but this task would require considering much larger systems and we leave it to future studies.

The above features are rather unusual with respect to the usual space-time chaotic system whereby dynamical invariants are extensive with the volume [25,26]. They are instead partially reminiscent of delayed dynamical systems, where, for large delays, the KY dimension is extensive (i.e., proportional to the delay), while the KS entropy remains finite [27,28]. Here, however, this is a true instance of space-time chaos and the nonextensive character of the KS entropy is not a formal consequence of the interpretation of the delay as a spatial extension.

Additional studies carried out for larger F values confirm the general validity of this mixed extensive and nonextensive behavior. One has only to be careful in selecting sufficiently long chains, so as to avoid the existence of a pointlike interfacial region: this phenomenon, which is suggestive of a second transition (see the open circles in Fig. 1), is instead a finite size effect that disappears for sufficiently large values of N (see the diamonds in Fig. 1).

Finite temperature.—We now explore the behavior for nonzero boundary temperatures (i.e., in the presence of an external source of noise). The results reported in Fig. 1 indicate that for $T = 0.5$ (crosses and plusses) both $\hat{T}$ and the momentum flux depend smoothly on F. Additionally, the momentum conductivity is normal, i.e., $j^p \sim 1/N$. For smaller temperatures, a residue of the transition is still present as a sudden increase of $\hat{T}$ at finite F [see Fig. 1(a)

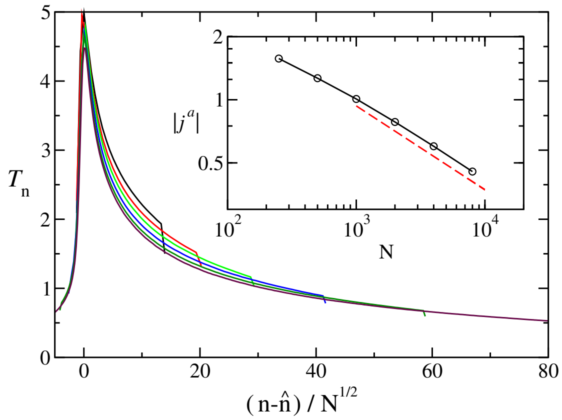

FIG. 4 (color online). Kinetic temperature profiles of the DNLS equation for $N = 250$, 500, 1000, 2000, 4000, and 8000 and $T = 0$, $\mu_1 = 2$ and $\mu_N = 5$. The spatial direction is rescaled in order to obtain a data collapse in the region around the point of maximal temperature $\hat{n}$. Inset: chemical-potential flux j_n^a vs system size N. The (red) dashed line corresponds to a slope $-2/5$.

for $T = 0.1$]. This is, nevertheless, a finite-size effect, as the pseudodiscontinuity disappears upon increasing N [compare squares and triangles in Fig. 1(a)]. This suggests that the fluctuations imposed on the boundaries induce phase slips, which are thereby responsible for the suppression of the synchronized state in the subcritical region. It is, however, interesting to notice the persistence of a bump in the temperature profile, although its width is now proportional to N.

DNLS model.—The above discussed nonequilibrium transition is not a peculiarity of the rotor model. Here below, we show that a similar scenario can be observed for the DNLS equation, $i\dot{z}_n = -2|z_n|^2 z_n - z_{n+1} - z_{n-1}$, where $z_n = (p_n + iq_n)/\sqrt{2}$ is a complex variable. The DNLS Hamiltonian has two conserved quantities, the mass or norm a and the energy density h [29,30], so that it is a natural candidate for describing coupled transport [10,31].

We have numerically studied a DNLS chain interacting with two Langevin thermostats at $T = 0$ and different chemical potentials μ_1 and μ_N imposed at the boundaries (see Ref. [31] for details). In this case, the control parameter, i.e., the driving force, is $\delta\mu = |\mu_N - \mu_1|/2$ [31]. When $\delta\mu$ is larger than a critical value (e.g., $\mu_1 = 2$ and $\mu_N = 5$), a bumpy temperature profile spontaneously emerges. In Fig. 4 one can see that the width of the peak scales as $N^{1/2}$, (as for the XY chain), while the left-right symmetry is lost and the mass (norm) flux $j_n^a = i\langle(z_n z_{n-1}^* - z_n^* z_{n-1})\rangle$ now scales as $N^{-2/5}$ instead of $N^{-1/5}$ as in the XY case (see the inset in Fig. 4).

Discussion and conclusions.—In this Letter we have shown that in the presence of coupled transport, the application of deterministic boundary forces may induce a nonequilibrium transition at zero temperature.

The different scaling behavior observed in two models (XY and DNLS), suggests the existence of multiple universality classes. We conjecture that, as in the context of (anomalous) heat conduction in one-dimensional systems, the discriminating factor is given by the presence of symmetries [24,32]. In the XY case, the average value of the torque is immaterial, since it can be removed by selecting a suitably rotating frame. This invariance implies that positive and negative frequency shifts are equivalent to one another and, as a result, symmetric profiles are expected and, indeed, observed. This symmetry is, however, not present in the DNLS dynamics, in spite of the fact that the DNLS equation can be effectively approximated by an XY model [31] in the limit of small gradients and large mass densities.

If finite-temperature heat baths are considered, the first-order transition is smoothed out and the anomalous superconductive behavior is replaced by a normal transport. A characterization of such a phase remains, however, nontrivial because of the underlying kink in the frequency or chemical potential profile, which induces a bump in the temperature and makes the implementation of a Green-Kubo formalism rather problematic. It will be instructive to explore the same problem in higher dimensions: one cannot exclude that the zero-temperature transition reported herein survives in the presence of finite fluctuations.

It is finally important to stress the anomalous properties of the supercritical phase in the context of nonlinear dynamics and synchronization phenomena. This regime is indeed characterized by a mixture of extensive (Kaplan-Yorke dimension) and nonextensive (Kolmogorov-Sinai entropy) properties, which make it atypical and different from (i) the standard extensive chaos typically observed in both dissipative and Hamiltonian models, and (ii) the localized chaotic states generated when all oscillators are damped and driven [33,34]. In other words, this regime provides an example of how complex dynamics can be in relatively simple models, characterized by nearest neighbor interactions.

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