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 non-trivial interfacial region where the kinetic temperature is finite. Dynamics in such supercritical state displays anomalous chaotic properties whereby some observables are non-extensive and transport is superdiffusive. At finite temperatures, the transition is smoothed, but the temperature profile is still non-monotonous.

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The characterization of steady-states is a widely investigated problem within non-equilibrium statistical mechanics, 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. Anyway, it is quite a non-trivial 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 (i.e. when two or more currents coexist, such as heat and electric ones in thermo-electric 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 discovering non-equilibrium transitions, such as those exhibited by TASEP-like models, that have been used to describe translation of proteins, or traffic flows.

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 subject to an applied mechanical torque and the Discrete NonLinear Schrödinger (DNLS) equation 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 there dynamical invariants have non-standard dependence on the system size, as the fractal dimension is extensive while the Kolmogorov-Sinai entropy is not.

Studies of unlocking transitions have been previously performed in purely dissipative chains of phase-oscillators, 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 nonequilibrium models like stochastic lattice gases. In the present case however the (zero-temperature) non-equilibrium 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
\[ p_n = \sin(g_{n+1} - g_n) - \sin(g_n - g_{n-1}) + \]
\[ (\delta_{1,n} + \delta_{N,n}) [\gamma(F_n - p_n) + \sqrt{2\gamma F} \eta_n] \]

where \( p_n = \dot{q}_n, F_n \) denotes a torque applied to the chain boundaries, \( \gamma \) is the coupling strength with two external baths and \( \eta_n \) 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 \( j^p_n = \langle \sin(g_{n+1} - g_n) \rangle \), while the energy flux is \( j^\epsilon_n = \langle (p_n + p_{n+1}) \sin(g_{n+1} - g_n) \rangle \) (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 \( n \)th 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 \( F = 0 \) case. As long as \( F = (F_1 - F_N)/2 < F_c = 1/\gamma \), the ground state is a twisted fully-synchronized state, whereby each element rotates with the same frequency \( \omega = (F_1 + F_N)/2 \) 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 fix \( \omega_n = 0 \) below threshold). As shown in Fig. 1, the maximum value \( \bar{T} \) 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 \( j^\epsilon \) 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).

A more detailed characterization of the supercritical phase is reported in Figs. 2 and 3. The temperature profiles above threshold \( (F = 1.05) \) are shown in Fig. 2a 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 \( \bar{T} \) 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 \( \bar{\omega}_{n} \) for \( F = 1.05 \). In Fig. 2c 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 \( \omega_n \) changes from \( F_1 \) to \( F_N \).

The supercritical phase is, however, more complex than revealed by this average characterization. In Fig. 2b we plot a space-time representation of the “instantaneous” 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 has 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. 2d corresponds 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. 3).
In order to further refine our understanding of the supercritical regime, we have computed the spectra of Lyapunov exponents $\lambda_n (n = 1, \ldots, 2N)$. As a first check we have verified that the sum of all $\lambda_n$ is equal to the dissipation $-2\gamma$, as it should. The spectra obtained for different system sizes reveal substantial differences from the standard (extensive) chaotic regime \cite{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 shrinks to zero as $\lambda_1$ and $\lambda_{2N}$ 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 non-equilibrium invariant measure extends along (almost) 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 non-extensive 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 usual space-time chaotic system whereby dynamical invariants are extensive with the volume \cite{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 \cite{27, 28}. Here, however, this is a true instance of space-time chaos and the non-extensive 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/non-extensive behavior. One has only to be careful in selecting sufficiently long chains, so as to avoid the existence of a point-like 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 non-zero boundary temperatures (i.e. in the presence of an external source of noise). The results reported in Fig. 4 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 synchronized state is still present as a sudden increase of $\hat{T}$ at finite $F$ (see Fig. 1 for $T = 0.1$). This is, nevertheless, a finite-size effect, as the pseudo-discontinuity disappears upon increasing $N$ (compare squares and triangles in Fig. 1). 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 non-equilibrium transition is not a peculiarity of the rotor model. Here below, we show that a similar scenario can be observed for the DNLS equation, $i\dot{z}_n = -2|z_n|^2z_n - z_{n+1} - z_{n-1}$, where $z_n = (p_n + iq_n)/\sqrt{2}$ is a complex variable. The DNLS Hamiltonian has two conserved quantities, the mass/norm $a$ and the energy density $\hbar$ [24, 50], so that it is a natural candidate for describing coupled transport [10, 51].

![Figure 4](image_url)

**FIG. 4:** (Color online) Kinetic temperature profiles of the DNLS equation for $N = 250, 500, 1000, 2000, 4000, 8000$ 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 $\tilde{n}$. Inset: chemical-potential flux $j^{\mu}_n$ versus system size $N$. The (red) dashed line corresponds to a slope $-2/5$.

We have studied a DNLS chain interacting with two Langevin thermostats at $T = 0$ and different chemical potentials $\mu_1$ and $\mu_N$ = imposed at the boundaries (see Ref. [51] for details). In this case, the control parameter, i.e. the driving force, is $\delta \mu = [\mu_N - \mu_1]/2$ [51]. In simulations with $\delta \mu$ larger than a critical value, e.g., $\mu_1 = 2$ and $\mu_N = 5$, a bumpy temperature profile spontaneously emerges. On the one hand, the data plotted in Fig. 4 indicate that the width of the peak scales as $N^{1/2}$, such as for the XY chain. On the other hand, the left-right symmetry is lost and the mass (norm) flux $j^{\mu}_n = i(\langle z_n^* z_{n-1}^* - z_n^* z_{n-1} \rangle)$ scales as $N^{-2/5}$ instead of $N^{-1/5}$ of 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 on oscillator chains may induce a non equilibrium transition at zero temperature. The supercritical phase is characterized by an unusual mixture of extensive (KY dimension) and non-extensive (KS entropy) properties, and by anomalous (superdiffusive) transport.

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 presence of symmetries is a crucial element [24, 32]. In the XY case, the average value of the mass flux $\langle j^{\mu} \rangle$ 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. It is known that the DNLS dynamics, in the limit of small gradients and large mass densities, can be effectively approximated by an XY model, where the application of a chemical potential corresponds to applying a torque [51]. The parameter values herein selected do not fall within such a parameter region, and, more important, the DNLS→XY mapping depends on the value of the chemical potential, so that the left-right symmetry cannot, any longer, hold. It is, therefore, reasonable to conjecture that such a symmetry determines the universality class, although this point needs further investigations.

It is also important to notice that the localized chaotic dynamics of the supercritical phase markedly differs from the localized chaotic state observed when all oscillators are damped and driven [33, 34]. First, the transition discussed here indeed occurs in an almost Hamiltonian setup. Moreover, the extensivity properties of the Lyapunov spectra are different indicating a complex interaction between the external forces and the bulk dynamics. 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. The development of theoretical arguments to describe such a phase is, however, hindered by the presence of an underlying kink in the frequency/chemical potential profile, which makes the development of a Green-Kubo formalism as well as of perturbative techniques rather problematic.

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