Simple Model for Active Nematics: Quasi-Long-Range Order and Giant Fluctuations

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We propose a simple microscopic model for active nematic particles similar in spirit to the Vicsek model for self-propelled polar particles. In two dimensions, we show that this model exhibits a Kosterlitz-Thouless-like transition to quasi-long-range orientational order and that in this nonequilibrium context, the ordered phase is characterized by giant density fluctuations, in agreement with the predictions of Ramaswamy *et al.* [Europhys. Lett. **62**, 196 (2003)].

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Over the last decade or so, physicists have been looking for common, possibly universal, features of the collective motion of animals, bacteria, cells, molecular motors, as well as driven granular objects [1,2]. Among the emergent properties of these groups of ''active'' or self-propelled particles (SPP), distinctively out-of-equilibrium features have been found, such as the existence of long-range orientational order in two-dimensional ''ferromagnetic'' flocks of polar SPP [3,4].

Another set of striking intrinsically nonequilibrium properties have recently been predicted by Ramaswamy and co-workers [1,5,6]. They considered, in particular, the case of apolar but oriented SPP and argued that such ''active nematics'' should differ dramatically from the usual (equilibrium) case [7]. In particular, their approach, based on the analysis of hydrodynamic equations derived from symmetry arguments, predicts that giant density fluctuations arise in the ordered phase of such media. In [1], it is also hinted at the possibility of true long-range order and of a different isotropic-nematic transition out of equilibrium, but no definitive statement is offered. Resolving these issues is nevertheless crucial, especially in view of the predicted giant density fluctuations, and all the more so since, in polar SPP, the transition to true long-range order was shown to be discontinuous [8].

In spite of the above-mentioned current surge of activity in nonequilibrium systems, the giant density fluctuations predicted by Ramaswamy and co-workers have not been observed so far, and the nature of the nematically ordered phase and of the transition leading to it have not been elucidated. Experimentally, relevant systems such as colonies of elongated cells [9] and ensembles of rodlike objects driven by vibration [10–12] have been studied, but with other issues at stake. On the theoretical side, no microscopic model has been proposed [13]. In this Letter, we fill this gap, confirm for the first time the predictions of Ramaswamy *et al.*, and investigate the nature of the isotropic-nematic transition in driven systems. We introduce a simple model for active nematics, and show numerically that its isotropic-nematic transition in two space dimensions does not differ significantly from the equilibrium case: only quasi-long-range (QLRO) order is attained, with scaling laws compatible with those of the Kosterlitz-Thouless (KT) transition. Nevertheless, giant density fluctuations are clearly observed in the ordered phase: the standard deviation Δn of n, the average number of particles in a given subsystem, is proportional to n and not to $\sqrt{n}$ as expected in equilibrium.

Our model is similar in spirit to the Vicsek model for polar SPP [3]. In a typical driven-overdamped dynamics, identical pointwise particles move synchronously at discrete time steps Δt by a fixed distance $v_0\Delta t$. In two space dimensions and for uniaxial nematics—the case to which we restrict ourselves in the following—each particle j is endowed with an orientation θ_j and moves along θ_j or $\theta_j + \pi$ with equal probabilities. At every time step, θ_j^{t+1} is given by $\Theta(\mathbf{Q}_j^t)$, the direction of the first eigenvector of the *local* tensorial traceless order parameter

$$\mathbf{Q}_j = \begin{pmatrix} \langle\cos^2\theta_k\rangle - \frac{1}{2} & \langle\cos\theta_k \sin\theta_k\rangle \\ \langle\cos\theta_k \sin\theta_k\rangle & \langle\sin^2\theta_k\rangle - \frac{1}{2} \end{pmatrix}, \qquad (1)$$

where the average is taken over all particles k within the interaction range $r_0 = 1 > v_0\Delta t$, including particle j (in this Letter, we use $v_0\Delta t = 0.3$). As for the Vicsek model, disorder arises from the addition of a random angle to this newly calculated orientation, and we have finally

$$\theta_j^{t+\Delta t} = \Theta(\mathbf{Q}_j^t) + \sigma\xi_j^t, \qquad (2)$$

where ξ_j^t is a delta-correlated white noise ($\xi \in [-\frac{\pi}{2}, \frac{\pi}{2}]$). The interaction introduces a tendency to align (nematically) with neighboring particles, so that two simple limits arise: complete orientational order settles in the absence of noise, whereas particles perform random walks for maximal noise ($\sigma = 1$). We first characterize the transition that necessarily lies in between these two regimes. To this aim, we calculate the total order parameter $\mathbf{Q}(N, L)$ measured for N particles in a square domain of linear size L with periodic boundary conditions. We use, in particular, the scalar order parameter

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$$S = 2\sqrt{(\langle\cos^2\theta\rangle - \tfrac{1}{2})^2 + \langle\cos\theta\sin\theta\rangle^2}, \qquad (3)$$

which is equal to twice the (positive) eigenvalue of $\mathbf{Q}$, so that $S = 1$ for perfect orientational order, and $S = 0$ for complete disorder. Starting from random positions and orientations, S typically grows in time and eventually reaches a statistically stationary state characterized by a well-defined distribution function of mean $\langle S\rangle$.

Varying the noise intensity σ, we observe a continuous change of $\langle S\rangle$. Increasing system size at fixed density $\rho = N/L^2$, the curves $S(N)$ versus σ reveal sharper transitions for larger sizes, but they do *not* cross each other [Fig. 1(a)]. Figure 1(b) shows that $\langle S(N)\rangle \sim N^{-\zeta(\sigma)}$. Increasing the noise strength from $\sigma = 0$ towards the transition zone, $\zeta(\sigma)$ increases from zero to take rather small values. Sufficiently deep in the transition zone, the effective exponent $\bar{\zeta}(\sigma, N) = -\frac{d\ln S}{d\ln N}$ can be observed to cross over, as $N \to \infty$, from these small values towards $\frac{1}{2}$ [Fig. 1(c)], the value observed at larger σ and characteristic of a completely disordered phase. All these observations are in qualitative agreement with an equilibrium KT transition [15], and signal that only QLRO order is present in the ordered phase. At the quantitative level, the location of the KT transition point in an equilibrium system is characterized by $\zeta = \frac{1}{16}$. Our data are consistent with this: for $\rho = \frac{1}{2}$, we find $\zeta \simeq \frac{1}{16}$ at $\sigma_c \simeq 0.113(5)$, and for larger noise values $\bar{\zeta}(\sigma, N)$ show signs of crossing over to $\frac{1}{2}$ (i.e., one is in the disordered phase).

These observations are strengthened by the study of the orientational spatial correlation functions $g_{2m}(r) = \langle\cos\{2m[\theta(0) - \theta(r)]\}\rangle$ (here m is integer and averages are taken both in space and time). They decay algebraically at low noise values [$g_{2m}(r) \sim r^{-m^2\eta}$ with η also increasing with σ] and exponentially in the disordered phase (with a diverging correlation length ξ as σ approaches the critical point) [Figs. 2(a) and 2(b)]. At a quantitative level, one expects that in equilibrium $\eta(\sigma) = 4\zeta(\sigma)$ in the ordered phase [15]. This is roughly borne out of our data, even though good estimates of the correlation functions are difficult to obtain close to the transition. In the disordered phase, in particular, the expected divergence of ξ is observed [Fig. 2(c)] but not in its expected functional dependence as ξ can only be safely estimated rather far away from threshold. Despite these difficulties, we can check

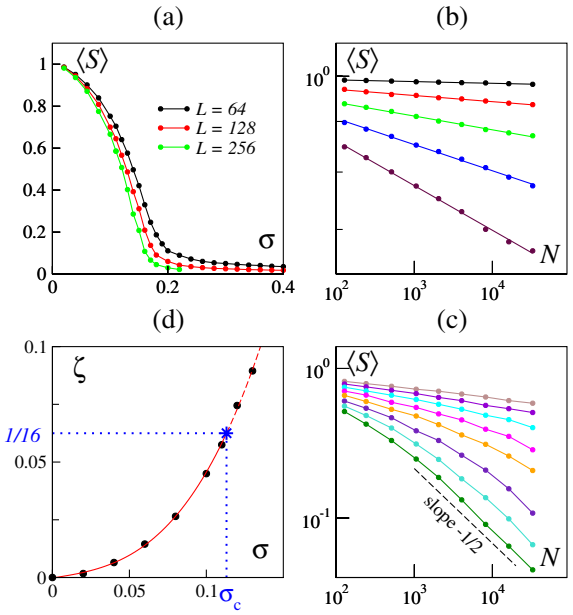

FIG. 1 (color online). Transition to nematic order at density $\rho = N/L^2 = \frac{1}{2}$. (a) (Time-averaged) scalar order parameter $\langle S\rangle$ vs noise strength σ for various sizes. (b) $\langle S\rangle$ vs N at $\sigma = 0.02$, 0.04, 0.06, 0.08, 0.1 from top to bottom; the lines are fitted power laws. Each point represents an average over 10^6–10^7 time steps after transients. (c) Same as (b) but for larger noise values: $\sigma = 0.11, 0.12, 0.13, 0.14, 0.15, 0.16, 0.17, 0.18$. For large σ values these curves cross over to $1/\sqrt{N}$ decay. (d) Exponents ζ extracted from the power laws shown in (b) and (c) vs σ. The line linking the symbols is a (cubic) fit. For the last 2 points, the exponent is only effective, as it was estimated from small N values, before signs of crossover appear. The dotted lines indicate the threshold $\sigma_c = 0.113(5)$ estimated from the condition $\zeta(\sigma_c) = \frac{1}{16}$ (see text).

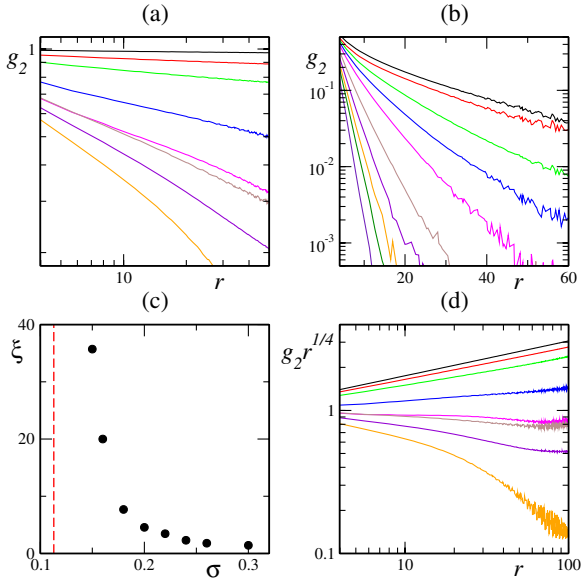

FIG. 2 (color online). Orientational correlation function $g_2(r)$ as calculated from the orientation field coarse grained over boxes of linear size 4 [$\rho = \frac{1}{2}$, time average over 10^6–10^7 time steps after transients for each run, $L = 256$ in (a), (d), and $L = 128$ in (b)]. (a) In log-log scales at small noise values $\sigma = 0.02$, 0.04, 0.06, 0.08, 0.10, 0.11, 0.12, and 0.13 from top to bottom. (b) In lin-log scales for $\sigma = 0.14$ to 0.3 from top to bottom. (c) Variation of the correlation length ξ extracted from the exponential tails in (b) as the transition point is approached (dashed line at the estimated threshold $\sigma_c = 0.113$). (d) Same as in (a), data multiplied by the expected exponent at threshold $\eta_c = \frac{1}{4}$: around the estimated threshold value $\sigma_c = 0.113(5)$, the curves are flat and straight.

that the critical noise level determined above is consistent with our correlation function data [Fig. 2(d)].

The above results are characteristic of QLRO order and of a KT-like phase transition. Further preliminary results [16] show that the disclination unbinding mechanism characteristic of the KT transition [17] is also at work in our nonequilibrium context. All this indicates the proper but costly methodology to locate the critical noise level σ_c. We have not, so far, used this protocol extensively, but ongoing simulations indicate that the critical line may scale like $\sigma_c \sim \rho^{3/4}$ and extend to arbitrarily small densities and noise levels.

In spite of the equilibriumlike properties of the transition to QLRO, the nonequilibrium character of the problem manifests itself in strong density fluctuations, as predicted by Ramaswamy *et al.* [6]: we measured, in the ordered phase, the density fluctuations in square boxes of linear size ℓ embedded in a square domain of linear size L. These boxes contain, on average, $\langle n \rangle = \rho \ell^2$ particles. As long as $\ell < L$, Δn, the rms of the fluctuations of n, scales linearly with $\langle n \rangle$ (and *not* $\sqrt{n}$), in agreement with [6] (Fig. 3). These giant number fluctuations are the statistical consequence of the complex, coupled, spatiotemporal dynamics of density and orientation in the system. After transients, low- and high-density regions emerge with the highly populated domains taking the form of bands inside which nematic order is strong (Fig. 4). These bands evolve (move, split, merge, dissolve, and form again along a new direction) over very long time scales. Typically, however, a single band is present at any given time, independently of the system size, and its characteristic evolution time grows with system size. Thus, contrary to what has been observed in the polar SPP case [8], these structures have no well-defined length or time scales. Ongoing work aims at quantifying these statements [16].

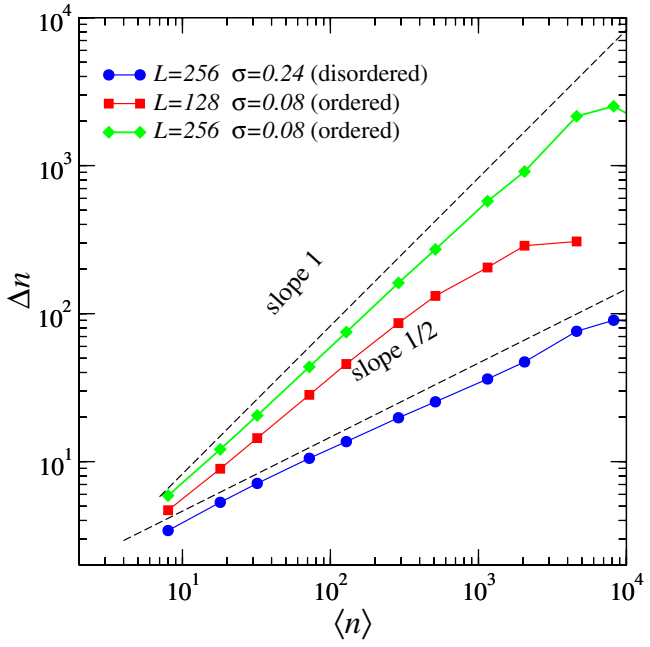

FIG. 3 (color online). Root mean square density fluctuations Δn in square boxes containing $\langle n \rangle$ particles on average (linear size $\ell = \sqrt{n/\rho}$, $\rho = \frac{1}{2}$, time average over 10^6–10^7 time steps after transients). The saturation at large $\langle n \rangle$ occurs when $\ell \simeq L$. Top two curves: giant fluctuations in the ordered phase at 2 different system sizes. Bottom curve: normal fluctuations in the disordered phase.

We now comment on our results. In our model, the density and orientation fields are coupled intimately. Whether the mechanism put forward in [6]—namely that the current in the conservation equation for the concentration has a contribution proportional to $(\partial_y \theta, \partial_x \theta)$—is actually present here remains to be seen explicitly, but we believe that this is the case because the general symmetry arguments invoked there must apply. As a matter of fact, in our model, intrinsically nonequilibrium features are still observed when the displacement of the particles is not made along their orientation—the "natural" case if one has in mind particles with an elongated physical shape—but, for instance, *perpendicularly* to their axis (not shown). On the other hand, displacing them randomly along one of the four directions defined by adding multiples of $\frac{\pi}{2}$ to their current angle yields normal fluctuations ($\Delta n \sim \sqrt{n}$) and no segregation (not shown). This is not surprising since then particles effectively perform random walks on scales larger than the elementary displacement. This case is thus equivalent to strictly decoupling density fluctuations from the orientation field by letting particles be noninteracting random walkers. Apart from such "equilibrium" cases, it seems that any coupling generically triggers giant fluctuations. In fact, it seems that this robust feature is also present when the orientation is imposed externally, influencing the particle motion without feedback [14].

Whereas giant number fluctuations are easily observed, we have not been able to measure the slow decay of tagged-particle velocity autocorrelations also predicted in [6]. We believe this is because the only significant motion in our model, apart from the microscopic random displacements, is due to the very slow dynamics of the high-density bands (Fig. 4). Thus, we expect such an effect to be only observable on time scales so large that they are not easily accessible.

The giant number fluctuations taken as the signature of the "nonequilibriumness" of the system are tantamount to the formation of the high-density ordered band described above (Fig. 4). Whether this is "true" macroscopic phase separation is thus a key question [14]. Here we have shown that despite this spectacular phenomenon, the phase transition is similar, as far as we can tell numerically, to the equilibrium one, with an ordered phase characterized by QLRO only. This has to be paralleled to the case of polar SPP, where true long-range order is ascertained [4], and the transition is discontinuous (i.e., first-order-like) [8]. At equilibrium, the Mermin-Wagner theorem states that true

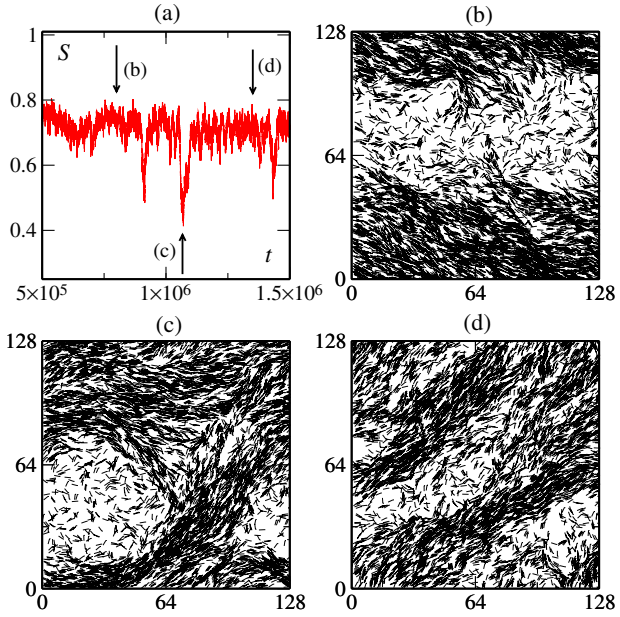

FIG. 4 (color online). Typical time series of S in the ordered phase. ($\rho = \frac{1}{2}$, $L = 128$, $\sigma = 0.1$). Note the large excursions to small S values which make time averaging difficult. (b)–(d) Snapshots taken during the run shown in (a) at the times indicated there. For each particle, a small segment (of arbitrary length) centered on its position and aligned on its orientation is drawn. (b), (d) are typical ordered states, while (c) represents the more disordered episodes when the macroscopic structure changes orientation.

LRO cannot arise from the spontaneous breaking of a continuous symmetry in two dimensions [18]. Out of equilibrium, this constraint disappears [1,4], and it is quite interesting to notice that polar and nematic SPP behave differently. Note also that for polar particles the ordered phase is *not* density homogeneous, but typically consists of well-defined solitary bands with high-density and strong order moving in a low-density disordered background [8]. These bands, which can appear in arbitrary numbers depending on the system geometry, are very different from the single, fluctuating, splitting, and merging object described here in Fig. 4. Thus, combining the present conclusions and the results obtained recently on polar SPP, we see clearly how the nonequilibrium nature of these nonlinear driven systems can emerge differently at the collective level.

To summarize, we have introduced a simple model for active nematic particles in which the density and orientation fields are coupled in a natural way. This nonequilibrium model exhibits a KT-like phase transition to a nematically ordered phase in which giant density fluctuations arise. This constitutes a first nontrivial confirmation of the intrinsically nonequilibrium properties predicted in [6] and calls for further experimental studies, either with assemblies of granular elongated particles or, better, in biological systems where such effects could play an important role. In view of the notorious difficulties encountered to decide about similar issues in the case of polar particles, our results will need to be confirmed by a proper renormalization group analysis. On the modeling side, finally, our approach can easily be extended to other space dimensions and/or to more complex types of interactions. Future work will explore these issues, in particular, three-dimensional systems and the nature of tetratic order out of equilibrium.

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