Active Nematics Are Intrinsically Phase Separated

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Two-dimensional nonequilibrium nematic steady states, as found in agitated granular-rod monolayers or films of orientable amoeboid cells, were predicted [Europhys. Lett. **62**, 196 (2003)] to have giant number fluctuations, with the standard deviation proportional to the mean. We show numerically that the steady state of such systems is macroscopically phase separated, yet dominated by fluctuations, as in the Das-Barma model [Phys. Rev. Lett. **85**, 1602 (2000)]. We suggest experimental tests of our findings in granular and living-cell systems.

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The ordering or "flocking" [1–3] of self-propelled particles obeys laws strikingly different from those governing thermal equilibrium systems of the same spatial symmetry. Even in two dimensions, the velocities of particles in such flocks show true long-range order [1,2], despite the spontaneous breaking of continuous rotational invariance. Density fluctuations in the ordered phase are anomalously large [2], and the onset of the ordered phase is discontinuous [4]. The ultimate origin of these nonequilibrium phenomena is that the order parameter is not simply an orientation but a macroscopic velocity. It is thus intriguing that even the nematic phase of a collection of self-driven particles, which is apolar and hence has zero macroscopic velocity, shows [5,6] giant number fluctuations [7], as a result of the manner in which orientational fluctuations drive mass currents. This Letter takes a closer look at these fluctuations and shows that they offer a physical realization of the remarkable nonequilibrium phenomenon known as fluctuation-dominated phase separation [8], hitherto a theoretical curiosity.

Before presenting our results, we make precise the term active nematic. An active particle extracts energy from sources in the ambient medium or an internal fuel tank, dissipates it by the cyclical motion of an internal "motor" coordinate, and moves as a consequence. For the anisotropic particles that concern us here, the direction of motion is determined predominantly by the orientation. Our definition encompasses self-propelled organisms, living cells, molecular motors, and macroscopic rods on a vertically vibrated substrate (where the tilt of the rod serves as the motor coordinate). An active nematic is a collection of such particles with axes on average spontaneously aligned in a direction $\hat{\mathbf{n}}$, with invariance under $\hat{\mathbf{n}} \rightarrow -\hat{\mathbf{n}}$. We know of two realizations of active nematics: collections of living amoeboid cells [9] and granular-rod monolayers [10,11].

We study active nematics in a simple numerical model described in detail below. Our results confirm (see Fig. 1) the giant number fluctuations (standard deviation $\propto$ mean) [6] predicted by the linearized analysis of Ref. [5] but are far richer: (i) A statistically uniform initial distribution of particles, on a well-ordered nematic background, undergoes a delicate "fluctuation-dominated" [8] phase separation, where the system explores many statistically similar segregated configurations. (ii) The equal-time two-point density correlator $C(\mathbf{r})$ (Fig. 5) shows a collapse when plotted as a function of $r/L(t)$, where $L(t)$ is the location of the first zero crossing of $C(\mathbf{r})$, with a cusp at small $r/L(t)$ signaling a departure from Porod's law, i.e., the absence of sharp interfaces. (iii) We confirm that the large density inhomogeneities are indeed best thought of as phase separation, by showing (1) that the saturation value of $L(t)$ is proportional to the linear size of the system and (2) that the phase-separation order parameter—the time-averaged first spatial Fourier component of the particle density—approaches a nonzero value in the limit of large system size (Fig. 6). (iv) $L(t)$ grows clearly faster than the $t^{1/3}$ for normal conserved-order-parameter coarsening (see inset in Fig. 2) and is consistent with $t^{1/2}$ as expected by analogy to Ref. [8]. Below, we show how these results were obtained, discuss them in detail, explain the analogy to the

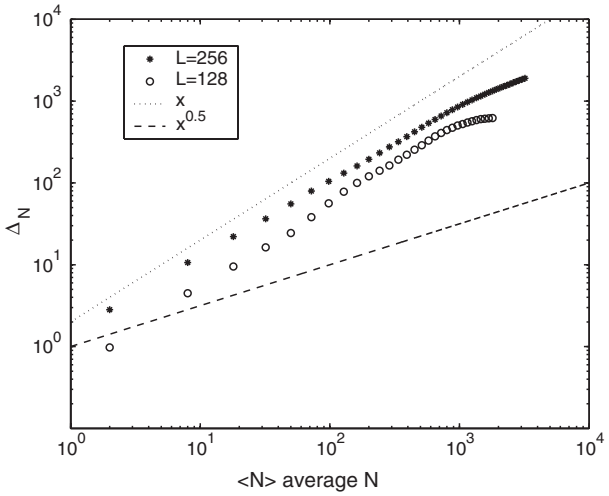

FIG. 1. Number standard deviation Δ_N scales roughly as the mean $\bar{N}$, for system sizes $L = 128, 256$.

work of Ref. [8], and suggest experimental tests for these striking phenomena.

We begin with some background information. An apolar, uniaxial, compressible nematic liquid crystal is described by director and number-density fields $\hat{\mathbf{n}}(\mathbf{r})$ and $c(\mathbf{r})$, with fluctuations $\delta\mathbf{n}(\mathbf{r})$ and $\delta c(\mathbf{r})$ about their uniform mean values $\hat{\mathbf{n}}_0$ and c_0. Let us review first what happens at thermal equilibrium. The system is then governed by an extended Frank [12] free-energy $F[\hat{\mathbf{n}}, c] = (1/2) \times \int d^d r[\mathbf{K}(\boldsymbol{\nabla}\hat{\mathbf{n}})^2 + A(\delta c)^2/c_0 + C_1\hat{\mathbf{n}} \cdot \nabla c \nabla \cdot \hat{\mathbf{n}} + C_2\hat{\mathbf{n}} \times \nabla c \cdot \nabla \times \hat{\mathbf{n}}]$, where $\mathbf{K}$ is an elastic tensor, A the compressional modulus at constant orientation, and $C_{1,2}$ couple orientation and density in the simplest symmetry-allowed fashion. Equipartition applied to F implies that the static structure factor $S_\mathbf{q} \equiv \int d^d r \exp(-i\mathbf{q} \cdot \mathbf{r})\langle \delta c(\mathbf{0}) \delta c(\mathbf{r})\rangle / c_0$ is finite for $q \to 0$; i.e., the mean $\bar{N}$ and standard deviation Δ_N of the number N of particles obey $\Delta_N \propto \sqrt{\bar{N}}$ at equilibrium even when $C_1, C_2 \neq 0$.

An active nematic is a steady state away from thermal equilibrium, in which not only dynamic correlators but equal-time quantities such as $S_\mathbf{q}$ or Δ_N as well must be inferred from equations of motion for $\hat{\mathbf{n}}$ and c. As shown in Ref. [5], the equation of motion for $\hat{\mathbf{n}}$ is qualitatively the same as for equilibrium nematics. The feature [5] that distinguishes active nematics crucially from their equilibrium counterparts is that the current $\mathbf{j}$ in the continuity equation $\partial_t c = -\nabla \cdot \mathbf{j}$ for the density has a contribution $\propto \nabla \cdot c(\hat{\mathbf{n}}\,\hat{\mathbf{n}})$ [13]. This term, which is ruled out at thermal equilibrium, has a simple, physically appealing origin: Spatial variation in the director field $\hat{\mathbf{n}}$ defines a curve; the normal to this curve defines a local vectorial asymmetry; for a driven system, such an asymmetry implies a current [14]. If $\hat{\mathbf{n}} = (\cos\theta, \sin\theta)$, then inhomogeneities in θ give a curvature-induced current $\mathbf{j} = (j_x, j_z) \propto (\partial\theta/\partial z, \partial\theta/\partial x)$ (see Fig. 3), analogous to Ref. [8] where particles slide with velocity $\propto \nabla h$ on a fluctuating interface with height field h, except that our current is not a gradient. Since the nematic order is a spontaneous breaking of rotation invariance, large fluctuations in θ at long wavelengths are expected to be present in abundance and to decay slowly, in any nematic, equilibrium or otherwise. We showed in the previous paragraph that the effect of these broken-symmetry modes on the density field was benign in an equilibrium nematic. In an active nematic, however, the same orientational fluctuations, because of the curvature-induced current we just mentioned, will affect the density fluctuations substantially. A linearized small-fluctuations analysis [5] showed that they to lead to giant fluctuations in the number of particles: $\Delta_N/\sqrt{\bar{N}} \propto \bar{N}^{1/d}$ in d dimensions, i.e., $\Delta_N \propto \bar{N}$ for $d = 2$.

Such large fluctuations prompt the suspicion that an analysis beyond Gaussian fluctuations would reveal that the system is, in fact, phase separated, as in Ref. [8]. There are two issues here: (i) whether the nonequilibrium coupling mentioned above inevitably arises in an active nematic and (ii) whether it leads to phase separation. Reference [6] effectively answers the first question in the affirmative; we focus on the second.

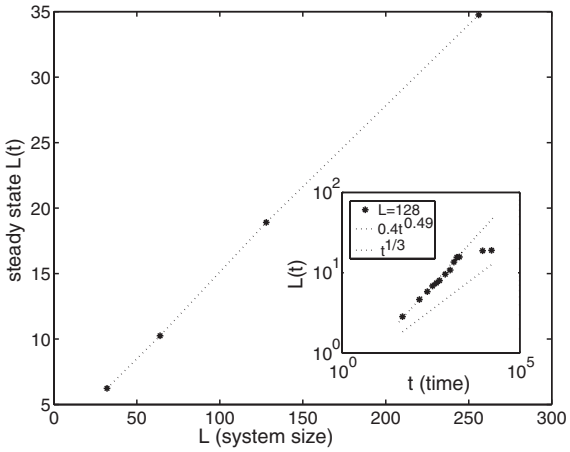

FIG. 2. Coarsening length $L(t)$ saturates to a value proportional to system size. Inset: $L(t)$ consistent with $t^{1/2}$ despite conservation law.

We find it convenient to separate the density and orientation degrees of freedom and employ a discrete model of lattice-gas particles coupled to an angle field, incorporating explicitly the nonequilibrium curvature-induced current $\mathbf{j} \propto (\partial_z\theta, \partial_x\theta)$ mentioned above, via a suitable choice of particle-hopping rates. We consider a two-dimensional lattice with angles $\theta_i \in [0, \pi]$ and noninteracting lattice-gas occupancy variables $n_i = 0, 1$ at each site i. The angles evolve by Metropolis Monte Carlo updates governed by the Lebwohl-Lasher [15] Hamiltonian $H = -K\sum_{\langle ij\rangle} \cos 2(\theta_i - \theta_j)$ yielding a nematic phase at low temperature. Particle motion is nonequilibrium: Hops of a particle at site i to a nearest-neighbor site in the $\pm x$ direction are attempted with probability $1/4 \pm \alpha(\theta_1 - \theta_2)$ and in the $\pm z$ direction with probability $1/4 \pm \alpha(\theta_3 - \theta_4)$, where θ_i are the angles at sites $i = 1$–4 as in Fig. 3, and α encodes the strength [16] of the active curvature-current coupling of Ref. [5]. In Ref. [5], the effect of the concentration field on the dynamics of the angle field is shown to play an insignificant role in the giant number fluctuations. Accordingly, we neglect it here, so that the particles are

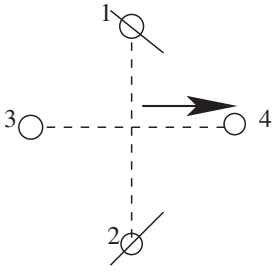

FIG. 3. Director variation from the bottom to the top of the picture gives rise to a current in a transverse direction.

advected passively by an autonomous angle field. This simplifying approximation should not make a qualitative difference deep in the nematic phase. We therefore work with $K = 10.0$ and let the angle field equilibrate until a well-ordered nematic is formed. An initial statistically uniform distribution of particles (mean occupancy = 50%) clusters and coarsens (Fig. 4), most strongly at $\pm 45°$ to the mean direction of nematic ordering. The anisotropic two-point density correlator $C(\mathbf{r}, \mathbf{t})$ shows a scaling collapse for a given direction for all t, if plotted as a function of $r/L(t)$ for a coarsening length $L(t)$, defined by the value of r at the first zero crossing, whose scaling is consistent with $t^{1/2}$ (see Figs. 2 and 5). The value at which $L(t)$ saturates is proportional to the system size L (see Fig. 2), which makes a strong case for true phase separation. The value of the saturation length is numerically small compared to L, probably because of the poorly defined clusters (Fig. 4) of fluctuation-dominated phase separation. That we work with hard-core particles, and on time scales on which the macroscopic variation of the mean nematic orientation is very small, also probably contributes. The exponent of $1/2$ is because the particles aggregate not by diffusion plus short-range capture but, rather, by analogy with Ref. [8] (see also [17]), because the broken-symmetry mode of the nematic order sweeps the particles over large distances via curvature-induced drift. A nematic fluctuation on a scale ℓ collects particles in a time of order ℓ. For two such domains to coalesce requires the nematic director field on that scale to turn over, which is a time $\sim \ell^z$, where $z = 2$ is the dynamic exponent of transverse fluctuations of the nematic director.

At long times a steady state is reached, and $C(r/L(t \to \infty))$ shows a cusp at small argument [$C(x) \propto x^a$, $a \simeq 0.33$], which can be seen in Fig. 5 as well, signaling the absence of sharp interfaces between regions rich and poor in particles, and a power-law distribution of cluster sizes. For a steady state in the largest system, we also measured the standard deviation Δ_N in the number of particles in an observation containing $\bar{N}$ particles on average. The plot of Δ_N vs $\bar{N}$ (Fig. 1) shows precisely the linear dependence predicted by Ref. [5]. Faced with these results, we ask: Is this phase separation or a single phase with large fluctuations? This is answered by measuring the magnitude of the time-averaged lowest spatial Fourier component $Q(1, 1)$ of the density, shown in Fig. 6. Although the data are not conclusive, the flattening of the semilog plot as a function of system size rules out an exponential decay to zero. Together with the proportionality of the coarsening length to the system size, and the nature of the mechanism, this suggests strongly that active nematics offer the most natural physical realization of macroscopic fluctuation-dominated phase separation [8]. As in Ref. [8], we find that the time series of $Q(1, 1)$ shows enormous fluctuations (Fig. 6, inset) with "crashes" during which other nearby Fourier components gain weight. Thus, as in Ref. [8], the system lurches from one macroscopically phase-separated configuration to another, spending very little time in non-phase-separated states. Last, the velocity autocorrelation of tagged particles at a low (15%) concentration agrees qualitatively with the $1/t$ tail (plot not shown) predicted by Ref. [5], over the range in which a given particle moves unimpeded by others.

What experiments can test these results? The best would be agitated layers of granular rods, for which nematic phases have been reported [11]. Although many features of these systems can be rationalized in terms of equilibrium hard-rod theories [18], some properties such as global circulation and swirls [10,11] are clearly very nonequilibrium. These systems as well as the living melanocyte nematic of Gruler *et al.* [9] remain the most promising

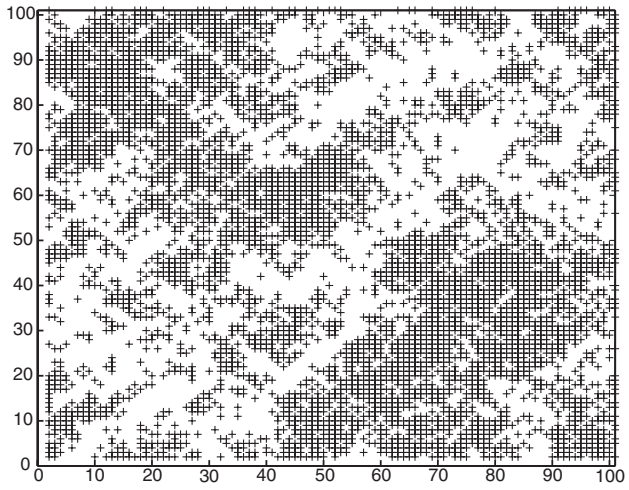

FIG. 4. Anisotropic clustering of particles, 20 000 time steps, system size 100, 50% occupancy.

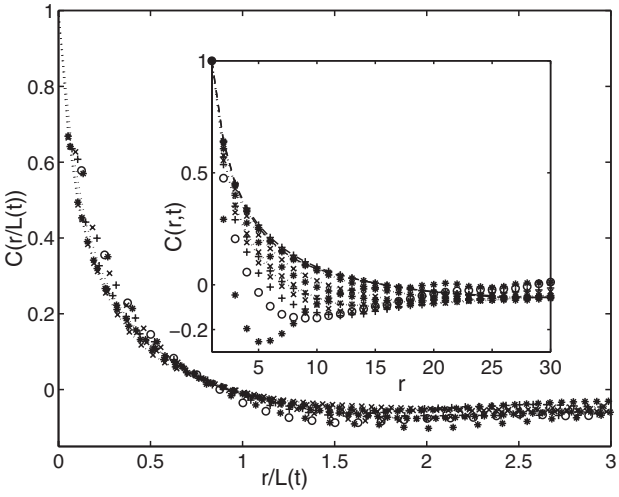

FIG. 5. Plots of the equal-time density correlator $C(r, t)$ at different times t collapse onto a single curve when r is scaled by the zero-crossing coarsening length $L(t)$; data shown for direction transverse to nematic ordering. Inset: $C(r, t)$ vs r.

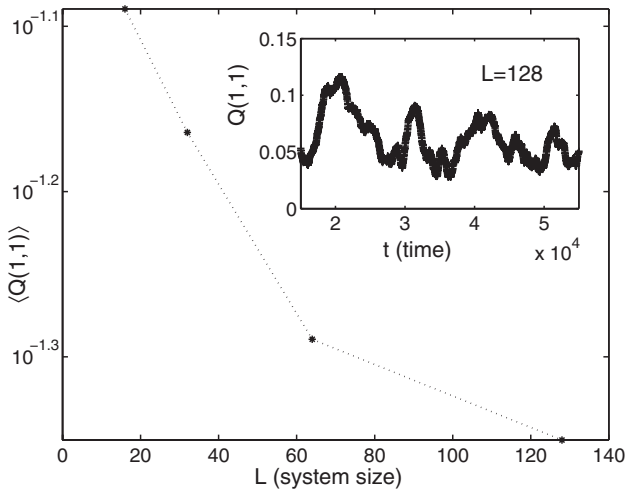

FIG. 6. Time-averaged Fourier component of the density profile vs wave vector k for wave vector direction (1, 1), for system sizes $L = 16, 32, 64$, and 128; flattening in a semilog plot at the largest size suggests a nonzero value for $L \to \infty$. Inset: Time series of Q for the (1, 1) direction.

candidates for experimental tests of the rich range of results made here and in Ref. [5]. The confirmation of giant number fluctuations in the numerical experiments of Ref. [6] is encouraging in this regard.

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