Active nematics on a substrate: giant number fluctuations and long-time tails

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Abstract

We construct the equations of motion for the coupled dynamics of order parameter and concentration for the nematic phase of driven particles on a solid surface, and show that they imply (i) giant number fluctuations, with a standard deviation proportional to the mean and (ii) long-time tails $\sim t^{-d/2}$ in the autocorrelation of the particle velocities in d dimensions despite the absence of a hydrodynamic velocity field. Our predictions can be tested in experiments on aggregates of amoeboid cells as well as on layers of agitated granular matter.

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Recent experiments [1, 2] offer evidence for long-ranged orientational order in collections of driven particles. The work of [1] is concerned with aggregates of living cells confined to a solid surface, whereas that of [2] studies vertically vibrated layers of granular rods. Two kinds of uniaxial orientational order are discussed in [1], and appear to arise in [2] as well: (i) *nematic* or *apolar*, where the axes of the elongated cells are oriented, say along a mean direction $\hat{\mathbf{n}}$, but $\hat{\mathbf{n}}$ and - $\hat{\mathbf{n}}$ are equivalent; and (ii) *vectorial* or *polar* order, where $\hat{\mathbf{n}}$ and - $\hat{\mathbf{n}}$ are not equivalent. On symmetry grounds [3], a vector-ordered nonequilibrium steady state should have a nonzero macroscopic drift velocity $\mathbf{v}_0$, while for true nematic order $\mathbf{v}_0 = 0$.

We shall be concerned here with strictly nematic order. In [2] a nematic phase is mentioned but not discussed much. In [1], there is particularly convincing evidence for a nematic, including images of classic strength -1/2 disclinations, from studies on melanocytes (cells which distribute pigment in the skin). In fact in this class of cells the individual particles themselves are head-tail symmetric, or *apolar*, so that the drift velocity is zero for each particle. The cells involved are tens to hundreds of microns in length, and the rods in [2] are 6 mm long, so that thermal Brownian motion plays no role in the dynamics of these particles. What distinguishes the particles in these experiments from conventional nematics is their *active* or *driven* character: they absorb energy from their surroundings (from nutrient in one case, shaking in the other) and transform it into motion in the plane. The dynamical behaviour of melanocytes, for example, involves rhythmic movements of the cell body as well as two long projections called dendrites which appear to be responsible for the inter-cell interaction and the level of fluctuations [1]. In granular rods the interaction and noise come from collisions. Ordered phases of particles on an air-table [4] would also obey our model, except for possible complications arising from the periodic array of air-holes.

As has been noted earlier [5, 6] the organization, dynamics, and fluctuation properties of such active, energy-dissipating objects cannot be described by equilibrium statistical physics. Continuum models appropriate for the dynamics of *polar* order wherein the particles are on average in motion were presented in [6]; the extension of those models to include momentum-conserving hydrodynamic flow and both polar and apolar order was discussed in [7]. The cells in [1] and the rods in [2], however, move on a solid surface which acts as a momentum sink for the velocity even at zero wavenumber.

In this paper we derive the most general *universal* equations of motion, valid for all systems of active nematogenic particles *without* total momentum conservation [8], for the

apolar order parameter and concentration fields in such systems, retaining all relevant terms allowed by symmetry. Our aim is to look for *universal* properties, independent of microscopic details, that distinguish these active nematics from their counterparts at thermal equilibrium.

Two predictions stand out as most striking: (i) The standard deviation in the number N of particles is *enormous,* scaling as N in the entire nematic phase for two dimensional systems. By contrast, in *any* thermal equilibrium system with a finite compressibility, which in practice means any equilibrium system not at a continuous phase transition, number fluctuations are far smaller, scaling as $\sqrt{N}$ as $N \to \infty$. (ii) The autocorrelation of the velocity of a tagged particle decays with time t as $t^{-d/2}$ for space dimension $d \geq 2$. It should be recalled that precisely this form of long-time tail [9] occurs in bulk fluids at thermal equilibrium, but as a result of advection of particles by thermal fluctuations in the hydrodynamic velocity field, which decays slowly because of momentum conservation. Here the total momentum of the particles is not conserved, since it is damped by friction with the substrate [10]. A collection of particles at thermal equilibrium on a substrate would show velocity autocorrelations decaying much more rapidly [11]; specifically as $t^{-(d+2)/2}$. It should be possible to test these predictions by studying large-scale real-space images and videos of the behavior of systems such as those in [1] as well as two-dimensional nematic phases in agitated layers of granular particles [2].

Our predictions for *nematically ordered* phases of powders stand in dramatic contrast to experimental results obtained on *disordered*, monodisperse powders (ping-pong balls) [4], which showed that the latter systems could be described surprisingly completely by equilibrium statistical mechanics, albeit with a very high fictive temperature [12]. The findings we've summarized above clearly show that nematic phases of rod-like powders *cannot* be described by equilibrium statistical mechanics *at all*, even at the crudest level of scaling [13].

We turn next to the construction of our equations of motion.

Since our nematogens are spread on a solid substrate, there is only one conserved quantity of relevance, namely, the number of particles. A description valid at sufficiently long length- and time-scales [14] needs then to include only the concentration field $c(\mathbf{r}, t)$ of particles and the orientational order parameter, described by the traceless symmetric tensor field $\mathbf{Q}$ with components $Q_{ij}(\mathbf{r}, t)$ at point $\mathbf{r}$ and time t. For uniaxial nematics, to which we restrict our attention here, we can write $\mathbf{Q} = [\mathbf{nn} - (1/d)\mathbf{I}]S$, where the unit vector $\mathbf{n}$ is the director

field, $\mathbf{I}$ is the unit tensor, and the conventional scalar order parameter S [15] measures the degree of order. It is however convenient to introduce and later eliminate a fast variable, the velocity field $\mathbf{v}(\mathbf{r},t)$ of the particles. Number conservation tells us that

$$\frac{\partial c}{\partial t} = -\nabla \cdot \mathbf{j} \tag{1}$$

where the number current $\mathbf{j} = c\mathbf{v}$. Newton's 2nd law for the local momentum density $m\mathbf{j}$, where m is the mass of a particle, gives

$$m\frac{\partial \mathbf{j}}{\partial t} = -\Gamma\mathbf{v} - \nabla \cdot \sigma + \mathbf{f}_R = -\Gamma\ \mathbf{v} - w_o\nabla c - w_1\nabla\cdot(\mathbf{Q}c) + \mathbf{f}_R \tag{2}$$

up to bilinear order in the fields. In (2), the term in Γ represents friction with the substrate, the stress tensor σ contains the effect of interparticle interactions, the w_0 term can be thought of as osmotic pressure, $\mathbf{f}_R$ is a random, nonconserving, spatiotemporally white Gaussian noise, not in general of thermal origin, and the w_1 term, unique to this driven system, says that inhomogeneities in the nematic order drive mass motion.

To see where this comes from, note first that, by definition, inhomogeneities in σ produce local acceleration. What is novel here is that there is a contribution to the stress tensor proportional to the nematic order parameter. This is allowed by symmetry here, and can be obtained by noting (see [7, 16]) that each active particle is a force dipole. Such a term is *not* allowed in an *equilibrium* nematic since the stress tensor in equilibrium must be derived from functional derivatives of the free energy. Since *that* free energy must be rotation invariant, it can only depend on *derivatives* of the nematic director $\hat{\mathbf{n}}$ (in fact, this argument leads to the familiar Frank free energy [15] for equilibrium nematics). Functional derivatives of this then lead to a stress σ which depends on *derivatives* of $\mathbf{n}$. Since we are considering *non-equilibrium* nematics, however, this constraint that σ be derived from a functional derivative of a rotation-invariant free energy does not apply. Hence, the only constraint on allowed terms is rotation invariance of the equations of motion, which is respected by a term in σ proportional to $\mathbf{Q}$ [17], since both objects are symmetric second rank tensors.

We now restrict our attention only to small fluctuations about the uniaxial nematic phase, aligned along the z axis, and denote vector components in directions normal to z by the subscript $\perp$. We assume the nematic order is well developed, so that S can be treated as constant, and consider spatial variations $c(\mathbf{r},t) = c_0 + \delta c(\mathbf{r},t)$, where c_0 is the mean concentration, and $\mathbf{n}(\mathbf{r},\mathbf{t}) = \hat{\mathbf{z}} + \delta\mathbf{n}(\mathbf{r},\mathbf{t})$. Since $\mathbf{n}$ is a unit vector, we need consider only the transverse components $\delta\mathbf{n}_\perp$.

To close our equations, we need the equation of motion for $\mathbf{n}$ [7], which is identical in form to that for an equilibrium nematic and reads, to linear order:

$$\partial_t \delta\mathbf{n}_\perp = \lambda_+ \partial_z \mathbf{v}_\perp + \lambda_- \boldsymbol{\nabla}_\perp v_z + K_1 \boldsymbol{\nabla}_\perp (\boldsymbol{\nabla}_\perp \cdot \delta\mathbf{n}_\perp) + K_2 \nabla_\perp^2 \delta\mathbf{n}_\perp + K_3 \delta_z^2 \delta\mathbf{n}_\perp + \mathbf{f}_\perp. \tag{3}$$

Here $\lambda_\pm = (\lambda \pm 1)/2$; λ is the "flow alignment parameter", familiar from equilibrium nematics, which affects the response of the nematic director to shear, and the noise $\mathbf{f}_\perp$ is delta-correlated in space and time:

$$\langle f_{\perp i}(\mathbf{r},t) f_{\perp j}(\mathbf{r}',t') \rangle = \delta_{ij}\, \Delta_n \delta^d(\mathbf{r}-\mathbf{r}') \delta(t-t') \tag{4}$$

We now use the equation of motion (2) to eliminate $\mathbf{v}$. For hydrodynamically slow processes, $\partial_t \mathbf{v} \ll \Gamma \mathbf{v}$, and so we can neglect the $\partial_t \mathbf{v}$ term in (2) and immediately solve for $\mathbf{v}$, finding, to linear order,

$$\mathbf{v} = -\alpha \left(\partial_z \delta\mathbf{n}_\perp + (\nabla_\perp \cdot \delta\mathbf{n}_\perp)\, \hat{\mathbf{z}} \right) - \gamma_1 \boldsymbol{\nabla}_\perp c - \gamma_2\, \partial_z\, c\, \hat{\mathbf{z}} + \frac{\mathbf{f}_R}{\Gamma} \tag{5}$$

where α and γ_i are related to c_o, S and the coefficients in (2). Inserting (5) into (1) gives, to linear order in fluctuations, the concentration equation of motion

$$\frac{\partial \delta c}{\partial t} = (D_z \partial_z^2 + D_\perp \nabla_\perp^2)\, \delta c + 2 c_0\, \alpha\, \partial_z (\nabla_\perp \cdot \delta\mathbf{n}_\perp) + \nabla \cdot \mathbf{f}_c \tag{6}$$

where the various coefficients in (6) and the noise $\mathbf{f}_c$ are derived from those in (2) and (5). The leading nonlinearities that arise in (6) are of the form $\nabla_\perp \cdot (\partial_z \delta\mathbf{n}_\perp \delta c)$ and similar terms, as well as $(\boldsymbol{\nabla}_\perp \cdot \delta\mathbf{n}_\perp)^2$ and similar terms. These nonlinearities as well as the couplings to the director in (6) are forbidden at thermal equilibrium.

The director dynamics obtained by inserting (5) into (3) is given to linear order by

$$\frac{\partial \delta\mathbf{n}_\perp}{\partial t} = (K_z \partial_z^2 + K_\perp \nabla_\perp^2 + K_L' \boldsymbol{\nabla}_\perp \boldsymbol{\nabla}_\perp \cdot)\, \delta\mathbf{n}_\perp + D_{cn} \partial_z \boldsymbol{\nabla}_\perp \delta c + \mathbf{f}_\perp \tag{7}$$

where, again, the phenomenological parameters and noise source $\mathbf{f}_\perp$ are derived from corresponding terms in (2) to (5). The leading nonlinearities which will appear in (7) are of the form $\partial_z \delta\mathbf{n}_\perp (\boldsymbol{\nabla}_\perp \cdot \delta\mathbf{n}_\perp)$, $\delta\mathbf{n}_\perp \partial_z (\boldsymbol{\nabla}_\perp \cdot \delta\mathbf{n}_\perp)$ and similar terms. These nonlinearities too are completely nonequilibrium in origin.

The concentration field as well as the nonlinearities mentioned above are absent in the treatment of Gruler et. al. [1]. The effect of the nonlinearities will be dealt with elsewhere

[18]. The inclusion of the concentration field leads to our most striking nonequilibrium effect, namely, the giant number fluctuations we predict below.

The linearized equations of motion are easily analyzed for their mode structure, possible instabilities, and fluctuation statistics. This is most conveniently done by Fourier-transforming in space and time, i.e., considering modes that go as $\exp(i\mathbf{q}.\mathbf{r} - i\omega t)$. Doing this enables us to rewrite (6) and (7) as

$$\left[-i\omega + D_c\left(\hat{\mathbf{q}}\right) q^2\right] \delta c\left(\mathbf{q},\omega\right) + 2c_0\alpha q_z\, q_\perp\, \delta n_L\left(\mathbf{q},\omega\right) = i\mathbf{q}\cdot\mathbf{f}_c\left(\mathbf{q},\omega\right) \tag{8}$$

$$D_{cn} q_z q_\perp \delta c\left(\mathbf{q},\omega\right) + \left[-i\omega + K_L\left(\hat{\mathbf{q}}\right) q^2\right] \delta n_L\left(\mathbf{q},\omega\right) = f_L\left(\mathbf{q},\omega\right) \tag{9}$$

$$\left[-i\omega + K_T\left(\hat{\mathbf{q}}\right) q^2\right] \delta \mathbf{n}_T = \mathbf{f}_T \tag{10}$$

where

$$f_L\left(\mathbf{q},\omega\right) \equiv \hat{\mathbf{q}}_\perp \cdot \mathbf{f}_\perp\,,\; \mathbf{f}_T = \mathbf{f}_\perp - \hat{\mathbf{q}}_\perp\left(\hat{\mathbf{q}}_\perp \cdot \mathbf{f}_\perp\right) \tag{11}$$

$$\delta\mathbf{n}_L(\mathbf{q},\omega) \equiv \hat{\mathbf{q}}_\perp\; \left(\hat{\mathbf{q}}_\perp \cdot \delta\mathbf{n}_\perp(\mathbf{q},\omega)\right) \tag{12}$$

and

$$\delta\mathbf{n}_T \equiv \delta\mathbf{n}_\perp - \delta\mathbf{n}_L \tag{13}$$

are, respectively, the components of $\mathbf{f}_\perp$ and $\delta\mathbf{n}_\perp$ along and transverse to $\hat{\mathbf{q}}_\perp$ [19] and we've defined the direction dependent diffusion constants

$$D_c\left(\hat{\mathbf{q}}\right) \equiv D_z \hat{q}_z^{\,2} + D_\perp \hat{q}_\perp^{\,2} \tag{14}$$

$$K_L\left(\hat{\mathbf{q}}\right) \equiv K_z \hat{q}_z^{\,2} + \left(K_\perp + K_L'\right) \hat{q}_\perp^{\,2} \tag{15}$$

$$K_T\left(\hat{\mathbf{q}}\right) \equiv K_z \hat{q}_z^{\,2} + K_\perp \hat{q}_\perp^{\,2} \tag{16}$$

The eigenfrequencies obtained from these equations are all diffusive. There are $d-2$ transverse diffusive modes coming from the $\mathbf{n}_T$ equation, all with identical imaginary frequencies

$$\omega_T = -iK_T\left(\hat{\mathbf{q}}\right) q^2 \tag{17}$$

and two coupled concentration - longitudinal modes with

$$\omega_{\pm} = -i\Gamma_{\pm}\left(\hat{\mathbf{q}}\right) q^2 \tag{18}$$

with

$$\Gamma_{\pm}\left(\hat{\mathbf{q}}\right) = \frac{1}{2}\left[D_c\left(\hat{\mathbf{q}}\right) + K_L\left(\hat{\mathbf{q}}\right) \pm \sqrt{\left(D_c\left(\hat{\mathbf{q}}\right) - K_L\left(\hat{\mathbf{q}}\right)\right)^2 + 8c_0\alpha D_{cn}\hat{q}_{\perp}^{\,2}\hat{q}_z^{\,2}} \,\right] \tag{19}$$

We shall assume linear stability, which is assured if the K_is and D_is are positive and the combination $c_0\alpha D_{cn}$ is not too large.

With these eigenfrequencies in hand, it is straightforward to solve (8) -(10) for δc, δn_L, and $\delta\mathbf{n}_T$ obtaining

$$\delta c = \frac{\left(2c_0\alpha q_{\perp} q_z\right) f_L}{\left(\omega + i\Gamma_+\left(\hat{\mathbf{q}}\right) q^2\right)\left(\omega + i\Gamma_-\left(\hat{\mathbf{q}}\right) q^2\right)} \tag{20}$$

$$\delta n_L = \frac{-\left(-i\omega + D_c\left(\hat{\mathbf{q}}\right) q^2\right) f_L}{\left(\omega + i\Gamma_+\left(\hat{\mathbf{q}}\right) q^2\right)\left(\omega + i\Gamma_-\left(\hat{\mathbf{q}}\right) q^2\right)} \tag{21}$$

$$\delta\mathbf{n}_T = \frac{\mathbf{f}_T}{-i\omega + K_T\left(\hat{\mathbf{q}}\right) q^2} \tag{22}$$

Autocorrelating these, using the known autocorrelations Eqn. (4) for the random forces gives

$$\left\langle \left|\delta c\left(\mathbf{q},\omega\right)\right|^2 \right\rangle = \frac{\left(2c_0\alpha q_{\perp} q_z\right)^2 \Delta_n}{\left(\omega^2 + \Gamma_+^2\left(\hat{\mathbf{q}}\right) q^4\right)\left(\omega^2 + \Gamma_-^2\left(\hat{\mathbf{q}}\right) q^4\right)} \tag{23}$$

$$\left\langle \left|\delta n_L\left(\mathbf{q},\omega\right)\right|^2 \right\rangle = \frac{\left(\omega^2 + D_c^2\left(\hat{\mathbf{q}}\right) q^4\right) \Delta_n}{\left(\omega^2 + \Gamma_+^2\left(\hat{\mathbf{q}}\right) q^4\right)\left(\omega^2 + \Gamma_-^2\left(\hat{\mathbf{q}}\right) q^4\right)} \tag{24}$$

$$\left\langle \delta n_L\left(\mathbf{q},\omega\right) \delta c\left(-\mathbf{q},-\omega\right)\right\rangle = \frac{2ic_0\alpha q_z q_{\perp}\left(\omega + iD_c\left(\hat{\mathbf{q}}\right) q^2\right) \Delta_n}{\left(\omega^2 + \Gamma_+^2\left(\hat{\mathbf{q}}\right) q^4\right)\left(\omega^2 + \Gamma_-^2\left(\hat{\mathbf{q}}\right) q^4\right)} \tag{25}$$

$$\left\langle \delta n_{T_i}\left(\mathbf{q},\omega\right) \delta n_{T_j}\left(-\mathbf{q},-\omega\right)\right\rangle = \frac{\Delta_n P_{ij}^{\perp}\left(\hat{\mathbf{q}}\right)}{\left(\omega^2 + K_T^2\left(\hat{\mathbf{q}}\right) q^4\right)} \tag{26}$$

with $\left\langle \delta n_{T_i} \delta n_L \right\rangle = \left\langle \delta n_{T_i} \delta c \right\rangle = 0$ for all i, $\mathbf{q}$ and ω.

In writing eqns. (23 - 26), we have neglected all of the contributions coming from the noise $\mathbf{f}_c$ in the concentration equation of motion (5), since these are all negligible, as $\mathbf{q} \to \mathbf{0}$, relative to those coming from the noise $\mathbf{f}_{\perp}$ in the director equation of motion (3).

Equations (23 - 26) can now be Fourier-transformed back to get real space-real time correlations functions. One quantity of particular interest are the equal-time, spatially fourier-transformed correlations of the concentration:

$$\langle \delta c(\mathbf{q},t)\delta c(-\mathbf{q},t)\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left\langle \left|\delta c(\mathbf{q},\omega)\right|^2 \right\rangle = \frac{(2c_0\alpha q_\perp q_z)^2 \Delta_n}{F\left(\hat{\mathbf{q}}\right) q^6} \propto \frac{1}{q^2} \tag{27}$$

where

$$F\left(\hat{\mathbf{q}}\right) \equiv 2\left(D_c\left(\hat{\mathbf{q}}\right) + K_L\left(\hat{\mathbf{q}}\right)\right)\left[D_c\left(\hat{\mathbf{q}}\right) K_L\left(\hat{\mathbf{q}}\right) - 2c_0\alpha D_{cn}\hat{q}_\perp^2 \hat{q}_z^2\right] \tag{28}$$

The important thing about this result is that the $(\delta c)^2$ fluctuations are *enormous* as $q \to 0$, diverging as $\frac{1}{q^2}$. This would be equivalent, in an equilibrium system, to having a compressibility which diverged as $\frac{1}{q^2}$ as $q \to 0$. To restate this in real space, it is as if the compressibility of a system of linear extent L diverged according to $\chi \propto L^2$ as $L \to \infty$. Independent of any connection to a response quantity like the compressibility, the rms number fluctuations $\sqrt{\delta N^2}$ in a volume V scale as $\sqrt{S(q \to 0)V}$. For active nematics this implies that

$$\sqrt{\delta N^2} \propto \sqrt{L^2 V} \propto L^{1+\frac{d}{2}} \propto N^{\frac{1}{2}+\frac{1}{d}} \tag{29}$$

where in the last step we've used the fact that $N \propto V \propto L^d$ and solved for L as a function of N. For $d = 2$ this recovers our earlier statement that $\sqrt{\langle \delta N^2 \rangle} \propto N$.

Lastly, Eqn. (5) for the velocity implies that the autocorrelation of a tagged particle will be controlled mainly by the effect of soft director fluctuations: a particle at a point in the nematic moves with a speed proportional to the local curvature of $\mathbf{n}_\perp$. This means the autocorrelation of the velocity $\mathbf{v}(t)$ of a particle with trajectory $\mathbf{R}(t)$ will be, schematically,

$$\langle \mathbf{v}(0) \cdot \mathbf{v}(t)\rangle \sim \langle \nabla \delta n_\perp(\mathbf{R}(0),0) \nabla \delta n_\perp(\mathbf{R}(t),t)\rangle, \tag{30}$$

Fourier transforming the $\mathbf{n}$ correlation functions (25) and (26) back to real space and time, and using the fact that, for a diffusing particle, $\left\langle \left|\mathbf{R}(t) - \mathbf{R}(0)\right|^2 \right\rangle \propto t$, implies that the correlation function (30) decays as $t^{-d/2}$, as claimed earlier [20].

We close with some comments on the experiments in [2]. Although the nematic "phase" in their images appears rather polydomain, it is likely that their system does display true nematic order in some parameter range. Perhaps the polydomain structures coarsen at long

times to a true nematic. Such a driven nematic would be the ideal place to test the predictions of this paper. If, for some range of parameters, they are able to find macroscopically aligned regions of *tilted* rods — which would constitute vectorial order and therefore, as explained in [2], move coherently in one direction — these would be examples of the moving XY-model of [5, 6]. Indeed, the coupled equations for tilt and concentration in [21], which analyzes the experiments of [2], are closely related to those of [6]. Lastly, the "vertical rods" phase, from the images, displays a good deal of order; one wonders whether it is a nonequilibrium realization of a crystal or hexatic.

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[19] Of course, in $d = 2$, there *are* no components of $\delta\mathbf{n}_\perp$ perpendicular to $\mathbf{q}_\perp$, since there is only one direction perpendicular to z. We include $\delta\mathbf{n}_T$ here to generalize the model to systems in $d > 2$, such as those mentioned in [8].

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