Deterministic endless collective evolvement in active nematics

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We propose a simple deterministic dynamic equation and reveal the mechanism of large-scale endless evolvement of spatial density inhomogeneity in active nematic. We determine the phase regions analytically. The interplay of density, magnitude of nematic order, and nematic director is crucial for the long-wave-length instability and the emergence of seemingly fluctuated collective motions. Ordered nematic domains can absorb particles, grow and divide endlessly. The present finding extends our understanding of the large-scale and seemingly fluctuated organization in active fluids.

Assemblies of active particles, which may be a physical abstraction of running animals\[1\], flying birds\[2\], swimming bacteria\[3\], migrating cells\[4\] or even cytoskeleton\[5\], have been served as a new building block for physicists over the last decade or so to understand the common collective behavior in these non-equilibrium systems\[6\]. Active nematic, a recently proposed concept for a kind of apolar active particles, is formed by driven rod-like particles with head-tail symmetry through the randomly driving force along the rod orientation axis at the single-particle level\[7(a)\]-\[7(f)]\]. The symmetry of the system is not broken by applying such micro-driven forces until spontaneous symmetry breaking occurs. Recently, simulations and experiments in active nematic system show well-organized collective motions with system-sized fluctuation\[7(b)\]-\[7(e)]\). For example, splitting and merging of large-scale self-organized structures are exemplified in the simulation on active nematics\[7(c)]\). Experiments also show large-scale collective swarming and swirling in driven granular rods monolayer\[7(d),7(e)\]. These observations lead us to think about the nature of such seemingly fluctuated collective motions. It is currently unclear whether these large-scale collective motions arise in a deterministic manner or as a result of noises applied upon the system. Moreover, are they genuinely restless on large scale and evolving without end? These important aspects are still not well addressed in previous studies.

In the present study, we start from a deterministic equation to study the mechanism of restless collective evolution in active nematics. We reveal a new phase that is characterized by the unattainability of stable steady state. We first identify that, if the steady state can be reached, the system investigated here favors spatially homogeneous state. On the other hand, by taking account of the interplay between particle density and local nematic order (i.e., magnitude and orientation), the linear stability analysis shows that homogeneous nematic state can be unstable to fluctuations of small wave number. Therefore, the system enters into a chaotic phase region with no stable steady state. Large-scale spatial inhomogeneity of density and nematic order is developed as a result of long-wavelength instability. The spatial inhomogeneity in turn changes the direction of the nematic director, leading to a non-ending evolvement of the system. Numerical flux analysis shows that the particle-rich nematic domains are surrounded by particles fluxes, and evolve via absorbing particles from low-density isotropic medium, growing, and extending itself and breaking into small pieces. More importantly, all these seemingly fluctuated collective motions giving rise to giant number fluctuations are governed by a deterministic equation which is essentially free of noises.

We notice that one salient feature of simulation rules for active nematics by Chate et al.\[7(c)]\) is that particle rotations are governed through inter-particle nematic interaction while spatial translational movements are free of such interactions. Experimentally particles are driven along their long axis, inducing strong longitudinal diffusion, and they can thrust into the media with the supply of kinetic energy\[7(e)]\). A simple diffusion equation which follows these observations can be written as(see \[8\]):

$$\partial_t f(r,u,t) = \nabla [D_iu_iu_j + D_\perp (1 - uu)\nabla]f(r,u) + \mathcal{R}[D_i \mathcal{R} f(r,u) + D_r \mathcal{R} w(r,u)f(r,u)],$$

(1)

where $D_i$ and $D_\perp$ are the parallel and perpendicular components of the translational diffusion constants. $D_r$ is the rotational diffusion constant, and the rotational operator $\mathcal{R}$ is defined by $\mathcal{R} = u \times \partial_u \mathcal{R}$, $f(r,u,t)$ is the particle number distribution function where the spatial coordinate $r$ and the unit vector $u$ denote the center-of-mass position and long-axis direction of particles, respectively. $w(r,u)$ is a self-consistent interacting potential which has $\pm u$-symmetry. In two-dimensional(2-D) case, the most common form of such interacting potential is the excluded-volume-like interaction $w(r,u) = l^2 \int du'|u \times u'|f(r,u'),$ where $l$ is the particle length.

The diffusion equation Eq.(1) for active nematics satisfies particle number conservation with the spatial translational current $J^t_i(r,u) = -D_iuu_i\nabla f(r,u) - D_\perp (1 - uu)\nabla f(r,u)$ and the local rotational current $J^r_i(r,u) = -D_r \mathcal{R} f(r,u)$ which are independent of each other. The translational current is purely diffusive. In the Fourier space as defined by $f(k,u) = \int dr f(r,u)e^{-ikr}$, the spatial fluctuation modes are governed by diffusive decaying term.
The truncated dynamic equation for the nematic order parameter can be written as:

$$\frac{\partial S(t)}{\partial t} = (\hat{\rho} - 1)S - \frac{3\hat{\rho}^2S^3}{4(5-\hat{\rho})},$$

where $\hat{\rho} = \rho/\rho^*$ is the rescaled number density, and the critical density $\rho^* = 3\pi/2D^2$, beyond which the system enters into a spatially homogeneous nematic state.

Next, we examine the linear stability of such spatially homogeneous nematic state above $\rho^*$, by expanding the number distribution function $f(\mathbf{r}, \mathbf{u}) = (2\pi)^{-1} \rho(\mathbf{r})[1 + 4(u_n u_\perp - \delta_{\alpha\beta}/2)Q_{\alpha\beta}(\mathbf{r})]$ with the inclusion of the alignment tensor $Q_{\alpha\beta}(\mathbf{r}) = S(\mathbf{r})[\hat{n}_\alpha \hat{n}_\beta - \delta_{\alpha\beta}/2]$ where $\hat{n}(\mathbf{r})$ is the unit vector of the nematic director. We assume that nematic director is along the $x$ axis of the system.

Small fluctuations of density and nematic director near the ordered nematic state are given by $\delta \hat{\rho}(\mathbf{r}) = \hat{\rho}(\mathbf{r}) - \hat{\rho}_0$ and $\delta \hat{n}_y(\mathbf{r}) = Q_{xy}(\mathbf{r})$, respectively. Here, $\hat{\rho}_0 = \rho_0/\rho^*$ is the reduced bulk particle density, and $\delta \hat{n}_y(\mathbf{r})$ is the $y$-component of the deviated nematic director. Noting that $\mathbf{n}_0(\mathbf{r}) = \hat{x}$ and $|\mathbf{n}| = 1$, $\delta \hat{n}_y(\mathbf{r})$ is the only possible small fluctuation of nematic director $\mathbf{n}(\mathbf{r})$. The resulting hydrodynamic equations can be obtained from Eq. (1), yielding

$$\partial_t \delta \hat{\rho} = \frac{D_p}{2} \partial^2_x \delta \hat{\rho} + \frac{D_n}{2}(\partial^2_z - \partial^2_y)(\delta \hat{S})$$

$$+ 2D_n \hat{\rho}_0 S \partial_x \partial_y \delta \hat{n}_y, \quad (2)$$

$$\partial_t \delta \hat{\rho}_0 S \partial_y \delta \hat{n}_y = \frac{D_p}{4} \partial^2_x \delta \hat{\rho}_0 + \frac{D_n}{2} \partial^2_y \delta \hat{\rho} S,$$

$$+ 4D_p \hat{\rho}_0 (\hat{\rho} - 1) S - D_p \frac{3\hat{\rho}^2 S^3}{5 - \hat{\rho}}, \quad (3)$$

where $D_p = D_{\parallel} + D_{\perp}$ and $D_n = D_{\parallel} - D_{\perp}$. It is easy to see that the homogeneous state is stable to fluctuations of coupled nematic director and density field. Here we consider the stability of the modes that couple fluctuations of density $\delta \hat{\rho}(\mathbf{r}) = \hat{\rho}(\mathbf{r}) - \hat{\rho}_0$ and magnitude of nematic order $\delta \hat{n}_y(\mathbf{r}) = \hat{n}_y(\mathbf{r}) S(\mathbf{r}) - \hat{n}_y S_0$ with $\delta \hat{n}_y = 0$ around the homogeneous state $\hat{\rho}_0, S_0$, where

$$S_0 = \sqrt{4(5 - \hat{\rho}_0)(\hat{\rho}_0 - 1)/3\hat{\rho}_0^2}.$$ 

The mode of fluctuations in Fourier components with wave vector $\mathbf{k}$, defined by $\delta \hat{\rho}(\mathbf{r}) = \int d\mathbf{k} \hat{\rho}_k e^{-i\mathbf{k} \cdot \mathbf{r}}$ and $\delta S_{\mathbf{k}}(\mathbf{r}) = \int d\mathbf{S} \hat{\rho}_\mathbf{k} e^{-i\mathbf{k} \cdot \mathbf{r}}$, is governed by

$$\partial_t \begin{bmatrix} \hat{\rho}_k \\ S_{\mathbf{k}} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \begin{bmatrix} D_p k^2 & D_n \cos 2\theta k^2 \\ D_n \cos 2\theta k^2 / 2 & D_p k^2 \\ -8D_r \hat{\rho}_0 S_0 \\ +16D_r \sigma \delta \end{bmatrix} \\ -8D_r \hat{\rho}_0 S_0 + 16D_r \sigma \delta \end{bmatrix} S_{\mathbf{k} \mathbf{S}}, \quad (5)$$

where $\sigma = (4 - \delta)/3$, the rescaled coefficient $D_0 = D_n/D_p$, and the wave number $\kappa = \sqrt{D_p / D_k}$. The real part of $\lambda_{\rho,S_\mathbf{k}}$ is always negative, representing stable decaying

FIG. 1: Three phases are separated by the blue curves. Polar plots (a)-(f) indicate the instability regime for $\kappa$ and $\theta$. The locations $(D_0, \delta)$ of their origins are used as the parameters to produce these plots. (a) $|D_0| = 0, \delta = 0.8$, (b) $|D_0| = 2/3, \delta = 0.4$, (c) $|D_0| = 0, \delta = 0.4$, (d) $|D_0| = 1/3, \delta = 0.01$, (e) $|D_0| = 2/3, \delta = 0.01$, and (f) $|D_0| = 0, \delta = 0.01$. The black and red branches in polar plots represent the cases of positive and minus $D_0$, respectively. The inset shows the corresponding instability modes $D_t^{-1} \lambda_{\rho,S_\mathbf{k}}|_{\mathbf{k}=0}$ for these polar plots.
mode. However, the mode \( \lambda_{p,0}^{\perp} \) becomes positive when
\( 3(2(D_0\sigma \cos 2\theta + \delta)\kappa^2 + (2 - D_0^2 \cos^2 2\theta)\kappa^4 < 0 \). The coefficient
of \( \kappa^4 \) is always positive since \( |D_0| \leq 1 \), signifying
that for large enough wave numbers, the fluctuations are
always stable. For small wave numbers which describe
large-scale fluctuations, the stability is controlled by the
coefficient of \( \kappa^2 \). Thus when \( (D_0\sigma \cos 2\theta + \delta) < 0 \), the
system becomes unstable on large scale.

The phase map for \((D_0, \delta)\) is given in Fig. 1. Be-
tween the isotropic and linearly stable nematic phases,
there is a region where spatially homogeneous nematic
state is unstable. It is denoted as a ‘phase with no sta-
bale state’ to emphasize that the only possible form of
steady-state solution is unachievable there. For different
\((D_0, \delta)\) within the ‘no stable state’ region, the instabil-
ity mode structures \((\kappa, \theta)\) are given by the polar plots
whose central positions represent \((D_0, \delta)\). Here, each po-
lar plot is composed of horizontal (black) and vertical
(red) branches enclosing unstable fluctuation modes, cor-
responding to \( D_0 < 0 \) and \( D_0 > 0 \), revealing that spatial
inhomogeneities are developed parallel and perpendicu-
lar to the nematic director, respectively. The maximum
values \( \kappa_m \) of \( \kappa \) for the instability regimes are always in
the directions \( \theta = \pi/2, 3\pi/2 \) for \( D_0 > 0 \) and \( \theta = 0, \pi \)
for \( D_0 < 0 \), respectively. Generally speaking, \( \kappa_m \) be-
comes larger when \((D_0, \delta)\) is far from the phase bound-
ary. The inset of Fig. 1 shows the value of \( D_0 - 1 \lambda_{p,0}^{\perp} \),
where for small \( \kappa \), \( D_0 - 1 \lambda_{p,0}^{\perp} > 0 \) corresponds to the long-
wavelength instability and the onset of large-scale spatial
inhomogeneity.

What will happen in the phase region where there is
no stable steady state? And how the system evolves in
time? To answer these questions we directly integrate
Eq. (1) numerically in this region using alternative im-
plex algorithm (see [3]). Starting from an isotropic and
spatially-homogeneous initial condition, local ordered ne-
matic domains form at the beginning, accompanied with
quick development of density inhomogeneity. Further
coursening of these structures leads to the coexistence of
particle-enriched nematic domains and particle-poor
isotropic region where \( \rho < \rho^* \) (Fig. 2a). However, such
a large-scale spatially inhomogeneous structure is insta-
ble, and it will evolve and become fragmented as shown in
Fig. 2b. The fragmented structure will again coa-
lesce and similar process will repeat aperiodically and
endlessly (see [3] M1.mov). In Fig. 2c-2k, we show how
a particle-rich nematic branch breaks into pieces and re-
unites into a structure with new morphology.

How does the fragmentation process occur? In Fig.
3a-c, we take a close look at the process that a nematic
band breaks up (for a more continuous process, see [3] M2.mov). In Fig. 3a, after the spontaneous formation of a nematic
band, initially, it is shown that the nematic director in the high-density ordered region is almost par-
allel to the density stripe boundary. In this case, the
nematic director is along the \( x \)-axis. For \( D_0 > 0 \), from
our previous stability analysis, the term \( -4D_0 \delta n \partial_y (\rho S) \)
in Eq. (2) is directly responsible for the development of
such density inhomogeneity. Now, we are interested if
such aligned director field is stable to small fluctuations
\( \delta n_{\perp}(\mathbf{r}) = n_{\perp}(\mathbf{r}) - n_0 = (0, \delta n_{\perp y}) \). To linear order, the
dynamic equation for \( \delta n_{\perp y}(\mathbf{r}) \) can be obtained from Eq. (1)
as \( \rho S \partial_t \delta n_{\perp y} = \frac{1}{2} D_0 (\rho S \partial_y^2 \delta n_{\perp y} + \delta n_{\perp y} \partial_y^2 \rho S) \), where we have assumed that there is no spatial variation of \( \rho S \)
along \( x \)-axis. The spatial variation of \( \rho S \) along the \( y \)-axis is significant since density inhomogeneity is developed in
that direction. Near stripe boundaries, we always have
\( \partial_y^2 \rho S > 0 \), which makes the fluctuations \( \delta n_{\perp y} \) unstable.
Such instability will induce the change of the nematic
orientation, and this explains why the nematic directors
in Fig. 2 and Fig. 3b are most likely to be oblique to the
density profile boundaries. When the nematic direc-
tors become oblique to the boundary, as shown in Fig.
3b, there is a leakage of particles from the high-density
region. As the particle density in the stripe falls into the
‘no stable state’ region as shown in Fig. 1, the spatial
instability takes place again. This leads to a fragmen-
tation event, as shown in Fig. 3c. It is shown that a
density crevice forms parallel with the nematic director
as spatial instability requires. In Fig. 3d, we show a

FIG. 2: Density and nematic order profiles are plotted. The
color scale shows the local relative rescaled density value
\( \delta(\mathbf{r}) = \rho(\mathbf{r}) - 1 \). The length and angle of white segments
show the magnitude and direction of nematic order, respec-
tively. The dynamic parameters are \( D_r = 2 \), \( D_\perp = 0.4 \),
and \( D_y = 2.4 \). The reduced instability dynamic parameter
\( D_0 = 5/7 \) and \( \delta = 0.01 \). The system size is \( 300 \times 300 \) with
the particle length \( l = 1 \). Periodic boundary condition is
implemented. Discrete time step \( \Delta t = 0.018 \) and spatial steps
\( \Delta_x = \Delta_y = \Delta_z = 3 \). (a)-(b) The snapshots are taken at
times \( 1.7 \times 10^6 \Delta t \) and \( 2.3 \times 10^6 \Delta t \). (c)-(k) A close look of the
breaking and coalescing processes of a nematic domain,
at times \( 1.6 \times 10^6, 1.7 \times 10^6, 1.71 \times 10^6, 1.72 \times 10^6, 1.73 \times 10^6,
1.74 \times 10^6, 1.75 \times 10^6, 1.76 \times 10^6 \) and \( 1.8 \times 10^6 \) in unit \( \Delta t \).
twisted-spindle shaped high-density region with local nematic order, which is commonly formed after it breaks off from a larger ordered structure in Fig. 2e.

We also perform simulations to examine the stability of homogeneous nematic state on the basis of Eq. (1) (see 8). Fig. 3e shows the formation of a particle-enriched nematic band. We find that such band is also unstable off from a larger ordered structure in Fig. 2e. The color scale shows the density inhomogeneity and similar restlessness evolvement in active nematics for $9.4 \times 10^4$ and $1.1 \times 10^5$ simulation sweeps.

As we show in Fig. 3a, inward currents, generated by van der Waals forces, of long-wavelength instability, density and order inhomogeneity develops as guided by nematic director field. The spatial inhomogeneity in turn changes the directions of local nematic directors. The changed nematic directors further guide the fragmentation events, leading to endless evolution of the system. Finally, it would be interesting to extend our analysis to other active fluids. This work was supported by the National Natural Science Foundation of China (No. 10974080).

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