Instabilities and chaos in a kinetic equation for active nematics

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Received 18 September 2013, revised 12 January 2014
Accepted for publication 28 January 2014
Published 13 March 2014

New Journal of Physics 16 (2014) 035003
doi:10.1088/1367-2630/16/3/035003

Abstract
We study dry active nematics at the kinetic equation level, stressing the differences with the well-known Doi theory for non-active rods near thermal equilibrium. By deriving hydrodynamic equations from the kinetic equation, we show analytically that these two description levels share the same qualitative phase diagram, as defined by the linear instability limits of spatially-homogeneous solutions. In particular, we show that the ordered, homogeneous state is unstable in a region bordering the linear onset of nematic order, and is only linearly stable deeper in the ordered phase. Direct simulations of the kinetic equation reveal that its solutions are chaotic in the region of linear instability of the ordered homogeneous state. The local mechanisms for this large-scale chaos are discussed.

Keywords: active nematics, kinetic equation, hydrodynamic equation, chaos
1. Introduction

The collective properties of assemblies of active particles are currently under intense scrutiny, both at the theoretical and experimental level. Following the seminal works of Vicsek et al., and Toner and Tu [1, 2], which were published in 1995, physicists have made progress towards uncovering and understanding universal, generic features of groups of interacting self-propelled particles, some of these results have started to be confronted to experimental data. This is the case, for instance, in the long-range correlations and anomalous fluctuations that are predicted by Toner and Tu [3] and by Ramaswamy et al. [4–6] to characterize most homogeneous, orientationally-ordered, fluctuating phases of flocks. They have been observed in numerical simulations of simple models [7] and they have been argued to have been seen in vibrated granular particles [8–10], bacterial swarms [11, 12], as well as in vitro motility assays, where grafted motor proteins displace biofilaments [13].

The Vicsek et al. model [1] now serves as the reference minimal model. In this context, the collective motion is reduced to the competition between noise and the local ferromagnetic alignment of the polarities of constant-speed particles. All other possible interactions are neglected, as is the fluid in which the particles evolve (as opposed to active suspensions). Even within this somewhat restrictive, ‘dry flocking’, minimal context, other classes of active particles systems can be defined, varying the symmetry of the particles (polar or apolar) and of the interaction (ferromagnetic versus nematic alignment). The case of active nematics [14] was considered very early on by Ramaswamy et al. [4–6], and has recently enjoyed a lot of attention. This may be understood here as assemblies of apolar particles that are forced to jiggle along their director and aligning nematically. Ramaswamy and collaborators, working on a linearized theory, predicted the existence of a non-equilibrium current at the origin of particularly strong number fluctuations [4–6].

The active nematics version of the Vicsek model was introduced in [15]. In this model, point particles possess a (uniaxial) nematic degree of freedom. They are displaced at discrete time steps along one of the two directions defined by the director and are calculated from the nematic average of local neighbors’ orientation, to which some random noise was added. This model can be seen as a toy model for active, self-propelled rod-like objects interacting by steric inelastic collisions. The numerical work of [15] revealed an isotropic/nematic transition to quasi-long-range order, similar to the equilibrium Kosterlitz-Thouless transition of the XY model. The quasi-ordered phase was found to be spontaneously segregated into a large high-density high-order band fluctuating in a sparse, disordered sea, and is shown to exhibit the strong number fluctuations predicted by Ramaswamy et al.

More recently [16], the hydrodynamic equations describing dry active nematics were derived from the Vicsek-like model of [15], and were found to coincide with those obtained by different approaches [19, 20]. These equations, derived via a Boltzmann equation obtained in the dilute limit by kinetic theory techniques, were found to possess features at odds with those reported in the original Vicsek-like microscopic model. For instance, a homogeneous ordered phase is predicted to exist deep in the ordered phase whereas it was not observed in the microscopic model.

Here, we study dry active nematics directly at the level of the Boltzmann kinetic equation level in order to clarify the above issues. We consider a slightly more complicated (but more realistic) case where particles also undergo positional diffusion. Stressing the differences with the well-known Doi theory for non-active rods near thermal equilibrium, we write a simple
kinetic equation (section 2) and study the linear stability of its homogeneous solutions (section 3). In the same section, we also derive the corresponding hydrodynamic equations governing the nematic order field and show analytically that these two description levels share the same qualitative phase diagram, but quantitatively diverge rather strongly as the global density is increased. We show, in particular, that the ordered, homogeneous state is unstable in a region bordering the linear onset of nematic order and is only linearly stable deeper in the ordered phase. In section 4, we perform direct simulations of the kinetic equation and reveal that its solutions are chaotic in the region of linear instability of the ordered homogeneous state. We discuss the local mechanisms at the origin of this large-scale chaos. In section 5, our results are summarized and discussed in view of the above-mentioned discrepancies between the reported behavior of the microscopic Vicsek-like model and the properties of continuous descriptions of active nematics.

2. Kinetic equation for dry active nematics

One salient feature of the Vicsek-style model for active nematics that was developed by Chaté et al [15] is that the rotations of particles are governed by local nematic alignment while the streaming (translational movement) is implemented at constant speed independently of interactions. Similarly, real ‘self-propelled’ particles are driven along their long axis, inducing strong longitudinal diffusion [21–26].

Let us thus consider elongated objects interacting by local nematic alignment and suppose that every particle is driven along its long axis at speed $v_0$, with the driving force switching the sign of the velocity randomly with rate $k$. One can then write, in the mean-field limit, the kinetic equations for the two one-particle number distribution functions $f_\pm(r, u, t)$ for particles of center of mass located at $r$ moving in $\pm u$ directions where $u \in [0, 2\pi]$ is the unit vector along their long axis. Given that the two subpopulations $f_+(r, u, t)$ and $f_-(r, u, t)$ constantly exchange members at rate $k$, we have:

$$\frac{\partial}{\partial t} f_+ (r, u, t) + v_0 (u \cdot \nabla) f_+ (r, u) = -k f_+ (r, u) + k f_- (r, u) + \mathcal{R} [D_r \mathcal{R} f_+ (r, u) + D_r \mathcal{R} w (r, u) f_+ (r, u)],$$

(1)

$$\frac{\partial}{\partial t} f_- (r, u, t) - v_0 (u \cdot \nabla) f_- (r, u) = k f_+ (r, u) - k f_- (r, u) + \mathcal{R} [D_r \mathcal{R} f_- (r, u) + D_r \mathcal{R} w (r, u) f_- (r, u)],$$

(2)

where $D_r$ is the rotational diffusion constant, the rotational operator $\mathcal{R}$ is defined by $\mathcal{R} = u \times \partial_u$, and $w (r, u)$ is a self-consistent interaction potential which has $\pm u$-symmetry [27–29]. In the two-dimensional case studied here, $w (r, u)$ commonly takes the form of the excluded-volume-like interaction for infinitely thin rods [27, 28],

$$w (r, u) = l^2 \int du' |u \times u'| (f_+ (r, u') + f_- (r, u')),$$

(3)

where $l$ is the particle length and we have neglected the high-order spatial derivatives in the integration.

Equations (1) and (2) can be rewritten in terms of $f (r, u) = f_+ (r, u) + f_- (r, u)$ and $f_M (r, u) = f_+ (r, u) - f_- (r, u)$:
When the switching rate $k$ is large, we expect the difference between $f_r(\mathbf{r}, \mathbf{u})$ and $f_-(\mathbf{r}, \mathbf{u})$ to be small. In particular, the damping term $-2kf_M(\mathbf{r}, \mathbf{u})$ is dominant in equation (5) when $k \gg D_r$ and $f_M$ relaxes quickly to a quasi-steady-state. In such a case, we can assume $\partial_t f_M = 0$ and obtain $f_M(\mathbf{r}, \mathbf{u}) \approx -v_0(\mathbf{u} \cdot \nabla)f(\mathbf{r}, \mathbf{u})/2k$ to the first order in spatial derivatives, which is assumed to be small if $k \gg v_0/l$. Substituting this result into equation (4) we have

$$\partial_t f(\mathbf{r}, \mathbf{u}, t) = \nabla [D_\parallel uu \nabla]f(\mathbf{r}, \mathbf{u}) + \mathcal{R}[D_\parallel \nabla f(\mathbf{r}, \mathbf{u}) + D_\perp \nabla w(\mathbf{r}, \mathbf{u})]f(\mathbf{r}, \mathbf{u}),$$

where $D_\parallel = v_0^2/2k$ is the effective longitudinal diffusion coefficient. Similarly, in the presence of some transverse diffusion perpendicular to particle’s long axis, we can write:

$$\partial_t f(\mathbf{r}, \mathbf{u}, t) = \nabla [D_\parallel uu \nabla + D_\perp (\mathbf{I} - uu) \nabla]f(\mathbf{r}, \mathbf{u}) + \mathcal{R}[D_\parallel \nabla f(\mathbf{r}, \mathbf{u}) + D_\perp \nabla w(\mathbf{r}, \mathbf{u})]f(\mathbf{r}, \mathbf{u}),$$

where $D_\perp$ is the perpendicular component of the translational effective diffusion rate referring to particle’s long axis and $w(\mathbf{r}, \mathbf{u}) = l^2 \int d\mathbf{u}' [\mathbf{u} \times \mathbf{u}']f(\mathbf{r}, \mathbf{u}')$. For simplicity, in the following we rescale length scales by the particle’s length and set $l = 1$.

Equation (7) confirms that the excluded-volume-like potential $w(\mathbf{r}, \mathbf{u})$ codes for nematic alignment but has no effect on the translational motion of particles. A system of physical rods interacting by volume exclusion can only exhibit this property if some driving forces are applied to the particles to overcome the effect of mutual interaction on their spatial translocation. This is different from the well-known dynamic mean field theory of non-active rods near thermal equilibrium [27], where excluded-volume interactions also affect translational motion.

### 3. Instabilities of homogeneous solutions

We now proceed to study the linear stability of the homogeneous solutions to the kinetic equation (7). We first note that equation (7) is invariant under reversal of $\mathbf{u}$, as expected for nematics. We can thus expand it in Fourier series of the angular variable $\theta$ (the argument of $\mathbf{u}$) as:

$$f(\mathbf{r}, \mathbf{u}, t) = \frac{1}{2\pi} \sum_{m=0}^{\infty} p_m(\mathbf{r}, t) \cos 2m\theta + q_m(\mathbf{r}, t) \sin 2m\theta,$$

where $p_0(\mathbf{r}, t) = \int d\mathbf{u}f(\mathbf{r}, \mathbf{u}, t) = 0, \quad q_0(\mathbf{r}, t) = 0, \quad p_m(\mathbf{r}, t) = 2 \int d\mathbf{u} \cos 2m\theta f(\mathbf{r}, \mathbf{u}, t)$ and $q_m(\mathbf{r}, t) = 2 \int d\mathbf{u} \sin 2m\theta f(\mathbf{r}, \mathbf{u}, t)$ for $m \geq 1$.

Note that the low-order fields $p_m(\mathbf{r})$ and $q_m(\mathbf{r})$ give the hydrodynamic variables: $p_0(\mathbf{r})$ is just the local particle density, while $p_1(\mathbf{r})$ and $q_1(\mathbf{r})$ are related to the nematic field (see below).

Integrating both sides with $\int d\mathbf{u} \cos 2m\theta$ and $\int d\mathbf{u} \sin 2m\theta$, equation (7) can be rewritten as a double hierarchy of equations [16, 30] given by:
\[ \partial_t p_0 (r, t) = \frac{1}{2} D_p \left( \partial_x^2 + \partial_y^2 \right) p_0 + \frac{1}{4} D_n \left[ \left( \partial_x^2 - \partial_y^2 \right) p_1 + 2 \partial_x \partial_y q_i \right]. \] (9)

\[ \partial_t p_m (r, t) = \frac{1}{2} D_p \left( \partial_x^2 + \partial_y^2 \right) p_m + \frac{1}{4} D_n \left[ \left( \partial_x^2 - \partial_y^2 \right) \left( p_{m+1} + p_{m-1} + p_{-m+1} + p_{-m-1} \right) \right] + 2 \partial_x \partial_y \left( q_{m+1} + q_{1-m} - q_{m-1} \right) - 4 D_m^2 p_m \]

\[ + 4 D_p \sum_{n=0}^\infty \frac{nm}{4n^2 - 1} \left[ p_n (p_{m-n} + p_{n-m} - p_{m+n}) + q_n \left( q_{m-n} - q_{m-n} - q_{n+m} \right) \right], \] (10)

\[ \quad \text{where } D_p = D_1 + D_2 \text{ and } D_n = D_1 - D_2. \]

We introduced \( p_m = 0 \) and \( q_m = 0 \) for \( m < 0 \) in above equations for compactness of expressions. The obtained hierarchy of equations has the same mathematical structure as that obtained in [16]. The diffusive coefficients are the same if we set \( D_1 = 0 \) and \( D_2 = 1 \). The coefficients controlling the isotropic/nematic transition differ because different interaction rules are implemented. Here we have only one control parameter for the transition, the particle density. For Vicsek-style models, the noise-level is also an explicit parameter that dominates the nematic ordering transition.

### 3.1. Spatially homogeneous solutions

We first determine the spatially-homogeneous solutions to the kinetic equation. An obvious example is the disordered homogeneous state \( p_0 = \rho \), \( p_{m>0} = q_{m>0} = 0 \).

To find the nematicely-ordered solution, we neglect all spatial derivatives in equations (9)–(11). Assuming that the nematic director is along the \( x \)-axis, we can further set \( q_n = 0 \), so that we are left with simple ordinary differential equations for coefficients \( p_n \):

\[ \frac{\partial p_n (t)}{4 D_p} = -n^2 p_n + p_0 \frac{n^2 p_n}{4n^2 - 1} \pi + \sum_{m=1}^{\infty} \frac{nm p_n (p_{m-n} - p_{m+n})}{4m^2 - 1} \pi. \] (12)

The fixed point solution \( p_n = p_n^* \) of this hierarchy can be found numerically by keeping a large number of modes and setting the others to zero.

At order 3, an explicit solution is easily found, which gives the density dependence of the magnitude of nematic order. Conventionally, the tensorial order parameter for homogeneous nematics is defined as

\[ Q_{afil} \equiv S \left( \hat{n}_a \cdot \hat{n}_i - \delta_{af} \right) = \int d\mathbf{u} \left( u_a u_i - \delta_{af} \right) f (\mathbf{u}) / \rho, \] (13)

where \( \rho = \int d\mathbf{u} f (\mathbf{u}) \) is the density and \( \hat{n} \) is the unit vector of the nematic director. If we let \( \hat{n} \) align with the \( x \)-axis, that is \( \hat{n}_x = 1 \) and \( \hat{n}_y = 0 \), from equation (13), we have \( S = \int d\mathbf{u} (2 \cos^2 \theta - 1) / \rho = p_1 / 2 \rho. \) Setting \( p_n = 0 \) for \( n > 3 \), we obtain an equation for
nematic order parameter $S(t)$,

$$\frac{\partial S(t)}{4D_r} = (\bar{\rho} - 1)S - \frac{3\bar{\rho}^2 S^3}{2(5 - \bar{\rho})}, \quad (14)$$

where $\bar{\rho} = \rho/\rho^*$ is the number density rescaled by the critical density $\rho^* = 3\pi/2$. For $\bar{\rho} < 1$, the disordered solution $S=0$ is stable. For $\bar{\rho} > 1$, it is unstable and is replaced by the homogeneous solution

$$S = \sqrt{2[5 - \bar{\rho}][\bar{\rho} - 1]/3\bar{\rho}^2}, \quad (15)$$

which is then stable. In other words, the transition is continuous in the mean field homogeneous limit and $S \propto \sqrt{(\bar{\rho} - 1)/\bar{\rho}}$. Since we only include the excluded-volume-like interaction equation (3) in equation (7), equation (15) shows that the magnitude of nematic order is independent of driven activity as given by parameters $D_\perp$ and $D_\parallel$. In dry active nematics, enhanced ordering effects can be accounted for if we explicitly write down how the active processes modify the rotation of particles upon collision, as done for example in [29, 31].

In figure 1, we show the difference between the ordered homogeneous solutions of the full kinetic equation (7) (obtained numerically) and solutions of the hierarchy (12) keeping 300 modes and 3 modes (solution (15) above). No difference can be seen between the full numerical solution and the high-order truncation but, as expected, the cubic solution only matches those near the transition line.

The stability of the homogeneous solutions can be studied at two levels: numerically at the ‘full’ kinetic equation level (with a high-order truncation), and analytically at the hydrodynamic
equations level (with an appropriate low-order truncation and closure scheme). Below we first proceed with the hydrodynamic approach, following closely the recent work of Bertin et al. [16] (see also [17–20, 30] for polar particle and other cases). We then treat the full kinetic equation level.

### 3.2. Stability at the hydrodynamic level

In order to work with a well-controlled expansion, we follow the ‘Boltzmann–Ginzburg–Landau’ approach used in [16, 30, 32]. We work in the vicinity of the main instability line: \( \delta = \bar{\rho} - 1 \sim \epsilon^2 \), where \( \epsilon \) is a small parameter. We further use the scaling ansatz \( \delta \rho \sim \epsilon \), \( \partial_t \sim \partial_x^2 \sim \partial_y^2 \sim \partial \partial_x \sim \epsilon^2 \) and \( \rho_m \sim q_m \sim |\epsilon|^n \), where \( \delta \rho \) is the local deviation from the average density. The simplest non-trivial closure is to discard terms that are higher than \( \epsilon^3 \). In this scenario, equation (9) is unchanged, and equations (10) and (11) are truncated according to the scaling ansatz, leaving four equations for \( p_1, q_1, p_2, q_2 \):

\[
\partial_p (r, t) = \frac{1}{2} D_p (\partial_x^2 + \partial_y^2) p_1 + \frac{1}{2} D_n (\partial_x^2 - \partial_y^2) p_0 - D_l \left( 4 - \frac{8}{3\pi} \rho_0 \right) p_1 - \frac{4D}{5\pi} (p_1 q_2 - q_1 p_2), \tag{16}
\]

\[
\partial_q (r, t) = \frac{1}{2} D_p (\partial_x^2 + \partial_y^2) q_1 + D_n \partial_x p_0 - D_l \left( 4 - \frac{8}{3\pi} \rho_0 \right) q_1 - \frac{4D}{5\pi} (p_1 q_2 - q_1 p_2), \tag{17}
\]

\[
0 = \frac{1}{4} D_l \left[ (\partial_x^2 - \partial_y^2) p_1 - 2\partial_x \partial_y q_1 \right] - 16D_p^2 + \frac{8D}{3\pi} \left[ (p_1^2 - q_1^2) + \frac{4}{5} p_1 q_2 \right], \tag{18}
\]

\[
0 = \frac{1}{4} D_l \left[ (\partial_x^2 - \partial_y^2) q_1 + 2\partial_x \partial_y q_1 \right] - 16D_q^2 + \frac{8D}{3\pi} \left[ 2p_1 q_1 + \frac{4}{5} p_1 q_2 \right]. \tag{19}
\]

From equations (18) and (19), we see that \( p_2 \) and \( q_2 \) are enslaved to \( p_1 \) and \( q_1 \) as long as \( \rho_0 \leq \frac{5\rho^*}{2} \). By solving equations (18) and (19) for \( p_2 \) and \( q_2 \), substituting their expressions into equations (16) and (17), and discarding \( \epsilon^4 \) terms, we have

\[
\partial_p (r, t) = \frac{1}{2} D_p (\partial_x^2 + \partial_y^2) p_1 + \frac{1}{2} D_n (\partial_x^2 - \partial_y^2) p_0 - D_l \left( 4 - \frac{8}{3\pi} \rho_0 \right) p_1 - \frac{\left( p_1^2 + q_1^2 \right) D_l}{5\rho^* - \rho_0} p_1, \tag{20}
\]

\[
\partial_q (r, t) = \frac{1}{2} D_p (\partial_x^2 + \partial_y^2) q_1 + D_n \partial_x p_0 - D_l \left( 4 - \frac{8}{3\pi} \rho_0 \right) q_1 - \frac{\left( p_1^2 + q_1^2 \right) D_l}{5\rho^* - \rho_0} q_1. \tag{21}
\]

Equations (9), (20) and (21) constitute the closed hydrodynamic description of equation (7). They are formally identical, up to the positional diffusion terms, to those derived in [16]. They can also be rewritten in tensorial notation. Similarly to equation (13), the local nematic order parameter tensor is given by \( Q_{\alpha \beta} (r) = S (r) (\hat{n}_r \partial_r) (\partial_r \delta_{\alpha \beta} / 2) = \int du (u_r \rho_r - \delta_{\alpha \beta} / 2) f (r, u) / \rho (r) \), where \( \rho (r) = \int uf (r, u) \) is the density and \( \hat{n} (r) \) is the unit vector of the nematic director [19, 28, 29, 33]. By comparing with the definition of \( p_1 (r) \) and
\[ q_i(r), \] it is easy to show that 
\[ p_i = 4\rho Q_{xx} = -4\rho Q_{yy} = 2\rho (Q_{xx} - Q_{yy}), \]
\[ q_i = 4\rho Q_{xy} = 4\rho Q_{yx} \]
and 
\[ p_i^2 + q_i^2 = 4\rho^2 S^2. \]
The hydrodynamic equations written in terms of the reduced density 
\[ \tilde{\rho}(r) = \rho(r)/\rho^* \]
and the alignment tensor \( Q_{q\rho}(r) \) then read:

\[ \partial_t \tilde{\rho}(r) = \frac{D}{2} \rho^2 \tilde{\rho} + D \tilde{\rho}_n \tilde{\rho}_n \partial_n \tilde{\rho}_n, \tag{22} \]

\[ \partial_t [\tilde{\rho} Q_{q\rho}(r)] = \frac{D}{4} \partial_n \tilde{\rho} - \frac{D}{8} \delta_{q\rho} \partial^2 \tilde{\rho} + \frac{D}{2} \rho^2 (\tilde{\rho} Q_{q\rho}) + D \left[ 4\tilde{\rho}(\tilde{\rho} - 1) - \frac{6\rho^3 S^2}{5 - \rho} \right] Q_{q\rho}. \tag{23} \]

These hydrodynamic equations are similar to those used by Baskaran and Marchetti for analyzing the stability of fluctuations in the nematic state \cite{[28]}, where they not only include the enhanced diffusion by self-propelled motion but also include normal passive diffusion coefficients. One major difference is that, while we explicitly include the density dependence of the magnitude of nematic order, they focus on the deep nematic state and suppose the strength of nematics is a constant parameter. As a result, they did not observe the instability we describe below.

We now turn to the linear stability analysis of the homogeneous solutions of equations (22) and (23). Let us assume that the nematic director \( \hat{n}(r) \) of the homogeneous ordered solution is along the \( x \)-axis of the system, that is \( \hat{n}(r) = \hat{x} \) so that \( Q_{xx} = -Q_{yy} = \frac{1}{2} S \). Since \( \hat{n} = 1 \), the only possible small fluctuations of the nematic director \( \delta \hat{n}(r) \) in this homogeneous state is given by \( \delta \hat{n}(r) = \delta n_x \hat{y} \), and we have \( Q_{rs}(r) = S \delta n_s(r) \). Apart from the fluctuations of the nematic director, we also have fluctuations of density \( \delta \tilde{\rho}(r) = \tilde{\rho}(r) - \tilde{\rho}_0 \) and of the magnitude of the nematic order parameter \( \delta S_{\rho}(r) = \tilde{\rho}(r) S(r) - \tilde{\rho}_0 S_0 \), where \( \tilde{\rho}_0 = \rho_0/\rho^* \) is the reduced bulk particle density and \( S_0 = \sqrt{2(5 - \tilde{\rho}_0)(\tilde{\rho}_0 - 1)/3\tilde{\rho}_0^2} \) is the nematic order parameter of homogeneous state.

The linearized hydrodynamic equations read:

\[ \partial_t \delta \tilde{\rho} = \frac{D}{2} \partial_n \partial_n \delta \tilde{\rho} + 2D \partial_n \tilde{\rho}_0 \partial_n \delta n_s + \frac{D}{2} \left( \partial^2 - \partial_n^2 \right) \delta S_{\rho}, \tag{24} \]

\[ \partial_t \delta S_{\rho} = \frac{D}{4} \left( \partial^2 - \partial_n^2 \right) \partial_n \partial_n \delta \tilde{\rho} + 8D \sigma \delta \rho + \frac{D}{2} \partial^2 \delta S_{\rho} - 8D (\tilde{\rho} - 1) \delta S_{\rho}, \tag{25} \]

\[ \tilde{\rho}_0 S_0 \partial_n \delta n_s = \frac{D}{4} \partial_n \partial_n \delta \tilde{\rho} + \frac{D}{2} \tilde{\rho}_0 S_0 \partial^2 \delta n_s, \tag{26} \]

where \( \sigma = (2 - \delta) \sqrt{2\delta/3(4 - \delta)} \) with \( \delta = \tilde{\rho} - 1 \). To keep \( \sigma > 0 \), which ensures that local nematic order grows with increasing local density, we restrict our analysis to the regime \( \delta < 2 \). It is convenient to study the stability of fluctuations in Fourier space. The Fourier modes of fluctuations \( (\tilde{\rho}_k, n_{k\rho}, S_{k\rho}) \) with wave vector \( k \), defined as \( \delta \tilde{\rho}(r) = \int dke^{-ik \cdot r} \),

\[ \delta n_s(r) = \int dke^{-ik \cdot r} \] and \( \delta S_{\rho}(r) = \int dke^{-ik \cdot r} \), are governed by
\[
\frac{\partial}{\partial t} \begin{bmatrix} \rho_k \\ S_{\rho k} \\ n_{y k} \end{bmatrix} = -\frac{D^2 k^2}{2} \begin{bmatrix} 1 & D_0 \cos 2\theta & 2D_0 \tilde{\rho}_0 S_0 \sin 2\theta \\ D_0 \cos 2\theta/2 - 16\sigma/k^2 & 1 + 16\delta/k^2 & 0 \\ D_0 \sin 2\theta/(4\tilde{\rho}_0 S_0) & 0 & 1 \end{bmatrix} \begin{bmatrix} \rho_k \\ S_{\rho k} \\ n_{y k} \end{bmatrix},
\]

(27)

where \( \theta \) is the angle between wave vector \( \mathbf{k} \) and the nematic director \( \hat{n} \), \( \kappa^2 = D_\parallel k^2/D_\parallel \) and \( D_0 = D_\rho k^2/D_\parallel \). Finding the eigenvalues of equation (27) is difficult since we need to solve a cubic equation. Here, we only determine the instability line. Let us define \( z = 1 + 2\lambda D_\parallel^{-1}k^2 \), where \( \lambda \) is an eigenvalue of the coefficient matrix of equation (27). The homogeneous nematic ordered state becomes linearly unstable if \( \text{Re}(\lambda) \geq 0 \); that is, \( \text{Re}(z) \geq 1 \). The characteristic polynomial of the coefficient matrix is

\[
g(z) = z^3 + \frac{16\delta}{k^2}z + \left( \frac{16D_0\sigma \cos 2\theta}{k^2} - \frac{D_0^2}{2} \right)z - \frac{8\delta D_0^2}{k^2} \sin^2 2\theta = 0.
\]

(28)

For the cubic equation \( g(z) = 0 \), the system either has: (i) one real root and two complex conjugate roots, (ii) one real root and two identical real roots, or (iii) three different real roots.

For cases (i) and (ii) we can prove that only the single real root (not the multiple real roots) of \( g(z) = 0 \) can cause the linear instability of the system. Let us suppose \( z_1 \), \( z_2 \) and \( z_3 \) are three roots of \( g(z) = 0 \), where \( z_2 \) and \( z_3 \) are the complex roots or the multiple roots and we have \( z_2 = z_3^* \). According to Vieta’s formula, we have:

\[
z_1 + z_2 + z_3 = z_1 + 2 \text{Re}(z_2) = -16\delta/k^2,
\]

(29)

\[
z_2z_2 + z_3z_3 + z_2z_3 = 2z_1 \text{Re}(z_2) + \text{Re}(z_2)^2 + \text{Im}(z_2)^2 = \frac{16D_0\sigma \cos 2\theta}{k^2} - \frac{D_0^2}{2},
\]

(30)

\[
z_2z_2z_3 = z_1(\text{Re}(z_2)^2 + \text{Im}(z_2)^2) = 8\delta D_0^2 \sin^2 2\theta/k^2.
\]

(31)

If the linear instability is caused by the complex root or the multiple roots, then \( \text{Re}(z_2) \geq 1 \) and it is easy to see that equation (29) and (31) contradict each other. Thus, if the linear instability takes place, it must be caused by a real but non-multiple root.

For case (iii), we can prove that only the largest real root of \( g(z) = 0 \) can cause the linear instability. Let us suppose \( z_1 \), \( z_2 \) and \( z_3 \) are three different roots of \( g(z) = 0 \), and we have \( z_1 > z_2 > z_3 \). According to Vieta’s formula, we have:

\[
z_1 + z_2 + z_3 = -16\delta/k^2,
\]

(32)

\[
z_2z_2z_3 = 8\delta D_0^2 \sin^2 2\theta/k^2.
\]

(33)

If \( z_2 \) is larger than 1, since \( z_1 > z_2 \), we find equations (32) and (33) contradict each other. This can be further shown when \( z_2 \leq 1 \) if \( z_1 \geq 1 \).

Thus, for cases (i), (ii) and (iii), the real root \( z_i \), as defined above, is the only root which may cause the linear instability. In such conditions, to have a real root \( z_i \geq 1 \) for function \( g(z_i) = 0 \), we must have \( g(1) \leq 0 \), and \( g(1) = 0 \) gives the instability line. By substituting it into the expression of \( g(z) \), we have
\[
\left(1 - \frac{D_0^2}{2}\right)\frac{\kappa^2}{8\delta} + \left(D_0 \cos 2\theta + \frac{\sigma}{\delta}\right)^2 + \left(2 - D_0^2 - \frac{\sigma^2}{\delta^2}\right) \leq 0. \tag{34}
\]

Since \(|D_0| \leq 1\), the first term is positive. If the second and third terms together are negative, the system can always be destabilized when \(\kappa \to 0\). To push the system into an instability regime, we try to minimize equation (34) with respect to \(\kappa\) and \(\theta\), which gives

\[
\begin{aligned}
2(1 - \sigma D_0/\delta) &\leq 0, \quad \frac{\sigma}{\delta D_0} \geq 1, \kappa = 0, \theta = \pm \frac{\pi}{2}; \\
2(1 + \sigma D_0/\delta) &\leq 0, \quad \frac{\sigma}{\delta D_0} \leq -1, \kappa = 0, \theta = 0, \pi; \\
2 - D_0^2 - (\sigma/\delta)^2 &\leq 0, \quad \frac{\sigma}{\delta |D_0|} \leq 1, \kappa = 0, \theta = \pm \frac{\pi}{2} \pm \frac{1}{2} \arccos \left(-\frac{\sigma}{\delta D_0}\right).
\end{aligned}
\tag{35}
\]

The third inequality cannot be satisfied since it contradicts the condition \(\sigma/(\delta|D_0|) \leq 1\). The instability line is given by

\[
\begin{aligned}
2(1 - \sigma D_0/\delta) &= 0, \quad \frac{\sigma}{\delta D_0} \geq 1, \kappa = 0, \theta = \pi, \frac{3\pi}{2}; \\
2(1 + \sigma D_0/\delta) &= 0, \quad \frac{\sigma}{\delta D_0} \leq -1, \kappa = 0, \theta = 0, \pi.
\end{aligned}
\tag{36}
\]

On the instability line, the instability takes place only when \(\theta = \pi/2, 3\pi/2\) for \(D_0 > 0\) and \(\theta = 0, \pi\) for \(D_0 < 0\). For such conditions, the coupling between \(\tilde{\rho}_k\) and \(n_{ik}\) vanishes. This suggests that the instability line could also be predicted by only considering the coupling between \(\tilde{\rho}_k\) and \(S_{ik}\). For such 2 × 2 coefficient matrix, the eigenvalues \(\lambda_{\tilde{\rho}, S_{ik}}\) are given by:

\[D_r^{-1}\lambda_{\tilde{\rho}, S_{ik}} = -(8\delta + \kappa^2)/2 \pm \sqrt{D_0^2\kappa^4 \cos^2 2\theta/8 - 4\sigma D_0 \kappa^2 \cos 2\theta + 16\delta^2}. \tag{37}\]

The real part of \(\lambda_{\tilde{\rho}, S_{ik}}\) is always negative, representing a stable decaying mode. However, the mode \(\lambda_{\tilde{\rho}, S_{ik}}^+\) becomes positive when

\[32(D_0\sigma \cos 2\theta + \delta)\kappa^2 + (2 - D_0^2 \cos^2 2\theta)\kappa^4 < 0. \tag{38}\]

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 that describe large-scale fluctuations, the stability is controlled by the coefficient of \(\kappa^2\). Thus, when

\[(D_0\sigma \cos 2\theta + \delta) \leq 0, \tag{39}\]

the system becomes unstable on a large scale. The instability line is thus given by

\[
\begin{aligned}
\delta - D_0\sigma &= 0, \quad D_0 \geq 0, \kappa = 0, \theta = \pi, \frac{3\pi}{2}; \\
\delta + D_0\sigma &= 0, \quad D_0 \leq 0, \kappa = 0, \theta = 0, \pi,
\end{aligned}
\tag{40}
\]

which is the same as predicted by equation (36).

Our results for the linear stability of homogeneous solutions at the hydrodynamic level are summarized in figure 2(a). The isotropic, disordered solution becomes linearly unstable for...
\[ \delta = \rho - 1 > 0. \] In this region, the homogeneous ordered solution (15) exists. This solution is linearly unstable to long wavelength modes below the orange line defined by equation (39). The unstable modes are transversal to the nematic order for \( D_0 = (D_{||} + D_{\perp})/2 \) and parallel to it for \( D_0 < 0 \). The most unstable mode is always strictly transversal (\( D_0 > 0 \)) or strictly parallel (\( D_0 < 0 \)). Some typical dispersion relation curves are shown in figure 2(b). Above the orange line, the homogeneous ordered solution (15) is linearly stable.

### 3.3. Stability at the kinetic equation level

The homogeneous ordered solution to the kinetic equation (7) is very well approximated by the fixed point solution \( (p_n^* = p_n^*, q_n^* = q_n^*) \) of the truncated hierarchy (12), where we have kept a large number of modes (figure 1). We thus study the linear stability of this solution by linearizing equations (9), (10) and (11) around it. Assuming, without loss of generality, that the order of the solution is along the x-axis, so that \( q_n^* = 0 \), the linearized equations read, in Fourier space:

[Further explanation and equations related to linearized equations and dispersion relations are provided here.]

**Figure 2.** (a) Left panel: Phase diagram for active nematics in the \( (\delta = \tilde{\rho} - 1, D_0 = D_{||}/D_{\perp} = (D_{||} - D_{\perp})/(D_{||} + D_{\perp})) \) parameter plane. Three regions are distinguished by the linear instability analysis of spatially-homogeneous solutions. The horizontal axis (blue line) marks the linear instability of the disordered homogeneous solution and the advent of the homogeneous ordered solution. The yellow curve is the line above which the homogeneous ordered solution of the hydrodynamic equations (22) and (23) is linearly stable. The green curve marks the same limit, but for the many-mode truncation of the kinetic equation as given in equations (41)–(43) up to \( m = 300 \). In the intermediate region where no homogeneous solution is linearly stable, the polar plots (a)–(f) indicate, for the homogeneous ordered solution of the hydrodynamic equations, the shape of the unstable region in the \((\kappa, \theta)\) space. Their origin is located at the \((D_0, \delta)\) values used for their calculation. (a) \( |D_0| = 1, \delta = 0.4 \), (b) \( |D_0| = 2/3, \delta = 0.2 \), (c) \( |D_0| = 1, \delta = 0.2 \), (d) \( |D_0| = 1/3, \delta = 0.01 \), (e) \( |D_0| = 2/3, \delta = 0.01 \), and (f) \( |D_0| = 1, \delta = 0.01 \). The black curves in polar plots are generated by equation (34) and the red curves are generated by equation (38). These branches in the polar plots show that the instabilities are developed perpendicular and parallel to the nematic director for positive and negative \( D_0 \), respectively. The red dots and blue circles near the yellow curve are located where numerical integration of equation (7) was performed. The blue circles represent the cases where the system ended up in the ordered homogeneous state. The red dots indicate where the system entered and remained in a chaotic regime. (b) Right panel: Corresponding growth rates \( D^{-1}_r \lambda_{\rho, \delta, \kappa} \) for the polar plots in the left panel.
space:
\[
\partial_t \delta \tilde{p}_0 = -\frac{1}{2} D \kappa \partial^2 \delta \tilde{p}_0 - \frac{1}{4} D_n \left( (k_x^2 - k_y^2) \delta \tilde{p}_1 + 2k_x \delta \tilde{q}_1 \right)
\]  
(41)

\[
\partial_t \delta \tilde{p}_m = -4D_m^2 \delta \tilde{p}_m - \frac{1}{2} D \kappa \partial^2 \delta \tilde{p}_m - \frac{1}{4} D_n \left( (k_x^2 - k_y^2) (\delta \tilde{p}_{m+1} + \delta \tilde{p}_{m-1} + \delta \tilde{q}_{m-1} - \delta \tilde{q}_{m+1}) \right) + \frac{4D_n}{\pi} \sum_{n=0}^{\infty} \frac{nm}{4n^2 - 1} \left[ \delta \tilde{p}_n \left( p_{m-n}^* + p_{n-m}^* - p_{m+n}^* \right) + p_{n}^* \left( \delta \tilde{p}_{m-n} + \delta \tilde{p}_{n-m} - \delta \tilde{p}_{m+n} \right) \right],
\]

(42)

\[
\partial_t \delta \tilde{q}_m = -4D_m^2 \delta \tilde{q}_m - \frac{1}{2} D \kappa \partial^2 \delta \tilde{q}_m - \frac{1}{4} D_n \left( (k_x^2 - k_y^2) (\delta \tilde{q}_{m+1} + \delta \tilde{q}_{m-1} - \delta \tilde{q}_{m+1} - \delta \tilde{q}_{m+1}) \right) + \frac{4D_n}{\pi} \sum_{n=0}^{\infty} \frac{nm}{4n^2 - 1} \left[ \delta \tilde{q}_n \left( p_{m-n}^* + p_{n-m}^* + p_{m+n}^* \right) + p_{n}^* \left( \delta \tilde{q}_{m-n} + \delta \tilde{q}_{n-m} - \delta \tilde{q}_{m+n} \right) \right],
\]

(43)

where \( \delta \tilde{p}_m = \delta \tilde{p}_m (\mathbf{k}, t) = \int d\mathbf{r} (p_m (\mathbf{r}, t) - p_m^*) \exp (-i\mathbf{k} \cdot \mathbf{r}) \) and \( \delta \tilde{q}_m = \delta \tilde{q}_m (\mathbf{k}, t) = \int d\mathbf{r} (q_m (\mathbf{r}, t) - q_m^*) \exp (-i\mathbf{k} \cdot \mathbf{r}). \)

We calculated numerically the maximum eigenvalue of the above system, truncated at the same high-order as for the solution, for wavenumbers \( k = |\mathbf{k}| \) close to zero. We find that this eigenvalue changes sign and becomes negative above the green line in figure 2(a). (These results were obtained by keeping 300 modes; we checked that no significant change occurs when keeping more modes.)

For large \( D_0 \), the region of linear instability of the homogeneous ordered solution is thus much larger for the kinetic equation (7) than for the hydrodynamic equations (22) and (23). The hydrodynamic description is quantitatively valid only in the near threshold region of isotropic-nematic transition.

4. Beyond linear instability: chaotic solutions of the kinetic equation

We now investigate numerically the solutions of the kinetic equation (7) in the parameter region where no homogeneous solution is linearly stable. We use an alternating-direction implicit algorithm, which is unconditionally stable and accurate to second-order for the linear part (see the appendix for details).

We first test the phase boundary predicted by linear instability analysis (green line in figure 2(a)). We integrate the kinetic equation for parameter values around the predicted line, starting from the disordered homogeneous state with small initial noise, in a domain of size 120 with periodic boundary conditions.

As shown in figure 2(a), all runs above the phase boundary (blue circles) end up in the homogeneous nematic state, while those below (red dots) never settle in a stationary state. This confirms the results of the linear stability analysis. Figure 3 shows the patterns found by numerical integration of the kinetic equation, starting from a slightly perturbed homogeneous
Figure 3. Phase diagram of the patterns found by numerical integration of the kinetic equation for various parameter values in the region of linear instability of the homogeneous nematic phase. Two consecutive snapshots are shown in each case: one for the transient regular nematic band eventually forming from a slightly perturbed isotropic homogeneous state, and one at a later time when this transient band has broken into several pieces. The color scale bar shows the local relative rescaled density value $\delta(r) = \tilde{\rho}(r) - 1$. The length and angle of white segments show the magnitude and direction of nematic order, respectively. System size $120 \times 120$ with the particle length $l = 1$ with periodic boundary conditions. Time step is $\Delta t = 0.01$, lattice steps $\Delta_x = \Delta_y = \Delta_z = 3$, and angular step $\Delta \theta = \pi/30$. Snapshots are taken at times: (a) $7.17 \times 10^5 \Delta t$ and $9.69 \times 10^5 \Delta t$, (b) $2.4 \times 10^5 \Delta t$ and $1.032 \times 10^5 \Delta t$, (c) $1.302 \times 10^6 \Delta t$ and $1.72 \times 10^6 \Delta t$, (d) $2.4 \times 10^5 \Delta t$ and $5.67 \times 10^6 \Delta t$, (e) $7.02 \times 10^5 \Delta t$ and $1.116 \times 10^6 \Delta t$, and (f) $5.61 \times 10^5 \Delta t$ and $6.69 \times 10^5 \Delta t$. 
isotropic solution. In the regime of linear instability of the homogeneous nematic state, the system tends to evolve first to a high density nematic band, which later breaks. The two snapshots shown for each run presented are taken in these two stages. The width of this transient nematic band increases with the global density $\delta$. Increasing the anisotropy of diffusion $D_0 = (D_\parallel - D_\perp)/(D_\parallel + D_\perp)$, the nematic band becomes highly concentrated and narrower. All these bands are unstable. The dynamical behavior is analyzed in detail in the next section using a larger periodic domain.

4.1. A chaotic, disordered phase?

Next, we investigate the dynamics of the system in the linear instability regime using larger domains. Starting from an isotropic and spatially-homogeneous initial condition, local ordered nematic domains form at the beginning, accompanied by the quick development of density inhomogeneities. Further coarsening of these structures leads to the coexistence of particle-enriched nematic domains (where $\rho > \rho^*$) in a particle-poor isotropic sea (where $\rho < \rho^*$). The system exhibits large-scale chaos with statistically stationary properties. In figure 4, we show snapshots of the reconstructed density and nematic order fields in this asymptotic chaotic regime. The rescaled density field $\delta(r) = \bar{\rho}(r) - 1$ represented by the color scale was obtained by integrating the distribution function $f(r, u)$ over the angular variable. The magnitude $S(r) = \sqrt{(Q_{xx} - Q_{yy})^2 + 4Q_{xy}^2}$ and direction $n(r)$ of the nematic order, where $Q_{\alpha\beta}(r) = \int u(u\alpha - \delta_{\alpha\beta}/2)f(r, u)/\rho(r)$, is represented by the length and orientation of local white segments. Large-scale spatially inhomogeneous structures form, but they systematically break into several thin pieces. These fragments, in turn, eventually coalesce and merge into a bigger band, which then breaks, etc.

Global nematic order fluctuates strongly, both in magnitude and direction during evolution (figure 5(a), (b) and snapshots in figure 5(d)-(f)), but keeps a fairly large average value ($\sim 0.4$) in spite of the chaos. Note that this behavior is similar to the observations of Chaté et al in their Vicsek-like active nematics model [15]. It is not clear at this stage whether or not this chaotic dynamics eventually gives rise to a bona fide disordered phase in the asymptotic large-size limit. Unfortunately, we are currently unable to simulate much larger systems.

Similarly, the two-point orientational correlation functions display, somewhat surprisingly, algebraic tails typical of quasi-long-range order (figure 5(c)). This may only be a finite-size effect: if the chaotic dynamics possesses a large but finite correlation length (something we are not able to probe yet), then we expect these correlation functions to have exponential tails.

4.2. Fragmentation of nematic bands

We now take a close look at how a nematic band along the $x$-axis breaks (see figure 6). For $D_0 > 0$, from our previous stability analysis, the density inhomogeneity develops along $\theta = -\pi/2$, that is, perpendicular to nematic director $n$. The term $-\frac{1}{2}D_\parallel \partial^2_\parallel(\delta\rho)$ in equation (24) is directly responsible for the development of density inhomogeneity.

Initially, the nematic director in the high-density region is almost parallel to the nematic ordered stripe boundary (see figure 6(a), where only a fraction of the space domain is shown). To illustrate the mechanism for the deviation of nematic director, we investigate whether this alignment is stable with respect to small fluctuations of the director.
δn_\perp (r) = n(r) - n_0 = (0, \delta n_\parallel). To linear order, the dynamic equation for \delta n_\parallel (r) in the present case can be obtained from equation (7) as \rho S \partial_t \delta n_\parallel = \frac{D}{2} \rho S \delta^2 n_\parallel + \delta n_\parallel \partial^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 the main density inhomogeneity is developed in that direction. Near the stripe boundaries, we always have a region with \partial^2 \rho S > 0, which makes the fluctuations \delta n_\parallel unstable. This instability induces changes of the order parameter’s orientation; thus, the nematic directors in figure 6(b) become oblique to the density profile boundaries after the band forms. This also explains why the nematic directors in figure 4(a), (b) are often found to be oblique to the domain boundaries. In figure 6(b), together with the obliqueness of directors, we observe a leakage of particles from the high-density region via the relatively faster diffusion along the director’s alignment. With this decrease the density of ordered nematic stripe enters into the unstable region, and the spatial instability takes place again. Figure 6(c)

Figure 4. Snapshots of density (color scale) and nematic order (white segments) obtained by numerical integration of the kinetic equation. The color scale bar shows the local relative rescaled density value \delta(r) = \bar{\rho}(r) - 1. The length and angle of the white segments show the magnitude and direction of the nematic order, respectively. The parameters are D_x = 2, D_y = 0.4, and D_z = 2.4. The reduced parameters are D_\rho = 5/7 and \delta = 0.01. System size is 300 x 300 with the particle length l = 1 with periodic boundary conditions. The time step is \Delta_t = 0.018, lattice steps \Delta_x = \Delta_y = \Delta_z = 3, and angular step \Delta_\theta = \pi/30. The snapshots are taken at times (a) 1.7 x 10^6 \Delta_t and (b) 2.3 x 10^6 \Delta_t. Snapshots (c)–(k) provide a close look at the breaking and coalescing processes of a nematic domain, at times (c) 1.6 x 10^6 \Delta_t, (d) 1.7 x 10^6 \Delta_t, (e) 1.71 x 10^6 \Delta_t, (f) 1.72 x 10^6 \Delta_t, (g) 1.73 x 10^6 \Delta_t, (h) 1.74 x 10^6 \Delta_t, (i) 1.75 x 10^6 \Delta_t, (j) 1.76 x 10^6 \Delta_t, and (k) 1.8 x 10^6 \Delta_t.
shows the band just after a fragmentation event: a narrow disordered channel appears along the direction perpendicular to the director. In figure 6(d), we show the typical ‘twisted-spindle’ shape commonly taken by fragments after they detach from the band. It is worth noticing that all of these highly dynamic structures are surrounded by particle fluxes around the density profile boundaries. The density currents can be defined as
\[
\frac{\partial \rho}{\partial t} - \mathbf{J} = \nabla \cdot \mathbf{J} = \frac{1}{2} \mathbf{D}\nabla \rho = \mathbf{D} \left( \nabla \rho + \nabla \rho^T \right) = \mathbf{D} \left\{ \nabla \rho + \nabla \rho^T \right\}
\]
where the first term is just an ordinary diffusive current and the second is generated by the nematic field. As shown in figure 6(a), currents into high density nematic band, generated by
\[
\rho \frac{\partial n}{\partial t} (0, (0, 0))
\]
which is included in the second term of \(\mathbf{J}\), are directly responsible for the development of the density inhomogeneity. In figure 6(b), along the two sides of the stripe boundaries, the system generates anti-parallel currents which also originate from \(-\nabla \rho \mathbf{Q}_{\rho\rho}(\mathbf{r})\). When the gap in the high density nematic region forms in figure 6(c), particles flow into the low density region, guided by the nematic directors with the formation of nematic tips near the gap. In figure 6(d), we also

\[\text{Figure 5. Time evolution and spatial correlation of order parameters in the chaotic regime. (a) Time series of nematic scalar order parameters } S_G \text{ and } S_L. \ S_G \text{ is a global quantity defined by } \langle \mathbf{Q}_{\rho\rho} \rangle = S_G (n_{\rho\rho} n_{\rho\rho} - \delta_{\rho\rho}/2) \text{ and obtained by averaging } \mathbf{Q}_{\rho\rho}(\mathbf{r}) = S(\mathbf{r}) (n_{\rho\rho} n_{\rho\rho} - \delta_{\rho\rho}/2) \text{ on every discrete site, where } n_{\rho\rho} = (\cos \theta, \sin \theta) \text{ and } n(\mathbf{r}) = (\cos \theta(\mathbf{r}), \sin \theta(\mathbf{r})). \ S_L \text{ is a direct average of the local nematic order parameter } S(\mathbf{r}) \text{ on every discrete site. We always have } S_L \geq S_G; S_L = S_G \text{ only when the system is aligned in the same direction. (b) Time series of the angle of global nematic order } \theta_G. \text{ Note the sudden and rather abrupt change of orientation around } t = 1.6 \times 10^7. \ (c) Two-point spatial correlation function of local nematic order parameters. The system shows evidence for quasi-long-range order, that is, \langle S(\mathbf{r}) S(0) \cos 2(\theta(\mathbf{r}) - \theta(0)) \rangle \text{ and } \langle \cos 2(\theta(\mathbf{r}) - \theta(0)) \rangle \text{ decay as } r^{-\alpha} \text{ in long range (dotted line marks } \alpha = 0.2). \ (d) Snapshot for small } S_G/\mathbf{L} \text{ corresponding to blue circle in (a). (e), (f) Snapshots taken during the sudden change of orientation of } \theta_G \text{ corresponding to the blue circles in (b).} \]

5. Summary and discussion

To summarize, we have studied the kinetic equation for active nematics in the dilute regime, both analytically and by direct numerical simulations. In deriving the kinetic equation, we deliberately stayed in the fast reversal limit, that is, the reversal rate $k$ in equations (1) and (2) is kept much larger than the self-diffusion rate $D$, which leads to a kinetic equation with pure nematic symmetry. When $k$ is comparable to, or even smaller than, $D$, such a simple kinetic equation is not expected to be valid. Since self-diffusion itself gives rise to an effective reversal rate, it contributes a term $v^2/D$ to the renormalized spatial diffusion coefficient. With small $k$, we can expect enhanced spatial diffusion, and the drift terms in equations (1) and (2) will induce local polarities enslaved to the nematic order. Furthermore, the implicit numerical algorithm we use to solve the kinetic equation (7) is not suitable for equations with drift terms.

At the level of the linear instability of spatially-homogeneous solutions of the kinetic equation (7), we have found that the homogeneous nematic solution is linearly unstable to long wavelength transversal modes in a region bordering the transition line defined by the instability of the homogeneous disordered solution (between the blue and green lines in figure 2). This scenario is in agreement with recent studies at the hydrodynamic level [16, 19]. Here, deriving and performing analytically the linear stability of the hydrodynamic equations,
we have quantified the consequences of the reduction to the hydrodynamic level (the difference between the green and orange lines in figure 2). To our knowledge, this is achieved for the first time in the context of active matter (see, however, the recent preprint by T Ihle [34]).

At the nonlinear level, we have found that in the region of instability of the homogeneous ordered solution, the kinetic equation exhibits chaotic behavior. We have described this chaos as the fragmentation of the larger high-density high-order structures formed by the instability mechanism and the subsequent renewal of such ‘spindle-shaped’ structures (figures 4 and 6). Clearly, more work will be needed to characterize the nature and the asymptotic properties of this chaos and, in particular, to determine whether or not it constitutes a disordered phase.

Indeed, the chaotic dynamics described above are different from the chaos found at the hydrodynamic level, but our findings are nevertheless reminiscent of the dynamics reported in [15] for the Vicsek-style microscopic model for active nematics, where intermittent destabilization events of a large high-density, high-order macroscopic band were described. As already suggested in the recent work of Bertin et al [16], this Vicsek-style microscopic model, which should be described at the kinetic level by a Boltzmann equation similar to the kinetic equation studied here, will have to be revisited. Indeed, no homogeneous ordered phase was reported for it and the segregated phase with its intermittent destruction of a single large, dense, ordered band was found to be quasi-long-range ordered. While this is not, strictly speaking, at odds with the results presented here (see the relatively-high order parameter values in figure 5(a), and the correlation function in figure 5(c)), this calls for larger-scale simulations of both the microscopic model and the kinetic equation. The hydrodynamic equations (22) and (23) have the same mathematical structure as those derived in [16] and used in [37], except for the difference in dynamic parameters. While these hydrodynamic equations also give rise to large scale chaotic behavior, as shown very recently in [37], the ordered structures found there are different from those arising in the full kinetic equations studied here. In the kinetic equation, the system generates twisted spindle shaped local ordering structures that are unlike the bow-like traveling structures found in hydrodynamic simulations. By keeping the higher modes in equations (9)-(11), we can recover similar division processes of ordered domains. Moreover, the chaos found in the nonlinear regime also differs from that found in the hydrodynamic description of active nematics suspensions, where interesting low Reynolds number turbulence has been reported [38–41]. The mechanism for linear instability, however, shares similarity, where the density dependence of nematic strength is required for the initiation of the destabilization of ordered state [40].

At this stage, we can nevertheless already come back to the question of ‘giant number fluctuations’ in active nematics systems. These anomalous fluctuations have become a landmark of active matter studies following the seminal works of Toner and Tu, as well as Ramaswamy and co-workers [2, 4, 5]. In their study of the Vicsek-style model for active nematics, Chaté et al reported that the standard deviation $\Delta n$ of the number of particles present in a sub-system containing on average $n$ particles scales anomalously: $\Delta n \sim n$, in agreement with predictions of Ramaswamy et al based on a simple linearized theory. We have performed the same measurement in the chaotic regime of the kinetic equation studied here, and found the same ‘anomalous’ scaling (figure 7). This may appear to be a surprising result since the kinetic equation is not supposed to incorporate noise terms at the origin of giant number fluctuations. In fact, the results obtained here are simply explained by the strong density segregation observed: having sharp interfaces delimiting dense-ordered regions moving in a sparse-disordered
medium trivially yields the above scaling without recursing to the Ramaswamy et al calculation. Also note that this calculation, as well as that of Toner and Tu for polar flocks, assumes that one is in the homogeneous ordered phase.

Again, the question of determining whether the chaotic phase reported here is asymptotically ordered or not, and/or whether the quasi-long-range ordered phase reported in [15] is in fact disordered, appears as the next crucial question down the road towards a comprehensive understanding of dilute active nematics.

**Acknowledgments**

We thank L Tang, C Ren, W Tian, L Xiong, K Yang and X Jiang for helpful discussions; E Bertin and F Ginelli for carefully reading the manuscript and helpful suggestions on the revision of calculations. We are grateful to the Max Planck Institute for the Physics of Complex Systems (MPIPKS) in Dresden, Germany, for providing the framework and support of the Advanced Study Group ‘Statistical Physics of Collective Motion’. This work was supported by the National Natural Science Foundation of China (Nos. 91027040, 11047027, 10974080, and 11204194 ) and the National Basic Research Program of China (No. 2012CB821500).
Appendix. Numerical method

Equation (7) can be solved by using the alternating-direction implicit method [42]. Using a uniform spatial and angular grid with \( x_i = x_0 + i \Delta_x \), \( y_j = y_0 + j \Delta_y \), and \( \theta_k = \theta_0 + k \Delta_\theta \), the discretized distribution function and interacting potential can be denoted as \( f_{i,j,k}^n \) and \( w_{i,j,k}^n \), where \( n \) denotes the discretized time step \( t_n = t_0 + n \Delta_t \). Applying operator-splitting and time-splitting methods, equation (7) can be discretized as

\[
\begin{align*}
\alpha_x f_{i,j,k}^{n+1} &= f_{i,j,k}^n + \alpha_x L_x f_{i,j,k}^{n+1/4} + \alpha_y L_y f_{i,j,k}^n + \alpha_{xy} L_{xy} f_{i,j,k}^n, \\
\alpha_y f_{i,j,k}^{n+1} &= f_{i,j,k}^n + \alpha_\theta L_\theta f_{i,j,k}^{n+1/2} + \alpha_{\theta y} L_{\theta y} f_{i,j,k}^{n+1/2}, \\
\alpha_x f_{i,j,k}^{n+3/4} &= f_{i,j,k}^{n+1/4} + \alpha_x L_x f_{i,j,k}^{n+1/2} + \alpha_y L_y f_{i,j,k}^{n+3/4} + \alpha_{xy} L_{xy} f_{i,j,k}^{n+1/2}, \\
\alpha_\theta f_{i,j,k}^{n+1} &= f_{i,j,k}^{n+3/4} + \alpha_\theta L_\theta f_{i,j,k}^{n+1} + \alpha_{\theta y} L_{\theta y} f_{i,j,k}^{n+1}, \\
\end{align*}
(A.1)
\]

where the operators are given by

\[
\begin{align*}
L_x f^{n+a} &= f_{j+1,i,j,k}^{n+a} + f_{j-1,i,j,k}^{n+a} - 2f_{i,j,k}^{n+a}, \\
L_y f^{n+a} &= f_{i,j+1,k}^{n+a} + f_{i,j-1,k}^{n+a} - 2f_{i,j,k}^{n+a}, \\
L_{xy} f^{n+a} &= f_{i,j+1,j,k}^{n+a} + f_{i,j-1,j,k}^{n+a} - f_{i+1,j,j,k}^{n+a} - f_{i-1,j,j,k}^{n+a}, \\
L_\theta f^{n+a} &= f_{i,j,k+1}^{n+a} + f_{i,j,k-1}^{n+a} - 2f_{i,j,k}^{n+a}, \\
L' \theta f^{n+a} &= (w_{i,j,k+1}^{n+a-1/4} - w_{i,j,k}^{n+a-1/4})(f_{i,j,k}^{n+a} + f_{i,j,k+1}^{n+a}) \\
&- (w_{i,j,k}^{n+a-1/4} - w_{i,j,k-1}^{n+a-1/4})(f_{i,j,k}^{n+a} + f_{i,j,k-1}^{n+a}),
\end{align*}
\]

and the coefficients are given by

\[
\begin{align*}
\alpha_x &= \frac{\Delta_x}{2 \Delta_x} (D_x \cos^2 \theta_k + D_\perp \sin^2 \theta_k), \\
\alpha_y &= \frac{\Delta_y}{2 \Delta_y} (D_\perp \sin^2 \theta_k + D_x \cos^2 \theta_k), \\
\alpha_{xy} &= \frac{\Delta_{xy}}{4 \Delta_x \Delta_y} (D_\perp - D_x) \cos \theta_k \sin \theta_k, \\
\alpha_\theta &= \frac{2 \alpha_\theta'}{2 \Delta_\theta^2} D_\perp.
\end{align*}
\]

Then, each substep in equation (A.1) requires only the solution of a simple tridiagonal system.

References

[1] Vicsek T, Czirok A, Ben-Jacob E, Cohen I and Shochet O 1995 Phys. Rev. Lett. 75 1226
[2] Toner J and Tu Y 1995 Phys. Rev. Lett. 75 4326
[3] Toner J and Tu Y 1998 Phys. Rev. E 58 4828
[4] Toner J 2012 Phys. Rev. E 86 031918
[4] Ramaswamy S, Simda R A and Toner J 2003 *Europhys. Lett.* **62** 196
[5] Toner J, Tu Y and Ramaswamy S 2005 *Ann. Phys.* **318** 170
[6] Mishra S and Ramaswamy S 2006 *Phys. Rev. Lett.* **97** 090602
[7] Chaté H, Ginelli F, Gregoire G and Raynaud F 2008 *Phys. Rev. E* **77** 046113
[8] Deseigne J, Dauchot O and Chaté H 2010 *Phys. Rev. Lett.* **105** 098001
[9] Deseigne J, Léonard S, Dauchot O and Chaté H 2012 *Soft Matter* **8** 5629
[10] Weber C A et al 2013 *Phys. Rev. Lett.* **110** 208001
[11] Chen X, Dong X, Be’er A, Swinney H L and Zhang H P 2012 *Phys. Rev. Lett.* **108** 148101
[12] Zhang H P, Be’er A, Florin E L and Swinney H L 2012 *Proc. Natl. Acad. Sci. USA* **107** 13626
[13] Schaller V and Bausch A R 2013 *Proc. Natl. Acad. Sci. USA* **110** 4488
[14] Giomi L, Bowick M J, Ma X and Marchetti M C 2013 *Phys. Rev. Lett.* **110** 228101
[15] Chaté H, Ginelli F and Montagne R 2006 *Phys. Rev. Lett.* **96** 180602
[16] Bertin E, Chaté H, Ginelli F, Mishra S, Peshkov A and Ramaswamy S 2013 *New J. Phys.* **15** 085032
[17] Bertin E, Droz M and Grégoire G 2006 *Phys. Rev. E* **74** 022101
[18] Bertin E, Droz M and Grégoire G 2009 *J. Phys. A: Math. Theor.* **42** 445001
[19] Baskaran A and Marchetti M C 2012 *Eur. Phys. J. E* **35** 95
[20] Marchetti M C et al 2013 *Rev. Mod. Phys.* **85** 1143
[21] Narayan V, Menon N and Ramaswamy S 2006 *J. Stat. Mech.* P01005
[22] Narayan V, Ramaswamy S and Menon N 2007 *Science* **317** 105
[23] Aranson I S, Volfson D and Tsimring L S 2007 *Phys. Rev. E* **75** 051301
[24] Kudrolli A, Lumay G, Volfson D and Tsimring L S 2008 *Phys. Rev. Lett.* **100** 058001
[25] Daniels L J, Park Y, Lubensky T C and Durian D J 2009 *Phys. Rev. E* **79** 041301
[26] Kudrolli A 2010 *Phys. Rev. Lett.* **104** 088001
[27] Shimada T, Doi M and Okano K 1988 *J. Chem. Phys.* **88** 7181
[28] Baskaran A and Marchetti M C 2008 *Phys. Rev. E* **77** 011920
[29] Baskaran A and Marchetti M C 2008 *Phys. Rev. Lett.* **101** 268101
[30] Peshkov A, Aranson I S, Bertin E, Chaté H and Ginelli F 2012 *Phys. Rev. Lett.* **109** 268701
[31] Shi X and Ma Y 2013 *Nat. Commun.* **4** 3013
[32] Peshkov A, Ngo S, Bertin E, Chaté H and Ginelli F 2012 *Phys. Rev. Lett.* **109** 098101
[33] Ahmadi A, Marchetti M C and Lippool T B 2006 *Phys. Rev. E* **74** 061913
[34] Ihle T 2013 *Phys. Rev. E* **88** 040303
[35] Aranson I S, Snezhko A, Olafsen J S and Urbach J S 2008 *Science* **320** 612c
[36] Narayan V, Ramaswamy S and Menon N 2008 *Science* **320** 612d
[37] Ngo S, Peshkov A, Aranson I S, Bertin E, Ginelli F and Chaté H 2013 arXiv:1312.1076
[38] Saintillan D and Shelley M J 2008 *Phys. Fluids* **20** 123304
[39] Wolgemuth C W 2008 *Biophys. J.* **95** 1564
[40] Giomi L, Mahadeva L, Chakraborty B and Hagan M F 2011 *Phys. Rev. Lett.* **106** 218101
[41] Giomi L, Mahadeva L, Chakraborty B and Hagan M F 2012 *Nonlinearity* **25** 2245
[42] Press W H, Teukolsky S A, Vetterling W T and Flannery B P 1992 *Numerical Recipes in C: The Art of Scientific Computing* 2nd edn (New York: Cambridge University Press)