Large scale ordering of active defects

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We use continuum simulations to study the impact of friction on the ordering of defects in an active nematic. Even in a frictionless system, +1/2 defects tend to align side-by-side and orient antiparallel reflecting their propensity to form, and circulate with, flow vortices. Increasing friction enhances the effectiveness of the defect-defect interactions, and defects form dynamically evolving, large scale, positionally and orientationally-ordered structures which can be explained as a competition between hexagonal packing, preferred by the -1/2 defects, and rectangular packing preferred by the +1/2 defects.

Active materials are out-of-equilibrium systems that continuously consume energy and exert stress on their environment [1]. Examples include bacterial suspensions [2–4], living cells [5–7] and vibrating granular rods [8]. The continuous injection of energy - or activity - and the resulting stress can lead to phenomena such as collective motion [9–11], and active turbulence [12, 13], behaviours which cannot be captured by conventional equilibrium statistical mechanics. [14–18].

Many active systems have nematic symmetry, and such active materials extend the physics of passive nematics [19]. The activity destroys long-range nematic order, resulting in the proliferation of topological defects in the orientation field. The defects annihilate in oppositely charged pairs as in a passive nematic [20], but they are also continuously created in pairs due to the activity [21]. Moreover, in active systems gradients in the director field induce stresses and hence +1/2 topological defects are self-propelled [22]. Flows driven by the defects, and by other gradients give rise to active turbulence (Figure 1a), a chaotic flow state characterised by short-range nematic order, high vorticity and localised bursts of velocity [23, 24].

A key experimental system for investigating the properties of active turbulence is a dense suspension of microtubules propelled by two-headed kinesin motors [10, 25]. Investigation of the defect motion in a thin layer of this material showed that the +1/2 topological defects can themselves display long-range nematic order while retaining their motile nature [26]. Very recent simulations of active nematics with hydrodynamics, wet systems, have shown short-range defect ordering [27, 28]. Simulations of active nematics with no hydrodynamics, dry systems, have reproduced +1/2 defect ordering, but this is polar rather than nematic [29–31]. Such polar defect ordering has been attributed to arch-like configurations of the nematic director field [32]. In other simulations of active systems, with hydrodynamics and strong friction the defects formed a static lattice with positional and orientational order [33, 34].

To clarify how defects order in active nematics, we perform large scale continuum simulations to measure both the positional and the orientational order of topological defects with varying friction. We confirm that +1/2 defects prefer to position themselves side by side and align anti-parallel [27, 28], while the −1/2 defects prefer to impose a three-fold symmetry on their surroundings. Increasing friction increases the effectiveness of the defect-defect interactions, and they start to form dynamically evolving orientationally and positionally ordered structures which can be explained in term of the competition between hexagonal packing preferred by the −1/2 defects and rectangular packing preferred by the +1/2 defects. Locally, the ordering of the +1/2 defects is either polar or anti-polar, depending on their relative position. However, we also observe a nematic order of defects that spans the system, even in the regime where defects are still motile. This increases with increasing friction, in agreement with the experiments [26].

To investigate the orientational arrangements of defects, we solve the continuum equations of motion for a 2D active nematic [23, 24, 35, 36]. These are now very well documented, so we summarise relevant points here, giving the full equations and simulation parameters in the SM. The relevant hydrodynamic variables are an orientational order parameter $\mathbf{Q}$, which describes the magnitude and direction of the nematic order, and the velocity. We consider very low Reynolds number and constant density. We work above the nematic transition temperature, so any nematic order is induced solely by the activity, and consider a flow-aligning fluid. The equations of motion are identical to those describing the nemato-hydrodynamics of passive nematic liquid crystals except for an additional term in the stress $-\zeta \mathbf{Q}$ which implies that any gradients in the nematic ordering drive flows and, for extensile activity, $\zeta > 0$, results in active turbulence. Lastly, we include a frictional damping term $f$ in our Navier-Stokes equation mod-
Defect ordering in wet active turbulence: (a) Snapshot of active turbulence for very low friction, \( f = 0.0007 \). The white (magenta) symbols are +1/2 (−1/2) defects. Background colour denotes the vorticity. (b) Schematic representation of +1/2 and −1/2 defects. +1/2 defects have a single polar axis (blue line) and −1/2 defects have three axes. (c) For a reference defect \( i \) we define an associated polar co-ordinate system, with \( \hat{y} \) in the direction of the defect. (d) Spacing between +1/2 defects (defined as the position of the maximum in \( g^{++} \)) as a function of the active length scale \( \sqrt{K/\zeta} \). Activity \( \zeta \) and elasticity \( K \) were varied. (e-h) Pair distribution function \( g_{ab}(r,\theta) \) showing the positional distribution of \( b \)-type defects around an \( a \)-type defect. The white arrows represent the orientational distribution vector \( S \) with arrow size normalized by the magnitude of \( S \).

**Defect distributions:** To measure positional and orientational correlations between defects, we treat the +1/2 and −1/2 defects as two different types of quasi-particle with different symmetries [37]. We consider a reference defect \( i \) and choose a Cartesian co-ordinate system with the \( y \)-axis along the polar axis of the defect as shown in Figure 1b. To define the relative position of the second defect, we use a polar co-ordinate system \( (r,\theta) \) with origin at the position of the \( i \)th defect and define \( \theta \) as the angle from the \( x \)-axis. We measure the relative position of the other defects \( j \) present at a given time step (Figure 1c), and then average over all the measured defect pairs to get the pair-wise positional distribution function:

\[
g_{\pm \pm}(r, \theta) = \frac{V}{N} \sum_i \sum_{j(i) < j(i)} \delta(r - r_{ij}, \theta - \theta_{ij}),
\]

where the subscripts of \( g \) indicate the type of the defects \( ij \), e.g. −+ refers to the positioning of +1/2 defects around a −1/2 defect. The normalization \( V/N \) is the area divided by the total number of defect pairs \( N \). We introduce this normalization to set \( g = 1 \) at \( r \to \infty \) to normalize to bulk densities at large distances.

In addition to the relative defect positions, we are also interested in the average defect orientation relative to the reference defect. To obtain this information, we calculate the orientation distribution vector,

\[
S_{\pm \pm}(r, \theta) = \frac{\mathcal{N}}{N} \sum_i \sum_{j(i) < j(i)} \delta(r - r_{ij}, \theta - \theta_{ij}) \left[ \frac{\cos \kappa_j \psi_j}{\sin \kappa_j \psi_j} \right],
\]

where \( \psi_j \) is the polar angle of the orientation of defect \( j \) in the co-ordinate frame defined by the reference defect \( i \) (Figure 1c). Here \( \kappa_j = 2(1 - k_j) \), where \( k_j \) is the charge of the \( j \)th defect, accounts for the three-fold rotational symmetry of the −1/2 defects. Taking the normalization constant as \( \mathcal{N} = V/(Ng_{\pm \pm}(r, \theta)) \) means that the magnitude of \( S \) is 0 in the absence of orientational correlations and 1 if the defect orientations are perfectly correlated. If
FIG. 2: (a) Snapshot of the defect structures at intermediate friction $f = 0.009$. +1/2 ($-1/2$) defects are shown in white (magenta). There is transient local defect ordering into a rectangular (green outline) or a hexagonal (magenta outline) pattern. The background colour represents the vorticity field. (b) Schematic of the rectangular ordering. (c) Schematic of the hexagonal ordering. This is chiral: $-1/2$ defects (in grey) have either a left or right neighbouring $-1/2$ defect (in green). The other position is filled by rotating $+1/2$ defects resulting in local zero charge.

$g(r; \theta)$ is zero, we set $S = 0$.

Emergent defect ordering at low friction:- We first consider very low friction, $f = 0.0007$, and high activity, $\zeta = 0.03$, recovering well-developed wet active turbulence (Figure 1a). Figure 1c shows how positive defects behave in the vicinity of another positive defect: even in this highly turbulent regime there is a clear preference for neighbouring $+1/2$ defects to line up along the $x$-axis in an anti-parallel configuration with a preferred distance between neighbours. This preferred defect spacing scales with the active nematic length scale, $\sqrt{K/\zeta}$ (Figure 1d), indicating that it results from a balance between elastic and hydrodynamic forces. As we will show later, these peaks are the result of the tendency of two $+1/2$ defects to orbit on the same vortex. Such behaviour is also a feature of the dancing state stabilised in narrow channels [38].

Figure 1h shows that $-1/2$ defects prefer not to lie too close to each other, and that there is no preferred length scale in contrast to the $+1/2$ defects. Interestingly, the $-1/2$ defects do impose an orientational structure on surrounding $-1/2$ defects even in this fully active turbulent regime. We already find six peaks where the neighbouring defects have a strong preference for anti-parallel alignment. This is due to the elastic torque [39]. However, the symmetry of the peak positions is caused by the flow fields which form six vortices around negative defects.

Finally Figure 1f,g show that positive and negative defects are preferentially found close together and aligned in the relative orientation associated with creation (shown schematically in Figure 1b) and annihilation events. Once the polar alignment has become established, the situation can persist as oppositely charged defects pairs have a tendency to line up their polar axis with the flow of the central defect [28].

Defect lattices at high friction:- As the friction is increased, the defect interactions result in large-scale ordering of the defects. As an example, Figure 2a presents a snapshot of the defect structure and corresponding vorticity field for $f = 0.009$, where the mean speed of the flow has been reduced by an order of magnitude with respect to the no friction regime. This figure and movie 1 show that $+1/2$ defects have a strong tendency to form anti-parallel pairs, which induce and orbit on vortices, as already apparent in the no friction limit. But much larger-scale defect arrangements also become apparent at high friction, as not only the interactions between the $+1/2$ defects but also those between the $-1/2$ defects result...
We show in significant ordering. To investigate this, we first consider the structure formed by the +1/2 defects (Figure 2b), and then the ordering preferred by the −1/2 defects (Figure 2c).

Figure 3a,b show positional distribution function of ±1/2 defects around a +1/2 defect at strong friction, \( f = 0.014 \). The preferred orientational ordering of the defects at each position is superimposed upon the plot. The first obvious feature of these correlations is that the anti-parallel ordering of the +1/2 defects along \( x \) is more pronounced and longer ranged than in the frictionless limit. This is confirmed by Figure 3c where we plot the pair-wise positional distribution function \( g_{++}(r, 0) \) showing how the strength and range of the correlations increase with increasing friction.

Figure 3d shows that +1/2 defects are also ordered along the \( y \)-axis. This ordering can be interpreted by comparing the distribution functions in Figure 3a,b which show that +1/2 and −1/2 defects alternate along the \( y \)-axis, and that they align parallel. The ordering increases with friction, but is less pronounced than that along \( x \). We show in the SM that the energy of two +/− defect pairs, each arranged as in Figure 2b and held at a fixed distance apart, is minimised if the pairs line up along the \( y \)-axis. Moreover, this configuration is favoured because it leads to non-conflicted flows. Together, the preferred ordering of +1/2 defects along \( x \) and \( y \), i.e. perpendicular and parallel to the polar axis of the defects, is satisfied by the rectangular packing of defects shown in Figure 2b.

In Figure 3e we plot the nematic order parameter, \( S_d = -\frac{2}{N} \sum_i \sum_{j \neq i} \sum_r (\hat{m}_i \cdot \hat{m}_j)^2 \) as the friction is increased. In this relation, \( \hat{m}_i \) is the polar axis of the \( j \)th +1/2 defect. \( S_d \) takes a non-zero value, even when the defects are still motile, and increases with increasing friction. It is reminiscent of the experimental system of microtubules driven by motor proteins where the nematic order of defects increases with decreasing film thickness [26]. However, the patterning also exhibits higher-order symmetry than just nematic as the ordering of defects is polar or anti-polar depending on their relative positions. Upon increasing the friction further (\( f = 0.015 \) in Figure 3e), the defects stop moving and a vortex lattice with perfect orientational order is established [33].

Figure 4 presents results for the ordering around negative defects showing a distinct difference between intermediate (\( f = 0.009 \), Figure 4a,d) and high friction (\( f = 0.014 \), Figure 4b,e). In the intermediate friction regime there are six first neighbour and six second neighbour peaks in the positional distribution function around the central defect, corresponding to a hexagonal packing of −1/2 defects. Both right-handed and left-handed lattices are possible (see Figure 2c and Movie 1). With increasing friction, however, the nearest neighbour peaks become less pronounced showing that it is increasingly difficult to form a hexagonal lattice.

Instead the secondary peaks become more pronounced. The reason for this is apparent from Figure 4c,f, which shows that the +1/2 defects increasingly line up along the polar arms of the −1/2 defects, and lie between two −1/2 defects. We show in the SM that this is the elastically preferred configuration of two defect pairs. It corresponds to the polar ordering of alternate +1/2 and -1/2 defects seen in the rectangular lattice (Figure 2b and Movie 1).

Conclusion:- We have numerically investigated defect ordering in an active nematic with hydrodynamic interactions and increasing friction. We show that friction can introduce a nematic order of defects that span the system, as observed in experimental systems [26]. A local measurement would,
however, give polar order of $+1/2$ defects in the direction of their polar axis (mediated by intervening $-1/2$ defects), and anti-polar order of the $+1/2$ defects perpendicular to this axis.

Weak signatures of this ordering are observed even in fully developed active turbulence with no friction. Upon increasing the friction they result in structures with longer-ranged order. The $-1/2$ defects tend to reorganize themselves into hexagons, where each hexagon encompasses two $+1/2$ defects which rotate on a vortex. However, this is not an ideal configuration for pairs of $\pm 1/2$ defects and, as a consequence, the hexagonal packing of defects coexists with the rectangular structure shown in Figure 2b. As the friction is increased, and the hydrodynamic interactions become weaker, the rectangular packing becomes dominant, and the system eventually freezes into the rectangular lattice [33, 34].

ACKNOWLEDGEMENTS

We thank Amin Doostmohammadi for fruitful discussions. K.T. received funding from the European Union’s Horizon 2020 research and innovation programme under Lubiss the Marie Skłodowska-Curie Grant Agreement No. 722497. M. R. N. acknowledges the support of the Clarendon Fund Scholarships.

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